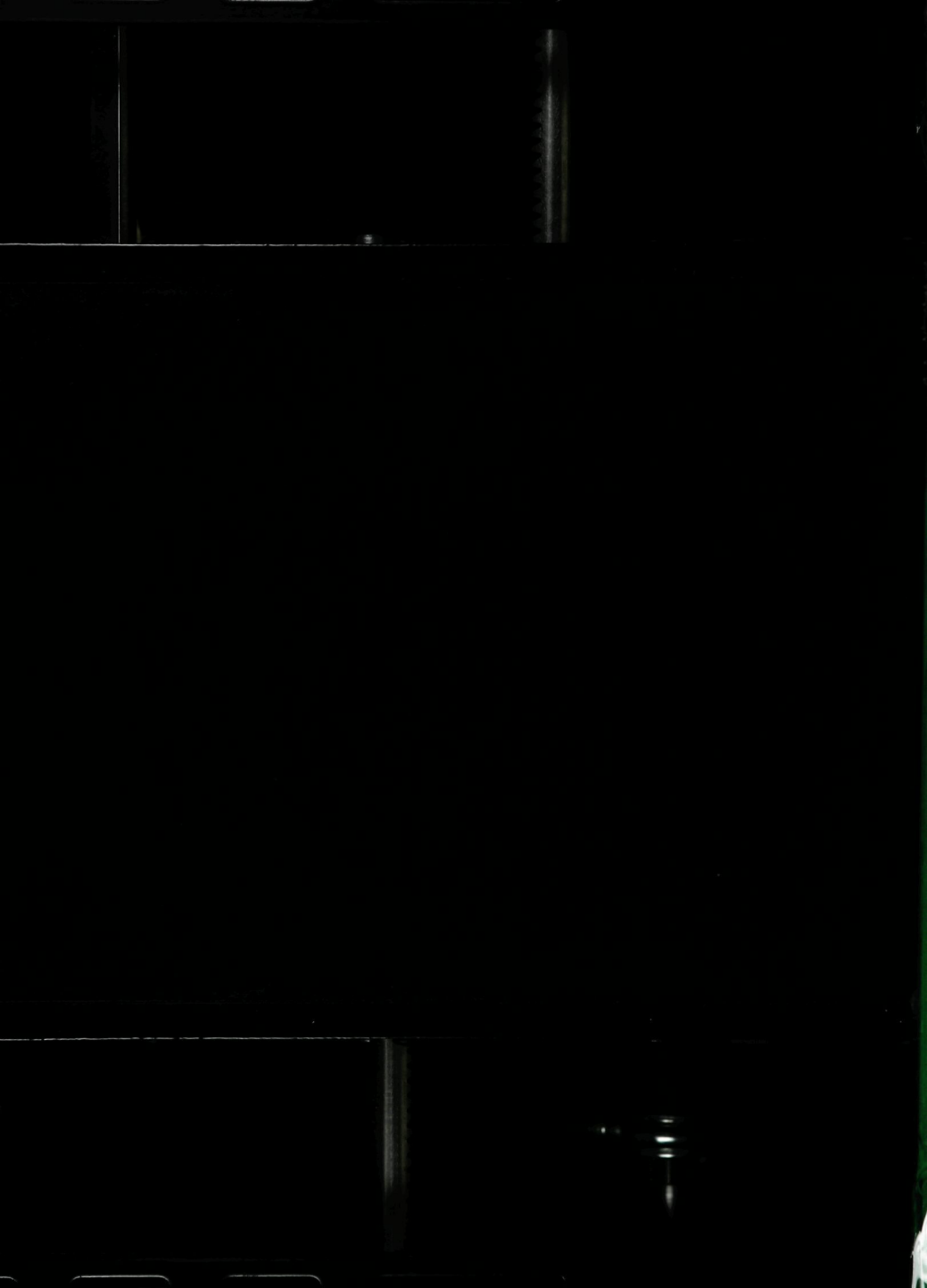

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NATIONAL ENERGY SOFTWARE CENTER: COMPILATION OF SOFTWARE ABSTRACTS

by

M. Birgersson, M. K. Butler, J. Carter,
M. M. De Bruler, F. K. Degges, C. E. Eyberger,
L. R. Eyberger, P. L. Johnson, and L. L. Reed

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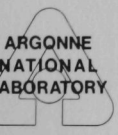

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NATIONAL ENERGY SOFTWARE CENTER: COMPILATION OF SOFTWARE ABSTRACTS

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M. Birgersson, M. K. Butler, J. Carter,
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March 1986

ANL-7411 REVISED SUPPLEMENT 2

This publication is the second supplement to ANL-7411 Revised which was published in May 1979. Supplement 1 was issued in September 1982.

Complete replacements are included for the Preface, and the following 148 NESC abstracts:

39, 246, 252, 253, 271, 275, 316, 350, 355, 358, 369, 375, 387, 408, 418, 420, 421, 423, 430-433, 447, 449, 482, 497, 498, 503, 505, 508, 510, 512, 517, 534, 551, 555, 561, 580, 586-588, 592, 593, 605, 618, 623, 633, 634, 637, 639, 647, 653, 658, 665, 670, 671, 676, 681, 686, 688, 689, 697, 703, 704, 709, 710, 716, 722, 727, 729, 730, 733, 734, 736, 739, 745, 759-761, 763, 767, 768, 770-772, 775, 776, 778-780, 782, 784, 791, 793, 794, 797, 798, 800, 806, 812, 818, 820, 823, 830, 832, 836, 844, 857-859, 861, 866, 870, 871, 877, 881, 886-889, 902, 905, 907, 912, 917, 919-921, 931-933, 939, 942, 943, 959, 963-965, 967, 972-975, 978-980, 983, 988.

In addition, new NESC abstracts 993, 994, 996-1000, 1002-1013, 1016-1018, 1020-1034, 1036-1038, 1056, 9673, 9674, 9676-9686, 9688-9915, 9917-9941, 9943-9952, 9954-9988, 9990, and 9992-9994 are included.

Complete replacements are also included for Appendix A: Library Software by Subject Classification, Appendix B: KWIC Index, and Appendix C: References.

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CINDER,M0102, point depletion fission product	BAPL	6600	F4	RS	P	D 313
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GAUGE, 2-d few-gp hex geom diffusion depletion	GGA	1108	F4	RS	P	D	339
GAUSS6, batch analysis of gamma-ray spectra	EG&G	360	F+P+A	RSBP	XC	W	622
GAUSS7, analysis of gamma-ray spectra from Ge	EG&G	C176	F4	RS	P X	U	605
GAZE2, 1-d multigroup diffusion slab, sph, cyl	GGA	1108	F+BAL	RS	P	C	430
GCFM5.0, geothermal field & power plant costs	MITR	370	F4	RS	L C	D	976
GEM, analysis of nuclear fuel cycle economics	UICS	360	F4	RS	P C	D	576
GEM, eigenvalue problem for vibrating systems	KAPL	6600	F+ASC	RS	P	I	R 344
GEM2D, 2-d electromagnetics Galerkin FEM	LLNL	CRA1	F	RS	P	X	9679
GENED ENVIRONMENTAL ROUTINES, subroutine lib	NED	635	F+GMP	RS		P	515
GENRD, free-format card input processor	LANL	360	F4	RS	P	L	530
GENRD, free-format card input processor	LANL	6600	F4	RS	P	L	530
GEOCITY, geothermal district heating economics	BNW	CY74	F4	RS	P	D	835
GEOCOST-BC, binary cycle geothermal cost study	BNW	6600	F4	RS	P	D	711
GEOCOST, geothermal energy cost analysis	BNW	6600	F4	RS	P	D	684
GEODYN, rock formation drill string dynamics	SNLA	VX11	F77	RS	P X	R	9781
GEOTEMP2, advanced wellbore thermal simulator	SNLA	C170	F5	RS	P	H	9771
GEOTHER, 2-phase fluid flow & heat transport	BPMD	C176	F4	RS	P	R	R9834
GETCOR,FRECOR, Fortran dynamic storage alloc	ORNL	360	BAL+F	RS	P C	P	644
GETOUT, radionuclide transport geologic media	BNW	1100	F	RS	PL C	R	887
GKS, minimal graphical kernel system C Binding	SNLA	VX11	C	RS	P X	P	9689
GLEN, group constant calc from TOR output data	LANL	6600	F4	RS	P	B	361
GLOVE CHANGE ANALYSIS SYSTEM, glove database	RFD	360	COBOL	RS	P	M	813
GLUB1, water-logged fuel element analysis	BAPL	6600	F4	RS	P	H	R 424
GNASH, particle induced x-sections & spectra	LANL	7600B	F+COM	RS	PL	A	757
GNATS,MESH2,GPRINT, 2-d nonlinear analysis	SNLL	6600	F+COM	RS	P	I	682
GRAFAID, interactive x-y data analysis & plots	SNLA	VX11	F	RSBP	LXC	N	9690
GRAFIX, general purpose graphics library	ORNL	MPL2	F+MAC	S	XC	N	9900
GRAIL, a device-independent graphics language	KAPL	6600	F+COM	RS	P X	N	910
GRAMP, R-M parameters of unresolved resonances	BAPL	6600	F4	RS	P	A	R 470
GRAPH, linear regression w/confidence limits	BKC	360	F4	RSBP		P	624
GRAV2D.REV2, models gravity data for anomalies	UUGG	400	F4	RS	C	R	9981
GRDWRK, grid generation for Safe programs	GGA	1108	F4	RS	P	L	296
GRFPAK, plot package for CORTES FEM programs	ORNL	360	F4	RS	P C	N	760
GROUP2, group theory of lattice dynamics	LANL	6600	F4	RS	P	Q	620
GROUP2, group theory of lattice dynamics	ANL	360	F4	RS	P	Q	620
GROUSE, space-dependent x-section generation	GEC	635	F4	RS	P	B	420
GRPNL2, fitting gamma & x-ray peak multiplets	MLMO	PD11	F3B	RS	X	U	9876
GSCRAP, LMFBR reactor core seismic analysis	FBRD	6000	F4	RS		I	R9816
GSM, Columbia plateau geologic site simulation	BPMD	C176	F77	RS	PLX	R	R9845

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GSMP, general systems analysis modeling code	ANL	370	P+F+A	RS	P C	T	882
GSSLRN1B, least squares photopeak spectra code	BNW	1108	F+BAL	RS	P	O	457
GWCORE, GSPC 79 core graphics routines package	GWSE	VX11D	F77+C	RS	PLXC	N	905
GWCORE, GSPC 79 core graphics routines package	GWSE	VX11C	F77+C	RS	PLXC	N	905
HAARM3, aerosol behavior log-normal dist model	BCL	6400B	F4	RS	P	G	797
HAA3B, aerosol behavior lognormal model	AI	370	F	RS	P	G	443
HAFMAT, system steady-state flow distribution	KAPL	6600	F4	RS	P	H	R 616
HAMMER, 1-dimensional critical analysis system	UNI	1110	F+ASM	RS	PLXC	B	9960
HAMMER,LITHE,HELP, critical analysis system	DP	360	F+BAL	RS	P XC	B	277
HAMOC, fluid hammer analysis of piping system	HEDL	6600	F4	RS	P	G	710
HAUSER5, nuclear reaction cross sections	HEDL	1100C	F+ASM	RS	P XC	A	830
HAUSER5, nuclear reaction cross sections	HEDL	7600	F4	RS	P XC	A	830
HAUSER5, nuclear reaction cross sections	NEA	370	F4	RS	P XC	A	830
HCT, hydrodynamics chemical kinetics transport	LLNL	7600	L+COM	RS	P X	U	9819
HEATING2, transient steady-state heat transfer	SSDC	370B	F4	RS	P C	H	198
HEATING3, 1,2, or 3-d heat conduction program	INER	CY73	F4	RS	P	H	517
HEATING5, 1,2, or 3-d heat conduction program	ORNL	360C	F+BAL	RS	P X	H	517
HEATMESH, geometrical data heat transfer study	SNLL	6600	F4	RS	P	N	434
HECTR, containment response to hydrogen event	SNLA	MPL3	F77	RS	P C	G	R9729
HELIOSTAT CONTROLLER, Solar 1 collector system	SAN	M680	ASM	R		T	9794
HEMP, hydrodynamic elasticmagneto plastic	LLNL	7600	F4	RS	P	H	775
HERESY3, 2-d heterogeneous reactor calculation	DP	360B	F4	RS	P C	C	136
HERMES, regional radiological effects analysis	HEDL	1108	F+SLE	RS	P XC	R	527
HETRAP, fuel rod response LOCA experiments	ORNL	360	F4	RS	P	H	730
HEXEREI2, HTGR thermal-hydraulic analysis	ORNL	360	F+BAL	RS	P	H	852
HEXSCAT, elastic scat x-sections hex lattice	GGA	1108	F4	RS		B	291
HFN, 1-d multi-gp diffusion slab cyl sphere	BNW	1107	F4	RS	P	C	241
HFN, 1-d multi-gp diffusion slab cyl sphere	BNW	6600	F4	RS	P X	C	241
HIDDEN, hidden surface processing algorithm	LLNL	7600	LRL+F	RS		P	996
HILITE, 3-d picture display with highlighting	LLNL	7600	F	S	X	P	9885
HISTAM2S, superheater sodium-water reaction	FBRD	6000	F4	RS	P C	G	R9751
HISTOGRAMS, quality control sample statistics	BKC	360	F4	RSBP		P	614
HONDO, a dynamic response finite-element code	UUCC	1100	F+ASM	RS	P	I	672
HONDO, a dynamic response finite-element code	SNLA	6600B	F4	RS	P	I	672
HONDO5, ab initio Hartree-Fock structure	BKY	7600	F+COM	S	P XC	W	1025
HOTDAMAGE, thermal transient structural damage	WAES	C170	F4	RS	P	I	R9783
HOTROD, rod bundle steady-state two-phase flow	BAPL	6600	F+COM	RS	P	H	R9855
HOT2, 2-d transient heat conduction program	BAPL	6600	F4	RS	P	H	R 286
HPXFER,HPOPEN,HPREAD, HP floppy data transfer	LLNL	LS11	F	RSB	C	P	9824
HRG3, slowing-down spectrum, multigp constants	TVA	360	F4	RS	PLX	B	467
HRG3, slowing-down spectrum, multigp constants	BNW	1108	F4	RS	PLX	B	467
HWOCR-SAFE, 2-d Monte Carlo cell calculation	AI	360	F+BAL	RS	P X	B	307
HYMAS, hydrodynamic mass matrix generation	BAPL	6600	F+COM	RS	P	H	R 560
ICANA, computer aided network analysis	BKC	MPL2	F77	RS		M	9815
ICARUS-LLNL, one-dimensional heat conduction	LLNL	7600	LRL	RS		H	9683
ICARUS, redundant system unavailability model	ANL	370	F4	RS	P	G	R 871
ICCG2, 2d PDE linear symmetric matrix solver	LLNL	CRA1	F	RS	X	X	9928
ICCG3, 3d PDE linear symmetric matrix solver	LLNL	CRA1	F	RS	X	X	9926
ICOP, financial model industrial cogeneration	ORNL	C170	F4	RS	P	D	971
IDAP, interactive decision analysis procedure	ANL	370	PL1	RS	PLXC	P	935
IGES/RIM PARSER & CONVERTER, IGES to RIM DBMS	SNLL	VX11	F77	RS	X	T	9712
IH, optical code solar central receiver system	SNLL	H66	F5	RS		T	9720
IHTSD, CRBRP heat transport system evaluation	FBRD	6000	F4	RS	P	H	R9743
ILUCG2, 2d PDE linear asymmetric matrix solver	LLNL	CRA1	F	RS	X	X	9929
ILUCG3, 3d PDE linear asymmetric matrix solver	LLNL	CRA1	F	RS	X	X	9927
ILUIR, incomplete LU with iterative refinement	LLNL	CRA1	LRL	S		P	9776
IMPAC2, B shipping container impact analysis	LANL	7600B	F4	RS	P	I	715
IMPORTANCE, FTA basic event & cut set ranking	ANL	370	F4	RS	P	G	779

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INCITE, thermal spectra & multi-gp constants	EG&G	360	F4	RS PL C	B	565
INDCEPT, industrial boiler plant capital cost	ORNL	3033	F4+A	RS P XC	D	1000
INDX, xray diffraction powder pattern indexing	LANL	6600	F+COM	RS P	Q	609
INGEN, finite element program mesh generator	LANL	7600B	F4	RS P	P	975
INSCAT, inelastic scattering method	CDCO	7600	F4	RS P XC	W	940
INTEG,INSPEC, Markov simulation of reactor opn	DP	360	F4	RS P	G	590
INTEROP, nonlinear optimization algorithms	EG&G	C173	F+COM	RS P	P	866
INVAR2, interactive nonlinear least squares	NBS	1100	F	RS XC	P	9925
IPINV.REV1, 2d dipole-dipole resistivity model	UUGG	400	F4	RS P C	R	9987
IP2D.REV1, resistivity & induced-polarization	UUGG	1108	F+ASM	RS C	R	990
ISDMS, INEL scientific data management system	EG&G	C176	F+COM	RS C	M	1034
ISOGEN, radionuclide generation and decay	BNW	1108	F5	RSBPL	D	367
ISOSEARCH, isotope production flux, x-sec calc	ORNL	360	F+BAL	RS P	D	322
ISOTAB, Pu power output from mixed isotopes	MLMO	360B	F4	RS P C	Q	R 619
ISOTOPES, maximum yield from reaction or decay	LMSC	1100	F5	RS P	D	179
ISTUM, industrial sector technology use model	DOEI	3033	APL	RS P	D	9895
JAKEF, symbolic function differentiation	ANL	MPLN	F77	RS P X	P	9877
JCLCROSS, DSN cross-ref list from JCL PROCLIBs	HCI	370	F+C+A	RS XC	P	725
JITER, fluctuation experiment analysis	BAPL	6600	F4	RS P	O	R 394
JOSHUA, data storage, retrieval, and display	DP	360B	F+ASM	RSBPLXC	M	490
JOURNAL CONTROL, library journal management	ORNL	360	C+BAL	RS PL C	M	660
JP1XR, coupled-channel scattering x-sec calc	KAPL	6600	F4	RS P	A	R 506
JUPITOR1, coupled channel x-sec evaluation	ENEA	360	F4	RS P C	A	308
K-FIX(3D), 3d extension 2-phase flow dynamics	LANL	7600	F4	RS P	H	877
K-FIX, transient 2-dimensional 2-fluid flow	LANL	7600	F4	RS P X	H	727
K-TIF, two-fluid PWR downcomer fluid dynamics	LANL	7600	F	RS P	H	876
KAPLPLOT, KAPL CalComp plotting routines	KAPL	6600	F+COM	RS	P	R 496
KAPPAS, semiclassical transmission probability	MINN	7600	F4	S P X	W	945
KEELE, linearly-constrained optimization	ORNL	360	F4	RS P	P	556
KEFF,MGBS,TGAN, nuclear criticality safety	DP	360	F4	RS P	C	617
KENO2, Monte Carlo multigroup criticality code	RFD	6600B	F+COM	RS PLX	C	450
KENO2, Monte Carlo multigroup criticality code	DP	360B	F+BAL	RSBP C	C	450
KENO4, Monte Carlo multigroup criticality code	ORNL	360C	F+BAL	RSBPLXC	C	450
KIVA, 2- & 3-d reactive flows with fuel sprays	LANL	CRA1	F	RS P X	U	9688
KNASA, multi-gas mixture component pressures	ANL	3033	F4	RS PL	U	9738
LADTAP2, liquid pathway dose calculations	ORNL	7600	F4	RS PL	R	992
LADTAP2, liquid pathway dose calculations	ORNL	360	F4	RS PL C	R	992
LANL-J501, SC-4020 emulation graphics library	LANL	6600	F4	RS P	P	633
LANL-J501, SC-4020 emulation graphics library	LANL	7600	F4	RS P	P	633
LANL-J501, SC-4020 emulation graphics library	LANL	7600B	F4	RS P	P	633
LANL-J501, SC-4020 emulation graphics library	LANL	CRA1	F4	RS P	P	633
LANL-J501, SC-4020 emulation graphics library	LANL	VX11	F4	RS P	P	633
LARCA, flux-weighting of DTF4 cross sections	LANL	6600	F4	RS P	N	409
LASER, spectrum calc with burnup cyl lattice	TVA	360B	F4	RSBPLXC	B	249
LASIP3, CCCC standard interface file processor	LANL	360	F4	RS P C	M	691
LASL XSEC SETS, Sn 18- 24- and 25-group sets	LANL	6600	BCD	R LX	Z	532
LASO, block Lanczos symmetric eigenvalue code	ORNL	370	F4	RS P	P	918
LATIN SQ, NxN Latin Square experimental design	MLMO	360	F4	RSBP C	P	630
LAYFLO, radionuclide transport geologic medium	BCL	CY74	F77	RS P	R	R1038
LCLSQ1, linear least squares with constraints	ANL	3033	F4	RS P	P	989
LCR-BASED DESIGN TOOL, LCR/SSF & energy plots	SSEC	1000	F4X	RS LX	M	9703
LCURVE, learning curve production calculations	GEPI	H66	BASIC	RS	M	936
LDEF-SS, two-phase fluid flow in spray dryers	DCRL	3033	F+BAL	RS P C	H	1027
LDEF-SS, two-phase fluid flow in spray dryers	LANL	7600B	F77	RS P	H	1027
LEAK, sodium flow heat transport system leaks	FBRD	6000	F	RS P	H	R9763
LENSDES, nonlinear least sq lens design system	LANL	6600B	F4	RS P C	W	602
LEOPARD,SPOTS, spectrum calc with depletion	WAPD	360C	F4	RS PLXC	B	279
LEOPARD,SPOTS, spectrum calc with depletion	JNC	1108B	F5	RS PLX	B	279

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LIFE3, mixed-oxide fuel element performance	ANL	7600	F4	RS	P			I		R 460
LIFE3, mixed-oxide fuel element performance	ANL	370	F4	RS	P		C	I		R 460
LIFE4.REV0, fast reactor fuel pin performance	WAES	7600	F4	RS	P			I		S9821
LINDA, evaluation of strain-gage data	ORNL	360	F+BAL	RS	P			I		657
LINEAR,SIGMA1, linearize & broaden ENDF/B data	LLNL	7600	F4	RS	P			B		747
LINPACK, simultaneous linear algebraic equatns	ANL	370	F4	RS	P	X		P		800
LINSED, 1d multireach sediment transport model	ORNL	360	F4	RS	P		C	R		930
LION, 3-d temperature distribution program	FW	1108B	F4	RS	P			H		R 299
LION, 3-d temperature distribution program	CHI	1108A	F4	RS	P			H		R 299
LION4, 3-d temperature distribution program	FW	360	F4	RS	P		C	H		R 299
LION4, 3-d temperature distribution program	KAPL	6600B	F+ASC	RS	P			H		R 299
LIZARD4, nonlinear differential eqns solution	KAPL	6600	F+ASC	RS	P			P		R 445
LMA,ITP, logic machine architecture for UNIX	ANL	VX11B	PAS	RS	BP	XC		P		9828
LMA,ITP, logic machine architecture for VMS	ANL	VX11	PAS	RS	BP	X		P		9828
LMA,ITP, logic machine architecture	ANL	3033	PAS	RS	BP	XC		P		9828
LOCK, few-channel coolant-flow blockage study	PNC	360	F4	RS	P			H		732
LOGD, multichannel log-derivative scattering	AERO	7600	F4	RS	P	XC		W		941
LOTS, Los Alamos optical transport simulator	LANL	7600	F4	RS	L	C		W		9857
LPMGB, linear programming subroutine w/bounds	SNLA	370	F4	RS	P			P		913
LPMGB, linear programming subroutine w/bounds	SNLA	7600	F4	RS	P			P		913
LR, LR(1) grammar analyzer & parser generator	LLNL	370	F4	RS	P	X		P		822
LRSYS, PASCAL LR(1) parser generator system	LLNL	MPL2	PAS	RS	P	X		P		9721
LRSYS, PASCAL LR(1) parser generator system	LLNL	PC__	PAS	RS	BP	X		P		9721
LSAP/DIGLIB, linear systems analysis program	LLNL	VX11	F+P+M	RS	BP	XC		N		1033
LSODA, ODE solver w/automatic method selection	LLNL	3033	F4	RS	P			P		9937
LSODA, ODE solver w/automatic method selection	LLNL	7600	F4	RS	P			P		9937
LSODAR, ODE system solver with rootfinding	LLNL	3033	F4	RS	P			P		9936
LSODAR, ODE system solver with rootfinding	LLNL	7600	F4	RS	P			P		9936
LSODE, ordinary differential eqn system solver	LLNL	7600B	F4	RS	P			P		592
LSODE, ordinary differential eqn system solver	LLNL	370B	F4	RS	P			P		592
LSODES, ODE system solver for sparse Jacobian	LLNL	3033	F4	RS	P			P		9938
LSODES, ODE system solver for sparse Jacobian	LLNL	7600	F4	RS	P			P		9938
LSODI, ODE system solver for implicit form	LLNL	3033	F4	RS	P			P		9939
LSODI, ODE system solver for implicit form	LLNL	7600	F4	RS	P			P		9939
LSODP, ODE system solver projection method	LLNL	3033	F4	RS	P			P		9686
LSODP, ODE system solver projection method	LLNL	7600	F4	RS	P			P		9686
LSOIBT, implicit ODE systems block-tridiagonal	LLNL	3033	F4	RS	P			P		9832
LSOIBT, implicit ODE systems block-tridiagonal	LLNL	7600	F4	RS	P			P		9832
LSTSQ, least squares gamma spectra analysis	ANL	360	F+BAL	RS				O		9896
LUGS, stress for integral attachments to pipe	ORNL	360	F4	RS	P			I		648
L2RMAT, coupled channel inelastic scattering	LANL	7600	F4	RS	P	XC		W		987
MACH1, 1-d multi-gp diffusion slab cyl sphere	MTS	360	F4	RS	BP	LX	C	C		262
MACH1, 1-d multi-gp diffusion slab cyl sphere	PURD	6500	F4	RS	PLX			C		262
MACKLIB4, CTR nuclear response function data	ANL	370	EBCDC	R		LX		Z		9898
MACK4, nuclear response functions from ENDF/B	ANL	370	F4	RS	P		C	B		9897
MACS LATTICE VIBRATION NEUTRON SCATTRING CODES	EG&G	360	F4	RS	P		C	W		574
MADS, JOSHUA module analysis & documentation	DP	360	F+BAL	RS			C	M		9869
MAEROS, multicomponent aerosol time evolution	SNLA	7600	F4	RS	P			R		1006
MAG2D.REV1, 2 1/2-dimension magnetic modeling	UUGG	400	F4	RS			C	R		9986
MALAPROP, light propagation in large lasers	LLNL	CRA1	F77	S	P			W		9840
MANE1, rectangular magnetic network solution	BAPL	6600B	F4	RS	P			I		R 412
MANTA, steady-state thermal-hydraulic analysis	NED	635	F4	RS	P			H		256
MANTA, steady-state thermal-hydraulic analysis	WARD	6600	F4	RS	P			H		256
MAPPER-GEPI, predicting equipment requirements	GEPI	GETS	BASIC	R				M		595
MAPPER, report quality graphics on command	LANL	VX11	F4	RS	P	X		N		939
MAPPER, report quality graphics on command	LANL	7600	F4	RS	P	XC		N		939
MAPPER, report quality graphics on command	ORNL	DE10	F4	RS	P			N		939
MAPPER, report quality graphics on command	ORNL	360	F4	RS	P		C	N		939

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MAPPER, report quality graphics on command	LANL	6600	F+COM	RS P XC	N	939
MAPPER, report quality graphics on command	LANL	CRA1	F4	RS P X	N	939
MARCH2, LWR meltdown accident response model	BCL	C180	F77	RS PL C	G	734
MARGE/SLUMP, maximum temperature LMFBR fuelpin	ANL	360	F4	RS P	H	677
MARLOWE, binary collision cascade simulation	ORNL	360C	F+BAL	RS P X	Q	680
MARLOWE, binary collision cascade simulation	ORNL	7600	F+BAL	RS P X	Q	680
MASEC1,MASEC2, multi-tech life cycle costing	MASE	C170	F+COM	RS PL	T	9870
MATADOR, radionuclide behavior in containments	BCL	C180	F5	RS P C	G	745
MATHDOC, VAX on-line SLATEC1.0 documentation	SNLL	VX11	F77	RSBPLXC	M	9933
MATLOC, thermal stress bilinear locking rock	BPMD	C176	F4	RS P	R	R9851
MATUS, 3-d finite-element elastic analysis	BAPL	6600	F+COM	RS P X	I	R 597
MAXPRES2, fluid flow & pressure during a HCDA	WAES	7600	F4	RS P	H	R9802
MAYU04, transient thermal hydraulic rod study	NED	6000	F4	RS P	H	9871
MAZE, input generation for DYNA2D & NIKE2D	LLNL	CRA1	F4	RS	L	9907
MAZE, input generation for DYNA2D & NIKE2D	LLNL	VX11	F77	RS X	L	9907
MC••2-2, fast neutron spectra & multigp x-secs	ANL	370C	F+BAL	RSBPL C	B	R 355
MC••2-2, fast neutron spectra & multigp x-secs	ANL	370D	F+BAL	RSBPL C	B	355
MC••2-2, fast neutron spectra & multigp x-secs	ANL	7600C	F+COM	RS PL C	B	R 355
MDSFP, FEM elastic solution of 3-d structures	BAPL	7600	F4	RS P	I	R9947
MEDPI, model of paper industry's energy demand	ORNL	360	F4	RS P	T	9883
MELD, ab initio SCF & CI method wavefunctions	UWCC	MPL2	F77	S PLX	W	9809
MELT3, fast reactor transient overpower study	HEDL	6600	F4	RS P C	F	700
MESA, maximum entropy time series analysis	ORNL	370	F4	RS P	P	825
MESH3D, 3-d finite-element mesh generation	PW	370	F4	RS P	I	R 597
MESOI2.0, puff dispersion model w/deposition	BNW	VX11	F77	RS P	R	9862
METACAD, AGS880 data structure usage routines	SNLA	VX11	F77	RS	T	9726
METER, MC simulation of complex interactions	BAPL	6600	F4	RS P	P	R9854
METRICATION, conversion to or from SI units	RDYN	370B	F4	RS P	P	G 668
MF.CH, Metafont change files typeface design	BKY	VX11	P+WEB	S X	P	9727
MFAULT, fault tree analysis cut set prediction	BNW	CY74	F4	RS P C	G	9975
MICHRD, microhardness measurement analysis	GEC	635	F4	RS P	O	421
MINPACK1, nonlinear equations & least squares	ANL	370B	F4	RS P X	P	888
MINX, multigroup xsections from ENDF/B V4 data	LANL	7600	F+COM	RS PL	B	851
MINX, multigroup xsections from ENDF/B V4 data	ORNL	370	F+BAL	RS PL C	B	851
MIRAB,MIRAP, containment system iodine removal	BCL	6400B	F4	RS P X	G	499
MMM3, coordinate analyses semi-rigid molecules	EG&G	360	F4	RS P	W	632
MMT, 1-d radionuclide ground water transport	BPMD	C176	FTN5	RS PLX	R	R9853
MNN, solution of close coupling equations	MINN	7600	F4	RS P XC	W	942
MOBY, mobile home heating & cooling energy use	ORNL	360	F4	RS P X	R	724
MOCARS, MC distribution & simulation limits	EG&G	CY76	F+COM	RS P C	G	912
MOCUS, minimal sets from fault trees	EG&G	360	F4	RSBP C	G	653
MODEL, modified Bettis envirnmntl lib SCOPE2.0	CEND	7600B	F4	RS	P	478
MODEL, modified Bettis envirnmntl lib SCOPE3.3	CDC	6600D	F+COM	RS	P	478
MODQKE,MDOF, generate design response spectra	HEDL	1100	F	RS P XC	I	R9930
MOD5, stochastic model of neutron slowing-down	NPGS	360	F4	RS P X	E	491
MOLSCAT, molecular scattering program	NASA	7600	F4	S P X	W	9984
MOL1D, partial differential equations solution	UBC	A470	F4	RS P	P	834
MOL1D, partial differential equations solution	LANL	6600B	F4	RS P	P	834
MONA, 1-d multigroup diffusion slab, cyl, sph	EG&G	360	F4	RSBP C	C	582
MOPAC, chemical quantum molecular orbitals	UTEX	VX11	F77	RS P XC	W	9913
MORSE-L, Monte Carlo multigroup transport code	LLNL	7600	F	RS	J	9912
MORTRAN2, macro-based structured Fortran	SLAC	360	F4	RSBP XC	P	678
MOST, a multidimensional optimization scheme	KAPL	6600	F4	RS P	P	R 446
MOXY/MOD032, BWR core heat transfer code	EG&G	7600	F+COM	RSBP C	H	551
MOXY/MOD032, BWR core heat transfer code	EG&G	360B	F4	RSBP XC	H	551
MRSPAK, combinatorial geometry PADL2 add-on	SNLA	VX11	FLEX	RSBP C	T	9730
MSCAT, slow neutron multiple scattering calc	MACU	360B	F4	RS P C	W	575
MSF21,VTE21, desalination plant optimization	ORNL	360	F+BAL	RS P	D	798

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MT2D.REV0, 2d FEM MT-line source resistivity	UUGG	1108	F5	RS P	R	9992
MT2D.REV1, 2d FEM MT-line source resistivity	UUGG	1108	F+ASM	RS XC	R	9992
MT2D.REV3.1, 2d FEM MT-line source resistivity	UUGG	400	F4	RS	R	9992
MT3D.REV2, 3d magnetotelluric modeling program	ANL	VX11	F77	RS PL	R	1005
MT3D.REV2, 3d magnetotelluric modeling program	UUGG	400	F4	RS PL C	R	1005
MUCHA1,MUCHA2, multiple channel analysis ECC	BCL	6400	F4	RS P X	G	508
MULTAN78, x-ray diffraction structure solution	UOYE	7600	F4	S X	W	9881
MULTAN78, x-ray diffraction structure solution	UOYE	VX11	F4	S X	W	9881
MULTAX-PLOT, multiaxis NC machine verification	SNLA	VX11	F77	RSBP C	T	9818
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MULTITASKER, multitasking environment kernel	LLNL	VX11	C	RSBP XC	P	9684
MUSCAT, view factor shielding code cavity geom	GGA	1108	F4	RS P	J	259
M0266, linear elastic structural dynamics	BAPL	6600	F4	RS P	I	R 383
M0457,PIPE, elastic stress of piping system	BAPL	6600	F4	RS P	I	R 329
M0552, dynamic analysis linear elastic systems	BAPL	6600	F4	RS P	I	R 283
M0555,ACT1, loss-of-coolant accident analysis	BAPL	6600	F4	RS P	G	R 284
M0648, 1-d slab transport with slowing down	BAPL	6600	F4	RS	C	R 342
M0661,M0657,M0626, polynomial curve fitting	BAPL	6600	F4	RS P	P	R 411
M0756,LETO, 1-d slab gamma-ray transport	BAPL	6600	F4	RS P	J	R 343
M0807, 2-d diffusion absorption removal x-secs	BAPL	6600	F4	RS	B	R 280
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NAHAMMER, fluid hammer analysis piping system	ANL	360	F4	RS P	G	717
NAHAMMER, fluid hammer analysis piping system	ANL	7600	F4	RS P	G	717
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NASSI, create & modify structured flowcharts	LLNL	PD11	F4	RS	P	9949
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NCAR GRAPHICS, graphics utilities and plot pkg	NCAR	3033	F+BAL	RS PLX	P	993
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NETFLO, network steady state groundwater flow	BPMD	C176	F4	RS P	R	R9831
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NPRFCCP, fuel cycle costs performance data	UEC	6600	F4	RS P	D	146
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ODEPACK, a collection of ODE system solvers	LLNL	7600	F4	RS	P		P	9935
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PASOLE, simulation of passive solar systems	LANL	7600	F4	RS	P		T	850
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RCTRMO, zinc ferrite coal-gas desulfurization	METC	VX11	F4	RS P	U	9767
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REBUS2, fuel cycle analysis for fast reactors	ANL	360C	F+BAL	RSBPL C	D	634
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RSX-MULTI, experiment control & data analysis	FNAL	PD11	F+MAC	RS P XC	O	9716
R101, space-independent kinetics kex options	ANL	360	F4	RS P	E	255
R102, space-independent inverse kinetics calc	ANL	360	F4	RS P	E	168
SABOR4, discrete-element analysis thin shells	MIT	360	F4	RS P	I	R 402
SAFE-AXISYM, stress analysis axisymmetric load	INER	CY73	F4	RS P	I	251
SAFE-CRACK, viscoelastic analysis of concrete	GGA	1108	F5	RS P	I	451
SAFE-CREEP, viscoelastic analysis of concrete	GGA	1108	F4	RS P	I	300
SAFE-PLANE, plane stress analysis, 2-d bodies	BNL	6600	F4	RS P	I	252
SAFE-PLANE, plane stress analysis, 2-d bodies	GGA	1108	F4	RS P	I	252
SAFE-SHELL, stress analysis thin shells	GGA	1108	F4	RS P	I	253
SAFE-SHELL, stress analysis thin shells	INER	CY73	F4	RS P	I	253
SAFE-2D, plane & axisymmetric stress analysis	GGA	1108	F4	RS P	I	379
SAFE-3D, 3-d composite structure stress study	GGA	1108	F4	RS P	I	332
SAFE-3D, 3-d composite structure stress study	ORNL	360	F+BAL	RS P	I	332
SAFE, fail-to-safe anal of protective networks	UWWA	1106	F4	RS P	G	890
SAFTAC, Monte Carlo fault tree simulation code	NEA	360	F4	RS P	G	674
SAFTAC, Monte Carlo fault tree simulation code	UNI	1108	F+SLE	RS P	G	674
SAGE-WASP, optimal electric utility expansion	TVA	370	F4	RS P C	D	S 744
SALE, analytical chemistry quality control	EG&G	360	F+BAL	RS P	U	919
SALE2D, general transient fluid flow algorithm	LANL	7600	F4	RS P	H	900
SALE3D, ALE treatment of 3-d fluid flows	LANL	CRA1	F4	RS P	H	9979
SALT-ANL, systems analysis process simulation	ANL	3033	PL1	RSBPL C	T	9695
SALT4, bedded salt radioactive waste storage	BPMD	C176	F4	RS P	R	R9849
SAMPLE TRANSACTION SYSTEM, analytical chemists	ORNL	DE10	C+ASM	RS C	M	1009
SAMPLE, Monte Carlo uncertainty analysis code	NRC	370	F4	RS P	P	879
SAMS, coupled channel molecular scattering	UICS	C175	F4	RS P XC	W	1026
SANDIA-ORIGEN, isotope generation & depletion	SNLA	7600	F	RS PL	D	874
SAP4, structural analysis of linear systems	ANL	370G	F4	RS P C	I	641
SAP4, structural analysis of linear systems	UUCC	1100	F+ASM	RS P C	I	641
SAS1A, fast reactor power and flow transients	ANL	360	F4	RS P	F	400
SAS1A, fast reactor power and flow transients	ANL	6600	F4	RS P	F	400
SATDSK, saturated iron magnetic field study	ORNL	360	F+BAL	RS P C	V	944
SCAP, point kernel single or albedo scatter	WARD	7600	F+COM	RS PLXC	J	R 933
SCHAFF, heat & water transfer in porous media	BKY	7600	F4	RS P	H	802
SCIENTIFIC WORKSTATION EVALUATION BENCHMARK	ANL	MPLN	F77	RS P	Z	9717
SCORE-EVET, 3d hydraulic reactor core analysis	EG&G	7600	F4	RS PLXC	G	931
SCORE3, SCISRS ENDF/B graphic x-sec evaluation	AI	360	F+BAL	RSB L C	M	375
SCRAM, control rod - guide duct interference	FBRD	6000	F4	RS P	I	R9754
SCREEN, identifying effective input variables	ANL	370	F+BAL	RS P X	G	1002
SEALSHELL2, shell stress analysis axisym load	WTSC	7600	F4	RS P	I	R 282
SEALSHELL2, shell stress analysis axisym load	SR	360	F4	RS P	I	R 282
SEALSHELL2, shell stress analysis axisym load	BAPL	6600	F4	RS P	I	R 282
SEAM1, Stirling engine analysis Rios solution	ANL	370	F4	RS P	H	9943
SECTION.REV1, plot geochemical drill hole data	UUGG	1108	F+ASM	RS X	R	977
SEDIS, social economic environmental data	BKY	VX11	F+R+C	R B LXC	M	9859
SEPHIS/MOD4, solvent extraction simulation	ORNL	360B	F4	RS P	U	R 690
SERI-RES, thermal analysis residential bldgs	SERI	C170	F77	RS PLX	T	9932
SERICOST, avoided costs of electric utilities	SERI	1100	F4	RS P	D	9964

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SERICPAC, electric utility avoided cost rates	SERI	VVIP	F4	RS	L	D	9963
SETS, set equation transformation system	SNLA	CY76	FTN4	RS	P XC	P	623
SHAFT79, 2-phase geothermal reservoir model	BKY	7600	F4	RS	PLX	H	893
SHAMT, steady forced-convection heat transfer	LLNL	7600	LRL	RS		H	9867
SHELL5, thin shell 3-d structural analysis	GGA	1108	F5	RS	P	I	452
SHLOG, data management, editing, & analysis	BAPL	6600	F4	RS	P	M	R 557
SHOCK, dynamic response of lumped-mass systems	SNLL	6600B	F4	RS	P	I	795
SIEX, LMFBR fuel pin thermal performance model	HEDL	6600	F	RS	P	H	673
SIG, signal processing, analysis, & display	LLNL	VX11B	F77	RSBP	XC	T	9787
SIGPLOT, resolved multilevel B-W x-sec calc	BNL	6600	F4	RS	P	A	377
SIMMER2, 2-d Sn neutronics & fluid dynamics	LANL	MPL4	F	RS	P X	F	R9965
SIMPLE1, time-sharing programming language	KAPL	6600	F+ASC	RS		P	R 442
SISAL,IF1, parallel machine data-flow language	LLNL	VX11	PAS	RSBP	X	P	9707
SITE2, energy facility siting assessment	ANL	360	F4	RS	P	R	687
SIZZLE, 1-d multigroup diffusion depletion	AI	360	F4	RSBP	X	D	58
SKILLS INVENTORY, personnel information system	H&N	6400	F4	RS	P C	M	801
SLAB, response in fluid sinusoidal temperature	WARD	7600	F4	RS	P	H	1018
SLACKLY, 1d multicavity Klystron tube analysis	SLAC	360	F4	RS	P	V	807
SLACMON 2.2, OS360 MVT/MFT performance monitor	SLAC	360	BAL	RS	C	P	635
SLACMON/370, Version 4.0 VS software monitor	SLAC	370	BAL	RSB	C	P	635
SLADE-D, dynamic analysis of thin shells	SNLA	6600	F4	RS	P	I	581
SLATEC2.0, mathematical subroutine library	SLAT	CRA1	F	RS	P X	P	820
SLGTR, slag transport models for duct surfaces	ANL	370	F4	RS	P	H	783
SLIB77, source library file maintenance system	WAPA	MPLNB	F77	RS	X	M	9770
SLIC, interactive graphics 3-d mesh generation	LLNL	7600	F+COM	RS	P X	P	968
SLIDES, for DISSPLA-lettered slides & posters	ANL	370	F4	RS	P C	P	728
SLOP,CROSS, IBM360 Fortran H program checker	ANL	360C	PL1	S	P C	P	647
SLUMB.REV0, 1-d Schlumberger inversion program	UUGG	1108	F+ASM	RS	PL	R	978
SMACS, probabilistic seismic analysis system	LLNL	7600	F4	RS	P XC	I	9706
SML, FORTRAN and CAL source library management	LLNL	MPL2	LRL	RS		P	9724
SNAP5.5, nuclear physics data acquisition	ANL	PD11	F+MAC	RS	X	O	9882
SNEQ, nonlinear algebraic eqn soln curve plot	KAPL	6600	F+ASC	RS	P	P	R 364
SNM, special nuclear materials accountability	ANID	7860	F	RS	X	M	9950
SOCOOL2, sodium-fuel interaction analysis	HEDL	1108	F4	RS	P	G	521
SOCOOL2, sodium-fuel interaction analysis	ANL	360	F4	RS	P	G	521
SOERP, second-order error propagation code	EG&G	360	F4	RS	P	P	764
SOERP, second-order error propagation code	EG&G	7600	F4	RS	P	P	764
SOFIRE2, sodium pool fire 1- & 2-cell analysis	AI	360	F4	RS	P	G	559
SOFTWARE TOOLS, program development environmnt	BKY	VX11	F+RAT	S	XC	P	967
SOFTWARE TOOLS, program development interface	BKY	BASE	F+RAT	S	X	P	967
SOLA-DF, transient 2-dimensional 2-phase flow	LANL	7600	F4	RS	P	H	832
SOLA-ICE, transient compressible fluid flow	LANL	7600	F4	RS	P	H	723
SOLA-LOOP, two-phase flow network analysis	LANL	7600	F4	RS	P	H	859
SOLA-VOF, transient fluid flow free boundaries	LANL	7600	F5	RS	P	H	948
SOLA,SOLA-SURF, transient fluid flow algorithm	LANL	7600B	F	RS	P	H	651
SOLAR HOT WATER MONITORING, image application	SSEC	1000	F4X	RS	P	M	9823
SOLCEL2, simulation of photovoltaic systems	SNLA	6600	F4	RS	P	T	937
SOLCOST3.0, solar heating & cooling design	SEEC	C172	F4	RS	PLX	T	907
SOLDATABQ62, Albuquerque 1962 solar data	SNLA	6600	BCD	R	L	Z	693
SOLDATABQ62, Albuquerque 1962 solar data	SNLA	6600B	BIN	R	L	Z	693
SOLGASMIX-PV, equilibria in chemical systems	ORNL	3033	F4	RS	P	U	9944
SOLSYS, solar energy system simulation program	SNLA	6600B	F4	RS	PL	R	692
SOLTES1, thermal energy systems simulation	SNLA	6600B	F+COM	RS	PL	R	841
SOLVEX, solvent extraction process simulation	DP	360	F4	RS	P	U	662
SOMIX1, sodium spray fires in cylindrical cell	AI	370	F4	RS	P	G	R 751
SORSDB, pressure vessel stress and fatigue	KAPL	6600	F4	RS		I	R 391
SOR3, stress analysis shells of revolution	KAPL	6600C	F4	RS	P	I	R 80
SPAN4, a point-kernel shield evaluation code	BAPL	6600B	F+ASC	RS	P	J	R 462

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SPAR1, shielding with analytic ray-tracing	BAPL	6600	F	RS	P	J	R 823
SPDFG, ab initio self-consistent field program	BKY	370	F4	S		W	9879
SPEAKEASY MU+ SOURCE, language processor	ANL	360B	F+BAL	S	P XC	P	S 593
SPEAKEASY MU+, language processor TSO or batch	ANL	360	F+BAL	RSBP	X	P	593
SPECIAL FUNCTIONS, Chebyshev approximations	LLNL	7600	F4	S	P	P	9886
SPECTR3T, 3-d time dependent resistive MHD	SAI	CRA1	LRL	S		X	9694
SPEKEN, Pearson Spearman & Kendall correlation	ORNL	360	F4	RS	P	P	781
SPIRAL, full-text storage, search & retrieval	SNLA	1108	F+BAL	RSBP		M	R 607
SPIRT, stress-strains from transient pressures	EG&G	CY76	F4	RS	PLX	G	927
SPLPKG,WFCMPR,WFAPPX, Wilson-Fowler spline use	SNLA	VX11	F77	RS	P	P	9736
SPOOL-FIRE, spray-pool burning of sodium	ANL	370	F+CSM	RS	P	G	R 714
SPRAY3, sodium spray release safety analysis	HEDL	CY74	F4	RS	P	G	716
SPRAY3B, sodium spray fires within containment	FBRD	7600	F4	RS	P C	G	R9744
SPXCPL, 2-d modeling of self-potential effects	UUGG	MPL2	F4	RS	P C	R	985
STAFAN, fluid flow, pressure, & stress in rock	BPMD	C176	F4	RS	P	R	R9850
STALS, control rod steady-state hydraulics	FBRD	6000	F4	RS	P C	H	R9753
STATLIB, conversational statistical library	SNLA	VX11	F77	RS		P	9749
STBRSIM, oil shale process simulation model	LLNL	7600	LRL	RS	P	H	9810
STEAM-67, 1967 ASME steam and water properties	DP	360D	F4	RS	P X	H	487
STEEP4, thermonuclear reaction rates	LANL	7600	F4	RS	P	X	749
STEFEG, analysis of PWR & BWR gaseous release	ORNL	360	F4	RS	P C	G	583
STEM, matrix generation for a system of beams	KAPL	6600	F4	RS	P	I	R 337
STESEP, solar total energy system evaluation	AI	6600	F4	RS	P	R	821
STESEP, solar total energy system evaluation	AI	370	F4	RS	P	R	821
STFLO, steady-state water flow in porous media	BPMD	C176	F4	RS	P	R	R9852
STFODE,COLODE, collocation soln of stiff ODE's	ANL	360	F	RSBP		P	652
STFODE,COLODE, collocation soln of stiff ODE's	SNLA	6600	F	RS	P	P	652
STINT3, single-channel space-time synthesis	KAPL	6600	F4	RS	P	F	R 389
STOPS, power system short-term optimization	ORNL	3033	F4	RS	P C	D	958
STRAP, static & dynamic structural analysis	EG&G	360	F4	RSBP	C	I	539
STRIPE, fuel rod clad strain & pellet cracking	BAPL	6600	F4	RS	P	I	R 570
SUBDOSA, external dose airborne radionuclides	BNW	1100	F	RS	PLXC	G	924
SUGAR-MD, 2-d natural gas reservoir simulator	METC	VX11	F4	RS	P	H	9890
SULCAL, model of sulfur chemistry in a plume	ORNL	360	F4	RS	P	R	788
SUMOR, s-wave neutron x-section calculation	BAPL	6600	F4	RS	P	A	R 399
SUPAN, analysis of beam-type piping supports	EG&G	7600	F	RS	P	I	842
SUPERENERGY2, steady-state LMFBR core analysis	BNW	7600	F4	RS	P X	H	R 904
SUPERTOG, ENDF/B fine-gp constants generation	ORNL	360	F4	RS	P	B	431
SUPORT, solution of boundary-value problems	SNLA	6600	F4	RS	P	P	731
SUPORT, solution of boundary-value problems	ANL	370B	F4	RS	P	P	731
SURGTANK, reactor steam surge tank dynamics	UOCC	360	F4	RS	P	H	853
SVDI, virtual device interface for graphics	SNLA	MPL3	F+ASM	RS	P	N	9985
SWAAM-LT, long-term sodium-water reaction	ANL	3033	F4	RS	P	G	R9718
SWAAM1, LMFBR sodium-water reaction analysis	ANL	370	F4	RSBP	C	G	R 885
SWAC13, sodium-water reaction two-phase flow	ANL	3033	F4	RSBP		G	R9691
SWAC13E, sodium-water reaction two-phase flow	ANL	3033	F4	RSBP	C	G	R9691
SWAP9, stress-wave analysis in 1-d strain	SNLA	6600	F4	RS	PL C	I	828
SWENT, 3d transport simulation geologic medium	BPMD	C176	F4	RS	PL	R	R9811
SWIFT, waste-isolation flow & transport model	SNLA	7600	F4	RS	P	H	973
SYN, 2d synthesis multigp diff & 1gp depletion	NED	635	F+GMP	RS	P	D	495
SYN3D, single-channel flux synthesis diffusion	ANL	7600	F+COM	RS	P XC	C	713
SYN3D, single-channel flux synthesis diffusion	ANL	370B	F+BAL	RS	P XC	C	713
SYSREL, reliability analysis of series systems	GEPI	H66	BASIC	RS	P	P	848
T-HEMP3D, elastic-plastic flow in 3-d & time	LLNL	750	F4	RS	LX	H	9766
TACASI, analysis of resonance measurements	GGA	1108	F4	RS	P	A	410
TACO3D, 3-d finite element heat transfer code	SNLL	CRA1	F77	RS	P C	H	9838
TAC2D, steady-state and transient temp calc	ENEA	360	F4	RS	P C	H	408
TAC2D, steady-state and transient temp calc	GGA	1110	F5	RS	P C	H	408

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TAC3D, transient 3-d heat transfer program	GGA	1108	F5	RS	P	H	414
TALKPLOT, plotting U.S. drill hole locations	LLNL	7600	F77	RS		R	9785
TASK, 1-d multigroup reactor kinetics program	ORNL	360	F4	RS	P XC	E	558
TAURUS, 3-d finite element code postprocessor	LLNL	VX11	F77	RS	X	N	9908
TAURUS, 3-d finite element code postprocessor	LLNL	CRA1	F4	RS		N	9908
TCB01, creep-buckling of tubes under pressure	BAPL	6600	F4	RS	P	I	R 604
TCU50, timing control unit for LSI-11 systems	LLNL	PD11	ASM	SB	X	P	1013
TDC, chemically reacting hydrodynamic flows	LLNL	CRA1	LRL	RS	P X	H	9892
TDELAY, scattering phase shifts & time delays	ANL	370	F4	RS	P X	A	928
TDELAY, scattering phase shifts & time delays	WAT	7600	F4	RS	P X	A	928
TDIST2, community energy consumption analysis	MIT	370	F4	RS	P	T	799
TDIST3, community energy consumption analysis	MIT	370	F4	RS	P	T	854
TDOWN4, spatial & composition-dependent x-secs	FBRD	6000	F+GMA	RS	PLXC	B	S 505
TEHM, terrestrial ecosystem hydrological model	ORNL	360	F+BAL	RS	P C	R	9873
TEMCO7, temperature coefficient calculation	GGA	1108	F4	RS	P	C	320
TEMPEST-BNW, transient 3-d thermal-hydraulic	BNW	7600B	F4	RS	P X	H	R9808
TEMPEST2, thermal neutron spectrum x-sections	BHSC	360	F4	RS	PL	B	50
TERRAIN.REV0, gravity data terrain corrections	UUGG	1108	F+ASM	RS	X	R	9955
TERZAGI, isothermal fluid flow & subsidence	BKY	7600	F4	RS	P	H	894
THERMIT2, BWR & PWR thermal-hydraulic analysis	MIT	370	F4	RS	P	H	9940
THERMOS LIBRARY, 30-gp ENDF/B scat kernels	DP	360	BCD	R	LX	Z	543
THERPP, thermodynamic properties hydrocarbons	EG&G	MPL2	F4	RS	P XC	H	869
THETA1-B, fuel rod thermal response LOCA	EG&G	360	F4	RSBP	X	G	512
THI3D, thermal-hydraulic multichannel analysis	ANL	370	F4	RS	P C	H	706
THREAD, concentration factors for bolt threads	BAPL	6600	F4	RS	P	I	R1012
THREDES, 1-d few-gp diffusion design system	AI	360	F4	RSBP		K	273
THRES2, statistical model reaction x-sections	ENEA	360	F4	RS	P	A	504
THRES2, statistical model reaction x-sections	BNL	6600B	F4	RS	P	A	504
TIDY-J, Fortran source code editing processor	DP	360	F4	RS	P C	P	896
TIDY3, utility to edit Fortran source programs	BCSR	CY74	F4	RS	P	P	857
TIDY4.63, utility to edit Fortran source code	BCSR	1100	F+ASM	RS	P	P	857
TIMEX, 1-d time-dep multigp discrete ordinates	LANL	360	F4	RS	P	F	756
TIMEX, 1-d time-dep multigp discrete ordinates	LANL	7600	F4	RS	P	F	756
TIPSY, PDQ8 power & fission/cc data processing	BAPL	7600	F+COM	RS		N	R9893
TOAD, processing of analyzer gamma-ray spectra	GGA	1108	F+BAL	RS	P	O	333
TOEPLITZ, Toeplitz & circulant linear systems	ANL	MPLN	F4	RS	P	P	9863
TOKMINA/TOKMINA2, Tokamak fusion reactor study	ANL	360	F4	RS	P	X	561
TOODY2, 2-d Lagrangian eqns of motion solution	SNLA	3600	F36	RS	P	I	627
TOOLPACK1, software tools for FORTRAN 77	ANL	VX11	F+C+P	RS	XC	P	1056
TOPAZ, 2d finite element heat conduction code	LLNL	PC__	F	RSBP	X	H	9801
TOPAZ, 2d finite element heat conduction code	LLNL	MPL2	F	RS	P	H	9801
TOPLYR2, power plant thermal discharge study	HEDL	1108	F5	RS	P	R	599
TOPS, transient thermodynamics of pressurizers	BAPL	6600	F4	RS	P	H	R 348
TOR, thermal scattering crystalline materials	LANL	6600	F4	RS	P	A	360
TOXRISK, toxic gas accident analysis release	SNLA	C170	FTN5	RS	LXC	R	9710
TPT01, 2-d few-group transport with depletion	BAPL	7600	F+COM	RS	P	D	R 669
TRAC-BD1, best estimate analysis BWR LOCA	EG&G	C176B	F+COM	RS	PL C	G	1031
TRAC-BD1, best estimate analysis BWR LOCA	EG&G	C176	F+COM	RSBP	LXC	G	1031
TRAC-PF1, best-estimate analysis PWR LOCA	LANL	7600	F4+C	RS	P X	G	836
TRAC-PF1, best-estimate analysis PWR LOCA	UFCC	370	F+BAL	RS	P XC	G	836
TRANSPORT, design of charged particle beams	FNAL	370B	F4	RS	P C	V	791
TRANSWRAP2, large scale sodium water reactions	FBRD	7600	F4	RS	P	G	G 962
TREDRA, drafting report quality fault trees	ORNL	360	F+ASM	RS	P C	N	1021
TRIAL, 3-d reaction rates from 2-d flux sets	FBRD	6000	F4	RS	P C	C	585
TRIDENT, 2d multigp transport triangular mesh	LANL	7600	F4	RS	P	C	741
TRIDENT, 2d multigp transport triangular mesh	LANL	360	F+BAL	RS	P C	C	741
TRIFIDO, pulsed neutron source data analysis	CNEA	360	F4	RS	P	E	489
TRIPLET, 2-d triangular mesh transport program	LANL	6600	F4	RS	P	C	608

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TRIPLET, 2-d triangular mesh transport program	LANL	360	F4	RSBP	C	C	608
TRIPLET, 2-d triangular mesh transport program	LANL	7600	F4	RS P		C	608
TRIPM, water & solute transport porous media	ANL	370	F4	RS P	XC	R	1028
TRITMOD, advection model of tritium dispersion	DP	360	CSMP	S		R	814
TRIXGL, general line-oriented text editor	LLNL	CRA1	LRL+A	RS		P	9807
TROUT, MUG multigroup xsec library maintenance	NED	1108	F5	RS P		M	493
TROUT, MUG multigroup xsec library maintenance	NED	635	F4	RS P		M	493
TRUMP, transient & s-state temperature dist	ORNL	7600	F4	RS P	X	H	771
TRUMP, transient & s-state temperature dist	ORNL	360	F+BAL	RS PL	XC	H	771
TRUST84, sat-unsat flow in deformable media	BKY	7600	F4	RS P	C	H	9788
TSN, spatially-dependent reactor kinetics	AI	360	F4	RS P		F	309
TSOAK-M1, analysis of fusion detritiation data	ANL	370	F4	RS P	XC	X	875
TUBE, U-tube heat exchanger stress analysis	KAPL	6600	F4	RS P		I	R 378
TVENT, ventilation system transient analysis	LANL	7600B	F4	RS P		H	809
TVENT, ventilation system transient analysis	LANL	360	F4	RS P	C	H	809
TWIGGLE, 2-d 2-gp space-time diffusion	ANL	360	F4	RS P		F	R 338
TWIGL, 2-d 2-gp space-time diffusion feedback	BAPL	6600	F4	RS P		F	R 338
TWODANT, 2d diffusion accelerated Sn transport	ANL	3033	F+BAL	RS P	XC	C	R9837
TWODANT, 2d diffusion accelerated Sn transport	LANL	7600	F4	RS P		C	R9837
TWODANT, 2d diffusion accelerated Sn transport	LANL	VX11	F77	RS P		C	R9837
TWODANT, 2d diffusion accelerated Sn transport	LANL	CRAX	F77	RS P	C	C	R9837
TWOHEX, 2-d x,y triangular mesh Sn transport	LANL	CRA1	F77	RS P	C	C	R9778
TWOTRAN-PNVW, 2-d particle transport xy rz rth	LANL	7600	F4	RS P		C	573
TWOTRAN2, 2-d multi-gp transport xy rz rtheta	LANL	360D	F4	RSBP	C	C	358
TWOTRAN2, 2-d multi-gp transport xy rz rtheta	LANL	7600D	F4	RS P		C	358
TWOTRAN2, 2-d multi-gp transport xy rz rtheta	LANL	6600D	F4	RS P		C	358
TXT, technical document word processing system	ANL	PD11	F+MAC	RSB	X	P	9919
UB1, HP subroutine name & location management	LLNL	1000	F+MAC	SB	XC	M	9734
UCMD108, AGS polyarc/path integrity verifier	SNLA	PD11	F+MAC	RS	C	T	9747
UCMD109, AGS880 x-y coordinate table generator	SNLA	PD11	F+MAC	RS	C	T	9746
UCMD92, mass properties analysis AGS/880 file	SNLA	PD11	F+MAC	RSB	C	T	9709
UDAD, uranium dispersion & dosimetry model	ANL	370	F+P+A	RS P	XC	R	824
UNIWIGL, 2-group time-dependent 1-d diffusion	BNW	6600	F+COM	RS P	C	F	R 870
UPD, source deck maintenance utility routine	TVA	360	F+BAL	RS P	XC	M	864
UPSON, natural scene ray-tracing graphics	LLNL	CRA1	LRL	RS		P	9733
UTAH2, thermoplastic response anisotropic rock	BPMD	C176	F4	RS P		R	R9848
UT200, DEC emulation of CDC200 user terminal	BNW	PD11	PAL	RS		P	916
U25DDS, MHD data acquisition & display system	ANL	370	F+P+A	RSBP	C	O	9880
U3R, unresol resonance xsec probability tables	AI	360	F+BAL	RS P	C	A	553
VARI-QUIR, time-dep 2-d multi-gp diffusion	WANL	6600	F4	RS P		C	212
VARI-QUIR, time-dep 2-d multi-gp diffusion	UMCC	360	F4	RS P		C	212
VARI-1D, 1-d variational sensitivity	ANL	360	F4	RSBPL	C	C	625
VARR2, CRBRP 2-d transient fluid flow analysis	WARD	7600	F+COM	RS P	XC	H	755
VELVET2, turbulent flow in LMFBR rod bundle	NED	635	F4	RS P		H	458
VENTURE, 1, 2, or 3-d multigroup diffusion	ORNL	360	F+BAL	RSBP	C	C	686
VENUS2, 2-d coupled neutronics-hydrodynamics	ANL	7600	F4	RS P		F	511
VENUS2, 2-d coupled neutronics-hydrodynamics	ANL	360	F4	RS P	C	F	511
VERTPAK1, code verification analytic solutions	BPMD	C176	F4	RS P		R	R9826
VIEWPIN, view factor calc for cylindrical pins	EG&G	360	F4	RSBP	C	J	569
VIM2/13, continuous energy MC neutron transprt	ANL	370B	F+BAL	S PL	XC	C	510
VIM2/13, continuous energy MC neutron transprt	ANL	7600	F+COM	S PL	XC	C	510
VISCOT, rock mass viscous mechanical behavior	BPMD	C176	F4	RS P	X	R	R9846
VIVAS2, A-BC exact coupled channel scattering	UOO	VX11	F77	RS P		W	966
VMCON, nonlinearly constrained optimization	ANL	370	F4	RS P		P	922
VUGRAPH, plots presentation-quality viewgraphs	LLNL	9825	HPL	RS P		P	884
WAMPUM, fuel cycle costs performance study	UEC	6600	F4	RS P		D	224
WAPPA, waste package performance assessment	BPMD	VX11	F77	RS PL		R	R9673
WASP2, water properties for safety analysis	BAPL	7600	F4	RS P		H	R 396

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WATER, steam tables 14.5-14,500psia 32-472degF	BAPL	6600	F4	RS			H	R 267
WATRE, heated concrete water and gas release	HEDL	1100	F77	RS	P		G	R9705
WECS, wind energy value to electric utilities	SERI	7600B	F4	RS	PL		D	932
WECSAM, wind energy conversion system analysis	SERI	7600	F5	RS	PL	C	T	9982
WELBORE, transient wellbore fluid flow model	BKY	7600B	F4	RS	P		H	895
WELLOG.REV1, well log data analysis & plotting	UUGG	1108	F+ASM	RS		C	R	9980
WELLOG.REV2, well log data analysis & plotting	UUGG	400	F4	RS		C	R	9980
WELWING, material buckling cyl fuel elements	AEB	360	F4	RS	P		B	362
WFLLL2B, wire configuration frequency domain	LLNL	7600	F4	RS	P		T	721
WHAM6, liquid-filled piping system analysis	EG&G	360B	F+BAL	RS	P		G	278
WHAM6, liquid-filled piping system analysis	ANL	7600B	F4	RS	P		G	278
WHIP1, structural deflection due to blowdown	BAPL	6600	F4	RS	P		G	R 863
WHTM, Wisconsin hydrologic transport model	ORNL	360	F+BAL	RS	P	C	R	808
WIGL2, 1-d 2-gp space-time diffusion 3-geom	UFCC	370	F4	RS	P		F	R 274
WIGL2, 1-d 2-gp space-time diffusion 3-geom	GGA	1108	F4	RS	P		F	R 274
WIGL2, 1-d 2-gp space-time diffusion 3-geom	BAPL	6600	F4	RS	P		F	R 274
WIGL3, 1-d space-time diffusion w/feedback	BAPL	6600	F4	RS	P		F	R 708
WOOD4.VER2, economics of wood energy systems	SSEC	C175	F4	RS	P		D	994
WORK SAMPLING, automated work sampling studies	GEPI	H66	COBOL	RS	P	C	M	9954
WRAPUP, LMFBR fuel cladding interactions	WAES	7600	F4	RS			I	R9806
WREM-TOODEE2/MOD3, 2d time-dep fuel elem study	NRC	370	F4	RSBP		C	G	712
WREM-TOODEE2/MOD3, 2d time-dep fuel elem study	NRC	7600	F4	RS	P		G	712
WSP-HASP/DOS, DOS-MFT remote workstation pkg	ANL	360B	F+ASM	RSB		C	P	541
WYLVAX, interactive line-oriented text editor	SLAC	VX11	F+MAC	RSB	L	C	P	1003
XASW, solves x-alpha scattered wave equations	HU	VX11	F4	S	PLX		W	9961
XCC, Sperry-Univac V77-600 C cross-compiler	SNLA	PD11	C	S	L	C	P	9822
XDTRAP, hydrogen permeation with trapping	DP	360	F4	RSBP			Q	655
XERROR, Fortran library error-handling package	SNLA	7600	F	RS	P		P	988
XOQDOQ, nuclear power plant effluent releases	NRC	370	F4	RS	P		R	964
XOQDOQ, nuclear power plant effluent releases	ESC	C175	F77	RS	P		R	964
ZONE, 2-d finite element mesh generator	LLNL	7600	F	RS	P		N	765
ZOOM, Omnimax view of diamond crystal lattice	LLNL	7600	LRL	S			P	9798
ZPR-III ASSEMBLY 48 GAFGAR ENDF/B DATA TAPES	GGA	1108	BIN	R		L	Z	356
1DX, 1-d diffusion fast x-section generation	BNW	1108	F4	RS	P	X	B	374
1DX, 1-d diffusion fast x-section generation	ANL	360	F+BAL	RSBP		XC	B	374
2DB, 2-d multigroup diffusion and depletion	LANL	6600	F4	RS	P		D	325
2DB, 2-d multigroup diffusion and depletion	BNW	1108	F4	RS	P		D	325
2DEPEP, elliptic parabolic & eigenvalue solns.	PURD	6500	F4	RS	P	C	P	806
2DF, 2-d multi-gp discrete ordinate code	GGA	1108	F5	RS	P		C	173
2DFLOW, 2-d drainage flow air pollution model	DP	VX11	F77	RS	PL		R	9739
3DB, 3-d multigroup diffusion burnup analysis	ANL	360	F4	RS	P	C	D	567
3DB, 3-d multigroup diffusion burnup analysis	HEDL	1108	F4	RS	P		D	567
3DDT, 3-d multigroup diffusion xyz r-theta-z	LANL	6600	F4	RS	P		D	463
3DXT,DEP3, 3-d xenon transient & depletion	KAPL	6600	F4	RS	P		D	R 477
6KILER, core heatup code for BWR/6 analysis	EI	360	F+BAL	RS	P	C	H	636

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NATIONAL ENERGY SOFTWARE CENTER: COMPILATION OF SOFTWARE ABSTRACTS

by

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PREFACE

As originally published, ANL-7411 was the second complete revision of program abstracts undertaken by the Center. ANL-7411 Revised, published in May 1979, represented the third such revision. With each revision, programs written for machines no longer in use were deleted, and other modifications were made to reflect current Center practice. In September 1982, ANL-7411 Revised Supplement 1 was issued. Supplement 1 contained additional abstracts to supplement or replace those contained in ANL-7411 Revised so as to bring the abstract compilation up-to-date. Supplement 2 is similar; its contents, collated with those of the two earlier ANL-7411 Revised reports, make up the Compilation of Software Abstracts for the current NESC software collection. Other changes introduced with Supplement 2 are the incorporation of screened or "As Is" software abstracts and the adoption of new information item titles to bring the Center's abstract format into closer conformance with the American National Standard.

The table of contents lists the current software collection in accession order, giving for each the KWIC-title of the package, the Center identification of the contributing installation, the computer and programming language used, symbols representative of the package contents, and the subject category of the program. The package contents symbols are defined as follows:

R = traditional hard-copy documentation or reference material,
S = compiler and assembly language source records,
B = object, executable image, or load module records,
P = sample problem input and output data,
L = library information or external data files, e.g., cross-section libraries, steam table or material properties data,
X = auxiliary routines or machine-readable information,
C = operating system control language records.

This collection includes programs in which the program number is preceded by the letter ***R***, ***G***, or ***S***. The letter ***R*** denotes ***restricted***, and U. S. citizens are required to file a release form with the Center for use of the program on either official U. S. government or commercial (nonmilitary) applications at a U. S. installation. The letter ***G*** designates programs which are limited to use on U. S. ***government*** contracts only. In addition to the release form requirement, the contract identification and the signature of the contracting officer must be furnished when requesting such programs. The Software Center is not authorized to distribute these programs outside the United States. The letter ***S*** is used to identify packages which are distributed to a ***special*** list of designated recipients only.

Abstracts for the OECD Nuclear Energy Agency (NEA) Data Bank programs in the National Energy Software Center collection are not included in this compilation. These, as well as the Center's abstracts are available in a database on the Department of Energy's on-line RECON system, and are distributed to NESC registered installations in a separate publication.

I. HISTORY AND ACKNOWLEDGMENTS

In 1956, at the Second Annual Meeting of the American Nuclear Society, the initial meeting of an informal group called the Nuclear Codes Group was held. This group was composed of "persons interested in the development and use of computer programs for reactor design." The group held regular meetings in conjunction with the semiannual ANS meetings and published and distributed a Newsletter containing code abstracts submitted by members. These abstracts followed the format of the Atomic Energy Commission document AECU-3078, *A Bibliography of Available Digital Computer Codes for Nuclear Reactor Problems*.[1]

From September 1956 to December 1959, ten Newsletters were published and distributed through the auspices of the AEC Computing Facility at New York University.[2] In 1959, Ward Sangren and personnel at General Atomics edited and published 300 abstracts collected from Group members.[3] A supplementary list of 100 abstracts was published the following year.[4]

In 1959 also, the Nuclear Codes Group became the nucleus of the American Nuclear Society's Mathematics and Computation Division. With stature came a desire for a central facility for the computer program library and the dissemination of information concerning programs written in the areas of nuclear physics, reactor design, and engineering. In 1960, a proposal was made whereby, with the cooperation of Division members and Installation Representatives, and the Atomic Energy Commission's approval, Argonne National Laboratory undertook to serve as this central agency and the Argonne Code Center was established.

Procedures were drafted defining the material to be collected--the abstract and the "package"--and the responsibilities of the Center and of the Installation Representatives. The submission of the material was made the responsibility of the authors, the developing organization, or the sponsor, either directly or through their designated Installation Representative. The Center was made responsible for editing and publishing the abstracts, and collecting, testing, maintaining, and distributing the packages. The representatives of registered installations--AEC laboratories, contractors, and universities--were to serve as a source of information to personnel at their organization concerning the Center operation and collection, and made responsible for library programs at their installations. In addition, they were asked to provide information to the Center concerning software or requests originating at their installations and, in collaboration with Center staff, to supply the answers to the questions and inquiries received concerning the software developed at their installations.

In 1965 the Argonne Center became a separately-budgeted operation of the Reactor Physics Branch of the USAEC Division of Reactor Development and Technology. In September of 1972 the Argonne Code Center was designated as the

AEC-wide computer program exchange and information center responsible for the dissemination of unclassified computer programs developed with AEC funds. The scope of the agency program was broadened later with the transfer from AEC to ERDA and then to the Department of Energy, and the agency administration of the program was centralized in the agency's Technical Information program. The name was changed to National Energy Software Center in July of 1978 to more adequately reflect the present program and current computing terminology.

From 1961 until issuance of the first edition of ANL-7411 in January 1968, the Argonne Code Center published 12 distributions containing abstracts of approximately 265 programs.[5] The ANL-7411 collection represented a complete revision of those previously published abstracts. The ANL-7411 Revised edition updated with existing Supplements represents the current NESC collection.

II. ABSTRACT FORMAT

The program abstract has been modified considerably over the years. Its evolution from the original AECU-3078 format is due primarily to our experience at the Center and cooperative efforts undertaken with NEA Data Bank personnel and the American Nuclear Society's ANS-10 subcommittee membership.[6] Present plans call for adoption of the American National Standard for a Computer Program Abstract, X3.88-1981, insofar as practicable.[7]

1. Identification and KWIC Title

This is the name or designation given the program(s) by the author, and the KeyWord-In-Context (KWIC) description.

2. Computer for Which Software is Written and Other Machine Versions Available

The computer hardware system for which the program or system was prepared is identified, and names of other computers for which versions are available are listed.

3. Description

A brief description of the problem being solved, the activity being modeled, or a definition of the data processing activity being carried out is given.

4. Method of Solution

A short summary of the mathematical methods employed, numerical algorithms adopted, or procedures incorporated in the program should appear under this entry.

5. Restrictions on the Complexity of the Problem

This item includes restrictions implied by storage allocation, such as maximum number of energy groups and mesh points, as well as those due to approximations used, such as implied argument-range limitations.

6. **Timing**

Information intended to enable the user to estimate machine time requirements is listed.

7. **Unusual Features of the Software**

Distinguishing features and special capabilities of the software are enumerated. Information given under this item should allow the user to select, from a number of similar programs, the one most suitable for a particular problem.

8. **Related and Auxiliary Software**

If this software supersedes or is an extension of an earlier program, this is noted here. Software used in conjunction with this program, e.g., for preparing input data, plotting results, or coupled through use of external data files, is identified.

9. **Status**

The Center lists here the initial date of publication of the abstract. Machine versions in the library are identified and the date they were submitted is given. If this accession number has been used for a number of editions of the program, a chronology of the various editions is included. The most recent testing completed at the Center is noted.

10. **References**

Available publications pertinent to the software are cited. All hard-copy documentation included in the software package is listed.

11. **Hardware Requirements**

This item lists the hardware components essential for full utilization of the software, including the amount of memory required to execute the program.

12. **Programming Language**

The programming language or languages in which the software was written are identified with an indication of the percentage of each used.

13. **Operating System**

This item identifies the operating system, associated subroutine or function library, and installation support software used by the program. The version used is identified and deviations or exceptions noted.

14. **Other Programming or Operating Information or Restrictions**

Additional information needed by the reader to install the software or determine the extent of the necessary implementation effort is summarized. If certain routines are in assembly rather than compiler language, or proprietary software is required, this information is noted.

15. **Name and Establishment of Author or Contributor**

The names and organizations of the software developers or contributors for the various machine versions or editions are listed.

16. **Material Available**

This lists the material being distributed, i.e., the contents of the software package.

17. **Category**

The subject classification chosen from the Center Subject Classification Guide is shown.

Keywords

This is a listing of the keywords associated with the software, supplied by the author or contributor and the Center based on the NESC Thesaurus.

18. **Sponsor**

This is the name of the agency and agency office or division, or other organization, responsible for funding the software development effort.

III. RECOMMENDED SOFTWARE PACKAGE CONTENTS

The "software package" is defined as the aggregate of all elements required for use of the software by another organization, or its implementation in a different computer environment. It is intended to include, insofar as practicable, all material, associated with a computer program, necessary for its modification and effective use by individuals other than the author, on a computer system different from the one on which it was developed.

The software package consists basically of two components--the computer-media material, and the traditional printed material or hard-copy documentation. The material required may include all of the following:

1. **Source Records** (S)

Compiler and assembly language source records.

2. **Executable Records** (B)

Object or load module records prepared by the language processors preliminary to execution of the software. If the program source cannot be distributed for proprietary or other reasons, executable or load modules may be substituted for interchange between users of like systems. This element provides redundancy when included in conjunction with the equivalent source material.

3. **Sample Problems** (P)

Test case input data together with output generated during problem execution, for use in checking program implementation.

4. **Data Libraries** (L)

External data files required for program operation, e.g., cross-section libraries, steam table or material properties data. It is preferable for exchange purposes to use decimal form for numerical data files.

5. **Control Information** (C)

Operating system control language records required for compilation or assembly of the program and execution of the sample problems. This information includes device assignments, format information, storage allocation, overlay structure definitions, etc.

6. **Auxiliary Information** (X)

Software package items for subsidiary programs used in preparing input information, processing results, maintaining data libraries, etc., for the program. Machine-readable documentation, when available.

7. **Documentation** (R)

The traditional documentation associated with the software and its application. This material may be compiled in a single comprehensive report or it may exist as several independent documents--published paper reprints, program reports, user's manuals, software maintenance manuals, installation memoranda, computer output listings, etc. It may, regardless of form, include all of the following:

a. *Problem definition or function description*
Information providing the *raison d'etre* for the computer program or system, a description of the problem solved, the process modeled, or of the processing performed. A description of the mathematical model used and the computational algorithms and techniques employed should be included.

b. *Application information*
Documentation directed to the software user, i.e., a User's Manual, if a separate publication. Operating instructions, program options, and a description of the input and output formats should be covered in sufficient detail to enable the user to specify a problem and interpret the results correctly. An example is helpful; if the identical sample problem of item 3 is used, the selected output for it can be shown in this document; otherwise, it is essential to include a copy of the computer output obtained from execution of the sample problem in the software package for checking implementation.

c. *Programming information*
A detailed description of the software addressed to the programmer responsible for maintenance or transfer of the program; i.e., a Software Maintenance Manual, if a separate publication. Material covered should include the overall program structure and logic, identification of subprograms and detailed information on their use, glossaries showing the relationship between problem variables and program symbols, definitions of external data files, system hardware and software requirements, shared storage assignments, overlay or segment structures, and system-dependent programming considerations.

d. *Installation environment information*
A description of the environment in which the software was developed and installation support facilities utilized such as installation-dependent library routines for mathematical functions, plotting, microfilm recording and the like. It is recommended that general Installation Environment Reports issued by individuals responsible for the computer environment at the software-originating installation be utilized for this part of the software documentation. Such documents can greatly simplify the preparation of portable software packages and facilitate effective software exchange.

Software package items 1 through 6 are most effectively maintained in machine-readable form and transmitted on magnetic tape; item 7 may be distributed either as printed material or on tape as machine-readable documentation. If a large quantity of sample problem output (item 3) is generated, selected hard-copy portions plus the complete output listing on microfiche or magnetic tape may be appropriate. Data libraries (item 4) are often computer-generated and exist only on tape. Control information (item 5) may, alternatively, be supplied as a computer output listing since this information is rarely identical at different installations.

IV. SUBJECT CLASSIFICATION GUIDE

The classification scheme is intended to serve as a guide to library software dealing with the solution of a specific physical problem or area of related applications. The category listed in Abstract Item 17 is selected from the Subject Classification Guide by the author of the software abstract or assigned by the Center staff.

A. Cross Section and Resonance Integral Calculations

Computation of reaction cross sections from nuclear theory such as the optical or Hauser-Feshbach models, resonance cross sections by Breit-Wigner or multilevel theory, determination of differential scattering cross sections, cross-section evaluation, and compilation programs.

B. **Spectrum Calculations, Generation of Group Constants, Lattice and Cell Problems**

Determination of the slowing-down density or thermal spectrum, weighting and averaging of cross sections and related quantities for the production of group constants, and evaluation of design parameters by lattice and cell calculation.

C. **Static Design Studies**

Calculation of the reactivity and flux distribution of the reactor system, and adjustment of design parameters to prescribed specifications, i.e., criticality and power distribution search procedures.

D. **Depletion, Fuel Management, Cost Analysis, and Power Plant Economics**

Includes burnup programs, isotope and fission-product buildup and decay computations, and optimization studies.

E. **Space-Independent Kinetics**

Studies of the time-behavior of reactors, including delayed-neutron effects and feedback mechanisms, and transfer-function evaluation.

F. **Space-Time Kinetics, Coupled Neutronics-Hydrodynamics-Thermodynamics and Excursion Simulations**

Software that considers spatial design characteristics and accompanying effects in studying the time behavior of the reactor.

G. **Radiological Safety, Hazard and Accident Analysis**

Calculation of internal and external dose rates, determination of reactor thermodynamic and hydrodynamic properties following an accident, e.g., release of radioactive materials, coolant system blowdown, steam generator rupture.

H. **Heat Transfer and Fluid Flow**

Steady-state and transient heat transfer computations, fluid-flow studies and calculations of thermodynamic properties.

I. **Deformation and Stress Distribution Computations, Structural Analysis, and Engineering Design Studies**

Includes fuel-element design evaluations, core-configuration studies, and composite structure analysis.

J. **Gamma Heating and Shield Design**

Gamma and photon transport calculations, computation of heat-generation rates, and penetration analysis and leakage calculations for shielding.

K. **Reactor Systems Analysis**

Combinations of programs, designed as systems, for solving correlated problems from several of the categories A through I.

L. **Data Preparation**

Generation of program parameters--checking, editing, and formatting of problem input information.

M. **Data Management**

Construction, maintenance, and retrieval of data files, e.g., cross section libraries, management systems such as payroll, personnel, and financial systems, property and equipment systems, network-oriented project management and indexing and retrieval systems, etc.

N. **Subsidiary Calculations**

Plotting, editing, and display routines that process output data from other programs.

O. **Experimental Data Processing**

Software designed to process data directly acquired from an experimental situation or to assist the experimenter in the design of the experiment.

P. **General Mathematical and Computing System Routines**

Calculation of mathematical functions, statistical analysis, special-language routines with general data-processing capabilities, and software systems.

Q. **Materials**

Measurements and computation of the physical and mechanical properties of materials, simulation of radiation damage processes, corrosion studies, and determination of crystallographic functions.

R. **Environmental and Earth Sciences**

Environmental impact studies, geology, seismology, geophysics calculations, hydrology and ground water studies, bioenvironmental systems analyses, meteorological calculations relating to the atmosphere and its phenomena, studies of airborne particulate matter, climatology, etc.

S. **Space Sciences**

Analysis of orbits and trajectories, astronomy and astrophysics computations, wave propagation studies, and the calculation of reentry parameters.

T. **Electronics, Engineering Equipment, and Energy Systems Studies**

Automated design of electronic equipment, computer-aided design (CAD) and manufacturing (CAM), process control programs, systems analysis, and engineering computations for numerically controlled machine tools and energy consumption analysis in buildings, industry, and transportation.

U. **Chemistry**

Chemical analysis, mass spectroscopy, radiation chemistry, radiolysis studies, etc.

V. **Particle Accelerators and High Voltage Machines**

Programs relating to the design, development and operation of high-voltage machines and particle accelerators such as Van de Graaff generators, linear accelerators, cyclotrons, synchrotrons, etc.

W. **Physics**

Calculations relating to theory of atomic or molecular structure or properties, charged particle collision studies that involve phenomena such as charge exchange, excitation, ionization, dissociation, etc., elementary particle theories and models, scattering theory, quantum field theory and quantum electrodynamics studies, general relativity and gravitation theory computations.

X. **Magnetic Fusion Research**

Electric discharge phenomena and plasma physics computations, electrodynamics and magnetic hydrodynamics studies.

Y. **Biology and Medicine**

Biological, medical and radiological studies of the structure, functions, chemistry, biophysics, reproduction, and heredity of bacteria, plants, laboratory animals, and humans.

Z. **Data**

Data prepared in specified program formats for software testing and evaluation, benchmark studies, or library use.

V. THESAURUS

A thesaurus has been prepared as a basis for the assignment of keywords to the library software. The keywords are taken from the Energy Data Base Subject Thesaurus[8] insofar as practicable. Accepted keywords not listed in the thesaurus include the names or acronyms identifying computer programs and reactors; these are always followed by the word "codes" or "reactors", e.g., AITP3 codes, HTGR reactors. Also accepted but not included in the thesaurus are element names and combinations of an element name and a mass number, e.g., hydrogen, uranium-238.

absorption
abstracts
acceleration
accelerators
accidents
accounting
acoustic monitoring
activated carbon
activation analysis
Adams method
adaptive random search method
adsorption
advection
adversaries
aerial monitoring
aerosols
after-heat removal
agglomeration
aging
air
air cleaning
air conditioning
air pollution
air quality
airfoils
Airy functions
albedo
alcohol fuels
algebra
algorithms
alpha decay
ammonia
ammonium sulfates
anaerobic digestion
analytical solution
angular correlation
angular distribution
angular momentum
anions
anisotropic scattering
anisotropy
annular space
antennas
APPLE computers
APT
aquatic organisms
aqueous solutions
aquifers
Arrhenius equation
artesian basins
aspect ratio
assembler
asymmetric matrices
atmospheric chemistry
atmospheric precipitations
atom collisions
atom impurities
atom-molecule collisions
atomic models
atoms
automated reasoning
availability
averages
background radiation
banded matrix
bandwidth minimization
Barstow solar pilot plant
BASIC
batch loading
beam dynamics
beam transport
beams
benchmarks
bending
Bessel functions
beta particles
bids
binary-fluid systems
biochemistry
biomass
biosphere
BL method
black shales
blackbody radiation
block-tridiagonal matrices
blowdown
body
Bohr-Wheeler theory
boilers
Boltzmann equation
Boltzmann statistics
boreholes
boundary conditions
boundary layers
boundary-value problems
Boussinesq approximation
breeding
breeding blankets
Breit-Wigner formula
brines
bubble growth
buckling
budgets
buildings
buildup
burnable poisons
burnup
C
C language
calculators
calorimetry
CAMAC system
capacity
capital
capitalized cost
capture
carbon dioxide
carbon dioxide injection
carbonization
Cartesian coordinates
Cauchy-Riemann equations
cavitation
cavities
CCCC
CDC computers
cell calculation
central heating plants
central receivers
centrifugal contactors
charge exchange
charged-particle transport
charges
chemical analysis
chemical composition
chemical effluents
chemical lasers
chemical reaction kinetics
chemical reactions
cladding
Clebsch-Gordan coefficients
climates
coal
coal gas
coal gasification
coal-fired MHD generators
cogeneration
Cohen equation
coking
collisions
collocation method
colloids
Columbia river
combustion
combustion control
combustion kinetics
combustion products
combustors
communications
comparative evaluations

composite materials
compound nuclei
compound-nucleus reactions
compressible flow
compression
compressor blades
computer calculations
computer graphics
computer networks
computer output devices
computer-aided design
computer-aided manufacturing
computerized control systems
computerized simulation
computers
concentrating collectors
concretes
condensers
cones
configuration
configuration interaction
construction
containers
containment
containment buildings
containment systems
contamination
contracts
control
control elements
control rod drives
control rod worths
control rooms
control systems
convection
coolant boiloff
coolant loops
coolants
cooling load
cooling systems
cooling towers
coordinates
core flooding systems
corrections
correlation functions
correlations
corrosion
corrosion fatigue
cost
cost benefit analysis
Coulomb field
counter current
coupled channel theory
coupling
cover gas
cracking
CRAY computers
creep
critical heat flux
criticality
criticality searches
cross sections
crystal defects
crystal lattices
crystal structure
crystallography
crystals
cutting
cutting tools
cyclotrons
cylinders
cylindrical configuration
D states
damage
damping
Dancoff correction
Darcy law
data
data acquisition
data acquisition systems
data analysis
data base management
data processing
data transmission
data-flow processing
daughter products
daylighting
DEC computers
decay
decision tree analysis
decomposition
decontamination
defects
deformation
delayed neutron precursors
delayed neutrons
deposition
desalination
design
design basis accidents
desulfurization
deuterium
devolatilization
diagnostic techniques
diagrams
dielectric materials
diesel engines
diesel fuels
difference equations
differential calculus
differential cross sections
differential equations
diffraction
diffraction models
diffusers
diffusion
digital filters
digital frequency analysis
digitizing
dipole moments
dipoles
Dirichlet problem
disadvantage factor
discrete ordinate method
dispersions
display devices
dissolution
distance
distribution
distribution functions
district cooling
district heating
documentation
Doppler broadening
Doppler coefficient
dose commitments
dose rates
doses
dosimeters
drainage
drift tubes
drill bits
drill cores
drilling
drilling equipment
drills
droplets
ducts
DWBA
dynamic loads
dynamic programming
dynamics
earth atmosphere
earthquake foci
earthquakes
economic analysis
economics
ECR heating
eigenvalues
eigenvectors
elastic scattering
elasticity
electric conductivity
electric fields
electric potential
electric power
electric power industry
electric utilities
electricity
electrodes
electromagnetic fields
electromagnetic interactions
electromagnetic pulses
electromagnetic radiation
electron beams
electron cyclotron-resonance
electron multipliers
electron spectra
electron-atom collisions
electron-ion collisions
electronic circuits
electronic equipment
electronic structure
electrons
elementary functions
elements
emergency plans
emission spectra
emissivity
ENDF/B
energy
energy accounting
energy analysis
energy conservation
energy consumption
energy conversion
energy demand
energy efficiency

energy levels
energy management
energy management systems
energy models
energy policy
energy shortages
energy storage
energy supplies
energy systems
energy transfer
energy transport
energy-level transitions
engineered safety systems
engineering
enrichment
enthalpy
environment
environmental effects
environmental impact statements
environmental impacts
environmental transport
epithermal neutrons
equations
equations of motion
equations of state
equilibrium
equipment
erosion
error function
errors
etching
evaluation
evaporation model
evaporative cooling
evaporators
excited states
excursions
expansion
experiment planning
experimental data
explosives
extraction apparatuses
F states
fabrication
failure mode analysis
failures
fallout
fallout deposits
fast fission factor
fast neutrons
Fastbus system
fasteners
fatigue
fault tree analysis
fcc lattices
feasibility studies
feedback
few-group
films
filters
financing
finite difference method
finite element method
finite-range interactions
fires
fission
fission barrier
fission products
fission spectra
flanges
flash heating
flat plate collectors
flexibility
flocculation
flow blockage
flow models
flow rate
flowcharts
flowmeters
flowsheets
fluctuations
flue gas
fluid flow
fluid injection
fluid mechanics
fluidized bed
fluids
flux synthesis
Fokker-Planck equation
foliar uptake
forced convection
forecasting
forests
form factors
FORTRAN
fossil-fuel power plants
Fourier analysis
Fourier transformation
fracture mechanics
fracture properties
fractured reservoirs
frequency response testing
fuel assemblies
fuel cans
fuel cycle
fuel cycle centers
fuel densification
fuel element clusters
fuel elements
fuel gas
fuel management
fuel pellets
fuel pins
fuel rods
fuel slurries
fuel substitution
fuel-cladding interactions
fuel-coolant interactions
fuels
fusion reactions
G states
gamma function
gamma radiation
gamma sources
gamma spectra
gas flow
gas fuels
gaseous wastes
gases
Gauss function
Gauss potential
Ge semiconductor detectors
gears
geochemical surveys
geochemistry
geography
geologic formations
geologic strata
geologic structures
geometry
geophysical surveys
geophysics
geothermal district heating
geothermal energy
geothermal exploration
geothermal fields
geothermal power plants
geothermal systems
geothermal wells
gloveboxes
gloves
government policies
graphs
gravity surveys
Great Lakes region
Green function
Green River formation
ground states
ground water
group constants
group theory
Hamilton-Jacobi equations
Hamiltonians
Hartree-Fock method
Hauser-Feshbach theory
health hazards
heat
heat distribution systems
heat engines
heat exchangers
heat flow
heat pumps
heat transfer
heaters
heating
heating load
heavy ions
heavy water
heliostats
heterogeneous effects
hexagonal configuration
hexagonal lattices
high temperature
high-level radioactive wastes
hot pressing
hot springs
HP computers
human populations
hydraulic conductivity
hydraulics
hydrocarbons
hydrodynamics
hydroelectric power plants
hydrology
hydrothermal systems
hydroxides
IBM computers
ice condensers

ICE method
illuminance
image processing
impact shock
implosions
in-service inspection
in-situ retorting
incoherent scattering
incompressible flow
indexes
induced polarization logging
industrial plants
industry
inelastic scattering
inertial confinement
information retrieval
information systems
ingestion
inhalation
initial-value problems
insolation
inspection
integral calculus
integral equations
integrals
integrated circuits
interactions
interactive computing
interactive display devices
interfaces
internal combustion engines
interpolation
interpreters
inventories
investment
ion beams
ion exchange
ion implantation
ion sources
ionic conductivity
iron oxides
irradiation
isothermal processes
isotope production
isotope separation
isotopes
isotropic scattering
iterative methods
jets
kerma
kernels
kerogen
kinetics
klystrons
Lagrange equations
laminar flow
land pollution
land use
Laplace equation
Laplace transformation
laser isotope separation
lasers
lathes
lattice vibrations
layers
leaks
learning
leasing
least square fit
Legendre polynomials
length
lenses
Li-drifted Ge detectors
libraries
licensing
life-cycle cost
lifetime
light transmission
lighting systems
linear programming
liquid fuels
liquid metals
liquid wastes
liquids
LISP
load collector ratio
load management
log gamma function
loss of coolant
low temperature
low-head hydroelectric power plants
low-level radioactive wastes
LRLTRAN
lubrication
machine tools
machining
magmatic water
magmatism
magnetic disks
magnetic fields
magnetic flux
magnetic surveys
magnetization
magnetohydrodynamics
magnetotelluric surveys
magnets
maintenance
man
management
manufacturing
maps
marginal-cost pricing
Markov process
mass
mass balance
mass spectrometers
mass transfer
materials testing
mathematical logic
mathematical models
mathematics
matrices
maximum entropy method
maximum-likelihood fit
Maxwell equations
measuring instruments
mechanical properties
mechanical structures
mechanical vibrations
mechanics
meetings
meltdown
melting
mesh generation
meteorology
metric system
metrics
MHD channels
MHD generator U-25
microanalysis
microhardness
microprocessors
mill tailings
minerals
mines
miscible-phase displacement
mixer-settlers
mixing ratio
mobile homes
moderators
modified in-situ processes
moisture
molecular biology
molecular models
molecular orbital method
molecular structure
molecule collisions
molecules
molten metal-water reactions
moment of inertia
moments method
monitoring
Monte Carlo method
motors
multi-channel analysers
multigroup theory
multilevel analysis
multiphase flow
multiple scattering
multiplication factors
multipolarity
multiprocessors
multivariate analysis
natural convection
natural gas fields
Navier-Stokes equations
network analysis
neutron absorbers
neutron age
neutron diffusion equation
neutron fluence
neutron flux
neutron reactions
neutron spectra
neutron transport
neutron transport theory
neutrons
Newton method
nitric acid
nondestructive analysis
nonlinear problems
nonlinear programming
nozzles
nuclear cascades
nuclear engineering
nuclear facilities
nuclear fuels

nuclear instrument modules
nuclear materials management
nuclear models
nuclear power plants
nuclear properties
nuclear reaction analysis
nuclear reaction kinetics
nuclear reaction yield
nuclear reactions
nuclear structure
numerical analysis
numerical data
numerical solution
ocean thermal power plants
oil fields
oil shale deposits
oil shales
oil wells
one-dimensional
one-group theory
open-cycle MHD generators
operating cost
operating systems
operation
optical models
optics
optimization
ordinary differential equations
organs
orifices
orthogonal transformations
oscillations
osmosis
oxidation
P states
paper industry
parallel processing
partial differential equations
particle interactions
particle resuspension
particle size
particles
Pascal
passive solar heating systems
pattern recognition
payback period
PDP computers
peak load
performance
performance testing
permeability
personnel
PERT method
perturbation theory
petroleum deposits
pH value
phase change materials
phase shift
phase space
phase transformations
phonons
photographic films
photoionization
photomultipliers
photon transport
photovoltaic conversion
photovoltaic power plants
photovoltaic power supplies
physical properties
physical protection
physical radiation effects
pipe fittings
pipe joints
pipes
PL method
planning
plant growth
plants
plasma
plasma heating
plasma seeding
plasma simulation
plasticity
plates
plotters
plugging
plumes
plutonium isotopes
point kernels
point sources
poisoning
Poisson equation
polarizabilities
polarization
pollution
polynomials
porosity
porous materials
Porter-Thomas distribution
positioning
potential flow
potential scattering
potentials
power distribution
power generation
power plants
power systems
power-cooling-mismatch accidents
precompound-nucleus emission
present worth method
presses
pressure
pressure dependence
pressure drop
pressure effects
pressure gradients
pressure release
pressure vessels
pressurizers
pressurizing
prestressed concrete
printed circuits
printing and publishing industry
probabilistic estimation
probability
process heat
processing
procurement
production
productivity
program management
programming
programming languages
prompt neutrons
public utility regulatory policies act
pulsed neutron techniques
pumped storage
pumped storage power plants
pumps
Purex process
pyrolysis
pyrolytic oils
quadratures
quality assurance
quality control
quantity ratio
quantum mechanics
R matrix
r-theta
r-theta-z
r-z
Racah coefficients
radiation detectors
radiation doses
radiation effects
radiation streaming
radiation transport
radio equipment
radioactive aerosols
radioactive clouds
radioactive effluents
radioactive waste disposal
radioactive waste facilities
radioactive waste management
radioactive waste storage
radioactivity
radioactivity transport
radioisotopes
radiolysis
radionuclide kinetics
radionuclide migration
randomness
Rankine cycle power systems
reaction kinetics
reactivity
reactivity insertions
reactor accidents
reactor channels
reactor components
reactor control systems
reactor cooling systems
reactor core disruption
reactor core restraints
reactor cores
reactor kinetics
reactor lattices
reactor licensing
reactor noise
reactor operation
reactor operators
reactor period
reactor protection systems
reactor safety
reactor stability
reactor vessels
reactors
real time systems

recombiners
recovery
rectangular configuration
redox potential
reflection
reflectivity
regeneration
regional analysis
regression analysis
Reich-Moore formula
reinforced concrete
reliability
relief valves
renewable energy sources
repair
reprocessing
reservoir engineering
reservoir pressure
reservoir rock
resistivity logging
resistivity surveys
resolution
resonance
resonance absorption
resonance escape probability
resonance integrals
resonance scattering
respiratory system
response functions
restraints
retorting
retrieval systems
reverse-field pinch
Ricatti equation
risk assessment
rock drilling
rock mechanics
rock-fluid interactions
rock-fluid mechanics
rockets
rocks
rod bundles
rod drop method
roofs
root absorption
rotational states
ruptures
rural areas
S matrix
S states
safeguards
safety
salt deposits
sampling
scattering
scattering law
SCEPTER project
schedules
Schroedinger equation
scintillation counters
SCISRS
scram
seawater
secondary emission
security
sediments
seismic detection
seismic effects
seismic events
self-consistent field
self-potential surveys
self-shielding
semiclassical approximation
semiconductor materials
sensitivity
sensitivity analysis
series expansion
shadow effect
shaped charges
shear
shell models
shells
shielding
shields
shock waves
SI units
signals
simulation
single-particle model
site selection
size
skin
sky
slabs
slags
slip flow
slowing-down
sodium phosphates
soil chemistry
soil mechanics
soil-structure interactions
soils
solar air conditioning
solar collectors
solar energy
solar heating systems
solar power plants
solar radiation
solar receivers
solar space heating
solar thermal power plants
solar water heating
solid state physics
solids
solutions
solvent extraction
Sommerfeld integrals
sorption
sorting
space dependence
space heating
space HVAC systems
space-time
special functions
specifications
spectra
spectra unfolding
spectral analysis
spectral density
spectral response
spectrometers
spent fuels
spheres
spherical configuration
spherical harmonics
spin
spline functions
spray drying
sprays
square configuration
stack disposal
standardization
standards
static loads
statistical models
statistics
steady flow
steady-state conditions
steam
steam generators
steam turbines
Stirling cycle
Stirling engines
stochastic processes
stoichiometry
storage
strain softening
strains
streams
stress analysis
stress corrosion
stress intensity factors
stress relaxation
stresses
structural beams
structural models
structure factors
structured programming
subsonic flow
sulfates
sulfites
sulfur dioxide
superheaters
supports
surface air
surface waters
surfaces
swelling
swimming pools
symmetric matrices
synthesis
system failure analysis
systems analysis
tables
tanks
taxes
technology assessment
temperature
temperature coefficient
temperature dependence
temperature distribution
temperature distributions
temperature effects
temperature feedback
temperature gradients
terrestrial ecosystems
testing
text editors

theorem proving
thermal analysis
thermal conduction
thermal conductivity
thermal diffusion
thermal energy storage equipment
thermal energy systems
thermal equilibrium
thermal expansion
thermal fatigue
thermal neutrons
thermal power plants
thermal radiation
thermal stresses
thermal utilization
thermalization
thermodynamic cycles
thermodynamic properties
thermodynamics
thermonuclear reactions
Thorex process
three-dimensional
three-dimensional calculations
three-nucleon transfer reactions
time dependence
time measurement
time-series analysis
tissues
topography
topological mapping
tornadoes
toroidal configuration
total cross sections
total energy systems
toxic materials
trace amounts
transfer functions
transient overpower accidents
transients
translators
transmission
transonic flow
transport theory
trapping
triangular configuration
triangular-z
tritium
trombe walls
tubes
turbine blades
turbines
turbulence
turbulent flow
two-dimensional
two-group
two-phase flow
UKNDL
underground storage
uranium isotopes
urban areas
US REA
utility routines
validation
vapor condensation
vapors
Varian computers
variations
vector processing
velocity
ventilation
ventilation systems
vibrational states
viewgraphs
viscosity
viscous flow
vortex flow
walls
washout
waste management
waste processing
waste-rock interactions
water
water chemistry
water hammer
water pollution
water quality
water vapor
waterflooding
watersheds
wave functions
wave propagation
weather
weight
weighting functions
Weisskopf model
welded joints
well drilling
well logging
well stimulation
Wigner-Wilkins model
Wilkins equation
wind
wind power
wind power plants
wind turbines
wires
wood fuels
Woods-Saxon potential
work functions
working fluids
x-ray diffraction
x-ray spectra
x-y
x-y-z
xenon oscillations
yield strength
yields
zero-range approximation
zircaloy

VI. ABSTRACT COLLECTION

When software is initially entered into the Center collection, it is assigned an accession number which is used to identify the software and its abstract. A separate numbering system is used for software which is evaluated and that which is screened and processed "As Is". The first proceeds in an ascending sequence from 1 while the second utilizes a descending sequence from 9999. When the abstract is prepared and thereafter whenever it is modified, the month and year are inserted in the abstract heading in the format MM/YY.

1. **IDENTIFICATION AND KWIC TITLE** - EQUIPOISE3
   EQUIPOISE3, 2-d 2-group diffusion slab cyl

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER73,175, CDC7600

3. **DESCRIPTION** - EQUIPOISE3 solves the two-group, two-dimensional, neutron diffusion equations in cylindrical or slab geometry.

4. **METHOD OF SOLUTION** - The EQUIPOISE method described by Tobias and Fowler in volume 12 of Nuclear Science and Engineering is used to solve the finite-difference analogs of the two-group neutron diffusion equations.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   2 groups
   2100 mesh points
   50 compositions
   100 regions

6. **TIMING** - NESC executed the sample problem in 9 seconds of CP time on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - EQUIPOISE3 is intended for rapid two-dimensional calculations suitable for survey calculations. The logarithmic derivative boundary condition is allowed, and adjoint fluxes and associated direct-adjoint flux region integrals may be calculated automatically, if desired.

8. **RELATED AND AUXILIARY SOFTWARE** - The original IBM7090 version of EQUIPOISE3 was prepared by T. B. Fowler and M. L. Tobias at Oak Ridge National Laboratory, Oak Ridge, Tennessee.

9. **STATUS** - Abstract first distributed April 1962.
   IBM7090 version submitted February 1962, deleted April 1978.
   CDC CYBER72 version submitted June 1975, replaced by CYBER73 version submitted February 1980, sample problem executed by NESC September 1980 on a CDC CYBER175.

10. **REFERENCES** - T. B. Fowler and M. L. Tobias, EQUIPOISE-3: A Two-Dimensional, Two-Group, Neutron Diffusion Code for the IBM-7090 Computer, ORNL-3199, February 1962.
    M. L. Tobias and T. B. Fowler, The Equipoise Method--A Simple Procedure for Group-Diffusion Calculations in Two and Three Dimensions, Nuclear Science and Engineering, Vol. 12, pp. 513-518, 1962.
    EQUIPOISE3, NESC No. 39.CY73, EQUIPOISE3 Sample Problem Output, National Energy Software Center Note 82-106, August 23, 1982.

11. **HARDWARE REQUIREMENTS** - 125,000 (octal) words of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS/BE 1.2, 1.3 (CDC CYBER73), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. L. Wang
    Institute of Nuclear Energy Research
    Atomic Energy Council
    Republic of China

16. **MATERIAL AVAILABLE** -
    Source (2750 lines)
    Sample problem (15 lines)
    Reference report, ORNL-3199, and NESC Note

17. **CATEGORY** - C
KEYWORDS - neutron diffusion equation, two-dimensional, two-group, slabs, cy
reactivity

18. **SPONSOR** - AEC
Republic of China - Institute of Nuclear Energy Research

1. **IDENTIFICATION AND KWIC TITLE** - FLOW-MODEL
   FLOW-MODEL, multi-channel 2-d 2-phase flow

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360, CDC CYBER73, CDC6600,7600

3. **DESCRIPTION** - FLOW-MODEL is a multi-channel, two-dimensional, two-phase flow model designed to compute the axial and radial coolant density and quality profiles, the axial pressure profile, and the weight flow distribution for an open matrix flow, boiling water reactor.

4. **METHOD OF SOLUTION** - The discontinuous nodal flow model approximation leads to a system of simultaneous nonlinear equations which are solved by iteration.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   20 channels
   100 axial nodes
   100 axial q points

6. **TIMING** - NESC executed the sample problem in 1 CPU minute on an IBM370/195 and in 4 CP seconds on a CDC6600 and 1 CP second on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The program can use an SC-4020 graphical display device for plotting results.

8. **RELATED AND AUXILIARY SOFTWARE** - The original IBM7094 version was prepared by R. F. Berland of the Mathematical and Computing Sciences Group, Atomics International, Canoga Park, California.

9. **STATUS** - Abstract first distributed July 1966.
   IBM7094 version submitted by AI May 1966, deleted July 1978.
   IBM360 version submitted January 1971, sample problem executed by NESC.
   CDC CYBER72 version submitted June 1975, replaced by CDC CYBER73 version submitted February 1980, sample problem executed by NESC February 1980 on a CDC6600 and a CDC7600.

10. **REFERENCES** - D. E. Schramm and R. F. Berland, A Multi-channel Two-dimensional, Two-phase Flow Model and IBM7090 Code, NAA-SR-MEMO-9444, December 31, 1963.
    M. Hoffman and W. A. Rhoades, AICRT 3 A General Code for Display of Digital Data, NAA-SR-MEMO-9069, October 1963.

11. **HARDWARE REQUIREMENTS** - 240K bytes of memory are needed for the IBM360 version. The CDC CYBER73 version requires 47,000 (octal) words of memory on the CDC6600 and 35,000 (octal) words of memory on the CDC7600.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360 (IBM360), SCOPE (CDC6600,7600), NOS 1.3 (CDC CYBER73).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The AICRT3 graphics subroutine is not included. A suitable alternative must be available in the user's computing environment to obtain graphical output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    360 G. W. Perry
    Middle South Services, Inc.

    CYBER73 C. L. Wang
    Institute of Nuclear Energy Research
    Atomic Energy Council
    Republic of China

16. **MATERIAL AVAILABLE** –
    Source (360–370 lines, CY73–408 lines)
    Sample problem (35 lines)
    Sample problem output (CY73–24 pages)
    Reference reports

17. **CATEGORY** – H
    KEYWORDS – two-dimensional, fluid flow, coolants, computer graphics, BWR reactors

18. **SPONSOR** – AEC
    Middle South Services
    Republic of China – Institute of Nuclear Energy Research

1. **IDENTIFICATION AND KWIC TITLE** - SAFE-PLANE
   SAFE-PLANE, plane stress analysis, 2-d bodies

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   UNIVAC1108, CDC6600

3. **DESCRIPTION** - SAFE-PLANE is applied to two-dimensional structures of arbitrary geometry under in-plane loads. Either plane stress or plane strain conditions may be imposed. Mechanical and thermal loads are permitted.

4. **METHOD OF SOLUTION** - The finite-element method is used to construct a mathematical model by assembling discrete elements. The total potential energy of the structure is determined and subsequently minimized by iteration on components of the displacement field until static equilibrium of the structure is attained. Strains and stresses are computed from the resulting displacements.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -
   Multi-material structures with varying rigidities converge very slowly.
   Not valid for incompressible materials.
   Maximum number of nodal points = 675.
   Maximum number of elements = 1350.

6. **TIMING** - Less than 3 minutes are required for a full capacity problem on the 1108.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Other programs useful for stress analysis of prestressed concrete reactor vessels are SAFE-AXISYM (NESC 251) and SAFE-PCRS for axisymmetric composite structures and SAFE-SHELL (NESC 253) for thin shells of revolution. On the 1108, ICON2 (a contour plotting program) plots the pointwise stress/strain output as a series of equal intensity contours.

9. **STATUS** - Abstract first distributed April 1967.
   IBM7044 version submitted August 1966, deleted October 1967.
   UNIVAC1108 version submitted October 1967.
   CDC6600 version submitted July 1970.

10. **REFERENCES** - Input Instructions for SAFE-PLANE Computer Program.
    Yusef R. Rashid, Analysis of Axisymmetric Composite Structures by the Finite Element Method, GA-6763, October 15, 1965.
    Prestress Concrete Reactor Vessels Analytical Methods Development, GACD-7258, June 1966.
    D. C. Cornell, SAFE-PLANE, A Computer Program for the Stress Analysis and Design of Two-dimensional Composite Bodies, A User's Manual, GA-7851, June 30, 1967.

11. **HARDWARE REQUIREMENTS** - Approximately 47000 words storage (decimal) plus the operating system (1108). Requirements can be easily reduced by simple adjustment of DIMENSION statements.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    1108 D. C. Cornell
    General Atomic Company

6600 M. Reich
Brookhaven National Laboratory

16. **MATERIAL AVAILABLE -**
Source (1108-1029 lines, 6600-1072 lines)
Sample problems (1108-142 lines, 6600-735 lines)
Reference reports and Input Instructions

17. **CATEGORY -** I
KEYWORDS - stresses, two-dimensional, strains, static loads, finite element method, ICON2 codes, PIZZA codes

18. **SPONSOR -**

1. **IDENTIFICATION AND KWIC TITLE** - SAFE-SHELL
   SAFE-SHELL, stress analysis thin shells

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   UNIVAC1108, CDC CYBER73, CDC7600

3. **DESCRIPTION** - SAFE-SHELL is used to design and analyze axisymmetric thin-shell structures of arbitrary generatrices under axisymmetric mechanical and/or thermal loading conditions. The intersection of two or more shells can be treated.

4. **METHOD OF SOLUTION** - The finite-element method is used to construct a mathematical model by assembling discrete elements. The total potential energy of the structure is determined and subsequently minimized by differentiating the energy function with respect to each displacement component. The equilibrium equations are then solved by tri-diagonalization. Strains and stresses are computed from the resulting displacement field.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   181 nodal points
   180 elements
   21 sections
   20 nodes per section
   Capacity can be easily increased at cost of storage requirements.

6. **TIMING** - Less than 3 minutes are required for a full capacity problem on the UNIVAC1108. NESC executed the sample problem in less than 1 second of CP time on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Other programs useful for stress analysis of prestressed concrete reactor vessels are SAFE-AXISYM (NESC 251) and SAFE-PCRS for axisymmetric composite structures and SAFE-PLANE (NESC 252) for plane structures involving in-plane stress distributions.

9. **STATUS** - Abstract first distributed April 1967.
   IBM7044 version submitted August 1966, deleted October 1967.
   UNIVAC1108 version submitted October 1967.
   CDC CYBER72 version submitted June 1975, replaced by CDC CYBER73 version submitted February 1980, sample problem executed by NESC March 1980 on a CDC7600.

10. **REFERENCES** - Input Instructions for SAFE-SHELL Computer Program.
    Finite Element Analysis of Axisymmetric Composite Structures, GA-6303, June 4, 1965.
    Yusef R. Rashid, Analysis of Axisymmetric Composite Structures by the Finite Element Method, GA-6763, October 15, 1965.
    Prestress Concrete Reactor Vessels Analytical Methods Development, GACD-7258, June 1966.
    D. C. Cornell, SAFE-SHELL, A Computer Program for the Stress Analysis of Thin-Shell Bodies of Revolution, A User's Manual, GA-7852, June 30, 1967.

11. **HARDWARE REQUIREMENTS** - The UNIVAC1108 version requires 26,000 words of memory and the CDC CYBER73 version requires 76,000 (octal) words of memory for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - EXEC8 (UNIVAC1108), NOS 1.3 (CDC CYBER73), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    1108 D. C. Cornell
    General Atomic Company

CYBER73 C. L. Wang
Institute of Nuclear Energy Research
Atomic Energy Council
Republic of China

16. **MATERIAL AVAILABLE** -
Source (1108-1195 lines, CY73-1235 lines)
Sample problems (1108-41 lines, CY73-39 lines)
Sample problem output (CY73-11 pages)
Reference reports, GA-6763, GACD-7258, GA-7852, and Input Instructions

17. **CATEGORY** - I
KEYWORDS - shells, stresses, mechanical structures, strains, finite element method

18. **SPONSOR** - AEC
Republic of China - Institute of Nuclear Energy Research

1. **IDENTIFICATION AND KWIC TITLE** - CLIP
   CLIP, FORM or THREDES library utility routine

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - CLIP is the cross section library preparation and maintenance program for FORM and THREDES.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - 1 to 2 minutes are required.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - CLIP -
   (a) creates a FORM and/or THREDES library from cards,
   (b) updates the FORM or THREDES library,
   (c) lists the FORM or THREDES library,
   (d) duplicates the FORM or THREDES library.
   The TEMPEST cross sections (for THREDES) may come from a decimal or hexadecimal library or an existing THREDES library. The FORM cross sections may come from cards or an existing FORM or THREDES library. The libraries may reside on disk or tape.

8. **RELATED AND AUXILIARY SOFTWARE** -
   (a) FORM library programs
   (b) TEMPEST (NESC 50) library programs
   (c) FORM (NESC 51)
   (d) THREDES (NESC 273)

9. **STATUS** - Abstract first distributed December 1967.
   IBM360 version submitted April 1967, revised January 1969.

10. **REFERENCES** - R. F. Berland and R. A. Blaine, CLIP, Conversion to IBM System/360, AI-66-MEMO-168, Vol. I and Flowcharts, Vol. II, December 1966.
    R. F. Berland and R. A. Blaine, CLIP, A Program to Construct, Update and List the FORM or THREDES Master Data Tape, AI-CE-MEMO-12, March 1966.
    R. A. Blaine, Atomics International Environment Report, May 1967.

11. **HARDWARE REQUIREMENTS** - 256K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. A. Blaine
    Mathematics and Computer Sciences
    Atomics International

16. **MATERIAL AVAILABLE** -
    Source (927 lines)
    TEMPEST and FORM decimal libraries (7077 lines)
    Reference reports (flowchart volume may be requested on a loan basis only)

17. **CATEGORY** - M
    KEYWORDS - cross sections, libraries, maintenance, information retrieval, data processing, FORM codes, THREDES codes, TEMPEST codes

18. SPONSOR -

1. **IDENTIFICATION AND KWIC TITLE** - PDQ8, PDQ7
   PDQ7, 1,2 or 3-d few-gp diffusion depletion
   PDQ8, 1,2 or 3-d few-gp diffusion depletion

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600,6600,CYBER175,170, IBM360,370,303x,308x

3. **DESCRIPTION** - The PDQ series of programs is designed to solve the neutron diffusion-depletion problem in one, two or three dimensions. Very large problems can be accommodated. The three-dimensional spatial calculation may be either explicit or discontinuous trial function synthesis. Up to five lethargy groups are permitted. The fast group treatment may be simplified P(3), and the thermal neutrons may be represented by a single group or a pair of overlapping groups. Adjoint, fixed source, one iteration, additive fixed source, eigenvalue, and boundary value calculations may be performed. The programs utilize the HARMONY system to allow for time-dependent representation of cross section variation and generalized depletion chain solutions. In PDQ8 the depletion is a combination gross block depletion for all nuclides as well as a fine block depletion for a specified subset of the nuclides. The geometries available include rectangular, cylindrical, spherical, hexagonal, and, in PDQ8 only, a very general quadrilateral geometry with diagonal interfaces. All geometries allow variable mesh in all dimensions. Various control searches as well as temperature and xenon feedback are provided.

4. **METHOD OF SOLUTION** - For the explicit spatial solution, difference equations are obtained at each point by integrating the differential equations over an appropriate mesh element. The resulting equations are three-point, five-point, seven-point, and nine-point for one dimension, two-dimensional rectangular, two-dimensional hexagonal and three-dimensional rectangular, two-dimensional quadrilateral and three-dimensional hexagonal. The group equations are solved directly using Gaussian elimination in one dimension, by use of the single-line cyclic Chebyshev semi-iterative method in two dimensions, and by use of the single-line successive overrelaxation method in three dimensions. The source iterations are accelerated by use of Chebyshev extrapolation applied to the group fluxes. The synthesis solution utilizes the axially discontinuous trial function formulation and solves the iterative problem by use of the Weilandt method. The feedback capabilities are implemented by utilizing a system of time-dependent cross sections and generalized depletion chains.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The total number of groups is limited to five, although six equations may be solved if the P(3) option is used. All storage is dynamic so no fixed problem size limits are imposed. However, as a general rule, the product of groups and points in an explicit solution is limited to roughly ten million due to disk capacity limitations. For synthesis calculations, the disk capacity limitation of about thirty million will limit the product of the number of gross blocks per plane and the number of trial functions or the product of the total number of gross blocks and the number of isotopes. These disk capacity limitations are for the CDC7600; the capacity of the CDC6600 is about one-tenth of the stated limitations.

6. **TIMING** - The PDQ8 program can solve two-dimensional problems at the rate of about one million group-points per hour and three-dimensional problems at the rate of about one-half to three-quarters of a million group-points per hour on the CDC7600. The CDC6600 PDQ8 times would be about five times the CDC7600 times. The synthesis spatial solution time is dependent on the number of trial functions used and the number of gross blocks. The actual running times may vary widely due to the convergence rate of the iterations, the use of control searches or feedbacks, or the complexity of the depletion formulation. PDQ7 running time in hours on a CDC6600 may be estimated by dividing the product of groups and points by 150,000. Running time for the sample problems on the IBM3033 is about 2 minutes.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Except for the group flux spatial calculation, both explicit and synthesis solutions utilize the same input, calculational, and edit portions of the program so that consistent comparisons of the two methods can be easily obtained.

8. **RELATED AND AUXILIARY SOFTWARE** - Cross sections, or tablesets, may be input on cards and/or may be obtained from a File Manager (reference 2) input file. Input card data may be merged with card data from one or more File Manager input files. The program will also accept input File Manager files containing pointwise flux, block concentrations, geometry, block flux, synthesis integrals, and, in PDQ8, quadrilateral geometry figures. On request, the program will prepare File Manager output files containing pointwise flux, block concentrations, partition power, various edit integrals, geometry, gross block power, block flux, synthesis mixing coefficients, synthesis integrals, fine block power, and PDQ8 quadrilateral geometry figures.

   The water properties required for thermal feedback calculations are obtained from a package of subroutines described in reference 3. PDQ8 uses the BETTIS ENVIRONMENTAL LIBRARY (NESC 665) and the M0899/HOH package (NESC 294). The EG&G CDC7600 version of PDQ7 uses a proprietary MODEL library from CDC. The EG&G IBM360 version of PDQ7 contains necessary NRTS Environmental Subroutines (NESC 613). The Boeing CDC CYBER175 version of PDQ7 contains necessary BETTIS ENVIRONMENTAL LIBRARY (NESC 665) routines.

9. **STATUS** - Abstract first distributed December 1967.

   CDC6600 (BETTIS) version of PDQ7 submitted May 1967, replaced by revised Edition C June 1971, replaced May 1979 by Edition B CDC7600 version of PDQ8 submitted November 1978, program compiled by NESC January-February 1979 on a CDC7600.

   IBM360 (IBM) version of PDQ7 submitted February 1969, deleted November 1971.

   CDC6600 (B&W) version of PDQ7 submitted February 1970, deleted May 1979.

   IBM360 (EG&G) version Edition B of PDQ7 submitted April 1970, revised to Edition C April 1971, replaced by Edition D August 1972, Edition E March 1973, Edition F March 1974, Edition G February 1977, revised to make it operable under MVS with Edition H December 1982, sample problems executed by NESC December 1982 on an IBM3033.

   CDC6600 KRONOS (Boeing) version of PDQ7 submitted July 1973, replaced August 1980 by CDC CYBER175 NOS version of PDQ7 submitted April and August 1980.

   CDC7600 (EG&G) version of PDQ7 submitted January 1977.

10. **REFERENCES** - C. J. Pfeifer and C. J. Spitz, PDQ-8 Reference Manual, WAPD-TM-1266, May 1978.

W. R. Cadwell, Ed., Reference Manual - Bettis Programming Environment, WAPD-TM-1181, September 1974.

L. L. Lynn, A Digital Computer Program for Nuclear Reactor Design Water Properties, WAPD-TM-680, July 1967.

PDQ8, NESC No. R275.7600B, Tape Description and Implementation Information, National Energy Software Center Note 79-43, March 31, 1979.

W. R. Cadwell, PDQ-7 Reference Manual, WAPD-TM-678, January 1967.

R. J. Breen, O. J. Marlowe, and C. J. Pfeifer, HARMONY - System for Nuclear Reactor Depletion Computation, WAPD-TM-478, January 1965.

R. J. Wagner, NESC No. R275 IBM Version, Operational Notes for PDQ7/14, ANC Note, August 25, 1972, revised January 14, 1983.

C. J. Pfeifer, PDQ-7 Reference Manual II, WAPD-TM-947(L), February 1971.

C. J. Pfeifer, CDC-6600 FORTRAN Programming - Bettis Environmental Report, WAPD-TM-668, January 1967.

PDQ7, NESC No. R275.370H, PDQ7 IBM Version Edition H Tape Description and Implementation Information, National Energy Software Center Note 83-23, December 14, 1982.

A. W. Brown, J. A. McClure, and R. J. Wagner, Summary of PDQ-7 (IBM-360-370 Version) Input Data Requirements and Operating Procedures, ANCR-1061, March 1972.

UPD, A Program to Update Source Decks, ANC Note P01750, March 1972.

NRTS Environmental Subroutine Manual, ANC Document, December 1972.

PDQ7, NESC No. R275.C175, PDQ7 CYBER175 Nos Version Transmittal Tape Description and Implementation Information, National Energy Software Center Note 80-58, August 12, 1980.

PDQ7, ACC No. R275.7600, Argonne Code Center Note 78-4, November 1, 1977.

R. J. Wagner, INEL Transmittal of PDQ7 Version 2, INEL Note, January 21, 1977.

R. J. Wagner, FAPFIM - Fortran Access to Permanent File Macros, INEL Note, October 11, 1976.

11. **HARDWARE REQUIREMENTS** - On CDC systems the central memory size should be at least 65K, and the program will utilize up to 1000K of extended core memory and up to four disks

transferring in parallel. The IBM360 version of PDQ7 requires at least 400K bytes of memory under MVT or 1000K under MVS and auxiliary disk storage.

12. **PROGRAMMING LANGUAGE** - PDQ8 - FORTRAN and COMPASS (RUN and FTN compatible); PDQ7 - FORTRAN IV and COMPASS (CDC CYBER175), FORTRAN FTN4.6 (CDC7600), FORTRAN IV (H) and BAL (IBM360)

13. **OPERATING SYSTEM** - PDQ8 - SCOPE 1.1 (CDC7600), SCOPE 3.3 (CDC6600); PDQ7 - NOS 1.2 (CDC CYBER175), SCOPE 2.1.4 (CDC7600), OS/MVT (IBM360), OS/MVS (IBM30xx).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The required PDQ8 software environment is described in reference 2 and that for PDQ7 in reference 9. It includes routines for program loading, free-field input conversion and processing, storage and retrieval of permanent File Manager files, scratch input/output, storage allocation, and plotting. All files used to communicate with other jobs, including other PDQ8 jobs, are in File Manager form.

The EG&G CDC7600 version of PDQ7 is also operable on a CDC6600 under the SCOPE 3.4 or NOS operating systems with the modifications described in reference 16.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

6600 PDQ7 W. R. Cadwell and C. J. Pfeifer

7600B PDQ8 C. J. Pfeifer and C. J. Spitz
Bettis Atomic Power Laboratory

360A PDQ7 R. J. Creasy
Palo Alto Science Center
International Business Machines Corporation

360B-G PDQ7 7600 R. J. Wagner and A. W. Brown
Computer Science Branch
EG&G Idaho, Inc.

360B-G PDQ7 J. A. McClure
Energy Incorporated

370H PDQ7 R. B. Lang and A. Serpas
Middle South Services, Inc.

6600 B&W PDQ7 M. L. Dech and R. W. McCraney
Control Data Corporation
G. R. Poetschat and G. L. Russell
Power Generation Division
Babcock & Wilcox Company

CYBER175 NOS PDQ7 S. J. Pruitt
Energy Technology Applications Division
Boeing Computer Services Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution

Source (PDQ8 96,804 lines, PDQ7 370H-38,268 lines, C175-51,305 lines)
Update files (EG&G UPDATE OLDPL of PDQ7 7600-519 records*, UPDATE OLDPL of INP subroutines 7600-29 records*, UPDATE OLDPL of INEL environmental library source 7600-80 records*, PDQ7 MVS 370H-427 lines)
2314 and 3330 load modules (PDQTRNMT 370H-1862 blocks)
3350 load module (PDQ7MVS 370H-2181 blocks)
Sample problems (PDQ8 518 lines, PDQ7 370H-478 lines, C175-2090 lines)
Auxiliary programs (PDQ7 BUFR 370H-246 lines, PDQDINIT 370H-31 lines, PDQD 370H-148 lines, PDQR 370H-107 lines, PDQTL 370H-53 lines, miscellaneous 370H-3135 lines, Bettis Environmental Library C175-11,779 lines, CPYPDQ C175-633 lines, PDQ C175-428 lines, MFN C175-447 lines, TPREL C175-26 lines, DCOPY C175-259 lines, TCOPY C175-294 lines)
Flux files (PDQ7 370H-137 blocks+)
Water property file (PDQ7 7600-15 records*)

Control information (PDQ7 loader directives 7600-2 records*, JCL and overlay line
370H-285 lines, MVS JCL and overlay lines 370H-250 lines)
Sample problem output (PDQ7 370H-196 pages, C175-59 pages)
Reference reports, WAPD-TM-678, WAPD-TM-668, WAPD-TM-947(L), WAPD-TM-1266, WAPD-TM-1181,
ANCR-1061, NRTS Manual, and Notes, as appropriate

* 512-word maximum length
+ RECFM=VS,LRECL=3628,BLKSIZE=3632

17. **CATEGORY** - D
KEYWORDS - burnup, neutron diffusion equation, one-dimensional, slabs, iterative methods,
cylinders, spheres, two-dimensional, x-y, r-z, three-dimensional, x-y-z, synthesis, few-
group, hexagonal configuration, HARMONY codes, UPD codes, BUFR codes, PDQDINIT codes, PDQD
codes, PDQR codes, PDQTL codes, TPREL codes, DCOPY codes, TCOPY codes

18. **SPONSOR** - DOE Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - GAFGAR, P3T, PROC, TAPCOP
   GAF,GAR, spectra and group-averaged x-sec calc

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - UNIVAC1108

3. **DESCRIPTION** - The problem is to obtain very detailed neutron flux and current distributions as functions of energy considering explicitly the possible overlap effects between resonances of a resonance absorber and of mixtures of resonance absorbers and to use these distributions to prepare group-averaged cross sections and transfer arrays for use in fast reactor analyses.

4. **METHOD OF SOLUTION** - The B1 approximation to the Boltzmann equation is solved for the neutron flux and current spectra. The GAF section uses a large number of fine energy groups to represent the cross sections above the resolved resonance region. The GAR section uses a very large number of discrete velocities in the resonance region along with slowing-down sources from the GAF section to treat leakage-dependent resonance absorption more rigorously than previous codes.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The maximum of 1740 fine groups in the GAF section may be subdivided into 10 or less sets of fine groups having a constant lethargy width. The GAR section requires a uniform spacing between the maximum of 14,700 discrete velocities. The maximum number of nuclides in a problem is 20, and the maximum total number of broad groups (output for nuclear design calculations) is 99 with a maximum of 20 broad groups in the GAR section.

6. **TIMING** - 4.6 minutes (1.1 minutes for GAF section and 3.5 minutes for GAR section) are required for a test problem involving hydrogen, carbon, oxygen, Pu239, and Pu240 with 731 fine groups above 10 keV in the GAF section (deltau=0.01), 12,367 velocities below 10 keV in the GAR section (deltav=110 m/sec), and 31 broad group output (11 in GAF section and 20 in GAR section).

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The GAF section allows downscatter by any process (anisotropic elastic scatter, inelastic scatter, (n,2n) processes, etc.) from any fine group to any lower energy fine group because the full P0 and P1 transfer arrays are used for all materials except hydrogen which is assumed to have only isotropic in the center-of-mass system elastic scatter. Data compression techniques are used to reduce the size of the transfer arrays. The GAR section uses a recursive scheme for the calculation of the P0 and P1 slowing-down source terms which decreases the running time for typical problems by a factor of 3 to 4 while still allowing isotropic in the center-of-mass system elastic scatter to any lower velocity to be treated rigorously. Either positive or negative buckling can be specified for each broad group in each section.

8. **RELATED AND AUXILIARY SOFTWARE** - Cross section input for the GAFGAR code is prepared by the GAND code from ENDF/B format nuclear data file tapes. Data on the GAFGAR cross section tapes may be printed with the P3T code. PROC is used to copy selected problems from 1 or 2 GAF and/or GAR problem tapes or to list the problem tapes. TAPCOP is used to copy GAFGAR (packed record) data tapes.

9. **STATUS** - Abstract first distributed June 1968.
   UNIVAC1108 version submitted January 1968, replaced by modified version August 1968.

10. **REFERENCES** - D. R. Mathews and R. J. Archibald, GAF, A Computer Program for Calculation of Neutron Spectra and Average Cross Sections in the High Energy Range, GA-7169, January 20, 1967.

C. A. Stevens and R. J. Archibald, GAR, A Computer Program for Evaluating Leakage Dependent Resonance Absorption, GA-6952, March 16, 1966.

R. J. Archibald and D. R. Mathews, The GAF/GAR/GAND Fast Reactor Cross Section Preparation System, GAFGAR - A Program for the Calculation of Neutron Spectra and Group-averaged Cross Sections, GA-7542, Vol. I, January 22, 1968, and Errata, May 1968.

11. **HARDWARE REQUIREMENTS** - 52K of available fast memory and 5 magnetic tape units plus 5 scratch files (drum files are used on the UNIVAC1108) totaling about 600K in capacity

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - EXEC2, GAX33A.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - GAFGAR is overlayed in three segments consisting of the GAF section, the GAR section, and a combining and punching section. The UNIVAC1107/1108 FORTRAN IV NTRAN I/O routines are used to buffer the I/O in parallel with computing and to reduce the number of record gaps on the data tapes.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. J. Archibald, D. R. Mathews, R. T. Shanstrom,
    C. A. Stevens, and R. M. Wagner
    General Atomic Company

16. **MATERIAL AVAILABLE** -
    Source (4699 lines)
    Sample problem input and output (240 lines)
    Auxiliary source (P3T 323 lines, PROC 192 lines, TAPCOP 139 lines)
    Reference reports and Errata

17. **CATEGORY** - B
    KEYWORDS - fast reactors, multigroup theory, cross sections, neutron flux, neutron spectra, resonance absorption, P3T codes, PROC codes, TAPCOP codes

18. **SPONSOR** -

. **IDENTIFICATION AND KWIC TITLE -** ETOE2
ETOE2, ENDF/B to MC**2-2 data conversion

. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -** IBM303x,370

. **DESCRIPTION -** ETOE2 (ENDF/B to MC**2-2 data conversion) accepts cross section data from an ENDF/B version 5 library tape in binary alternate form and prepares the binary cross section and Legendre polynomial tape for the MC**2-2 code (NESC 355). The MC**2-2 library generated consists of eight files containing (1) the administrative file, (2) function table file, (3) unresolved resonance data, (4) resolved resonance data, (5) smooth tabulated non-resonant data, (6) inelastic and n,2n distributions, (7) fission spectra data, and (8) Legendre data. File 2 may or may not be present.

. **METHOD OF SOLUTION -**

. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** The restrictions as to storage limitations and options are basically those imposed by the ENDF/B restrictions and the MC**2-2 program.

. **TIMING -** The average running time varies by material processed. It is dependent on resonance scattering calculations and Legendre polynomial calculations. About one minute of CPU time is required for each material.

. **UNUSUAL FEATURES OF THE SOFTWARE -**

. **RELATED AND AUXILIARY SOFTWARE -** ETOE2 prepares MC**2-2 binary libraries using a binary alternate form ENDF/B library tape. RIGEL (NESC 915) can be used to create the ENDF/B version 5 binary alternate tape. MERMC2-2 merges, deletes, or renames materials from one or two input MC**2-2 binary libraries and forms an output MC**2-2 binary library.

. **STATUS -** Abstract first distributed March 1969.
CDC3600 version submitted by APDA September 1968, deleted July 1978.
IBM360 version submitted April 1971, replaced by revised edition submitted June 1972, deleted June 1979.
IBM3033 version submitted August 1982, sample problem executed by NESC October 1982 on an IBM370/195.

. **REFERENCES -** ETOE2, NESC No. 350, ETOE2 Documentation, National Energy Software Center Note 83-84, August 25, 1983.

H. Henryson II, B. J. Toppel, and C. G. Stenberg, MC**2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections, ANL-8144, June 1976.

R. Kinsey, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF, BNL-NCS-50496 (ENDF-102), second edition (ENDF/B-V), October 1979.

Odelli Ozer, Ed., Description of the ENDF/B Processing Codes and Retrieval Subroutines, BNL 50300 (ENDF-110), September 1967, revised June 1971.

D. M. Green and T. A. Pitterle, ETOE, A Program for ENDF/B to MC**2 Data Conversion, APDA-219 (ENDF-120), June 1968.

. **HARDWARE REQUIREMENTS -** 1000K bytes of memory

. **PROGRAMMING LANGUAGE -** FORTRAN IV (90%) and BAL (10%)

. **OPERATING SYSTEM -** OS/MVT,MVS.

. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

C. G. Stenberg
Applied Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE –**
    Source (FORTRAN 21,367 lines, BAL 2,666 lines)
    Load modules (565 records•)
    Control information and sample problem (299 lines)
    Binary alternate form ENDF/B library data (62 records•)
    Sample problem output (22,932 133-character records+)
    Reference NESC Note
    • DCB=(RECFM=FB,LRECL=80,BLKSIZE=800)
    + DCB=(RECFM=VBS,LRECL=X,BLKSIZE=7600)

17. **CATEGORY – M**
    KEYWORDS – cross sections, libraries, data processing, Legendre polynomials, ENDF/B MC••2-2 codes, RIGEL codes, MERMC2-2 codes

18. **SPONSOR –** DOE Division of Reactor Research and Technology

IDENTIFICATION AND KWIC TITLE – MC••2-2
MC••2-2, fast neutron spectra & multigp x-secs

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE – IBM360,370, CDC7600

DESCRIPTION – MC••2-2 solves the neutron slowing-down equations using basic neutron data derived from ENDF/B data files to determine spectra for use in generating multigroup neutron cross sections. The current edition includes the ability to treat all ENDF/B-V representations, high-order PL scattering representations, a free-format input processor, isotope mixing, delayed neutron processing, and flexibility in output data selection.

METHOD OF SOLUTION – The extended transport P1, B1, consistent P1, and consistent B1 fundamental mode ultra-fine-group equations are solved using continuous slowing-down theory and multigroup methods. Fast and accurate resonance integral methods are used in the narrow resonance resolved and unresolved resonance treatments. Multigroup neutron cross sections are generated for arbitrary group structures. A hyper-fine-group integral transport slowing-down calculation is available as an option.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM – The program uses variable dimensioning throughout so that computer storage requirements depend on a variety of problem parameters. Space requirements range from approximately 400K to 1000K bytes on IBM equipment depending on the complexity of the problem.

TIMING – A 1740-group consistent P1 homogeneous twelve-isotope problem with 27 broad groups requires about 6.5 minutes of CPU time on an IBM370/195. The same problem requires approximately 30% less CP time on the CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE – Extreme flexibility is provided in specifying the rigor of a calculation including a choice of four distinct slowing-down treatments: multigroup, improved and standard Greuling-Goertzel continuous slowing-down, and integral transport theory. All binary data transfers are localized in CCCC standard subroutines REED/RITE. Broad group cross section files may be generated in the ARC System XS.ISO (reference 2) and CCCC ISOTXS (reference 3) formats.

RELATED AND AUXILIARY SOFTWARE – This edition supersedes previous releases of the MC••2-2 program and the earlier MC••2 program. Improved physics algorithms and increased computational efficiency are incorporated. Input data files required by MC••2-2 may be generated from ENDF/B data by the code ETOE2. The hyper-fine-group integral transport theory module of MC••2-2, RABANL, is an improved version of the RABBLE/RABID codes. Many of the MC••2-2 modules are used in the SDX code.

STATUS – Abstract first distributed March 1969.
CDC3600 version of MC••2 submitted November 1968, deleted December 1977.
IBM360 version of MC••2 submitted July 1970, replaced December 1977 with IBM370 version of MC••2-2, replaced May 1981 by Edition B, replaced February 1982 by Editions C and D submitted November 1981, sample problems executed by NESC January 1982 on an IBM3033 and an IBM370/195.
CDC7600 version of MC••2-2 submitted June 1976, replaced May 1981 by Edition B, replaced March 1982 by Edition C submitted November 1981, sample problem executed by NESC March 1982 on a CDC7600.

REFERENCES –
H. Henryson, II, B. J. Toppel, and C. G. Stenberg, MC••2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections, ANL-8144, June 1976.

L. C. Just, H. Henryson, II, A. S. Kennedy, S. D. Sparck, B. J. Toppel, and P. M. Walker, The System Aspects and Interface Data Sets of the Argonne Reactor Computation (ARC) System, ANL-7711, April 1971.

Standard Interface Files and Procedures for Reactor Physics Codes, Version III, LA-5486-MS, February 1974.

C. G. Stenberg and H. Henryson, II, MC••2-2 Information on IBM and CDC Implementation, Use of ENDF/B-V Library, and Added Capabilities, ANL/AP Memorandum, January 13, 1981.

C. G. Stenberg and A. Lindeman, The ARC System Cross Section Generatio Capabilities, ARC-MC••2, ANL-7722 excerpt pp. 571-576, June 1973.

11. **HARDWARE REQUIREMENTS** - A large amount of fast peripheral storage is required. Storag requirements depend on problem complexity but virtually any reasonable problem may b executed on IBM equipment with 800K bytes or CDC equipment with 50,000 words of SCM an 100,000 words of directly addressable LCM.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (99%) and Assembly language (1%) (IBM370), FORTRAN IV (99%) and COMPASS (1%) (CDC7600).

13. **OPERATING SYSTEM** - The IBM version of MC••2-2 may be executed under OS or VS operating systems and compiled using the FORTRAN H or program product compilers with the highest level of optimization. The CDC7600 version of MC••2-2 has been implemented on both the Lawrence Berkeley Laboratory and Brookhaven National Laboratory computers with their respective COKE/SCOPE operating systems. The SEGMENTATION LOADER is required and directly addressable LCM is used. The code was compiled using the FORTRAN Extended compiler under OPT=2 optimization.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subsequent CDC7600 system changes at BNL reduced the size of the directory tables used, obsoleting the operating instructions given on pages 221-229 and Appendix F of ANL-8144.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

H. Henryson, II, B. J. Toppel,
and C. G. Stenberg
Applied Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution (IBM370C, CDC7600C) (IBM370-2 tapes, CDC7600-3 tapes)

Source (370-FORTRAN 77,072 lines, Assembler 752 lines, 7600-FORTRAN 77,800 lines, COMPASS 101 lines)
3330 load module (370-MCC2.OBJLIB 1494 blocks)
Sample problems and control information (370-706 lines, 7600-205 lines)
Libraries (370-8 binary files•, 370-1 EBCDIC file 1274 lines, 7600 Tape 1-5 binary files+, Tape 2-4 binary files+)
Sample problems output (370-70 selected pages and 3 microfiche, 7600-59 selected pages)
Reference report, ANL-8144, ANL-AP Memorandum, and ANL-7722 excerpt

• RECFM=VBS,LRECL=X,BLKSIZE=6447
+ variable-length records, maximum=5120 characters

17. **CATEGORY** - B
KEYWORDS - multigroup theory, cross sections, group constants, spectra, resonance, BL method, PL method, slowing-down, ENDF/B, cell calculation, MC••2 codes, ETOE2 codes, RABANL codes, SDX codes

18. **SPONSOR** - DOE Division of Reactor Research and Technology

1. **IDENTIFICATION AND KWIC TITLE** - TWOTRAN2
   TWOTRAN2, 2-d multi-gp transport xy rz rtheta

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,6600, IBM360/195

3. **DESCRIPTION** - TWOTRAN2 solves the two-dimensional multigroup transport equation in (x,y), (r,theta), and (r,z) geometries. Both regular and adjoint, inhomogeneous and homogeneous (keff and eigenvalue searches) problems subject to vacuum, reflective, periodic, white or input-specified boundary flux conditions are solved. General anisotropic scattering is allowed and anisotropic inhomogeneous sources are permitted.

4. **METHOD OF SOLUTION** - The discrete ordinates approximation for the angular variable is used in finite difference form which is solved with the central (diamond) difference approximation. Negative fluxes are eliminated by a local set-to zero and correct algorithm. Standard inner (within-group) and outer iterative cycles are accelerated by a coarse-mesh rebalancing on a coarse mesh which may be independent of the material mesh.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Variable dimensioning is used so that any combination of problem parameters leading to a container array less than MAXLEN can be accommodated. On IBM machines, TWOTRAN2 will execute in the 4-byte mode so that any combination of problem parameters leading to a container array less than MAXLEN can be accommodated. MAXLEN can be several hundred thousand and most problems can be core-contained. On the CDC machines MAXLEN can be slightly greater than 40,000 words and peripheral storage is used for most group-dependent data.

6. **TIMING** - A six-group, S4, 42 x 42 mesh point, keff calculation of an EBR-II model requires about 3.9 minutes of CDC7600 time. The sample problems require 6 minutes on the IBM360.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Provision is made for creation of standard interface output files for SN constants, angle-integrated fluxes and angular fluxes. Standard interface input files for sources, fluxes, cross sections and SN constants may be read. All binary operations are localized in subroutines called REED and RITE. Detailed edit options, including angular fluxes, dumps and restart capability are provided. Optional use of an arbitrary rebalance mesh independent of the material mesh is allowed.

8. **RELATED AND AUXILIARY SOFTWARE** - TWOTRAN2 is an improved version of the TWOTRAN program. Many comment cards were added and much simplifying programming was performed to make TWOTRAN2 as easy to understand as possible.

9. **STATUS** - Abstract first distributed September 1969.
   UNIVAC1108 X-Y version submitted December 1968, replaced by updated edition June 1970, deleted June 1973.
   UNIVAC1108 R-Z version submitted October 1969, deleted June 1973.
   IBM360 X-Y version submitted April 1969, replaced by TWOTRAN2 June 1973, revised version B April 1974, revised version C December 1974, revised version D January 1975, sample problem executed by NESC.
   CDC6600 General Geometry version submitted July 1970, replaced by TWOTRAN2 July 1973, revised version B April 1974, revised version C December 1974, revised version D January 1975.
   CDC7600 version of TWOTRAN2 submitted June 1973, revised version B April 1974, revised version C December 1974, revised version D January 1975.

10. **REFERENCES** - K. D. Lathrop and F. W. Brinkley, TWOTRAN-II, An Interfaced, Exportable Version of the TWOTRAN Code for Two-dimensional Transport, LA-4848-MS, July 1973.
K. D. Lathrop and F. W. Brinkley, Theory and Use of the General-Geometry TWOTRAN Program, LA-4432, April 1970.
K. D. Lathrop, F. W. Brinkley, and P. Rood, Theory and Use of the Spherical Harmonics, First Collision Source, and Variable Weight Versions of the TWOTRAN Transport Program, LA-4600, March 1972.

11. **HARDWARE REQUIREMENTS** - Five output units, five interface units (use of interface units is optional) and two system input/output units are required. A large bulk memory is desirable, but it can be replaced by disk, drum or tape storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
K. D. Lathrop and F. W. Brinkley
Los Alamos Scientific Laboratory

16. **MATERIAL AVAILABLE** -
Source (7600-7076 lines, 6600-7077 lines, 360-7495 lines)
Sample problems (7600-1985 lines, 6600-685 lines, 360-1986 lines)
Control information (JCL 360-61 lines)
IBM 2314 load module (360-330 blocks)
Sample problem output (360-50 selected pages, 6600,7600-51 selected pages)
Reference report, LA-4848-MS

17. **CATEGORY** - C
KEYWORDS - two-dimensional, transport theory, x-y, r-z, r-theta, discrete ordinate method, criticality searches, neutron flux, anisotropic scattering, 2DF codes, TWOTRAN codes

18. **SPONSOR** - AEC

1. **IDENTIFICATION AND KWIC TITLE** - RELAP4/MOD7/101
   RELAP4/MOD7/101, thermal & hydraulic phenomena

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER176, CDC7600

3. **DESCRIPTION** - RELAP4/MOD7/101 performs best estimate analyses of nuclear reactors or related systems undergoing a transient. Transient thermal-hydraulic, two-phase phenomena are calculated from formulations of one-dimensional, homogeneous, equilibrium conservation equations for water mass, momentum, and energy. Heat structures are modeled using a transient one-dimensional heat conduction solution that is coupled to the fluid through heat transfer relations. Various explicit models are used to calculate nonhomogeneous, nonequilibrium behavior including a phase separation model, a vertical slip model, and a nonequilibrium model. Other models are used to represent critical flow, reactor kinetics, pressurized water reactor reflood behavior, nuclear fuel rod swelling and blockage, and components such as pumps, valves, and accumulators.

4. **METHOD OF SOLUTION** - The RELAP4 user must define the geometric features of the system to be analyzed as well as an appropriate set of initial conditions. RELAP4 then solves an integral form of the fluid conservation and state equations applied to each user-defined control volume.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   - 9 minor edit variables
   - 20 time-step cards
   - 20 trip control cards
   - 100 junctions (flow paths) between volumes
   - 5 bubble-parameter sets
   - 5 time-dependent volume descriptions on cards
   - 12 pumps
   - 99 control volumes
   - 10 check valve types
   - 5 normalized leak-area-versus-time curves
   - 20 fill system curves
   - 50 heat slabs
   - 20 heat slab geometries
   - 7 heat slab materials
   - 50 core sections
   - 99 data sets for heat exchangers without conduction

6. **TIMING** - For a PWR modeled with 30 to 40 fluid volumes, running time through reflood may range from 30 to 90 minutes or more on the CDC7600. The four sample problems require a total of 55 CP seconds to run on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - RELAP4 provides the following features: a fully-implicit integration technique, steam tables that contain derivatives, heat conduction between fluid volumes, momentum flux terms in the hydraulic equations, a pump model with inertia and friction, a limited air flow capability, a separate hot channel calculation, core cross flow, a boron tracking model, and a multinode steam generator self-initialization capability.
   RELAP4/MOD7 contains the following four program operations - standard RELAP4 (minimum controls), RELAP4-EM (a part of the NRC evaluation model), RELAP4-FLOOD (reflooding rates), and RELAP4-CONTAINMENT (special containment models).

8. **RELATED AND AUXILIARY SOFTWARE** - RELAP4/MOD7 uses PLOTR4M to produce microfilm plots of appropriate variables versus time from data stored on a RELAP4 output data tape. PRELOAD reduces the amount of storage required to run RELAP4.

9. **STATUS** - Abstract first distributed September 1969.
   IBM7044 version of RELAP2 submitted February 1969, deleted December 1971.

IBM360 version of RELAP3 submitted December 1971, 1st revision June 1972, 2nd revision January 1973, 3rd revision July 1973, replaced March 1974 by RELAP4, replaced by Edition B July 1974, revised August 1974, replaced by Edition C January 1975, replaced by Edition D May 1975, replaced by RELAP4/MOD5 Edition E December 1976, replaced December 1978 by RELAP4/MOD6 Edition F submitted April 1978, deleted October 1982.
UNIVAC1108 version of RELAP3 submitted December 1971, deleted March 1974.
CDC6600 version of RELAP3 submitted December 1971, deleted March 1974.
CDC7600 version of RELAP4/MOD5 submitted September 1976, replaced by revised Edition B October 1977 and by Edition C August 1977, replaced December 1978 by RELAP4/MOD6 revised Edition D submitted February 1978 and Edition E submitted April 1978, replaced October 1982 by CDC CYBER176 version and Edition B of RELAP4/MOD7/101 submitted October 1981, sample problems executed by NESC August 1982 on a CDC7600.

10. **REFERENCES** - Stephen R. Behling, et al., RELAP4/MOD7 - A Best Estimate Computer Program to Calculate Thermal and Hydraulic Phenomena in a Nuclear Reactor or Related System, NUREG/CR-1998 (EGG-2089), August 1981.

Steven R. Behling, Ming T. Hsu, Charles A. Dobbe, and Stewart R. Fischer, RELAP4/MOD7 - A Best Estimate Computer Program to Calculate Thermal and Hydraulic Phenomena in a Nuclear Reactor or Related System, Supplement 1, NUREG/CR-1998 (EGG-2089), Supplement 1, November 1981.

RELAP4/MOD7/101, NESC No. 369.C176, Description of RELAP4/MOD7/101 Tape for Use on CDC Cyber176 and CDC-Compatible Systems and Implementation Information, National Energy Software Center Note 83-04, August 24, 1982.

RELAP4/MOD7/101, NESC No. 369.C176B, Description of RELAP4/MOD7/101 Tape for Reading on Non-CDC Systems and Implementation Information, National Energy Software Center Note 83-05, August 24, 1982.

G. D. Brown, C. H. Bush, and R. A. Berman, The Integrated Graphics System for the SC4060: I. User's Manual, Memorandum RM-5660-PR, December 1968.

11. **HARDWARE REQUIREMENTS** - 160,000 (octal) words of SCM and 200,000 (octal) words of LCM (CDC7600), 3 tape drives, and a plotter

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (95%) and COMPASS (5%)

13. **OPERATING SYSTEM** - NOS/BE (CDC CYBER176), SCOPE 2.1.5 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - PLOTR4M as executed at NRTS makes use of the SC-4060 integrated graphics system for microfilm output.

The RELAP4/MOD7/101 Edition B package is provided for those wishing to obtain this CDC Cyber176 program for implementation on other than CDC systems.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

S. R. Behling, C. H. Burgess, H. Chow, K. G. Condie, T. L. DeYoung, S. R. Fischer, C. E. Hendrix, M. Hsu, G. A. Jayne, G. W. Johnson, D. M. Kiser, S. D. Kucharski, G. E. McCreery, C. M. Mohr, R. A. Nelson, R. J. Sand, G. L. Singer, D. L. Siegel, H. Stadtke, J. E. Tolli, and L. R. Fitch
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -

Source (C176-RELAP4 1515 records*, Environmental subroutines 285 records*, C176B-RELAP4 177,403 lines, Environmental subroutines 30,187 lines)
Sample problems (C176-RELAP4 6 records*, PLOTR4M 2 records*, C176B-RELAP4 227 lines, PLOTR4M 8 lines)
Water property library (C176-52 records*, C176B-3232 lines)
Auxiliary source (C176-PLOTR4M 23 records*, conversion program 2 records*, PRELOAD 34 records*, C176B-PLOTR4M 2206 lines, conversion program 8 lines, PRELOAD 2065 lines)
Sample problems output (C176-67 records*, C176B-3068 records+)

Reference reports, NUREG/CR-1998, NUREG/CR-1998 Suppl. 1, Memorandum RM-5660-PR, and NESC Note appropriate to edition

* 512-word maximum length

\+ 140-byte records, maximum of 10 records/block

17. **CATEGORY** - G
KEYWORDS - accidents, blowdown, excursions, heat transfer, hydrodynamics, power plants, reactor safety, transients, BWR reactors, PWR reactors, PLOTR4M codes, RELAP2 codes, RELAP3 codes, RELAP4 codes, PRELOAD codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE -** SCORE3
   SCORE3, SCISRS ENDF/B graphic x-sec evaluation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   IBM360

3. **DESCRIPTION -** SCORE3 is an interactive neutron cross section evaluation system.

4. **METHOD OF SOLUTION -** Experimental neutron cross section data can be retrieved and displayed on an active graphics console. Many bookkeeping operations may be initiated by option selection at the console. Evaluated data analysis modules, permitting the production of evaluated data curves or resonance parameters, are available. The evaluated data curve module includes linear, cubic spline, or least squares cubic spline (see reference 2) curve generation. The resonance analysis module permits single-level, Reich-Moore or Adler multilevel analysis.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** SCORE can display up to 500 experimental data points with their associated error bars. Up to 2 smooth curves may be overlayed on a display of experimental data points. Each curve is restricted to 150 points.

6. **TIMING -** Approximately 6 to 12 minutes per hour at the console are required on an IBM360/50.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** SCORE employs interactive graphics for control of execution paths.

8. **RELATED AND AUXILIARY SOFTWARE -** Three programs are needed to produce the required data libraries. SAP is used to construct experimental data libraries from SCISRS. SCOFF constructs evaluated data libraries from ENDF/B. RAP constructs the resonance parameter library.

9. **STATUS -** Abstract first distributed September 1969.
   IBM360 version of SCORE2 submitted April 1969, replaced by SCORE3 June 1971.

10. **REFERENCES -** C. L. Dunford, SCORE, An Interactive Cross Section Evaluation System, Volume I. Operator's Guide, AI-AEC-12994, Vol. 1, May 15, 1971.
    C. L. Dunford, SCORE, An Interactive Cross Section Evaluation System, Volume II. System Guide, AI-AEC-12994, Vol. 2, June 15, 1971.
    A. Horsley, J. B. Parker, K. Parker, and J. A. Price, Curve Fitting and Statistical Techniques for Use in the Mechanized Evaluation of Neutron Cross Sections, Nuclear Instruments and Methods, Vol. 62, p. 29, 1968.
    J. M. Friedman and M. Platt, SCISRS, Sigma Center Information Storage and Retrieval System, BNL-885, July 1964.
    H. C. Honeck, Specifications for an Evaluated Nuclear Data File for Reactor Applications, ENDF/B, BNL-50066, July 1967.

11. **HARDWARE REQUIREMENTS -** IBM360 Model 50 or higher with 125,000 bytes of fast memory, an IBM2250 graphics console, Models 1, 2, or 3, 2 9-track tape drives, and 1 disk

12. **PROGRAMMING LANGUAGE -** FORTRAN IV and BAL

13. **OPERATING SYSTEM -** OS/360, Version 14 or higher.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    C. L. Dunford
    Atomics International

16. **MATERIAL AVAILABLE -**
    Source (13,265 lines, PDS SCORE.SOURCE 1378 blocks)
    Load module (SCORE.GO 459 blocks)

Libraries (SCISRS data tape-7 files of 3744-character records, ENDF/B data tape-5 fi
of 3608-character records, Resonance Parameters-1 file of 400-character maxi
length records)
DADS libraries (SCISRS 520 blocks of 3520-bytes maximum length records, ENDF/B 40 bloc
of 3600-bytes maximum length records)
Control information (JCL to move data sets from transmittal tape 84 lines, JCL f
execution 137 lines)
Reference reports AI-AEC-12994, Vols. 1 and 2

17. **CATEGORY** - M
KEYWORDS - cross sections, computer graphics, ENDF/B, SCISRS, libraries, Reich-Moo
formula, multilevel analysis, SAP codes, SCOFF codes, RAP codes

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - CITATION
   CITATION, 1,2,3-d diffusion depletion multi-gp

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,303x

3. **DESCRIPTION** - CITATION is designed to solve problems using the finite-difference representation of neutron diffusion theory, treating up to three space dimensions with arbitrary group-to-group scattering. X-y-z, theta-r-z, hexagonal-z, and triagonal-z geometries may be treated. Depletion problems may be solved and fuel managed for multi-cycle analysis. Extensive first-order perturbation results may be obtained given microscopic data and nuclide concentrations. Statics problems may be solved and perturbation results obtained with microscopic data.

4. **METHOD OF SOLUTION** - Explicit, finite-difference approximations in space and time have been implemented. The neutron-flux-eigenvalue problems are solved by direct iteration to determine the multiplication factor or the nuclide densities required for a critical system.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - CITATION has been designed to attack problems which can be run in a reasonable amount of time. Storage of data is allocated dynamically to give the user flexibility in dimensioning. Typically, a finite-difference diffusion problem could have 200 depleting zones, 10,000 nuclide densities, and 30,000 space-energy point flux values.

6. **TIMING** - The two-dimensional finite-difference diffusion theory eigenvalue problems iterate at a rate of about 0.1 millisecond per point per iteration with alternating-direction line relaxation (two sweeps per iteration) with 8-byte words on the IBM360/91 (0.5 on the 360/75). Since about 30 iterations are required for each succeeding eigenvalue problem, machine time for a depletion problem is about 0.003 second per point per time-step. Machine time for most auxiliary calculations is usually insignificant. For a representative fast breeder depletion problem, 68 percent of the machine CPU time is spent in solving eigenvalue problems.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - CITATION is considered unusual in that it should be relatively easy to modify the contents or to add routines. Effective techniques are incorporated to determine a critical system. More than one set of microscopic cross sections may be used in a system and nuclide behavior can be followed on a sub-zone scale within depletion regions. The user has flexible control over the route of a calculation as well as the edit of results.

8. **RELATED AND AUXILIARY SOFTWARE** - The microscopic cross section tape for this program may be generated by various codes, but XSDRN is designed specifically for this purpose. The microscopic cross section routines, formerly an auxiliary program, were integrated into the code to permit such data to be supplied from cards or modified in the same run in which the problem is solved.

9. **STATUS** - Abstract first distributed May 1970.
   IBM360 version submitted July 1969, revised January 1970, replaced May 1970 by 2nd revision, replaced by 3rd revision November 1971, replaced by 4th revision April 1972, replaced by 5th revision July 1972, replaced by 6th revision October 1972, replaced by 7th revision, Edition G, November 1972, replaced by 8th revision, Edition H, September 1974, replaced by 9th revision, Edition I, December 1976, replaced June 1980 by 10th revision, Edition J, submitted August 1979, replaced July 1981 by 11th revision, Edition K, submitted September 1980, sample problem executed by NESC June 1981 on an IBM370/195.

10. **REFERENCES** - T. B. Fowler, D. R. Vondy, and G. W. Cunningham, Nuclear Reactor Core Analysis Code CITATION, ORNL-TM-2496, Revision 2, July 1971, Supplement 1, October 1971, Supplement 2, March 1972, Supplement 3, July 1972.

N. M. Greene and C. W. Craven, Jr., XSDRN, A Discrete Ordinates Spectral Averaging Code, ORNL-TM-2500, July 1969.

D. R. Vondy and T. B. Fowler, Job Stream of Cases for the Computer Code CITATION, ORNL-TM-3793, July 1972.

CITATION, NESC No. 387.360K, CITATION Tape Description and Implementation Information, National Energy Software Center Note 81-66, July 17, 1981.

11. **HARDWARE REQUIREMENTS** - IBM360/91 or equivalent with at least 128,000 32-bit words of directly-addressable main storage, 7 to 32 I/O devices depending upon the calculation, excluding input and output devices and system requirements.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - CITATION contains about 28,700 source statements. Without overlay, storage for the code instructions would approach 574,000 32-bit words, but with overlay the storage requirement is about 90,000 for the program and fixed storage, 10,000 of this 90,000 is used for system library routines.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
T. B. Fowler, D. R. Vondy, and G. W. Cunningham
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 28,521 lines, Assembly language 193 lines)
Sample problem (850 lines)
Control information (JCL 204 lines)
Reference report, ORNL-TM-2496, Rev. 2, Supplements 1, 2, and 3, and NESC Note

17. **CATEGORY** - K
KEYWORDS - one-dimensional, two-dimensional, three-dimensional, multigroup theory, diffusion, criticality searches, buckling, hexagonal configuration, x-y-z, r-theta, burnup, fuel management, XSDRN codes

18. **SPONSOR** - DOE Office of Reactor Research and Technology,
Safety and Physics Division

IDENTIFICATION AND KWIC TITLE - TAC2D
TAC2D, steady-state and transient temp calc

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
UNIVAC1110,1100, IBM360,370,303x

DESCRIPTION - TAC2D is designed to treat transient, two-dimensional heat transfer problems. Steady-state problems are treated by considering the problem to be a transient, starting with an assumed temperature distribution and running until equilibrium conditions are established. Geometrically, rectangular (x,y), cylindrical (r,z), or circular (r,theta) coordinates may be used.

METHOD OF SOLUTION - The heat conduction equation is replaced by an equivalent set of linear finite-difference equations. This set of equations is then solved by the Peaceman-Rachford implicit alternating direction method.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -
(a) The grid line system must be orthogonal in the rectangular, cylindrical, or circular coordinate system. Therefore, the sides of the nodal elements must be orthogonal. The entire problem must be bounded by four grid lines in one of the coordinate systems. Difficulties in treating irregular boundaries can be overcome to some extent through the use of materials having specially chosen properties.
(b) All radiation is treated one-dimensionally.
(c) There is no provision for change of phase. This special heat transfer situation could be included by extension of the existing programming.

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -
(a) The geometrical input is simple.
(b) The input of thermal parameters is by FORTRAN arithmetic statement functions. Many of the calculation variables (time, local temperature, local position) are available for use in these functions.
(c) Internal and external flowing coolants may be used.
(d) There may be internal and external thermal radiation.
(e) There is a wide selection of optional output.
(f) There is a special option which may be used for obtaining steady-state results efficiently.

RELATED AND AUXILIARY SOFTWARE - TAC3D (NESC 414), which is three-dimensional and has many of the features of TAC2D described in this abstract.

STATUS - Abstract first distributed May 1970.
UNIVAC1108 version submitted October 1969, replaced November 1984 by UNIVAC1110 version submitted August 1981, sample problem executed by NESC September 1983 on a UNIVAC1100/44.
IBM360 version submitted June 1980, sample problem executed by NESC August 1981 on an IBM3033 and an IBM370/195.

REFERENCES - R. H. Boonstra, TAC2D, A General Purpose Two-Dimensional Heat Transfer Computer Code, User's Manual, GA-A14032, July 15, 1976.
J. F. Petersen, TAC2D, A General Purpose Two-Dimensional Heat Transfer Computer Code - User's Manual, GA-8868, September 6, 1969.
S. S. Clark and J. F. Petersen, TAC2D, A General Purpose Two-Dimensional Heat Transfer Computer Code - Mathematical Formulations and Programmer's Guide, GA-9262, September 1969.

TAC2D, NESC No. 408.1110, TAC2D Tape Description and Implementation Information, National Energy Software Center Note 85-32, November 30, 1984.

TAC2D, NESC No. 408.360, TAC2D Tape Description and Implementaiton Information, National Energy Software Center Note 82-95, August 25, 1982.

S. M. Morcos and K. A. Williams, The TAC2D Code, Version TFMABC-75-1, Part C: Code Verification and Benchmark Problems, GA-A13415, June 1975.

D. W. Peaceman and H. H. Rachford, The Numerical Solution of Parabolic and Elliptic Differential Equations, Society for Industrial and Applied Mathematics, Vol. 3, pp. 28-41, March 1955.

J. F. Petersen, TAC3D, A General Purpose Three-Dimensional Heat Transfer Computer Code - User's Manual, GA-9263, September 1969.

S. S. Clark, J. V. Del Bene, and J. F. Petersen, TAC3D, A General Purpose Three-Dimensional Heat Transfer Computer Code - Mathematical Formulations and Programmer's Guide, GA-9264, September 1969.

11. **HARDWARE REQUIREMENTS** - 65K words are required on the UNIVAC1110 and 380K bytes on the IBM360. In addition to input/output, a maximum of four and a minimum of no tapes are required depending upon the code options being used.

12. **PROGRAMMING LANGUAGE** - FORTRAN V (UNIVAC1110), FORTRAN IV (IBM360)

13. **OPERATING SYSTEM** - EXEC8 (UNIVAC1110), OS/360 (IBM360).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The FORTRAN H compiler was used to produce the sample output included in the IBM360 package. Use of the H-Extended compiler resulted in a larger number of iterations with the associated variation in the printed results.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    1110 R. H. Boonstra, S. S. Clark, J. V. Del Bene, D. W. Graumann, R. Katz, J. F. Petersen, J. C. Saeger, and M. Troost
    GA Technologies

    360 NEA Data Bank

16. **MATERIAL AVAILABLE** -
    Source (1110-10,678 lines, 360-10,175 lines)
    Sample problems (1110-113 lines, 360-242 lines)
    Control information (1110-150 lines, JCL 360-52 lines)
    Sample problem output (360-41 records*, 40 selected pages)
    Reference reports, (1110 GA-A14032, 360 GA-8868 and GA-9262), and NESC Note appropriate to version
    * 132-byte records

17. **CATEGORY** - H
    KEYWORDS - heat transfer, two-dimensional, coolants, temperature distribution, TAC3D codes

18. **SPONSOR** - DOE
    General Atomic Technologies
    OECD Nuclear Energy Agency

IDENTIFICATION AND KWIC TITLE - CHAINS
CHAINS, analysis of radioactive decay chains

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
GE625,635

DESCRIPTION - CHAINS computes the atom density of members of a single radioactive decay chain. The linearity of the Bateman equations allows tracing of interconnecting chains by manually accumulating results from separate calculations of single chains. Re-entrant loops can be treated as extensions of a single chain. Losses from the chain are also tallied.

METHOD OF SOLUTION - The Bateman equations are solved analytically using double-precision arithmetic. Poles are avoided by small alterations of the loss terms. Multigroup fluxes, cross sections, and self-shielding factors entered as input are used to compute the effective specific reaction rates. The atom densities are computed at any specified times.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
50 members in a chain
100 energy groups
100 time values

TIMING - Less than 10 seconds are required on a GE625.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - CHAINS is similar to CRUNCH and ISOCRUNCH.

STATUS - Abstract first distributed December 1970.
GE635 version submitted December 1969.

REFERENCES - W. B. Henderson, Program CHAINS (NMP-856), GEMP-490, March 27, 1967.

HARDWARE REQUIREMENTS - 16K memory

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - GECOS.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
W. B. Henderson
PWR Systems Division
Westinghouse Electric Corporation

MATERIAL AVAILABLE -
Source (228 lines)
Sample problem (53 lines)
Reference report

CATEGORY - D
KEYWORDS - isotopes, production, decay, reaction kinetics, radioactivity, CRUNCH codes, ISOCRUNCH codes

SPONSOR -

IDENTIFICATION AND KWIC TITLE - GROUSE
GROUSE, space-dependent x-section generation

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - GE625,635

DESCRIPTION - GROUSE computes effective multigroup cross sections as a function of position in the core of a reactor or the absorber region of a fuel or control element. The flux weighting uses synthesized fluxes generated in fine energy detail from parametric flux traverses supplied as input as a function of the core absorption and scatter cross sections.

METHOD OF SOLUTION - Core cross sections in sufficiently fine energy detail to perform numerical Doppler-broadening are generated from single-level Breit-Wigner parameters over the specified energy range. Input parametric flux traverses are computed externally to GROUSE by any appropriate monoenergetic transport approximation, with a trial source in the core for which a correction in GROUSE is subsequently made. The moderator (reflector) and clad (structure) cross sections are supplied as constant scatter and absorption in the monoenergetic flux traverse calculations, but 1/v absorption in those regions is allowed in computing the energy dependence of the moderator flux. The spatial flux shape at each energy in the fine energy lattice is synthesized by interpolation in the parametric values using the value of the core absorption and scatter cross sections at those energies. The group reduction uses these fluxes to generate the effective multigroup reaction rates in specified zones in the core. The multigroup effective cross sections are computed to reproduce the effective reaction rates by again using the parametric flux data.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -

99 groups
40 core zones
20 parametric values of core absorption cross section
3 parametric values of scattering cross section
25 isotopes
2600 fine energy lattice points

The core can contain a mixture of isotopes if the isotopic composition is not a function of position. If isotopic composition varies, effective cross reactions for each isotope can be carried out on one isotope at a time, using the average non-resonant cross section of all others as part of the background cross section.

TIMING - About 20 minutes are required to process 2600 energies and 40 core zones to obtain multigroup cross sections involving 7 isotopes. Generation of Doppler-broadened isotopic library tape is proportional to the number of isotopes and the number of energies for each isotope. One isotope at 2600 energies can be added in about 4 minutes.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - The monoenergetic parametric flux distributions must be calculated and processed externally to GROUSE.

STATUS - Abstract first distributed December 1970.
GE635 version submitted December 1969.

REFERENCES - W. B. Henderson, Development and Correlation of a Method for Generating Space-dependent Multigroup Effective Core Cross Sections for 710 Reactor Analysis, GEMP-548, September 25, 1967.
W. B. Henderson, User's Data for the GROUSE Code, GEMP Note, December 2, 1969.

HARDWARE REQUIREMENTS - 38K memory, 6 tapes or disk

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - GECOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS –** Energy lattices are ordered the analogue of a card sorter. The floating numbers are sorted bit by bit. The sort algorithms (ORDER and ORDER 1) are therefore machine-dependent and are coded for GE625,635 machines.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

W. B. Henderson
PWR Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE –**
Source (1812 lines)
Sample problem (953 lines)
Reference report and Note

17. **CATEGORY –** B
KEYWORDS – cross sections, Breit-Wigner formula, Doppler broadening, flux synthesis, ce calculation, multigroup theory, group constants

18. **SPONSOR –**

1. **IDENTIFICATION AND KWIC TITLE** - MICHRD
   MICHRD, microhardness measurement analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   GE625,635

3. **DESCRIPTION** - The Vickers pyramid number and the microhardness increment fraction are computed from filar micrometer eyepiece readings. These readings are made on indents, which have been made by an indenter, in the material being tested.

4. **METHOD OF SOLUTION** - The Vickers pyramid number is a function of the included angle between two opposite faces of the indenter, the load on the indenter, and the diagonal of the indent. The microhardness increment fraction is a relationship between the Vickers pyramid numbers of two specimens, both being tested at the same temperature. If readings from both specimens are not available at the same temperatures, linear interpolation on the given readings is used to obtain readings at the desired temperatures.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   100 temperatures for each specimen
   1000 indents, summed over all temperatures, for each specimen
   4 readings per indent

6. **TIMING** - Less than 3 seconds per case are required.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - MICHRD is written to use a GE635 subroutine PLOP to plot results with a CalComp plotter. This is a program option. The PLOP subroutine for the GE635 is maintained by General Electric Aircraft Engine Group.

9. **STATUS** - Abstract first distributed December 1970.
   GE635 version submitted December 1969.

0. **REFERENCES** - N. R. Baumgardt and J. L. Kamphouse, Hot Microhardness Program, MICHRD, GEMP-725, December 1, 1969.

1. **HARDWARE REQUIREMENTS** - 27K memory

2. **PROGRAMMING LANGUAGE** - FORTRAN IV

3. **OPERATING SYSTEM** - GECOS.

4. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

5. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   N. R. Baumgardt
   Aircraft Engine Group
   General Electric Company

6. **MATERIAL AVAILABLE** -
   Source (754 lines)
   Sample problem (193 lines)
   Reference report

7. **CATEGORY** - O
   KEYWORDS - radiation effects, temperature, computer graphics, microhardness

8. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - DOS
   DOS, neutron flux-dosimeter activity relation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   GE625,635

3. **DESCRIPTION** - DOS computes the local neutron flux per reference reactor power level which will produce the measured activity of a dosimeter. Alternatively, if the flux value is supplied, the corresponding dosimeter activity will be calculated.

4. **METHOD OF SOLUTION** - The types of dosimeters treated are those in which neutron irradiation of the parent isotope leads to a ground state and a metastable state of the radioactive daughter, or to a ground state only. The Bateman equations are solved directly if the flux is given and iteratively if the activity is given.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maximum of -
   100 power cycles

6. **TIMING** - 0.25 seconds per dosimeter are required.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed December 1970.
   GE635 version submitted December 1969.

10. **REFERENCES** - N. R. Baumgardt and W. B. Henderson, Program DOS, NSP-874, A FORTRAN IV Program to Compute the Flux or Specific Activity Associated with a Dosimeter, GEMP-729, December 1969.

11. **HARDWARE REQUIREMENTS** - 25K memory

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GECOS III.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    W. B. Henderson
    PWR Systems Division
    Westinghouse Electric Corporation
    N. R. Baumgardt
    Aircraft Engine Group
    General Electric Company

16. **MATERIAL AVAILABLE** -
    Source (454 lines)
    Sample problem (93 lines)
    Reference report

17. **CATEGORY** - D
    KEYWORDS - isotopes, production, decay, dosimeters, daughter products

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - GAZE2
   GAZE2, 1-d multigroup diffusion slab, sph, cyl

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   UNIVAC1108

3. **DESCRIPTION** - GAZE2 is a one-dimensional, multigroup, neutron diffusion theory program. It includes all four of the standard one-dimensional geometries - slab, sphere, radial cylinder, and axial cylinder, the last of which is identical to slab geometry except when the ZOOM albedo-type transverse boundary condition is used.

4. **METHOD OF SOLUTION** - Third-order finite difference equations are used at exterior boundaries and material interfaces with fourth-order differencing at interior points. Criticality searches are performed by repetition of pairs of direct and adjoint flux calculations, each pair followed by a first-order perturbation to derive an estimate of the parameter variation required to achieve the desired system multiplication factor.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Optional treatment of the transverse boundary by use of energy- and material-dependent bucklings, leakage cross sections, or ZOOM albedo type boundary conditions.

8. **RELATED AND AUXILIARY SOFTWARE** - ZOOM

9. **STATUS** - Abstract first distributed December 1970.
   UNIVAC1108 version submitted January 1970.

0. **REFERENCES** - S. R. Lenihan, GAZE-2, A One-dimensional, Multigroup, Neutron Diffusion Theory Code for the IBM-7090, GA-3152, August 3, 1962.

1. **HARDWARE REQUIREMENTS** -

2. **PROGRAMMING LANGUAGE** - FORTRAN IV (95%) and Assembly language (5%)

3. **OPERATING SYSTEM** - EXEC2.

4. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

5. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   S. R. Lenihan
   General Atomic Company

6. **MATERIAL AVAILABLE** -
   Source (6118 lines)
   Sample problem (203 lines)
   Reference report

7. **CATEGORY** - C
   KEYWORDS - one-dimensional, multigroup theory, diffusion, slabs, spheres, cylinders, criticality searches, ZOOM codes

8. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - SUPERTOG
   SUPERTOG, ENDF/B fine-gp constants generation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360

3. **DESCRIPTION** - SUPERTOG accepts nuclear data in either a point by point or parametric representation as specified by ENDF/B. This data is averaged over each specified group width. The explicit assumption is made that the flux per unit lethargy is constant or that a suitable weight function will be supplied by the user. When resonance data is available, resolved and unresolved resonance contributions are calculated and used as specified by input options. Fine group constants such as one-dimensional reaction arrays (absorption, fission, etc.), PN elastic scattering matrices, and inelastic and (n,2n) scattering matrices are generated and placed on tapes in formats suitable for use by the GAM1, GAM2, ANISN, or DOT programs.

4. **METHOD OF SOLUTION** - The single-level Breit-Wigner formalism is used for calculation of cross sections in the resolved resonance region. Cross sections in the unresolved resonance region are computed by taking averages over suitable Porter-Thomas distributions of the neutron and fission widths. Smooth cross sections are calculated by integration of point-cross-section data given in ENDF/B File 3. Elastic scattering matrices are computed from Legendre coefficients of the scattering angular distribution data. Inelastic scattering and (n,2n) matrices are computed from excitation functions for individual levels and by using a nuclear evaporation model above the region of resolved levels.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   199 groups
   4000 data points for each reaction type
   30 Legendre coefficients

6. **TIMING** - On the IBM360/65 running time varies from 5 to 25 minutes per nuclide and is a function, primarily, of the number of groups, the number of resolved resonances, and the length of the elastic scattering matrix.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SUPERTOG employs a rather elaborate overlay structure and extensive use of EQUIVALENCE statements to minimize core requirements.

8. **RELATED AND AUXILIARY SOFTWARE** - Three programs are available which extend the flexibility of SUPERTOG. The SUPERTOG data retrieval program retrieves SUPERTOG output from a card image tape written in the ANISN format. This program will retrieve data from a maximum of four tapes and merge this data onto one tape. The program will then, by input option, edit the data, punch cards in either the ANISN or DTF4 format, or write an unformatted tape for use by ANISN. Another program is available which will merge up to a maximum of four card-image tapes written in the GAM2 update format onto a single tape. This program can also take the one-dimensional arrays from one tape and the two-dimensional arrays from another tape and merge this information onto a single tape. The single tape is input to the SUPERTOG version of the GAM2 update program. The GAM2 update program has been modified to accept output from SUPERTOG on either punched cards or magnetic tape.

9. **STATUS** - Abstract first distributed December 1970.
   IBM360 version submitted February 1970, replaced by version 2 January 1971, executed by NESC.

0. **REFERENCES** - R. Q. Wright, J. L. Lucius, N. M. Greene, and C. W. Craven, Jr., SUPERTOG A Program to Generate Fine Group Constants and Pn Scattering Matrices from ENDF/B, ORNL-TM-2679, September 1969, and Addendum, 1970.

1. **HARDWARE REQUIREMENTS** - 65K memory, 6 scratch disks, and 1 tape

2. **PROGRAMMING LANGUAGE** - FORTRAN IV (ANSI FORTRAN)

3. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – SUPERTOG is presently us
a two-level overlay structure consisting of seven separate links.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
R. Q. Wright, J. L. Lucius, N. M. Greene,
and C. W. Craven, Jr.
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** –
Source (Version 1 1192 lines, Version 2 9883 lines)
Sample problems (Version 1 5 lines, Version 2 43 lines)
Libraries (Version 1 1038 lines, Version 2 2231 lines)
Reference report and Addendum

17. **CATEGORY** – B
KEYWORDS – averages, group constants, inelastic scattering, elastic scattering, B
Wigner formula, Porter-Thomas distribution, cross sections, GAM1 codes, GAM2 codes,
codes, DOT codes, DTF4 codes, ETOG codes

18. **SPONSOR** –

1. **IDENTIFICATION AND KWIC TITLE -** COBRA4I
   COBRA4I, rod bundle & core thermal-hydraulics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC6600,7600,CYBER175, Cray1, IBM360,3033,4331

3. **DESCRIPTION -** COBRA4I performs steady-state and transient thermal-hydraulic analysis of rod bundle nuclear fuel elements and cores via the subchannel analysis method.

4. **METHOD OF SOLUTION -** The conservation equations of flow and energy are solved for interconnected subchannel control volumes via conventional finite differencing techniques. The steady-state calculations are solved by implicit finite differencing whereas the transient calculations are performed by either an implicit or explicit finite difference scheme. Internal rod temperatures are calculated by an orthogonal collocation approximation to the heat conduction equation.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** Using the COBRA4I code option to store variables on peripheral storage devices eliminates any practical limit as to maximum problem size. However, computer core requirements and code execution time is always a consideration when determining the complexity of the problem to be solved.

6. **TIMING -** On a CDC7600 running time is 0.004 seconds per cell-iteration using the implicit solution scheme and 0.00006 seconds per cell-iteration using the explicit scheme. The number of cells is determined as the number of subchannels times the number of axial nodes. The number of iterations required per time-step varies according to convergence criteria and complexity of physics; however, typical values are from 10 to 20 iterations for the implicit scheme and 10 to 50 iterations for the explicit scheme. The three sample problems run in less than 30 seconds on the Cray1. The U-tube and fuel thermal sample problems each run in less than 2 minutes and the 7-pin sample problem in less than 1 minute on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** The improved capabilities of COBRA4I over its predecessor COBRA3C include:
   (a) A new explicit solution scheme to calculate severe transients involving flow reversals, recirculations and expulsion and reentry flows with either a flow or pressure boundary condition specified.
   (b) Improved storage allocation to reduce central memory requirements and improved running time.
   (c) Improved fuel rod heat conduction model to calculate interior-rod temperatures with axial conduction and variable thermal conductivity included. Each rod may now consist of axially-varying materials.
   (d) Addition of a set of correlations to calculate the properties of superheated steam and a set of heat transfer correlations covering the complete range of heat transfer from subcooled through boiling.
   (e) Problem "Dump and Restart" capabilities which allow the solution to be saved for subsequent use either to continue calculations or to be used as an initial guess for a different problem which can result in significant time savings for similar problems.
   (f) Auxiliary program to re-dimension COBRA based on user specified input defining problem size and code options desired, thus minimizing storage requirements.
   (g) Auxiliary program to generate COBRA input for hexagonal rod-bundle geometry. Input for card groups 4, 7, and 8 can be generated, thus greatly reducing the amount of input required.
   (h) Line-printer plotting capability to display pressure drop, mass flux, enthalpy and crossflow versus axial position for all or a specified number of gaps and

channels.

(i) A thermally-conducting wall model which can conduct heat between two channels on opposite sides of a wall.

8. **RELATED AND AUXILIARY SOFTWARE** - COBRA4I is an extended version of the COBRA3C computer program. The auxiliary program SPECSET re-dimensions COBRA4I according to user-specified problem size, and the auxiliary program GEOM calculates COBRA input for data groups 4, 7, and 8 for hexagonal rod bundles. The IBM version also contains auxiliary program CSPECS which replaces pseudostatements of the form •CALL SPECx in COBRA4I with the correctly sized set of FORTRAN declarative statements comprising COMDECKx.

9. **STATUS** - Abstract first distributed December 1970.
UNIVAC1108 version of COBRA2 submitted December 1970, replaced by COBRA3 in June 1971, replaced by COBRA3C in April 1973, deleted August 1977.
IBM360 version of COBRA2 submitted February 1970, replaced by COBRA3 in September 1971, replaced by COBRA3C in April 1973, deleted August 1977.
CDC6600 version of COBRA3C submitted June 1973, replaced by CDC7600 version of COBRA4I in August 1977.
CDC7600 version of COBRA4I submitted June 1976, replaced by revised Edition B December 1977, replaced by revised Edition C April 1978, replaced by revised Edition D August 1978, replaced by revised Edition E October 1979, replaced by revised Edition F June 1980, replaced by revised Edition G May 1981, sample problems executed by NESC February and March 1981, on a CDC7600 and CYBER175.
Cray1 version of COBRA4I submitted April 1981, sample problems executed by NESC June 1981 on a Cray1.
IBM360 version of COBRA4I submitted February 1979, sample problems executed by NESC August 1985 on an IBM3033.

10. **REFERENCES** - C. L. Wheeler, C. W. Stewart, R. J. Cena, D. S Rowe, and A. M. Sutey, COBRA-IV-I: An Interim Version of COBRA for Thermal-hydraulic Analysis of Rod Bundle Nuclear Fuel Elements and Cores, BNWL-1962, March 1976.

C. W. Stewart, C. L. Wheeler, R. J. Cena, C. A. McMonagle, J. M. Cuta, and D. S. Trent, COBRA-IV: The Model and the Method, BNWL-2214, July 1977.

C. W. Stewart, C. A. McMonagle, M. J. Thurgood, T. L. George, D. S. Trent, J. M. Cuta, and G. D. Seybold, Core Thermal Model: COBRA-IV Development and Applications, BNWL-2212, January 1977.

D. M. Lister and P. A. Jallouk, COBRA IV-I An IBM-Compatible Version, NUREG/CR-0519 (ORNL/NUREG/CSD-9), December 1978.

COBRA4I, NESC No. 432.7600G, Tape Contents Description, National Energy Software Center Note 77-37, Revised May 23, 1981.

COBRA4I, NESC No. 432.CRA1, COBRA4I Tape Description, National Energy Software Center Note 82-108, August 20, 1982.

COBRA4I, NESC No. 432.3033, COBRA4I Tape Description and Implementation Information, National Energy Software Center Note 86-05, October 25, 1985.

11. **HARDWARE REQUIREMENTS** - 202,000 (octal) words and 4 scratch units besides the standard input/output units (CDC7600), 450K bytes and 6 units besides the standard input/output units (IBM3033).

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE (CDC6600,7600), NOS (CDC CYBER175), COS (Cray1), MVS (IBM3033), VM/CMS (IBM4331).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600 C. L. Wheeler, C. W. Stewart, J. F. Cena, D. S. Rowe, and A. M. Sutey
Pacific Northwest Laboratory

Cray1 T. Hosokawa

Century Research Center Corporation
Japan

3033 D. M. Lister and P. A. Jallouk
Oak Ridge National Laboratory
E. Pezzoni
Comision Nacional de Energia Atomica
Argentina

. **MATERIAL AVAILABLE** -
Source (COBRA4I 7600-6754 lines, CRA1-6780 lines, 3033-8436 lines)
Sample problems (COBRA4I 7600-214 lines, CRA1-213 lines, 3033-216 lines, SPECSET 7600-281 lines, CRA1-225 lines, 3033-244 lines, GEOM 7600-8 lines, CRA1-8 lines, 3033-8 lines, CSPECS 3033-1 line)
Auxiliary programs (SPECSET 7600-210 lines, CRA1-210 lines, 3033-214 lines, GEOM 7600-622 lines, CRA1-622 lines, 3033-617 lines, CSPECS 3033-225 lines)
Control information (7600-94 lines, CRA1-97 lines, 3033-220 lines)
Sample problem output (7600 and CRA1-58 selected pages, 3033 U-TUBE 1693 132-character records, FUEL THERMAL 1740 132-character records, 7-PIN 487 132-character records)
Reference reports, BNWL-1962, BNWL-2212, and BNWL-2214 (all versions), NUREG/CR-0519 (IBM version), and NESC Note, appropriate to version

. **CATEGORY** - H
KEYWORDS - blowdown, reactor cores, enthalpy, hydraulics, rod bundles, fluid flow, heat transfer, reactor safety, transients, LMFBR reactors, water reactors, COBRA codes, SPECSET codes, GEOM codes

. **SPONSOR** - ERDA Division of Reactor Development and Demonstration
NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research
Japan - Century Research Center Corporation

1. **IDENTIFICATION AND KWIC TITLE -** CONTEMPT-LT/028, CONTEMPT-LT/026
   CONTEMPT-LT/026, pressure-temperature response
   CONTEMPT-LT/028, pressure-temperature response

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -** CDC7600,CYBER176, IBM360

3. **DESCRIPTION -** CONTEMPT-LT was developed to predict the long-term behavior of water-cooled nuclear reactor containment systems subjected to postulated loss-of-coolant accident (LOCA) conditions. CONTEMPT-LT calculates the time variation of compartment pressures, temperatures, mass and energy inventories, heat structure temperature distributions, and energy exchange with adjacent compartments. The program is capable of describing the effects of leakage on containment response. Models are provided for fan cooler and cooling spray engineered safety systems. One to four compartments can be modeled, and any compartment except the reactor system may have both a liquid pool region and an air-vapor atmosphere region above the pool. Each region is assumed to have a uniform temperature, but the temperatures of the two regions may be different. The user determines the compartments to be used, specifies input mass and energy additions, defines heat structure and leakage systems, and prescribes the time advancement and output control.

4. **METHOD OF SOLUTION -** The initial conditions of the containment atmosphere are calculated from input values, and the initial temperature distributions through the containment structures are determined from the steady-state solution of the heat conduction equations. A time advancement proceeds as follows. The input water and energy rates are evaluated at the midpoint of a time interval and added to the containment system. Pressure suppression, spray system effects, and fan cooler effects are calculated using conditions at the beginning of a time-step. Leakage and heat losses or gains, extrapolated from the last time-step, are added to the containment system. Containment volume pressure and temperatures are estimated by solving the mass, volume, and energy balance equations. Using these results as boundary conditions, the heat conduction equations describing structure behavior are advanced using an implicit technique. The resulting heat transfer rates are used to correct the previous estimates of the water and energy storage in the containment volume, and the containment conditions are obtained by solving for the second time the containment balance equations. The pressure suppression routines use the conditions at the beginning of a time-step to calculate both the initial expulsion of water from the vents and the flow through the vents. From the calculated flow rates, mass and energy are removed from the dry well and added to the wet well.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** Maxima of -
   20 heat conducting structures
   101 mesh points for each structure
   20 regions for each structure
   50 flow elements in one segment of the horizontal vent pressure suppression system
   10 horizontal vents (or branches) in a segment
   50 reductions within an input time-step
   CONTEMPT-LT can be used for analyzing the transient containment behavior of boiling-water reactors (BWRs) including Mark I, Mark II, and Mark III systems; pressurized-water reactors (PWRs), and experimental water reactor simulators or related experiments.

6. **TIMING -** On the CDC7600, CONTEMPT-LT/028 requires less than 30 seconds to run the two sample problems. On the IBM360/75, CONTEMPT-LT/026 requires approximately 0.021 second per time advancement with 90 mesh points for heat structures without pressure suppression. The pressure suppression timing is not easily predicted but run time for two sample problems ranged from 0.3 to 2 seconds per time advancement.

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -** CONTEMPT-LT/028 is the most recent of a series of computer programs developed to describe the thermal-hydraulic conditions attendant to various postulated transients in the containment of light-water reactor systems. CONTEMPT-LT/026

replaced CONTEMPT (NESC 297), CONTEMPT-CONPS, CONTEMPT-PS, CONTEMPT-LT/022, and CONTEMPT-LT/025 (which contained known errors and was never distributed by the Center).

9. **STATUS** - Abstract first distributed December 1970.
CDC7600 version of CONTEMPT-LT/028 submitted March 1979, revised August 1979, revised November 1979, revised April 1980, replaced by revised Edition B October 1984, sample problems executed by NESC April 1984 on a CDC7600.
IBM360 version of CONTEMPT-CONPS submitted February 1970, replaced by CONTEMPT-PS April 1971, replaced by CONTEMPT-LT/020 August 1973, replaced by CONTEMPT-LT/022 December 1973, replaced by Edition B July 1974, replaced by CONTEMPT-LT/026 April 1976, revised to Edition B July 1977, sample problem executed by NESC September 1977 on an IBM370/195.

10. **REFERENCES** - D. W. Hargroves and L. J. Metcalfe, CONTEMPT-LT/028 - A Computer Program for Predicting Containment Pressure-Temperature Response to a Loss-of-Coolant Accident, NUREG/CR-0255 (TREE-1279), March 1979.

CONTEMPT-LT/028, NESC No. 433.7600B, CONTEMPT-LT/028 Tape Description and Implementation Information, National Energy Software Center Note 85-14, October 22, 1984.

L. L. Wheat, R. J. Wagner, G. F. Niederauer, and C. F. Obenchain, CONTEMPT-LT - A Computer Program for Predicting Containment Pressure-Temperature Response to a Loss-of-Coolant Accident, ANCR-1219, June 1975.

K. D. Richert, BUFIO, A Subroutine to Permit FORTRAN Access to IOOP, Phillips Petroleum Note, February 1966.

A. J. Smith, Standard Package Description, CalComp Plotter Subroutines (S0010.0), Appendix D, January 1971.

W. H. Rettig, R. C. Young, and N. H. Marshall, UPD - A Program to Update Source Decks, P01751, and Addendum.

R. J. Wagner, STH2O, A Subroutine Package to Compute the Thermodynamic Properties of Water, ANCR Note, 1975.

NRTS Environmental Subroutine Manual, ANC Document, December 1972.

W. J. Mings, Fan Cooler Containment Model in CONTEMPT-LT/025, SRD-25-76, November 1975.

W. J. Mings, Correction to Uchida Model of CONTEMPT-LT/025 Program, SRD-43-76, December 1976.

W. J. Mings, Version 26 Modifications to the CONTEMPT-LT Program, SRD-83-76, April 1976.

11. **HARDWARE REQUIREMENTS** - 58K (octal) bytes and a CalComp or microfilm plotter (CONTEMPT-LT/028); 430K bytes and a CalComp or SC4060 plotter for graphical output (CONTEMPT-LT/026)

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and COMPASS (CDC7600), FORTRAN IV and BAL (IBM360)

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), OS/MVT (IBM360).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The thermodynamic properties of water and steam required by the program are generated by the STH2O program and made available as a library data set.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600 D. W. Hargroves, L. J. Metcalfe, and Teh-Chin Cheng
EG&G Idaho, Inc.

7600B C. C. Lin
Department of Nuclear Energy
Brookhaven National Laboratory

360 L. L. Wheat and W. J. Mings
Idaho National Engineering Laboratory
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE -**
Source (CONTEMPT 7600B-10,622 lines, CONTEMPT UPDATE 7600B-10,657 lines, INEL Environmental Library (SCOPE1) 7600B-26,658 lines, INEL Environmental Library (SCOPE2) 7600B-26,677 lines, INEL Environmental Library UPDATE 7600B-27,631 lines, CONTEMPT 360-9954 lines, NRTS Environmental Subroutines 360-22,103 lines)
Sample problems (7600B-84 lines, 360-52 lines)
Libraries (7600B-2544 lines, 360-476 blocks•)
Auxiliary source (7600B-8 lines, 360-35 lines)
Control information (7600B-71 lines, segload lines 7600B-27 lines, JCL 360-110 lines)
Sample problems output (7600B-5436 132-character records)
Reference reports, Subroutine Descriptions, SRD Notes, and NESC Note, as appropriate
For 360 use:
Load modules (CNTMPT for both 2314 and 3330 disks 476 blocks, ENVIR for both 2314 and 3330 disks 559 blocks)
• DCB=(RECFM=VS,LRECL=796,BLKSIZE=800)

17. **CATEGORY** - G
KEYWORDS - accidents, temperature distribution, pressure, containment, water, thermodynamics, heat transfer, CONTEMPT codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
Division of Systems Safety

1. **IDENTIFICATION AND KWIC TITLE** - ETOG1 Data for MUFT and GAM Libraries
   ETOG1 DATA LIBRARIES, MUFT4 or 5, GAM1 or 2

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC6600

3. **DESCRIPTION** - The data required for the creation of MUFT4, MUFT5, GAM1, and GAM2 libraries were generated from the Brookhaven National Nuclear Data Center ENDF/B tapes 114 through 117 by the ETOG1 program (NESC 437).

4. **METHOD OF SOLUTION** - The original ENDF/B data tapes 114, 115, and 116 received from the Brookhaven Center were altered. The CRECT program (NESC 384) was used to make corrections to mu bar, the average cosine of the scattering angle, xi, the logarithmic energy decrement, and gamma, the anisotropic Grueling-Goertzel parameter. Points were inserted into elastic scattering angular distribution tables so that anisotropy did not extend down to thermal energies, and the secondary distribution data for material numbers 1018 and 1021 were changed. The materials for which library data were generated are -

1001	H	1019	Mn55	1037	Au197	1056	Am241
1003	D	1020	Fe	1042	U233FP	1057	Am243
1005	Li6	1021	Ni	1043	U234	1058	Cm244
1006	Li7	1024	Nb	1044	U235	1059	Na23
1007	Be9	1025	Mo	1045	U235FP	1060	W182
1009	B10	1026	Xe135	1046	U236	1061	W183
1010	C12	1027	Sm149	1047	U238	1062	W184
1012	N14	1028	Eu151	1048	Np237	1063	W186
1013	C16	1029	Fu153	1050	Pu238	1066	U233SFP
1014	Mg	1030	Gd	1051	Pu239	1067	U233NFP
1015	A127	1031	Dy164	1052	Pu239FP	1068	U235SFP
1016	Ti	1032	Lu175	1053	Pu240	1069	U235NFP
1017	V51	1033	Lu176	1054	Pu241	1070	Pu239SFP
1018	Cr	1035	Ta181	1055	Pu242	1071	Pu239NFP

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

Library	No. of groups
GAM1	68
GAM2	99
MUFT4,5	54

A 1/E weighting function joined to the fission spectrum was used. A 1.0•10••7 value was used as the non-resonance potential scattering cross section per absorber atom. For MUFT libraries the 26th group was the lowest group number in the resonance region, the 25th group was the highest in the inelastic region.

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The CRECT code was used to make the necessary alterations to the ENDF/B tapes. The data decks were created for the MUFT4, MUFT5, GAM1, and GAM2 programs.

9. **STATUS** - Abstract first distributed December 1970.
   CDC6600 version submitted February 1970.

10. **REFERENCES** - S. Kellman and D. E. Kusner, Description of the Generation of Data Decks by ETOG-1 for Use in Creating MUFT and GAM Libraries, WCAP-3845-2 (ENDF-133), January 1970.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** -

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

S. Kellman and D. E. Kusner
PWR Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE -**

MUFT4 (7,414 lines)
MUFT5 (10,438 lines)
GAM1 (15,393 lines)
GAM2 (36,970 lines)
Reference report

17. **CATEGORY -** Z
KEYWORDS - cross sections, libraries, MUFT4 codes, MUFT5 codes, GAM1 codes, GAM2 codes, ETOG codes, CRECT codes

18. **SPONSOR -**

1. **IDENTIFICATION AND KWIC TITLE** - CYGRO5
   CYGRO5, oxide fuel rod stress & deformation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600,6600,CYBER175

3. **DESCRIPTION** - CYGRO5 is the latest in the CYGRO series of fuel rod analysis programs. The program calculates the axisymmetric temperatures, deformations, and stresses in fuel rods. Significant developments in CYGRO5 include a comprehensive model for temperature and deformation analysis of radially-zoned fuel with separate or bonded zones having distinct material properties, provision for simultaneous, coupled analysis of a number of rod slices, a time- and temperature-dependent fission gas release model with a coupled swelling model, and improved cladding growth and creep representations. Either single-zone or dual-zone fuel can be analyzed.

   Input to CYGRO5 consists of rod data and operating history. The rod data characterize the geometry and physical properties of the rod, including the cladding diameter and thickness, fuel zone dimensions, and relevant mechanical and physical properties of the fuel and cladding. The operating history consists of the measured or predicted values of coolant pressure and temperature, reactor power level, and relevant relationships between power level, fission rate, and neutron flux. The program computes the corresponding history of rod temperature, dimensional changes, and stresses.

   Temperature computations assume thermal equilibrium. The temperature distribution is thus a function of current reactor power level, gamma heating and nuclear self shielding, and the thermal conductivities of fuel, clad, fuel-clad gap, and rod-coolant interface. Fuel conductivity is calculated from the input data as a function of the current, local temperature, porosity, fission depletion, and cracking. Gap conductivity depends on gap size, thermal radiation, conduction at points of fuel-clad contact, and the conductivity of the fluid in the gap. This conductivity depends on composition, on temperature, and, where appropriate, on pressure.

   Deformation of the fuel and clad, the stresses in both, and the forces of interaction between fuel zones, between fuel and clad, and between rod and support are computed from a Large Deflection Finite Element model incorporating representations for thermo-elasticity, creep resulting from thermally-activated mechanisms or mechanisms associated with bombardment by high energy particles, fuel swelling and densification, clad growth resulting from neutron bombardment, and fuel cracking and crack healing. In keeping with the Finite Element representation, the program accounts for the effects of spatial, as well as temporal, variation of temperature, stress, strain, cracking, and densification.

   Another important feature of CYGRO5 is the comprehensive model used for fuel-fuel, fuel-clad, and rod-support interaction. In addition to interacting through radial stresses, the two fuel zones and the fuel and clad can interact through axial forces. The axial strain rates may be the same or different depending on gap size, the direction and magnitude of the axial interaction force, and the effects of pellet "hourglassing", eccentric pellets, lodged chips, and clad collapse, where relevant. Similarly, the rod axial strain rate may be the same as, or different from, the rate of support extension. Relative motion between rod and support depends on the magnitude of the axial interaction force and the force needed for slippage. The support extension includes the effects of flexibility and thermal expansion, as well as user-input extension as might arise, perhaps, from the representation of support extension associated with neutron-flux-induced growth. The comprehensive form of the fuel-clad and rod-support interaction model is particularly important in the correct representation of rod behavior in response to reactor power changes such as those encountered in "swing load" operation.

4. **METHOD OF SOLUTION** - Each axial segment of the fuel and clad is divided into a number of concentric, ring-shaped finite elements. Equations for balance of forces and continuity of displacement between the rings determine the principal unknowns. Plastic flow (creep) is treated on an incremental basis. The required sizes of time-steps are calculated internally on the basis of specified accuracy limits.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   30 axial segments
   30 rings (fuel plus clad) in each axial segment

6. **TIMING** - Running time depends on complexities of history input and number of elements. The running time is roughly proportional to the number of axial segments. For a one-segment problem the program completes about 1500 time-steps per central processor minute on the CDC7600. The number of steps per reactor hour depends on the complexity of power history and the severity of the reactor environment. Practical problems display a range from about 0.5 reactor hours per step to about 10 hours per step.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - CYGRO5 has been developed from the CYGRO1, CYGRO2 (NESC 266), CYGRO3, and CYGRO4 programs. CYGRO5 uses routines from the BETTIS PROGRAMMING ENVIRONMENT LIBRARY (NESC 665). The IBM360 conversion of CYGRO3 was done by R. N. Hagen of EG&G Idaho, Inc., Idaho Falls, Idaho and D. C. Bell and T. R. Walker of the Tennessee Valley Authority, Chattanooga, Tennessee.

9. **STATUS** - Abstract first distributed December 1970.
   CDC6600 version of CYGRO3 submitted July 1970, replaced by corrected version August 1971, deleted June 1983.
   CDC7600 version of CYGRO5 submitted March 1983, source deck compiled by NESC April 1983 on a CDC CYBER175.
   IBM360,370 preliminary version of CYGRO3 submitted February 1973, replaced by Edition B March 1975, deleted June 1983.

10. **REFERENCES** - J. B. Newman and S. E. Kovscek, The CYGRO5 Fuel Rod Analysis Computer Program, WAPD-TM-1504, October 1982.
    W. R. Cadwell, (Ed.), Reference Manual - Bettis Programming Environment, WAPD-TM-1181, September 1974.
    J. B. Newman, J. F. Giovengo, and L. P. Comden, The CYGRO4 Fuel Rod Analysis Computer Program, WAPD-TM-1300, July 1977.
    S. E. Kovscek, CYGRO5 Compliance with American Standard FORTRAN, BAPL Note, March 21, 1983.
    CYGRO5, NESC No. R449, CYGRO5 Tape Description, National Energy Software Center Note 83-66, June 1, 1983.

11. **HARDWARE REQUIREMENTS** - 140,000 (octal) words of central memory; 10,000 plus 30,000 (octal) words of large core memory per axial segment

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.3 (CDC6600), SCOPE 2.0 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. B. Newman and S. E. Kovscek
    Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (22,772 lines)
    Sample problem (190 lines)
    Reference report, WAPD-TM-1504, and Notes

17. **CATEGORY** - I
    KEYWORDS - stresses, fuel elements, deformation, bubble growth, temperature, pressure, CYGRO codes

18. **SPONSOR** - DOE Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - COMNUC, CASCADE
   COMNUC,CASCADE, compound nucleus reaction

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - COMNUC calculates neutron reaction cross sections using a statistical model for decay of the compound nucleus. Competing reaction types permitted are elastic, discrete and continuum inelastic, gamma ray emission, capture, fission, and n,2n.
   CASCADE solves the intranuclear gamma ray cascade equation to determine secondary particle emission probabilities. Competing processes considered are gamma ray emission, neutron emission and fission.

4. **METHOD OF SOLUTION** - In COMNUC Hauser-Feshbach theory as modified by Moldauer is used to determine competition in the decay of the compound nucleus. Physical models for the various reaction types permit the user to input parameters for those models. Direct reaction components may be provided by card input. These cross sections are combined with calculated compound nucleus cross sections to provide a complete self-consistent set of neutron cross sections at each incident neutron energy.
   In CASCADE a coupled set of inhomogeneous Volterra equations of the second kind describing the energy dependence of the probability for particle termination of a gamma ray cascade is solved numerically. Branching ratios determined from these probabilities may be used as input to the COMNUC program.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -
   COMNUC - Only reaction types listed above may be analyzed, but other reactions such as n,p and n,alpha may be included easily.
   CASCADE - Only dipole radiation is permitted in the gamma ray cascades. No discrete channels are permitted - only continuum particle emission.

6. **TIMING** - For low incident-neutron energies and few open channels COMNUC running time is about 15 seconds per case on an IBM360/65. Cases of the complexity of the sample cases can take as much as 1.5 minutes. Approximately 15 minutes are required on an IBM360/65 for a CASCADE case exercising all options and incident neutrons up to 5 MeV in energy.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - CASCADE generates gamma ray cascade branching ratios for input to COMNUC. Output from CASCADE can be used as input for COMNUC when calculating neutron capture cross sections.

9. **STATUS** - Abstract first distributed January 1972.
   IBM360 version submitted April 1971.

10. **REFERENCES** - C. L. Dunford, A Unified Model for Analysis of Compound Nucleus Reactions, AI-AEC-12931, July 1970.
    C. L. Dunford, Compound Nucleus Reaction Analysis Programs COMNUC and CASCADE, AI-TI-707-130-013, March 1971.

11. **HARDWARE REQUIREMENTS** - 150K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV with one Assembler language subroutine for performing internal I/O.

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. L. Dunford
    Atomics International

16. **MATERIAL AVAILABLE -**
Source (COMNUC 2240 lines, CASCADE 1110 lines)
Sample problems (COMNUC 219 lines, CASCADE 29 lines)
Reference reports

17. **CATEGORY** - A
KEYWORDS - compound nuclei, cross sections, capture, fission, elastic scattering, inelastic scattering

18. **SPONSOR -**

IDENTIFICATION AND KWIC TITLE - RELO2
REL02, failure probability calculation by MC

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC6600,7600

DESCRIPTION - RELO2 computes the failure probability for a single failure mode. Six options are available: option 1 calculates the interaction of two normally-distributed variates, option 2 calculates the interaction of two truncated normally-distributed variates, option 3 calculates the interaction of a normal variate with a Weibull variate, option 4 calculates the interaction of two Weibull distributions, option 5 calculates the interaction of a truncated normal variate with a Weibull variate, and option 6 calculates the interaction of a truncated normal and uniform variate.

METHOD OF SOLUTION - The failure probability is calculated by means of a simplified Monte Carlo technique which randomly selects a value of the applied stress and calculates the probability that the strength is smaller than the stress. The density of the failure distribution and the average failure probability are calculated for N such selections.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The number of random selections of the applied stress is restricted to 2000.

TIMING - Less than 1 minute is required. NESC executed the sample problem in 30 CP seconds on a CDC6600 and 3 CP seconds on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE - Options 2, 5, and 6 of RELO2 offer the estimate of the interaction of truncated variates.

RELATED AND AUXILIARY SOFTWARE - RELO2 uses the Bettis Environmental Library (NESC 665). RELO2 is an extension of RELO1 which contained options 1 and 2 only.

STATUS - Abstract first distributed January 1972.
CDC6600 version of REL01 submitted September 1971, replaced August 1980 by REL02 submitted January 1979, sample problem executed by NESC January 1980 on a CDC6600 and CDC7600.

REFERENCES - D. R. Rauth, C. M. Smith, and E. C. Strothers, RELO1 - A Reliability Program for a Single Failure Mode, WAPD-TM-1009, May 1971.
D. R. Rauth and C. M. Smith, RELO2 - A Monte Carlo Technique to Calculate Failure Probability, WAPD-TM-1233, August 1978.
W. R. Cadwell, Editor, Reference Manual - Bettis Programming Environment, WAPD-TM-1181, September 1974.
C. Lipson and N. J. Sheth, Statistical Design and Analysis of Engineering Experiments, McGraw-Hill, New York, New York, 1973.

HARDWARE REQUIREMENTS - 74,000 (octal) words of memory are required for execution on the CDC6600 or 55,000 (octal) words of memory for execution on the CDC7600.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - SCOPE 3.1.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The Bettis Environmental Library routines used by REL02 are not included in the package. These routines would either have to be acquired and modified, or replaced for implementation in the local computing environment. They are heavily-dependent on the operating system under which they were developed.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
D. R. Rauth and C. M. Smith
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (1147 lines)
    Sample problem (4 lines)
    Sample problem output (41 pages)
    Reference report, WAPD-TM-1233

17. **CATEGORY** - P
    KEYWORDS - Monte Carlo method, statistics, stresses, failures

18. **SPONSOR** - DOE Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - CONCEPT5, CONCEPT3
   CONCEPT3, power plant conceptual cost estimate
   CONCEPT5, power plant conceptual cost estimate

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM3033,360,370,4331, UNIVAC1108

3. **DESCRIPTION** - The CONCEPT computer code system was developed to provide conceptual capital cost estimates for nuclear and coal-fired power plants. Cost estimates can be made as a function of plant type, size, location, and date of initial operation. The output includes a detailed breakdown of the estimate into direct and indirect costs similar to the accounting system described in document NUS-531. Cost models are provided in CONCEPT5, the fifth generation in the development of the CONCEPT package, for single-unit coal-fired plants, pressurized-water reactors, boiling-water reactors, liquid-metal-cooled reactors, and multi-unit coal-fired plants based on today's average or best operating experience. Costs may be obtained for any of twenty U. S. cities, a hypothetical Middletown site, and two Canadian cities. CONCEPT5 models are updated models of those available in CONCEPT3 and, in addition, this edition contains historical factory equipment cost data for the generation of cost indices and escalation rates; indirect costs are calculated as a function of unit size rather than a function of direct costs; and an indirect cost account for owner's costs and an improved time-dependent escalation feature are included.
   The CONCEPT3 models and cost data are outdated; the package is being retained in the library since it is the only UNIVAC1108 machine version of CONCEPT available and could prove helpful in converting the latest IBM release.

4. **METHOD OF SOLUTION** - CONCEPT is based on the premise that any central station power plant involves approximately the same major cost components regardless of location or date of initial operation. The program has detailed cost models for each plant type at a reference condition. Through use of size, time, and location-dependent cost adjustments, a reference cost model is modified to produce a specific capital cost estimate.
   CONCEPT is supported by two auxiliary programs--CONTAC, which generates and maintains the cost-model data file, and CONLAM, which generates and maintains the equipment, labor, and materials historical cost data file.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - CONCEPT5 accepts power levels of 500 to 1500 MW(e) for nuclear plants and 300 to 1000 MW(e) for coal-fired plants, while CONCEPT3 accepts levels of 500 to 2000 MW(e). The auxiliary program CONLAM is limited to 30 time periods of cost history for 23 locations without program alterations.

6. **TIMING** - A single CONCEPT5 or CONCEPT3 cost estimate is generated in less than 1 minute.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - CONCEPT utilizes execution-time NAMELIST variations of stored constants, printer plotting of cash flow curves, and numerous output and solution options.

8. **RELATED AND AUXILIARY SOFTWARE** - CONCEPT requires the use of CONLAM to generate a user file of labor and materials cost history and CONTAC to generate a user file of cost models.

9. **STATUS** - Abstract first distributed January 1972.
   IBM360 version of CONCEPT submitted September 1971, replaced by CONCEPT2 March 1973, replaced by CONCEPT3 March 1974, replaced by CONCEPT4 April 1976, replaced by Edition B February 1977, replaced by Edition C May 1978, replaced May 1979 by CONCEPT5 submitted February 1979, replaced September 1980 by Edition B submitted June 1980, replaced April 1982 by Edition C submitted February 1982, replaced by IBM3033 version May 1985, sample problem executed by NESC February 1985 on an IBM4331.
   UNIVAC1108 version of CONCEPT3 submitted May 1975.

10. **REFERENCES** - C. R. Hudson, II, CONCEPT-5 User's Manual, ORNL-5470, January 1979, with Addendum, June 26, 1980, Revised February 1985.

CONCEPT5, NESC No. 498.3033, CONCEPT5 Tape Description and User Information, National Energy Software Center Note 85-70, May 17, 1985.

H. I. Bowers, R. C. DeLozier, L. D. Reynolds, and B. E. Srite, CONCEPT - Computerized Conceptual Cost Estimates for Steam-Electric Power Plants - Phase II User's Manual, ORNL-4809, April 1973, as amended by CONCEPT User's Memoranda 1-4, April-June 1973.

CONCEPT III Supplemental User's Instructions, ORNL Note, March 25, 1974.

R. J. Barnard, CONCEPT User's Memo #6, March 27, 1974.

R. J. Barnard, CONCEPT User's Memo #8, April 30, 1974.

H. I. Bowers, CONCEPT User's Memo #9, October 28, 1974.

11. **HARDWARE REQUIREMENTS** - Less than 270K bytes, four scratch files, two support files, and the standard I/O units are required for CONCEPT5; 150K bytes, one scratch disk or tape, two support tapes, and the standard I/O units are needed for CONCEPT3.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (98%) and Assembly language (2%) (IBM3033); FORTRAN IV (UNIVAC1108)

13. **OPERATING SYSTEM** - MVS (IBM3033), VM/CMS (IBM4331), EXEC8 (UNIVAC1108).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The CONCEPT5 main program and the CONTAC5 auxiliary program use a local BAL subroutine called IDAY. The routine is used to obtain the date of the run. The ORNL routine is included in the package but should be replaced with the equivalent subroutine in the local environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    3033 CONCEPT5 H. I. Bowers
    Oak Ridge National Laboratory

    1108 CONCEPT3 J. B. Gratteau and T. J. Zielinski
    General Atomic Company

16. **MATERIAL AVAILABLE** -

    Source (CONCEPT5 3033-2177 lines, IDAY 3033-63 lines, CONCEPT3 1108-1672 lines)

    Sample problems (CONCEPT5 3033-12 lines, CONLAM5 3033-3473 lines, CONTAC5 3033-8615 lines; CONCEPT3 1108-8 lines, CONLAM3 1108-3359 lines, CONTAC3 1108 42 files-737 lines each)

    Control information (CONCEPT3 1108-47 lines)

    Auxiliary programs (CONLAM5 3033-484 lines, CONTAC5 3033-644 lines, CONLAM3 1108-499 lines, CONTAC3 1108-647 lines)

    Sample problem output (CONCEPT5 3033-3000 133-character records, CONLAM5 3033-22 selected pages, CONTAC5 3033-28 selected pages, CONCEPT3 1108-79 selected pages)

    Reference reports, Addendum, Supplemental User's Instructions, User's Memos, and NESC Note, appropriate to version

17. **CATEGORY** - D
    KEYWORDS - economics, power plants, capital, cost, PWR reactors, BWR reactors, LMR reactors, CONCEPT codes, CONLAM codes, CONTAC codes

18. **SPONSOR** - DOE Office of Nuclear Energy Programs

IDENTIFICATION AND KWIC TITLE - DUZ2
DUZ2, 2-d axisymmetric & plane elastic-plastic

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC6600

DESCRIPTION - DUZ2 performs two-dimensional elastic-plastic stress calculations. The program treats axially symmetric bodies or plane regions (plane stress or plane strain) assuming deformation theory. Loading conditions may be a non-uniform temperature distribution, body forces, and boundary displacements or stresses.

METHOD OF SOLUTION - A cyclic Chebyshev semi-iterative method is used. A symmetric nonnegative definite matrix which relates displacement components is derived by the finite element method. The elastic displacement solution is obtained using cyclic Chebyshev with simultaneous iterations. Plastic problems are solved by the initial strain method, whereby plastic strains are treated as thermal strains in an outer iteration, and the elastic solution constitutes an inner iteration. Stresses and other edit quantities are then calculated from elastic displacements and plastic strains.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The program provides for up to 99 regions, to describe material properties and boundary conditions. There may be up to 5000 points in a rectangular array, with at most 250 mesh rows or columns. Because of the initial strain method, plastic strains should not be significantly larger than elastic strains.

TIMING - Over a two-month period, successful user runs were observed to average 282 seconds, ranging from 37 to 1786 seconds. Most long jobs are not run all at once, but in 500-second shots with force-offs and restarts.

UNUSUAL FEATURES OF THE SOFTWARE - he program treats nonhomogeneous material properties which are temperature dependent. Temperature profiles may be obtained from HOT2 which uses an identical rectangular mesh-point grid and region overlay. Boundary displacements and stresses may be linear functions of r and z. Inelastic stress-strain relations may be input as piecewise linear curves or power fits. Several edit quantities including stress intensity, generalized stress, and principal stresses, can be plotted in contour or perspective, or printed.

RELATED AND AUXILIARY SOFTWARE - Temperature files from HOT2 (NESC 286) can be read. Displacement files can be requested for restarting DUZ2 or for use with other programs. A file of stresses and strains can also be requested for use with other programs. DUZ2 uses the Bettis Environmental Routines (NESC 478).

STATUS - Abstract first distributed October 1972.
CDC6600 version submitted October 1971.

REFERENCES - C. M. Friedrich, W. H. Guilinger, L. A. Hageman, C. Jeffrey, W. D. Peterson, DUZ-2 A Program for Solving Axisymmetric and Plane Elastic-Plastic Problems on the CDC-6600, WAPD-TM-926, September 1970.

C. J. Pfiefer, CDC-6600 FORTRAN Programming - Bettis Environmental Report, WAPD-TM-668, January 1967.

W. D. Peterson and J. Spanier, HOT2 - A Two-dimensional Transient Heat Conduction Program for the CDC-6600, WAPD-TM-669, June 1967.

HARDWARE REQUIREMENTS - The program was written for a CDC6600 with a central memory size of at least 64K, reader, printer, a system disk and 4 non-system disks each on its own channel. The program makes optional use of extended core storage and CDC-280 microfilm output.

PROGRAMMING LANGUAGE - Although the program is written primarily in FORTRAN IV, certain inner loop routines were optimized using COMPASS. Also, the program calls on COMPASS routines which are a part of the Bettis computing environment.

OPERATING SYSTEM - SCOPE 3.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – The program is organized for overlay loading under the SCOPE 3.1 system. There is a main overlay, or root, which resides in central memory at all times, and fourteen primary overlays and three secondary overlays. The root contains many of the FCHIP routines, including NEXT, which loads each overlay as needed. The two secondaries contain mutually exclusive routines for the input primary–INPF for card input and IFM for file input. The root declares a blank common array of length one. If there are m words from the start of blank common to the field length, and n words of text in whatever primary and secondary are executing, the storage space actually available totals m–n words. The root contains these parameters in the labeled common block /SIZE/M,N. All available blank common space is allocated by FTB, which also handles all temporary disk or extended core files.

Eight subroutines are missing and may be handled in the following ways. Calls to subroutines PEEP, UNPEEP, MESAGE, and NEXTIN are not necessary and may be eliminated. Subroutine REMARK writes a message in the day file or on the operator console. This subroutine can be replaced with a dummy subroutine. Subroutine SHIFT is described in WAPD-TM-668 on page 68. Subroutines WRITEC and READEC will not be called if sufficient storage and disk space is provided and they may remain as unsatisfied externals.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
W. D. Peterson and C. Jeffrey
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (25,631 lines)
Sample problem (72 lines)
Reference report, WAPD-TM-926

17. **CATEGORY** – I
KEYWORDS – stresses, two-dimensional, finite element method, deformation, HOT2 codes, BETTIS ENVIRONMENTAL ROUTINES codes

18. **SPONSOR** –

IDENTIFICATION AND KWIC TITLE - TDOWN4
TDOWN4, spatial & composition-dependent x-secs

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
Honeywell 6000

DESCRIPTION - TDOWN4 generates spatialand composition-dependent neutron cross section sets for both core and shielding analysis from a Bondarenko-type, generalized cross section library called GMUG, or alternatively, from the CCCC standard interface files ISOTXS and BRKOXS. Additional cross section libraries may be produced as output from TDOWN4 by condensing the primary output library to fewer neutron groups. Input to TDOWN4 can be as simple as a description of material compositions with an input flux spectrum or as complex as a description of a multi-region, two-dimensional reactor or shield and associated cells with several zero- or one-dimensional diffusion or transport theory flux solutions (keff or fixed source) to provide the flux for spectral adjustments of the cross section sets.

METHOD OF SOLUTION - TDOWN4 uses a rapid cross section adjustment procedure and a generalized library. For each material, the library contains the group values of: infinitely-dilute cross sections; resonance self-shielding factors which are tabulated for temperatures and a range of sigma(o) - the material composition dependent parameters; P(n)-scattering matrices; and, if the GMUG library is used, neutron cross sections for photon production.

Self-shielding of a cross section is accomplished by computing sigma(o) for either homogeneous compositions or multizone cells and using interpolation routines to determine the self-shielding factor for the sigma(o) and input temperature. Self-shielding is an iterative procedure with the convergence criteria specified in the input data. Spectral adjustments to the elastic removal are carried out directly, if the flux sets are given as input. Zero- and one-dimensional flux solutions may be specified to generate the flux sets. The flux solutions are iterated until spectral adjustments converge to user-specified input criteria.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The only major limitation is the maximum of 100 energy groups for the GMUG library. There is no group limit when using the CCCC libraries.

TIMING - Problems with all the flux spectra input use a maximum of a few minutes on the H6000. A 50-energy-group problem generating 27 materials in 11 compositions with the flux spectra computed by one transport theory cell and two one-dimensional diffusion theory flux solutions, taking a total of 14 flux iterations, required 13 minutes of processor time.

UNUSUAL FEATURES OF THE SOFTWARE - TDOWN4 gives the user flexibility in determining the detail a particular output cross section library will have with respect to composition and spatial effects. Output cross section sets from the compositions are not produced automatically; each set is selected from particular compositions and then the user can apply any spectral set to correct the elastic removal. If the problem requires flux solutions, and consequently regional descriptions, compositions may be defined outside of the regions.

RELATED AND AUXILIARY SOFTWARE - TDOWN4 evolved from the earlier TDOWN, TDOWN2, and TDOWN3 codes. Data for the generalized library GMUG are generated by the ENDRUN2 program (NESC 501) and modified using the PUNT program. Alternatively, a GMUG library can be generated from the CCCC standard interface files ISOTXS and BRKOXS using the BIGMUG program. BINX converts the BCD ISOTXS and BRKOXS files to binary for use by TDOWN4.

STATUS - Abstract first distributed October 1982.
GE635 version of TDOWN submitted October 1971, deleted October 1982.
H6000 version of TDOWN4 submitted June 1982.

REFERENCES - R. Protsik, E. Kujawski, and C. L. Cowan, TDOWN-IV: A Computer Code to Generate Composition and Spatially Dependent Neutron Cross Sections for Multigroup Neutronics Analysis, GEFR-00485, September 1979.

TDOWN4, NESC No. S505, Description of TDOWN4 Tapes and Implementation Information Including Function and Subroutine Specifications, National Energy Software Center Note 83-08, October 29, 1982.

B. A. Hutchins, C. L. Cowan, M. D. Kelley and J. E. Turner, ENDRUN-II, A Computer Code to Generate a Generalized Multigroup Data File from ENDF/B, GEAP-13704, March 1971.

I. I. Bondarenko, Group Constants for Nuclear Reactor Calculations, Consultants Bureau, New York, NY, 1964.

B. M. Carmichael, Standard Interface Files and Procedures for Reactor Physics Codes, Version IV, LA-6941-MS, September 1977.

11. **HARDWARE REQUIREMENTS** - TDOWN4 requires 27K words of computer memory for program storage on the H6000; for data storage, the program acquires whatever is needed. In addition to the card reader and printer devices, one tape handler, six random access scratch files on peripheral devices (discs on the H6000), and a variable number of sequential files for CCCC and SNLIB file input and output are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN-Y (95%) and GMAP (5%)

13. **OPERATING SYSTEM** - GECOS Release J with the optimized FORTRAN-Y compiler.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - All input and output conforms to CCCC recommendations, using the subroutines SEEK, REED, RITE, TIMER, DOPC, DRED, and DRIT as defined in the CCCC specifications. The GMAP routines are used to obtain additional core memory and peripheral storage.

    A number of routines used by TDOWN4 were not supplied including CASE, F4TRBK, BLKSIZ, RWD, SBITF, SBITB, RDBT, WTBT, IDFTAP, LIMRTN, ZERO, ISUP, ISUPC, ERRSYS, ERRUNS, F4TRAC, FSTACK, FSTAGE, MYTIM, NASTRK, YASTRK, TYPOT, CKRING, DUMP, PDUMP, EXIT, FCLOSE, FXEM, FXALT, FXOPT, .FGTFB, LLINK, SORT, and FSNOW. Copies of the first 9 were taken from the GENED ENVIRONMENTAL ROUTINES (NESC 515) and added to the package. Descriptions of all of the identified routines are included with NESC Note 83-08, which is part of the package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    R. Protsik, E. Kujawski, and C. L. Cowan
    Advanced Reactor Systems
    General Electric Company

16. **MATERIAL AVAILABLE** - Special Distribution
    - Source sample problem, and control information (TDOWN4 18,333 lines, environmental routines 605 lines)
    - Data libraries (ISOTXS 181,276 lines, BRKOXS 95,513 lines)
    - Auxiliary program, sample problems, and control information (BINX 960 lines)
    - Sample problem output (TDOWN4 74,821 records*, TDOWN4 Library 34,901 records*)
    - Reference report, GEFR-00485, and NESC Note

    * 132-character print records

17. **CATEGORY** - B
    KEYWORDS - multigroup theory, cross sections, self-shielding, neutron flux, CCCC, ENDRUN2 codes, BIGMUG codes

18. **SPONSOR** - DOE Division of Reactor Research & Development

1. **IDENTIFICATION AND KWIC TITLE** - MUCHA1, MUCHA2
   MUCHA1,MUCHA2, multiple channel analysis ECC

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC6400

3. **DESCRIPTION** - MUCHA1 predicts the thermal and hydraulic behavior of any two reactor fuel rods and their associated parallel flow channels during a loss-of-coolant accident using as boundary conditions plenum fluid conditions determined by MUCHA2 or a system-oriented code. MUCHA2 predicts the thermal and hydraulic behavior of the primary coolant within the reactor pressure vessel during a loss-of-coolant accident. The heated core is represented by two equivalent fuel rods and their associated parallel flow channels. A plenum model has been developed to predict the upper and lower plenum fluid conditions throughout the accident sequence for use as boundary conditions for the parallel core channels.

4. **METHOD OF SOLUTION** - In MUCHA1 an explicit, finite-difference technique is used to solve the conservation equations describing the fluid behavior in the parallel core channels. Fluid thermodynamic properties are determined from property tables using an explicit, finite-difference technique. In MUCHA2 an explicit finite-difference technique is used to solve the conservation equations describing the fluid behavior in parallel core channels and plena. Fluid thermodynamic properties are determined from property tables incorporated in the code. Heat conduction in the fuel rod is determined using an explicit, finite-difference technique.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - In MUCHA1 the two fuel rods can be represented by up to a total of 15 radial nodes. Each fuel rod and its associated flow channel may be represented by up to 12 axial segments. MUCHA2 applies the same restrictions to each pair of equivalent fuel rods.

6. **TIMING** - MUCHA1 running time varies between 200 to 300 times real time, using 2-foot axial segments in each flow channel. Doubling the number of axial segments will increase the running time by approximately a factor of 4. MUCHA2 running time varies between 200 to 400 times real time, using 2-foot axial segments in each flow channel. Doubling the number of axial segments will increase the running time by approximately a factor of 4.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - With MUCHA1 the thermal and hydraulic behavior of any two fuel rods and their associated flow channels can be predicted during all phases of a loss-of-coolant accident. MUCHA2 provides a detailed description of the core and plenum thermal-hydraulic behavior during all phases of a loss-of-coolant accident, including the emergency core coolant injection phase.

8. **RELATED AND AUXILIARY SOFTWARE** - MUCHA1 requires as input time-dependent plenum fluid conditions determined by MUCHA2 or a system-oriented code.

9. **STATUS** - Abstract first distributed October 1972.
   CDC6400 version submitted November 1971.

10. **REFERENCES** - R. A. Cudnik, ECCSA and MUCHA - Computer Codes for the Analysis of Emergency Core Cooling Systems, BMI-1916, September 1971.
    Battelle 6400 Programming Bulletin, No. 11, UNILIN, March 21, 1967.
    Battelle 6400 Programming Bulletin, No. 12, BILIN1, March 24, 1967.

11. **HARDWARE REQUIREMENTS** - MUCHA1 requires 120K (octal) memory and one tape for restart capability. MUCHA2 requires 120K (octal) memory, one tape for restart capability, and one tape for storing plenum boundary conditions.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - MUCHA1 and MUCHA2 require the use of CDC6400 FORTRAN function subprograms UNILIN and BILIN1. UNILIN performs linear interpolation from a table of values of y versus x. BILIN1 performs linear interpolation from a table of values of z versus x and y. MUCHA1 calls UNILIN from HTCHG and MUCHA2 calls it from HTCHG, FLUID, and PLENA. MUCHA1 calls BILIN1 from PHISQ and MUCHA2 also calls it from PHISQ.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

R. A. Cudnik
Columbus Laboratories
Battelle Memorial Institute

16. **MATERIAL AVAILABLE** -

Source (MUCHA1 1722 lines, MUCHA2 3067 lines)
Sample problems (MUCHA1 436 lines, MUCHA2 69 lines)
Block data and auxiliary routines (2111 lines)
Reference report and Bulletins

17. **CATEGORY** - G
KEYWORDS - reactor safety, heat transfer, accidents, coolants, thermodynamics, water

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - VIM2/13
   VIM2/13, continuous energy MC neutron transprt

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM370,303x

3. **DESCRIPTION** - VIM solves the three-dimensional steady-state multiplication eigenvalue or fixed source neutron transport problem. It was designed for the analysis of fast critical experiments.

4. **METHOD OF SOLUTION** - VIM uses the Monte Carlo technique to estimate eigenvalues by collision, track length, and analog methods. Geometry options include plate cell lattice, general combinatorial geometry, and repeating lattices of hexagonal or rectangular cells constructed using combinatorial geometry. ENDF/B cross section data are used, including thermal scattering law data. Variance reduction options available include several splitting and Russian roulette techniques, any linear combination of analog and absorption neutron weighting, and combined eigenvalue estimators. An easy-to-use restart option is also available.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Variable dimensioning is used throughout VIM2/13. A small problem requires 600K bytes on the IBM370 or 3033. Storage requirements depend linearly on the number of isotopes in the problem and also on the edit detail in space and energy.

6. **TIMING** - The running time of VIM2/13 varies widely with problem characteristics. It depends linearly on the number of isotopes and is also dependent on the number of geometrical zones. A small problem may run 10 seconds per batch of 1000 neutron histories on the IBM370/195. NESC executed the sample problem in approximately 500 CPU seconds on the IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - VIM uses continuous energy cross section data with very fine energy detail rather than multigroup cross sections. It has been extensively benchmarked on fast reactor problems using both experimental measurements and analytical comparisons.

8. **RELATED AND AUXILIARY SOFTWARE** - VIM2/13 supersedes earlier releases of VIM. The package includes a number of auxiliary codes: XSEDIT, a BCD-to-binary or binary-to-BCD cross section editing program; FILEONE, a cross section library preparation code which develops variable dimensioning information for BANDIT, a program to select the isotopes for a specific set of problems and split the cross section data into energy bands to reduce memory requirements; RETALLY, a code to reprocess VIM history data, collapsing the edit energy groups and homogenizing regions for processing selected batches; and KEFCODE, which reedits the eigenvalue estimators for a subset of batches.

9. **STATUS** - VIM1 abstract first distributed October 1972.
   VIM1 CDC7600 version submitted November 1971, deleted January 1983, replaced October 1984 by VIM2/13 submitted March 1980, revised April 1984.
   VIM1X IBM360 version submitted January 1972, revised February 1973, replaced January 1983 by VIM2/13 submitted March 1980, sample problems executed by NESC November 1981 to January 1982, replaced October 1984 by revised Edition B, member VIMUTL03 compiled by NESC.

10. **REFERENCES** - L. J. Milton, VIM Users' Guide, ANL Applied Physics Division Memorandum, June 24, 1981.

R. E. Prael, Cross Section Preparation for the Continuous-Energy Monte Carlo Code VIM, Proc. Conf. on Nuclear Cross Sections and Technology, March 3-7, 1975, NBS Special Publication 425, pp. 447-450.

R. E. Prael and H. Henryson, II, A Comparison of VIM and MC**2-2 - Two Detailed Solutions of the Neutron Slowing-Down Problem, Proc. Conf. on Nuclear Cross Sections and Technology, March 3-7, 1975, NBS Special Publication 425, pp. 451-454.

VIM2/13, NESC No. 510.370B, VIM2/13 IBM Version Tape Description and Implementation Information, National Energy Software Center Note 85-21, October 31, 1984.

VIM2/13, NESC No. 510.7600, VIM2/13 CDC Version Tape Description and Implementation Information, National Energy Software Center Note 85-23, October 31, 1984.

L. B. Levitt, R. C. Lewis, VIM1, A Non-multigroup Monte Carlo Code for Analysis of Fast Critical Assemblies, AI-AEC-12951, May 15, 1970.

11. **HARDWARE REQUIREMENTS** - Approximately 750K bytes of memory, 3 million bytes of direct access storage, and 1 tape drive are required for the IBM version.

12. **PROGRAMMING LANGUAGE** - FORTRAN H Extended and BAL (370), FORTRAN IV (FTN 4.8 compiler) and COMPASS (7600)

13. **OPERATING SYSTEM** - OS/370 (IBM370), SCOPE 2.1.5 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The original VIM system was developed at Atomics International by L. B. Levitt and R. C. Lewis.

The IBM370 routine TLEFT is part of the ANL computing environment. It returns to a calling program the difference, in hundredths of a second, between the time estimate on the job card and the total elapsed CPU and voluntary wait time. The function is called with one dummy argument. The value returned is a single-precision, floating-point variable. The value of the dummy argument remains unchanged. TLEFT is not included in the package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

R. E. Prael and L. J. Milton
Applied Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -

Source (370B-IEHMOVE unloaded dataset 25,241 lines, 7600-FORTRAN and COMPASS 19,007 lines)
Sample problems (370B-173 lines, 7600-164 lines)
Libraries (274,645 80-character records)
Control information (370B-JCL 394 lines, 7600-segload directives 33 lines)
Sample problem output (68 selected pages)
Auxiliary information (machine-readable User's Guide 9941 133-character records, 370B-NESC test JCL 1418 lines)
NESC Note, appropriate to version

17. **CATEGORY** - C
KEYWORDS - cell calculation, criticality, ENDF/B, hexagonal lattices, Monte Carlo method, neutron transport theory, reactor lattices, slowing-down, ZPR-3 reactors, ZPPR reactors, ZEBRA reactors, VIM1 codes, VIMIX codes

18. **SPONSOR** - AEC
ERDA
DOE Division of Reactor Development and Technology

1. **IDENTIFICATION AND KWIC TITLE** - THETA1B
   THETA1-B, fuel rod thermal response LOCA

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360/75

3. **DESCRIPTION** - THETA1B computes the thermal response characteristics of a nuclear fuel rod subjected to a loss-of-coolant accident environment.

4. **METHOD OF SOLUTION** - THETA1B solves the two-dimensional diffusion equation for a single fuel rod and the one-dimensional conservation of energy equation for the associated fluid channel. The two solutions are linked at the fuel rod-fluid interface by the boundary conditions of surface temperature and heat flux. The energy equations in the fuel rod and fluid channel are solved by several numerical differencing techniques. Normally the fuel rod equation is solved explicitly and the fluid equation is solved by the method of characteristics. The heat transfer model considers forced convection in subcooled liquid and superheated vapor, nucleate boiling, forced convection vaporization, transition boiling, and stable film boiling.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Small time-steps are used, resulting in long running times.

6. **TIMING** - Approximately 30 minutes are required for a 30-second transient.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Various options are available for heat transfer correlations in the different heat transfer regions. The code may also be used to model electrically-heated test elements used in out-of-pile decompression experiments.

8. **RELATED AND AUXILIARY SOFTWARE** - CINDA3G (reference 2) is used to solve the conduction equation.

9. **STATUS** - Abstract first distributed October 1972.
   IBM360 version submitted December 1971, sample problem executed by NESC.

10. **REFERENCES** - C. J. Hocevar and T. W. Wineinger, THETA1B, A Computer Code for Nuclear Reactor Core Thermal Analysis, IN-1445, February 1971.
    J. D. Gaski, Chrysler Improved Numerical Differencing Analyzer for Third Generation Computers, Chrysler Corporation Technical Note TN-AP-67-287, October 1967.
    ACC Programming Note 72-23, THETA1B Transmittal Tape, April 1972.

11. **HARDWARE REQUIREMENTS** - 400K bytes of core memory are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. J. Hocevar and T. W. Wineinger
    EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
    Source (THETA 3325 lines, CINDA1 9741 lines, CINDA2 7307 lines)
    Sample problem (700 lines)
    Load modules (THETA 1887 records, CINDA1 1221 records, CINDA2 4261 records)
    Sample problem output (24 pages)
    Reference report, IN-1445, and ACC Note 72-23

17. **CATEGORY** - G

KEYWORDS - thermal reactors, coolants, accidents, fluid flow, fuel elements, loss of coolant, water reactors, heat transfer

18. SPONSOR -

1. **IDENTIFICATION AND KWIC TITLE -** HEATING5, HEATING3
   HEATING5, 1,2, or 3-d heat conduction program
   HEATING3, 1,2, or 3-d heat conduction program

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
IBM360,370,303x, CDC CYBER73, CDC7600

3. **DESCRIPTION -** HEATING5 is designed to solve steady-state and/or transient heat conduction problems in one-, two-, or three-dimensional Cartesian or cylindrical coordinates or one-dimensional spherical coordinates. The thermal conductivity, density, and specific heat may be both spatially and temperature-dependent. The thermal conductivity can be anisotropic. Materials may undergo a change of phase. Heat generation rates may be dependent on time, temperature, and position, and boundary temperatures can be time-dependent. The boundary conditions, either surface-to-boundary or surface-to-surface, may be fixed temperatures or any combination of prescribed heat flux, forced convection, natural convection, and radiation. The boundary condition parameters are permitted to be time- and/or temperature-dependent. The mesh spacing can be variable along each axis.

   HEATPLOT is a temperature distribution plotting program which may be used with a plotting data set produced by HEATING5 to plot temperature contours (isotherms), temperature-time profiles, and temperature-distance profiles from a temperature distribution or from temperature changes relative to an initial temperature distribution.

   REGPLOT is a pre-processor graphics program which generates maps of the regions with labels for the materials, the heat generation function numbers, the initial condition function numbers, and the boundary condition function numbers specified by the input data to permit the user to visually check the HEATING5 input data.

   HEATING3 is designed to solve steady-state and/or transient heat conduction problems in one-, two-, or three-dimensional Cartesian or cylindrical coordinates. Thermal conductivity, density, and specific heat may be dependent on temperature. Heat generation rates may be dependent on position and time, and the boundary temperatures may be time-dependent. The boundary conditions may be fixed temperature or any combination of constant heat flux, forced convection, natural convection, and radiation. They can be from surface-to-boundary, surface-to-surface, or surface-to-surface plus conduction. The mesh spacing can be variable along each axis.

4. **METHOD OF SOLUTION -** The point successive overrelaxation iterative method and a modification of the "Aitken delta**2 extrapolation process" are used by HEATING5 to solve the finite difference equations which approximate the partial differential equations for a steady-state problem.

   The transient problem may be solved using any one of several finite difference schemes. These include an implicit technique which can range from Crank-Nicolson to the classical implicit procedure, an explicit method which is stable for a time-step of any size, and the classical explicit procedure which involves the first forward time difference. The solution of the system of equations arising from the implicit technique is accomplished by point successive overrelaxation iteration, and includes procedures to estimate the optimum acceleration parameter. The time-step size for implicit transient calculations may be varied as a function of the maximum temperature change at a node.

   HEATPLOT approximates contour points by using the quadrilaterals formed by four nodes. The temperature at the center of the quadrilateral is taken as the average of the temperatures at the four nodes. Then the quadrilateral is further divided into four triangles, and each side of the triangle is tested to determine if the contour line passes through that side.

   The extrapolated Liebmann method and a modification of the Aitken delta**2 extrapolation process are used by HEATING3 to solve the finite difference equations which approximate the partial differential equations for a steady-state problem. The difference equations for a transient problem involve the first forward time difference, and thus, the solution is expressed explicitly in terms of the temperatures at the previous time level. For transient calculations, a modified explicit method is incorporated into the program as an option which allows the use of an arbitrary time increment while maintaining stability.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**
   HEATING5 maxima of -
   3700 lattice points per 1 megabyte of core

100 regions
50 materials
50 boundary conditions
100 fine lattice lines along any axis
50 gross lattice lines along any axis
20 heat generation functions
25 initial temperature functions
25 analytical functions
5 materials with change-of-phase capabilities
20 nodes in special temperature table
25 points per tabular function
25 tabular functions
100 printout times
2000 surface-to-surface connectors

Transient problems involving materials with change-of-phase capabilities cannot be solved using the implicit technique with this version of HEATING5.

HEATPLOT maxima of -
1650 nodes
55 r, theta, or z values
75 horizontal or vertical plot axis values
5 profiles

Changes to these parameters can be affected by altering the appropriate parameter values and container array sizes in a BLOCK DATA routine.

HEATING3 maxima of -
100 lattice points
100 regions
50 materials
50 boundary conditions
100 fine lattice lines along any axis
50 gross lattice lines along any axis
20 heat generation functions
25 initial temperature functions
25 points per temperature-dependent conductivity function
25 points per temperature-dependent density function
25 points per temperature-dependent specific heat function
25 points per time-dependent function
50 position-dependent functions
100 printout times
500 surface-to-surface connectors
20 time-dependent functions

6. **TIMING** - Estimates for the CPU time (in seconds) required for HEATING5 problems run on the IBM360/91 for steady-state and explicit transient calculations are given by:

CPU(SS) = (1.0*10**(-4))*(No. of Nodes)*(No. of Iterations)
CPU(T) = (5.0*10**(-5))*(No. of Nodes)*(No. of Time-Steps)

It is emphasized that these equations are merely estimates, and the actual CPU time may be considerably different from the estimate depending on the options which are used. For the implicit transient algorithm, the amount of CPU time per time-step will be much larger than that for one of the explicit techniques since the code must do a lot more computation. However, one should be able to use a time-step much larger than would be required in the explicit technique, especially for later times in the transient. Frequently, the implicit algorithm is more than an order of magnitude faster than the explicit algorithm in solving a problem. Temperature-dependent thermal properties and/or boundary conditions can increase the running time by up to an order of magnitude depending on how many nodes are associated with the temperature-dependent parameters.

The HEATPLOT execution time depends on the size of the HEATING5 model and on the number of plots being created. On the average, 1 to 5 seconds is required for each plot. In NESC testing the DISSPLA sample problems required a total of about 15 seconds of CPU time, and the CalComp sample problems about 10 seconds on an IBM3033.

REGPLOT typically requires less than 1 second of CPU time per plot on an IBM3033.

The HEATING3 sample problem requires about 30 seconds on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** HEATPLOT allows the time and distance axes of the profile plots to be drawn with a logarithmic scale. Contour plots may be made for two- or three-dimensional nodes and profile plots may be made for one-, two-, or three-dimensional models. Plot-dependent scale factors can be computed by the program or specified as input data by the user.

8. **RELATED AND AUXILIARY SOFTWARE -** HEATING5 is the latest edition of the HEATING program originally developed by Liguori and Stephenson from Fowler and Volk's generalized heat conduction code, GHT. HEATING is an acronym for Heat Engineering And Transfer In Nine Geometries. HEATING5 is a modification of HEATING3. The major improvement is the incorporation of an implicit scheme to solve transient problems and the addition of change-of-phase capabilities.

9. **STATUS -** Abstract first distributed October 1972.
   IBM360 version of HEATING3 submitted January 1972, replaced by revised Edition B June 1975, replaced by HEATING5 August 1977, revised September 1977, replaced May 1980 by Edition B submitted October 1979, replaced May 1983 by revised Edition C submitted December 1981, HEATPLOT and REGPLOT submitted July 1978, revised June 1979, sample problems executed by NESC November 1982 on an IBM370/195.
   CDC CYBER72 version of HEATING3 submitted May 1975, replaced by CDC CYBER73 version February 1980, revised April 1980, sample problem executed by NESC May 1980 on a CDC7600.

10. **REFERENCES -** W. D. Turner, D. C. Elrod, and I. I. Siman-Tov, HEATING5 - An IBM 360 Heat Conduction Program, ORNL/CSD/TM-15, March 1977.

D. C. Elrod and W. D. Turner, HEATPLOT: A Temperature Distribution Plotting Program for HEATING5, K/CSD/TM-11, July 1977.

D. C. Elrod, REGPLOT: A Plotting Program to Graphically Check HEATING5 Input Data, K/CSD/TM-12, August 1977.

HEATING5, NESC No. 517.360C, HEATING5 Tape Description, Implementation Information, and Report Erratum, NESC Note 83-57, January 27, 1983.

HEATING5, NESC No. 517.360, HEATPLOT Non-DISSPLA Version - Additional Documentation on Input Data, Model-Dependent Dimensioning, Output for Sample Problems, CalComp CRT and EAI Routines, NESC Note 80-35, May 28, 1980.

HEATING5, NESC No. 517.360, HEATPLOT DISSPLA Version - Sample Problem 3 Output, NESC Note 80-36, May 28, 1980.

W. D. Turner and M. Siman-Tov, HEATING3 - An IBM 360 Heat Conduction Program, ORNL-TM-3208, February 1971.

W. D. Turner and J. S. Crowell, Notes on HEATING - An IBM 360 Heat Conduction Program, CTC-INF-980, 1969.

S. Levy, Use of Explicit Method in Heat Transfer Calculations with an Arbitrary Time Step, GE-98-C-282, 1968.

T. B. Fowler and E. R. Volk, Generalized Heat Conduction Code for the IBM-704 Computer, ORNL-2734, October 1959.

11. **HARDWARE REQUIREMENTS -** HEATING5 requires from 250K for one lattice point to 1256K bytes for 6000 lattice points.
   Storage requirements for HEATPLOT range from 400K to 700K bytes depending on the size of the HEATING5 model. In NESC testing of HEATPLOT the DISSPLA sample problems used less than 450K bytes and the CalComp sample problems less than 325K bytes of storage. REGPLOT used less than 180K bytes of storage to execute the sample problems. Standard input/output units are required in addition to the plot information file unit.

12. **PROGRAMMING LANGUAGE -** FORTRAN IV (95%) and Assembly language (5%) (HEATING5), FORTRAN IV (HEATING3)

13. **OPERATING SYSTEM -** OS/360 (IBM360), OS/370 (IBM370), NOS/BE 1.2 (CDC CYBER73), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -** Assembly language routines are included with HEATING5 to provide time and date information, to convert from integer to

character format, to provide model identification of the IBM360 used, and to compare character strings. These routines IDAY, TIME, TICK, INTOBCD, MODEL, and ICOMPARE are part of the ORNL environment and may require replacement by their counterparts at other installations.

Dummy subroutines are included in the HEATING5 package for the intended user-supplied functions defining the thermal conductivity (CONDTN), density (DNSITY), specific heat (CPHEAT), initial temperature distribution (INITTP), volumetric heat generation rate (HEATGN), boundary temperature (BNDTMP), film coefficient for forced convective heat transfer (CONVTN), coefficient for radiative heat transfer (RADITN), coefficient and exponent for natural convective heat transfer (NATCON and NCONEX), and the flux across a boundary (BNFLUX).

HEATPLOT exists in two versions. The DISSPLA version is compatible with the proprietary DISSPLA software marketed by Integrated Software Systems and the non-DISSPLA or CalComp version is designed for use with CalComp and EAI plotting equipment and the proprietary California Computer Products and EAI software. The DISSPLA HEATPLOT requires installation specific routines PRTPL, FILM, and COMPRS to perform printer-plotting, film-plotting, and DISSPLA post-plotting functions, respectively. These appear as dummy subroutines in the DISSPLA version. In addition, several installation-specific plotting routines for the CalComp CRT and EAI flatbed plotters appear as dummy subroutines in the CalComp version.

The HEATING3 CDC version lattice-point restriction can be easily modified to its original value of 1750, or some other value.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

360 HEATING5 W. D. Turner, D. C. Elrod, and I. I. Siman-Tov
Union Carbide Corporation, Nuclear Division

CYBER73 HEATING3 C. L. Wang
Institute of Nuclear Energy Research
Atomic Energy Council
Republic of China

16. **MATERIAL AVAILABLE -**

Source (HEATING5 7018 lines, Assembly routines 413 lines, HEATGN 82 lines, HEATING5 MAIN for HEATPLOT CalComp 8 lines, HEATPLOT DISSPLA 2798 lines, HEATPLOT CalComp 2638 lines, REGPLOT 846 lines, HEATING3 2583 lines)
Sample problems (HEATING5 163 lines, binary files 122 blocks* and 1 block*, HEATPLOT DISSPLA 26 lines, HEATPLOT CalComp 23 lines, REGPLOT 98 lines, HEATING3 59 lines)
Sample problems output (HEATING5 47 pages, HEATING3 16 pages)
Reference reports, ORNL/CSD/TM-15, K-CSD/TM-11, K/CSD/TM-12 (HEATING5), ORNL-TM-3208, CTC-INF-980 (HEATING3), and NESC Notes, appropriate to version

* RECFM=VBS,BLKSIZE=7294

17. **CATEGORY** - H
KEYWORDS - heat transfer, diffusion, thermal conductivity, iterative methods, x-y, x-y-z, r-z, r-theta, r-theta-z, HEATING codes, HEATPLOT codes, REGPLOT codes

18. **SPONSOR** - NRC Office of Nuclear Material Safety and Safeguards
DOE Office of Waste Isolation
Oak Ridge National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - EISPACK3
   EISPACK3, matrix eigenvalue/vector package

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Designed to be machine-independent

3. **DESCRIPTION** - EISPACK3 is a collection of 75 FORTRAN subroutines, both single- and double-precision, that compute the eigenvalues and eigenvectors of nine classes of matrices. The package can determine the eigensystem of complex general, complex Hermitian, real general, real symmetric, real symmetric band, real symmetric tridiagonal, special real tridiagonal, generalized real, and generalized real symmetric matrices. In addition, there are two routines which use the singular value decomposition to solve certain least squares problems. The individual subroutines are -

IDENTIFICATION	DESCRIPTION
BAKVEC	Back transform vectors of matrix formed by FIGI
BALANC	Balance a real general matrix
BALBAK	Back transform vectors of matrix formed by BALANC
BANDR	Reduce sym. band matrix to sym. tridiagonal matrix
BANDV	Find some vectors of symmetric band matrix
BISECT	Find some values of symmetric tridiagonal matrix
BQR	Find some values of symmetric band matrix
CBABK2	Back transform vectors of matrix formed by CBAL
CBAL	Balance a complex general matrix
CDIV	Perform division of two complex quantities
CG	Driver subroutine for a complex general matrix
CH	Driver subroutine for a complex Hermitian matrix
CINVIT	Find some vectors of complex Hessenberg matrix
COMBAK	Back transform vectors of matrix formed by COMHES
COMHES	Reduce complex matrix to complex Hess. (elementary)
COMLR	Find all values of complex Hessenberg matrix (LR)
COMLR2	Find all values/vectors of complex Hess. matrix (LR)
COMQR	Find all values of complex Hessenberg matrix (QR)
COMQR2	Find all values/vectors of complex Hess. matrix (QR)
CORTB	Back transform vectors of matrix formed by CORTH
CORTH	Reduce complex matrix to complex Hess. (unitary)
CSROOT	Find square root of complex quantity
ELMBAK	Back transform vectors of matrix formed by ELMHES
ELMHES	Reduce real matrix to real Hessenberg (elementary)
ELTRAN	Accumulate transformations from ELMHES (for HQR2)
EPSLON	Estimate unit roundoff relative to argument size
FIGI	Reduce nonsymmetric tridiag. matrix to sym. tridiag.
FIGI2	Reduce nonsymmetric tridiag. matrix to sym. tridiag.
HQR	Find all values of real Hessenberg matrix
HQR2	Find all values/vectors of real Hessenberg matrix
HTRIBK	Back transform vectors of matrix formed by HTRIDI
HTRIB3	Back transform vectors of matrix formed by HTRID3
HTRIDI	Reduce Hermitian matrix to symmetric tridiagonal
HTRID3	Reduce Hermitian packed matrix to sym. tridiagonal
IMTQLV	Find all values of symmetric tridiagonal matrix
IMTQL1	Find all values of symmetric tridiagonal matrix
IMTQL2	Find all values/vectors of sym. tridiagonal matrix
INVIT	Find some vectors of real Hessenberg matrix
MINFIT	Singular value decomposition & least squares soln.
ORTBAK	Back transform vectors of matrix formed by ORTHES
ORTHES	Reduce real matrix to real Hessenberg (orthogonal)
ORTRAN	Accumulate transformations from ORTHES (for HQR2)
PYTHAG	Find square root of sum of squares of two quantities
QZHES	Reduce real generalized matrix system
QZIT	Further reduce real generalized matrix system
QZVAL	Find all values of reduced real generalized system
QZVEC	Find all vectors of real generalized matrix system
RATQR	Find extreme values of symmetric tridiagonal matrix

REBAK	Back transform vectors of matrix formed by REDUC
REBAKB	Back transform vectors of matrix formed by REDUC2
REDUC	Reduce sym. generalized matrix system to standard
REDUC2	Reduce sym. generalized matrix system to standard
RG	Driver subroutine for a real general matrix
RGG	Driver subroutine for a real generalized system
RS	Driver subroutine for a real symmetric matrix
RSB	Driver subroutine for a real symmetric band matrix
RSG	Driver subroutine for a real sym. generalized system
RSGAB	Driver subroutine for a real sym. generalized system
RSGBA	Driver subroutine for a real sym. generalized system
RSM	Driver subroutine for a real symmetric matrix
RSP	Driver subroutine for a real symmetric packed matrix
RST	Driver subroutine for a real sym. tridiagonal matrix
RT	Driver subroutine for a real nonsym. tridiag. matrix
SVD	Singular value decomposition of rectangular matrix
TINVIT	Find some vectors of symmetric tridiagonal matrix
TQLRAT	Find all values of symmetric tridiagonal matrix
TQL1	Find all values of symmetric tridiagonal matrix
TQL2	Find all values/vectors of sym. tridiagonal matrix
TRBAK1	Back transform vectors of matrix formed by TRED1
TRBAK3	Back transform vectors of matrix formed by TRED3
TRED1	Reduce symmetric matrix to sym. tridiagonal matrix
TRED2	Reduce symmetric matrix to sym. tridiagonal matrix
TRED3	Reduce sym. packed matrix to sym. tridiagonal matrix
TRIDIB	Find some values of symmetric tridiagonal matrix
TSTURM	Find some values/vectors of sym. tridiagonal matrix

4. **METHOD OF SOLUTION** – Almost all the algorithms used in EISPACK are based on similarity transformations. Similarity transformations based on orthogonal and unitary matrices are particularly attractive from a numerical point of view because they do not magnify any errors present in the input data or introduced during the computation. Most of the techniques employed are constructive realizations of variants of Schur's theorem, 'Any matrix can be triangularized by a unitary similarity transformation'. It is usually not possible to compute Schur's transformation with a finite number of rational arithmetic operations. Instead, the algorithms employ a potentially infinite sequence of similarity transformations in which the resultant matrix approaches an upper triangular matrix. The sequence is terminated when all of the subdiagonal elements of the resulting matrix are less than the roundoff errors involved in the computation. The diagonal elements are then the desired approximations to the eigenvalues of the original matrix and the corresponding eigenvectors can be calculated. Special algorithms deal with symmetric matrices. QR, LR, QL, rational QR, bisection, QZ, and inverse iteration methods are used.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** –

6. **TIMING** – Running time varies and detailed information appears in references 2 and 3. The amount of time required to run the sample cases is small. On the IBM3033 NESC executed each of the sample cases in from 2 to 10 CPU seconds.

7. **UNUSUAL FEATURES OF THE SOFTWARE** –

8. **RELATED AND AUXILIARY SOFTWARE** – The subroutines are based mainly on the ALGOL procedures published by Wilkinson and Reinsch in Volume II of the Springer-Verlag Handbook series and the QZ algorithm of Moler and Stewart.

9. **STATUS** – Abstract first distributed October 1972.
   EISPACK3 submitted August 1983, sample cases executed by NESC August 1983 on an IBM370/195 and an IBM3033.
   IBM360 version of EISPACK submitted May 1972, replaced by IBM360,370 version of EISPACK2 July 1975, revised February 1976, revised to Edition B February 1977, replaced by EISPACK3 April 1984.

CDC6600,7600 version of EISPACK submitted May 1972, replaced by EISPACK2 July 1975, revised February 1976, revised to Edition B February 1977, replaced by EISPACK3 April 1984.

UNIVAC1108 version of EISPACK submitted May 1972, replaced by UNIVAC1108,1110 version of EISPACK2 July 1975, revised February 1976, revised to Edition B February 1977, revised to Edition C April 1981, replaced by EISPACK3 April 1984.

DEC PDP10 and Honeywell635 version of EISPACK submitted May 1972, replaced by DEC PDP10 and Honeywell635,6070 version of EISPACK2 July 1975, revised February 1976, revised to Edition B February 1977, replaced by EISPACK3 April 1984.

Burroughs6700 version of EISPACK2 submitted July 1975, revised February 1976, revised to Edition B February 1977, replaced by EISPACK3 April 1984.

Harris/7 version of EISPACK2 submitted June 1981, replaced by EISPACK3 April 1984.

REFERENCES - J. J. Dongarra and C. B. Moler, EISPACK - A Package for Solving Matrix Eigenvalue Problems, ANL Mathematics and Computer Science Division Technical Memorandum 12, revised April 1984.

B. T. Smith, J. M. Boyle, J. J. Dongarra, B. S. Garbow, Y. Ikebe, V. C. Klema, and C. B. Moler, Matrix Eigensystem Routines-EISPACK Guide, Lecture Notes in Computer Science, Volume 6 2nd Edition, G. Goos and J. Hartmanis, Springer-Verlag, New York, Heidelberg, Berlin, 1976.

B. S. Garbow, J. M. Boyle, J. J. Dongarra, and C. B. Moler, Matrix Eigensystem Routines-EISPACK Guide Extension, Lecture Notes in Computer Science, Volume 51, G. Goos and J. Hartmanis, Springer-Verlag, New York, Heidelberg, Berlin, 1977.

J. H. Wilkinson and C. Reinsch, Handbook for Automatic Computation, Volume II, Linear Algebra, Springer-Verlag, New York, Heidelberg, Berlin, 1971.

C. B. Moler and G. W. Stewart, An Algorithm for Generalized Matrix Eigenvalue Problems, SIAM Journal of Numerical Analysis, Vol. 10, pp. 241-256, 1973.

HARDWARE REQUIREMENTS - Vary according to usage. Previous releases of EISPACK used two machine-dependent parameters, RADIX and MACHEP. In EISPACK3 the relative precision of floating-point arithmetic parameter, MACHEP, has either been eliminated or replaced by the EPSLON function, which returns an estimate of the roundoff unit relative to the size of the argument. The parameter, RADIX, which specified the base of the machine floating-point representation in routines BALANC and CBAL has been replaced by the constant, 16.

PROGRAMMING LANGUAGE - The EISPACK3 subroutines are written in standard ANSI 1966 FORTRAN. The sample cases (testing aids) use the OPEN statement in FORTRAN 77 to associate the data file with the appropriate logical unit.

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - An auxiliary routine is provided to help in extracting individual routines from the transmittal tape on non-IBM systems, and the UNIX script for testing on a UNIX system is included. The set of sample cases consists of drivers, data input subroutines, residual calculation routines, and test data. Small changes may be required in the sample cases, e.g., to change the logical input and output unit or to include a PROGRAM statement. The FORTRAN 77 OPEN statement is used to associate the test data file with the appropriate logical unit number.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -

B. S. Garbow
Mathematics and Computer Science Division
Argonne National Laboratory

MATERIAL AVAILABLE -

Source (S-11,444 lines, D-11,444 lines)
Sample cases and data (S-6017 lines, D-6017 lines, data 3304 lines)
Auxiliary routines (133 lines)
Control information (UNIX 234 lines)
Machine-readable documentation (tape contents 201 lines, S-4143 lines, D-4143 lines)
Reference Memorandum

17. **CATEGORY** - P
KEYWORDS - eigenvalues, eigenvectors, matrices, numerical solution

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Engineering, Mathematical and Geo-sciences
NSF Mathematical and Computer Science Division

1. **IDENTIFICATION AND KWIC TITLE** - MOXY/MOD032
   MOXY/MOD032, BWR core heat transfer code

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360, CDC7600

3. **DESCRIPTION** - MOXY is used for the thermal analysis of a planar section of a boiling water reactor (BWR) fuel element during a loss-of-coolant accident (LOCA). The code employs models that describe heat transfer by conduction, convection, and thermal radiation, and heat generation by metal-water reaction and fission product decay. Models are included for considering fuel-rod swelling and rupture, energy transport across the fuel-to-cladding gap, and the thermal response of the canister. MOXY requires that time-dependent data during the blowdown process for the power normalized to the steady-state power, for the heat-transfer coefficient, and for the fluid temperature be provided as input. Internal models provide these parameters during the heatup and emergency cooling phases.

4. **METHOD OF SOLUTION** - An implicit numerical solution of the one-dimensional Fourier heat-conduction equation is used to compute heat conduction in fuel rods, solid inactive rods, and hollow inactive rods. Interchange of thermal radiation among surfaces is calculated using the network method described by Sparrow and Cess (see reference 5).

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   10 time-step sets
   10 print-interval sets
   50 normalized power-time pairs in considering time-dependent heat source
   50 convection heat transfer coefficient-time pairs in considering time-dependent convection
   50 fluid temperature-time pairs in considering time-dependent fluid temperature

6. **TIMING** - Approximately 3 minutes of CPU time are required to execute the sample problems on an IBM370/195 and 2 minutes on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - MOXY allows the use of fairly large (i.e., greater than 1 second) time-steps.

8. **RELATED AND AUXILIARY SOFTWARE** - MOXY/MOD032 is part of the Water Reactor Evaluation Model (WREM) as are RELAP4/MOD5 (NESC 369) and WREM-TOODEE2/MOD3 (NESC 712). View factors are computed using an extension of the method used in the VIEWPIN code (NESC 569). The model for fuel-to-cladding gap heat transfer coefficient was adapted from the GAPCON-THERMAL1 code.

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version of MOXY/MOD001 submitted June 1972, replaced by MOXY/MOD032 revised Edition B February 1977, sample problems executed by NESC April 1977 on an IBM370/195.
   UNIVAC1108 version submitted June 1972, deleted April 1977.
   CDC7600 version of MOXY/MOD032 submitted February 1977, sample problems executed by NESC February 1980 on a CDC7600.

10. **REFERENCES** - D. R. Evans, MOXY, A Digital Computer Code for Core Heat Transfer Analysis, IN-1392, August 1970.
    D. R. Evans, The MOXY Core Heat Transfer Code: Model Description and User's Guide, PG-R-76-003, December 1976, with Revision 1, February 14, 1977.
    D. R. Evans, The MOXY Core Heat Transfer Program: View Factor Model Improvements, RE-E-77-114, February 8, 1977.
    WREM: Water Reactor Evaluation Model, Revision 1, NUREG-75/056, May 1975.
    E. M. Sparrow and R. D. Cess, Radiation Heat Transfer, Belmont, California, Brooks-Cole, 1966.
    NRTS Environmental Subroutine Manual, ANC Document, December 1972.

MOXY/MOD032, ACC No. 551.360B, Tape Contents Description, Argonne Code Center Programming Note 77-23, April 29, 1977.

MOXY/MOD032, NESC No. 551.7600, MOXY/MOD032 CDC7600 Version Tape Description and Conversion Program Listing for Use on CDC7600-Compatible Systems, National Energy Software Center Note 81-58, March 15, 1980.

11. **HARDWARE REQUIREMENTS** - 300K bytes of storage (IBM360) or 110,000 (octal) words of small core memory (SCM) (CDC7600), standard input/output units, and 5 other units are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and Assembly language (IBM360), FORTRAN IV and COMPASS (CDC7600)

13. **OPERATING SYSTEM** - OS/360 (IBM360) and SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. R. Evans
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -

Source (360-3905 lines, 7600-3905 records*)
2314 load modules (MOXY32LM 360-261 blocks+, ENVIR 360-479 blocks+)
Absolute module (7600-18 records*)
Object module (7600-80 records*)
Sample problems (360-96 lines, 7600-146 records*)
Auxiliary source (Conversion program 360-24 lines)
Environmental subroutines (360-22,152 lines, 7600-70 records*)
Control information (JCL 360-114 lines, LIBEDIT lines 7600-7 records*, SEGLOAD lines 7600-10 records*)
Sample problems output (360-55 selected pages, 360-1292 blocks++, 7600-66 selected pages, 7600-49,908 records*)
Reference reports, PG-R-7600-003, RE-E-77-114, ANC document, ACC Programming Note, or NESC Note, as appropriate to version

* 512-word maximum length
\+ DCB=(RECFM=FB,LRECL=80,BLKSIZE=800)
++DCB=(RECFM=FBA,LRECL=133,BLKSIZE=1596)

17. **CATEGORY** - H
KEYWORDS - heat transfer, fuel elements, loss of coolant, accidents, molten metal-water reactions, thermal analysis, blowdown, thermal radiation, BWR reactors, RELAP4 codes, TOODEE2 codes, GAPCON-THERMAL1 codes, VIEWPIN codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
Division of Systems Safety

IDENTIFICATION AND KWIC TITLE - PARET-ANL
PARET-ANL, reactor core transient analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370,303x

DESCRIPTION - This program is designed for use in predicting the course and consequences of nondestructive reactivity accidents in research and test reactor cores. It can be used for both steady-state and transient analysis.

METHOD OF SOLUTION - PARET provides a hydrodynamic and point kinetics capability. The core can be represented by four or fewer regions, each having different power generation, coolant mass flow rate, and hydraulic parameters as represented by a single fuel pin or plate with its associated coolant channel. The heat transfer in each fuel element is computed on the basis of a one-dimensional conduction solution in each of up to a maximum of 21 axial sections. The hydrodynamics solution is also one-dimensional for each channel at each time node. The heat transfer may take place by natural or forced convection, nucleate, transition, or stable film boiling. The coolant is allowed to range from subcooled liquid, through the two-phase regime, up to and including superheated steam, and coolant flow reversal is allowed. PARET-ANL also has an optional "voiding model" which estimates the voiding produced by subcooled boiling.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The PARET model is subject to several recognized limitations which may limit the applicability in any specific situation, depending on the nature of the transient under consideration. The code employs steady-state heat transfer correlations throughout, possibly being unrealistic in certain transient situations. Any complete description of a severe transient must include provision for some sort of thermal or hydraulic crisis. PARET is limited in predicting such a crisis by the fact that it employs only steady-state correlations; no transient correlations with demonstrated reliability have been developed. Accurate description of hydraulic instability depends upon accurate calculation of transient pressure and flow fluctuations. PARET is limited in this respect because it employs an incompressible model and a simplified void volume generation equation. Also, the magnitude of local pressures predicted to accompany coolant expulsion is strongly affected by the number of axial sections chosen in the computations. As a result, the hydrodynamic output should be interpreted as a qualitative indication of a possible crisis rather than a reliable quantitative prediction.

PARET is not applicable to either destructive excursions or situations in which there is a space-time effect in neutron flux.

TIMING - The sample problem requires less than 18 seconds of CPU time to process 320 time-steps with 2 channels on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - This program is an extension of CHIC-KIN (NESC 473). The original PARET program was developed by P. D. Adolf and C. F. Obenchain at EG&G Idaho.

STATUS - Abstract first distributed December 1973.
IBM360 version of PARET submitted August 1972, replaced by revised version May 1973, replaced by revised Edition B January 1982, replaced October 1984 by IBM370 version of PARET-ANL submitted December 1982, sample problem executed by NESC February 1983 on an IBM3033.

REFERENCES - W. L. Woodruff, A Users Guide for the Current ANL Version of the PARET Code, Argonne National Laboratory memorandum, December 16, 1982.
C. F. Obenchain, PARET -- A Program for the Analysis of Reactor Transients, IDO-17282, January 1969.
C. J. Smith and W. A. Cody, ANL DATE Routine, ANL Subroutine Description Q054S, February 1968.
Excerpts from NRTS Environmental Subroutine Manual, December 1972.

William L. Woodruff, The PARET Code and the Analysis of the SPERT I Transients, Proceedings of the International Meeting on Research and Test Reactor Core Conversions from HEU to LEU Fuels, Argonne, Illinois, November 8-10, 1982, ANL/RERTR/TM-4 (CONF-821155), pp. 560-579, September 1983. (Also published as A Kinetics and Thermal-hydraulics Capability for the Analysis of Research Reactors, Nuclear Technology, Volume 64, pp. 196-206, February 1984).

PARET-ANL, NESC No. 555, PARET-ANL Tape Description and Implementation Information, National Energy Software Center Note 85-02, October 4, 1984.

J. A. Redfield, CHIC-KIN - A FORTRAN Program for Intermediate and Fast Transients in a Water-moderated Reactor, WAPD-TM-479, January 1965.

11. **HARDWARE REQUIREMENTS** - 240K bytes plus one magnetic tape

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (91%) and BAL (9%)

13. **OPERATING SYSTEM** - OS/MVT (IBM370), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - A generalized input processor in IBM assembly language is included. Auxiliary Fortran routines for processing and editing the summary plot file generated by PARET-ANL and for generating an updated properties library are also included. Subroutine INLK was compiled with the FORTX450 compiler with 450K. The normal compiler could not process OPT=2 because this routine is too large. The SIZE parameter of the linkage editor must be set to (300K,24K).

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

W. L. Woodruff
Applied Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -

Source (FORTRAN 7045 lines, BAL 679 lines)
Sample problem (78 lines)
Properties library (31 records•)
Auxiliary routines (PLOTPROS 181 lines, data 3 lines; PROPGENER 685 lines, output 3375 133-character records)
Sample problem output (3540 133-character records)
Reference report, IDO-17282, Users Guide, Subroutine Description, Manual Excerpts, ANL/RERTR/TM-4 Excerpt, and NESC Note

• DCB=(RECFM=VBS,LRECL=X,BLKSIZE=6136)

17. **CATEGORY** - G
KEYWORDS - reactivity insertions, accidents, reactor safety, heat transfer, hydrodynamics, reactor kinetics, feedback, CHIC-KIN codes, PARET codes

18. **SPONSOR** - AEC
ANL Reduced Enrichment Research and Test Reactor Program

1. **IDENTIFICATION AND KWIC TITLE** - TOKMINA, TOKMINA2
   TOKMINA/TOKMINA2, Tokamak fusion reactor study

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360

3. **DESCRIPTION** - TOKMINA finds the minimum magnetic field, Bm, required at the toroidal coil of a Tokamak type fusion reactor when the input is beta(ratio of plasma pressure to magnetic pressure), q(Kruskal-Shafranov plasma stability factor), and y(ratio of plasma radius to vacuum wall radius: rp/rw) and arrays of PT(total thermal power from both d-t and tritium breeding reactions), Pw(wall loading or power flux) and TB(thickness of blanket), following the method of Golovin, et al. TOKMINA2 finds the total power, PT, of such a fusion reactor, given a specified magnetic field, Bm, at the toroidal coil.

4. **METHOD OF SOLUTION** - TOKMINA: the aspect ratio(a) is minimized, giving a minimum value for Bm. TOKMINA2: a search is made for PT; the value of PT which minimizes Bm to the required value within 50 Gauss is chosen.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Input arrays presently are dimensioned at 20. This restriction can be overcome by changing a dimension card.

6. **TIMING** -
   TOKMINA - approximately 30 seconds for 100 sets of input values.
   TOKMINA2 - approximately 1 minute for 700 sets of input values.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Output for each set of input values are TB, Bt(toroidal magnetic field on the minor axis), R(major radius of the toroid), rp, Rm(distance between the major axis and the blanket in the midplane), n(density of the plasma) and I(plasma current). These values, as well as Bm and PT may be studied as a function of blanket thickness.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version submitted August 1972, sample problems executed by NESC.

10. **REFERENCES** - I. N. Golovin, Yu. N. Dnevstrovsky and D. P. Kostomarov, Tokamak as a Possible Fusion Reactor - Comparison with Other C. T. R. Devices, BNES Nuclear Fusion Reactor Conference at Culham Laboratory, September 1969.
    A. J. Hatch and J. Etzweiler, A Simplified Parametric Study of Tokamak Fusion Reactors, Proceedings of the Texas Symposium on Fusion Reactors, November 22-23, 1972, CONF-721111.

11. **HARDWARE REQUIREMENTS** - 160K bytes of core

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    A. J. Hatch
    Physics Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (TOKMINA 153 lines, TOKMINA2 198 lines)
    Sample problems (TOKMINA 4 lines, TOKMINA2 5 lines)
    Sample problem output (TOKMINA 2 pages, TOKMINA2 28 pages)
    Reference reprint, CONF-721111

17. CATEGORY - X
KEYWORDS - aspect ratio, Tokamak type reactors, tritium, breeding, magnetic fields, fusion reactions, plasma, toroidal configuration

18. SPONSOR -

1. **IDENTIFICATION AND KWIC TITLE** - ASTEM
   ASTEM, thermodynamic properties water & steam

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370/195, CDC6600,7600

3. **DESCRIPTION** - ASTEM is a modular set of FORTRAN IV subroutines to evaluate the Gibbs, Helmholtz, and saturation line functions as published by the American Society of Mechanical Engineers (1967). Any thermodynamic quantity including derivative properties can be obtained from these routines by a user-supplied main program. PROPS is an auxiliary routine available for the IBM360 version which makes it easier to apply the ASTEM routines to power station models.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Unless redimensioned by the user, the highest derivative allowed is order 9. All arrays within ASTEM are one-dimensional to save storage area.

6. **TIMING** - The sample problem requires less than a minute.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The main program is the sample problem.

8. **RELATED AND AUXILIARY SOFTWARE** - STEAM-67 (NESC 487)

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version submitted June 1973, PROPS routine added to package August 1978, sample problem executed by NESC August 1978 on an IBM3033.
   CDC6600 version submitted October 1973, sample problem executed by NESC May 1975 on a CDC6600 and a CDC7600.

10. **REFERENCES** - K. V. Moore, ASTEM - A Collection of FORTRAN Subroutines to Evaluate the 1967 ASME Equations of State for Water/Steam and Derivatives of these Equations, ANCR-1026, October 1971.
    C. A. Meyer, R. B. McClintock, G. J. Silvestri, and R. C. Spencer, Jr., 1967 ASME Steam Tables - Thermodynamic and Transport Properties of Steam, The American Society of Mechanical Engineers, New York, 1967.
    P. W. Bridgman, The Thermodynamics of Electrical Phenomena in Metals and a Condensed Collection of Thermodynamic Formulas, New York, Dover Publications, Inc., 1961.
    M. P. Burgess, G. L. Fuller, and A. H. Kaiser, Thermodynamic Properties of Steam and Water Adapted for the IBM 360/195 Computer, DPSPU 76-11-3, September 1976.

11. **HARDWARE REQUIREMENTS** - 68K bytes (IBM370/195), 21,000 (octal) words (CDC6600,7600). When using PROPS, 90K bytes of memory is required on the IBM system.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360,370 (IBM360,370), SCOPE (CDC6600,7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - In moving ASTEM to the CDC6600 the variable argument list calls to the CONU subroutine were converted to fixed to conform to CDC conventions, and double-precision data statements and arithmetic functions were changed to single-precision. The rounded arithmetic option of the FTN compiler was necessary for execution of the sample problem on the CDC7600. To relieve convergence failure in subroutine ROOT during CDC executions, the convergence criterion may be relaxed, but with caution.
    The output values from the PROPS routine are returned through the labeled COMMON block /CPROPS/. When using PROPS in conjunction with the ASTEM routines, a "larger" H or H-extended compiler is needed requiring 450K at SYSGEN time. The G and G1 compilers will compile in a normal region. These compilers, however, will delete some of the beginning comments of the ASTEM routine BINOMX, as there are more than 30 consecutive comments. Variables passed to PROPS must be either non-zero (INPUT) or zero.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

360 K. V. Moore
EG&G Idaho, Inc.

360 PROPS M. P. Burgess, G. L. Fuller, and A. H. Kaiser
Savannah River Plant

6600 D. L. Jaeger
Boeing Commercial Airplane Company

16. **MATERIAL AVAILABLE -**

Source (360-1551 lines, 6600-1531 lines)
Sample problems (360-83 lines, 6600-84 lines)
Auxiliary information (360 PROPS source-227 lines, sample problem-154 lines)
Reference reports, ANCR-1026 and DPSPU 76-11-3, as appropriate to machine version

17. **CATEGORY** - H
KEYWORDS - thermodynamics, water, pressure, temperature, liquids, vapors, STEAM-67 codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - PLENUM
   PLENUM, flow dist in cyl coolant inlet plenum

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - Bulk flow distribution in a cylindrical reactor coolant inlet plenum is calculated using potential flow theory.

4. **METHOD OF SOLUTION** - The Laplace equation for the velocity potential is solved for general, symmetric boundary conditions and one inlet nozzle by Gauss-Seidel relaxation (part 1). Nonsymmetric, dimensional solutions are then formed by superposition of the general solution (part 2).

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The code is dimensioned for 8000 mesh points in an (r,theta,z) array. Dimensions can be expanded at the expense of run time and core size.

6. **TIMING** - Run time for part 1 is proportional to n**2, where n is the number of mesh points. With 2299 mesh points CPU time is 42 seconds on a 360/195. Run time for part 2 is 1 second per problem. Sample problem running time is 2 minutes for part 1 and 1 minute for part 2.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The code approximates bulk fluid motion through large cylindrical headers in circumstances where details of the flow, such as boundary layer effects, may be neglected. Three-dimensional effects are calculated, so that asymmetric fluid input and output problems may be calculated. Use of a linear field equation permits rapid solution by superposition of many combinations of input and output boundary conditions. First order effects of friction may be included by addition of constant coefficients in the finite difference formulations.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version submitted June 1973, sample problem executed by NESC.

10. **REFERENCES** - S. D. Harris and J. W. Reece, Application of Potential Flow Theory to Reactor Coolant Circulation, Proceedings of the Eighth Southeastern Seminar on Thermal Sciences, DP-MS-71-13, March 23-24, 1972.

11. **HARDWARE REQUIREMENTS** - 240K bytes of storage and an on-line punch and printer

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - PLENUM is written as two separate programs. Part 1 provides a general dimensionless solution to the field equation. For a given header this code need only be executed once. Part 2 uses punched output from part 1 to determine solutions for a variety of user-specified boundary conditions by dimensionalization and superposition.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   S. D. Harris
   Savannah River Laboratory

16. **MATERIAL AVAILABLE** -
   Source (part1 312 lines, part2 220 lines)
   Sample problems (part1 3 lines, part2 16 lines)
   Punched output (part1 419 lines)
   Sample problem output (part1 31 pages, part2 11 pages)
   Reference report

17. **CATEGORY** - H
KEYWORDS - cylinders, coolants, r-theta-z, Laplace equation, potential flow

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - AEC-ALO FAU
   AEC-ALO FAU, radio frequency management system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360/50

3. **DESCRIPTION** - The AEC-ALO Radio Frequency Assignments and Uses program (FAU) provides for maintaining radio frequency assignment and transaction records. It lists all radio frequency assignments and uses from initial application (AEC-310) through authorizations (IRAC docket). The program allows for sorting by office, system number, location, frequency, expiration date, ALO or AEC serial number, and IRAC docket number.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - A general familiarity with AEC Appendix 0270, Part IV and the OTP Manual is assumed.

6. **TIMING** - 5 minutes are required for seven reports, 1000 records.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - An earlier version of this program was written for the Burroughs B-5500. This is a modified COBOL version of a USAEC NUO FORTRAN program.

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version submitted February 1973, sample problem executed by NESC.

10. **REFERENCES** - AEC-ALO Memorandum, AEC-ALO Radio Frequency Assignments and Uses (FAU), 1973.
    AEC-ALO Memorandum, Description of Radio Frequency Bookkeeping Program, 1973.

11. **HARDWARE REQUIREMENTS** - This system requires disk-sort of input data and the master tape records. Peripheral equipment required is card reader, line printer (132 character/line), and two magnetic tape units.

12. **PROGRAMMING LANGUAGE** - COBOL

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The system consists of two programs, M2501 the tape update program, and M2502 the report preparation program.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. H. Grayson, G. S. Hearron,
    and G. Kojima
    Albuquerque Operations Office
    U.S. Department of Energy

16. **MATERIAL AVAILABLE** -
    Source (M2501 485 lines, M2502 374 lines)
    Sample problems (M2501 43 lines, M2502 1 line)
    Sample problem output (M2501 11 pages, M2502 10 pages)
    Reference memoranda

17. **CATEGORY** - M
    KEYWORDS - maintenance, sorting, information systems, radio equipment

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - ORCOST2
   ORCOST2, power plant capital cost estimating

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - ORCOST2 estimates the cost of electrical energy production from single-unit steam-electric power plants. Capital costs and operating and maintenance costs are calculated using base cost models which are included in the program for each of the following types of plants: PWR, BWR, HTGR, coal, oil, and gas. The user may select one of seven input/output options for calculation of capital cost, operating and maintenance cost, levelized energy costs, fixed charge rate, annual cash flows, cumulative cash flows, and cumulative discounted cash flows. Options include the input of capital cost and/or fixed charge rate to override the normal calculations. Transmission and distribution costs are not included. Fuel costs must be input by the user.

4. **METHOD OF SOLUTION** - The code follows the guidelines of AEC Report NUS-531. A base capital-cost model and a base operating- and maintenance-cost model are selected and adjusted for desired size, location, date, etc. Costs are discounted to the year of first commercial operation and levelized to provide annual cost of electric power generation.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The capital cost models are of doubtful validity outside the 500 to 1500 MW(e) range.

6. **TIMING** - Execution time for a single case is less than one second on the IBM 360/91.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Capital cost calculations are based on the cost-model data developed for the CONCEPT program (NESC 498). A separate code OMCST (NESC 688) can be used to calculate nonfuel operation and maintenance costs.

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 version of ORCOST submitted March 1973, replaced by revision B July 1973, replaced by ORCOST2 March 1976, sample problem executed by NESC May 1976 on an IBM370/195.

10. **REFERENCES** - S. T. Brewer, L. C. Fuller, M. L. Meyers, L. L. Bennett and H. I. Bowers, ORCOST2 - A Computer Code for Estimating the Cost of Power for Steam-Electric Power Plants, ERDA 76-38, October 1975.

11. **HARDWARE REQUIREMENTS** - 90K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and Assembly language

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - ORNL environment subroutines IDAY, ICOMPARE, and TIME are supplied in Assembly language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. C. Fuller and M. L. Myers
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (ORCOST2 2283 lines, IDAY 63 lines, ICOMPARE 39 lines, TIME 28 lines)
    Sample problem (8 lines)
    Reference report

17. **CATEGORY** - D

NESC 588

KEYWORDS - economics, capital, cost, charges, power plants, PWR reactors, BWR reactors, HTGR reactors, CONCEPT codes, OMCST codes

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - LSODE
   LSODE, ordinary differential eqn system solver

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM370,303x, CDC7600,CYBER175

3. **DESCRIPTION** - LSODE is a package of subroutines for the numerical solution of the initial value problem for systems of first order ordinary differential equations. The package is suitable for either stiff or nonstiff systems. For stiff systems the Jacobian matrix may be either full or banded. LSODE can also be used when the Jacobian can be approximated by a band matrix.

4. **METHOD OF SOLUTION** - LSODE contains two variable-order, variable-step (with interpolatory step-changing) integration methods. The first is the implicit Adams or nonstiff method, of orders one through twelve. The second is the backward differentiation or stiff method (or BDF method, or Gear's method), of orders one through five.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The differential equations must be given in explicit form, i.e., dy/dt = f(y,t). Problems with intermittent high-speed transients may cause inefficient or unstable performance.

6. **TIMING** - NESC executed the sample problem in less than 4 CP seconds on a CDC CYBER175, and less than 6 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - LSODE offers a great deal of flexibility as to choice of basic method, either stiff or nonstiff, nonlinear corrector iteration method - 6 choices, error tolerances including componentwise relative and absolute tolerances, stopping criterion - at a specified time, t, or after every step, possibly with a critical t, optional input controls, e.g. maximum order or print flags, optional output controls, e.g. step and function evaluation counts and derivatives of the solution, interrupt and restart capabilities, etc. Work space arrays and the names of the user-supplied routines are passed as subroutine arguments for flexibility. User-controlled dynamic work space, real and integer, can also be passed to the user routines.

8. **RELATED AND AUXILIARY SOFTWARE** - LSODE supersedes both GEAR (NESC 592) and GEARB (NESC 661). For problems with intermittent high-speed transients, see EPISODE (NESC 675) for the case of a full Jacobian or EPISODEB (NESC 705) for the case of a banded Jacobian. LSODE uses routines from LINPACK (NESC 800) and several of the Basic Linear Algebra Subprograms (BLAS) to solve linear algebraic systems.

9. **STATUS** - Abstract first distributed December 1973.
   CDC6600,7600 version of GEAR submitted July 1973, replaced by Edition B February 1975, replaced by Edition C April 1976, replaced August 1981 by CDC7600 (long word-length) version of LSODE submitted February 1980, revised March 1980, May 1980, June 1980, September 1980, changes incorporated November 1980, replaced September 1983 by Edition B, sample problems executed by NESC July 1983 on a CDC CYBER175.
   IBM360 version of GEAR submitted September 1974, replaced by Edition B February 1975, replaced by Edition C April 1976, replaced August 1981 by IBM370 (short word-length) version of LSODE submitted February 1980, revised March 1980, May 1980, June 1980, September 1980, changes incorporated March 1981, replaced September 1983 by Edition B, sample problem executed by NESC July 1983 on an IBM3033.

0. **REFERENCES** - LSODE, NESC No. 592.370B, User's Manual for LSODE, National Energy Software Center Note 83-89, July 20, 1983.
   LSODE, NESC No. 592.7600B, User's Manual for LSODE, National Energy Software Center Note 83-90, July 20, 1983.
   A. C. Hindmarsh, Instructions for Installing LSODE, LLNL Memorandum M-4162, May 1983.

KEYWORDS - economics, capital, cost, charges, power plants, PWR reactors, BWR reactors, HTGR reactors, CONCEPT codes, OMCST codes

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - SPEAKEASY MU+ Level
   SPEAKEASY MU+, language processor TSO or batch
   SPEAKEASY MU+ SOURCE, language processor

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370,3033

3. **DESCRIPTION** - SPEAKEASY is a user-oriented language. It is intended to provide its users with the means of quickly formulating problems for computer processing and for obtaining answers to those problems in a minimum of time.

4. **METHOD OF SOLUTION** - The language syntax closely resembles that of mathematics. User-defined variables are classified as scalars, arrays, vectors, or matrices. Class-oriented operators simplify the language.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SPEAKEASY is an extensible library-directed processor. Available facilities include array algebra, complete matrix algebra, statistical packages, and assorted special functions. SPEAKEASY also offers HELP documents and TUTORIAL sessions.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed December 1973.
   IBM360 IOTA 3F Level submitted November 1973, replaced by revised IOTA Level edition March 1974, deleted January 1975.
   IBM360 MU+ Level submitted January 1979, sample problems executed by NESC February 1979 on an IBM360,370,3033.
   IBM360 MU+ Level Source made available upon special request November 1979, sample problems executed by NESC October 1979 on an IBM360,370,3033.

10. **REFERENCES** - S. Cohen and S. Pieper, The SPEAKEASY-3 Reference Manual, Level MU, IBM OS/VS Version, ANL-8000 Rev. 2, August 1977.
    G. Gordon, LECTURES ON SPEAKEASY, Communications Satellite Corporation-ANL Speakeasy Center Memorandum, August 1977.
    B. Williams, The SPEAKEASY Example Documents, ANL-CEA Program Report, Spring 1977.
    Installation Instructions for MU+ Level SPEAKEASY, ANL Memorandum, February 1979.
    Notes on the SPEAK.SOURCE PDS, NESC Note 79-25, February 26, 1979.
    SPEAKEASY MU+ Level, NESC No. S593.360B, Implementation Instructions for MU+ Level SPEAKEASY Source, NESC Note 80-10, December 5, 1979.
    SPEAKEASY MU+ Level, NESC No. S593.360B, SPEAKEASY MU+ Level Source Tape Description, NESC Note 80-09, December 5, 1979.

11. **HARDWARE REQUIREMENTS** - A minimum of 130K of memory is needed for the MU090 processor, 190K for the MU150 processor, and 300K for the MU260 processor for the MU+ Level of SPEAKEASY.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (95%) and Assembler (5%)

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - MU+ Level SPEAKEASY is distributed on a standard-labeled tape containing 18 files, and is intended for use only on IBM360,370,303x computers operating under OS/MVT or VS systems. Source decks are supplied (SPEAK.SOURCE) only for those utility routines which may require modification for local implementation. Sixteen of the 18 files are partitioned data sets (PDSs); the remaining two contain machine-readable documentation.

The IBM360 MU+ Level Source (as submitted at the termination of the ANL SPEA project) is supplied on an "as-is" basis with the SPEAKEASY MU+ Level package on specifically requested.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

S. Cohen
Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE -**

Source (PDS SPEAK.SOURCE)
Load modules (PDSs SPEAK.MU090, MU150, MU260, LINKULES, DATAMANG, FORTLIB, UTI VSCOPY)
Test data (PDSs SPEAK.EXAMPLES, TESTCASE)
Processor interface and initialization (PDS SPEAK.PROCLIB)
Auxiliary information (PDSs SPEAK.HELP, TUTOR, DOCUMENT, DATA)
Sample output (TESTCASE-25 pages)
Machine-readable documentation (SPEAK.MANUAL, HELPLIST)
Reference documents, ANL-CEA Program Report, ANL Memorandum, and NESC Note 79-25
Special Request -
Source (130,102 lines)
Control information (2776 lines)
Sample output (37 pages)
Reference notes, NESC Notes 80-10 and 80-09

17. **CATEGORY** - P
KEYWORDS - programming languages, numerical solution, libraries

18. **SPONSOR** - ERDA Division of Physical Research
Argonne National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - GAUSS7
   GAUSS7, analysis of gamma-ray spectra from Ge

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC CYBER176,CYBER175

3. **DESCRIPTION** - GAUSS7 is used to determine gamma-ray energies and intensities from a spectrum obtained with a Ge semiconductor detector and a multichannel pulse-height analysis system.

4. **METHOD OF SOLUTION** - The spectrum analysis is carried out in some or all of the following steps: a) Peaks in the spectrum are selected and used for internal energy and width calibrations. b) Significant peaks are determined by means of an auto-correlation routine. c) Spectral regions that are significantly above the background are identified as peak regions. d) These lists of peaks and peak regions can be modified by the user to fit particular needs. e) Each peak region is analyzed to determine the area and position of each peak component. This step can be repeated for additional peak components. The peak components can be represented by a Gaussian function; a Gaussian function with one or two additive, exponential low-energy tails; or either of the two previous functions with an additive, exponential high-energy tail. The background is a linear function with or without a step-like increase at the center of each peak component. f) The energy and intensity of each peak component is computed.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - GAUSS7 will handle spectra of up to 4096 channels, 300 peak regions, a total of 300 peaks in the search and required peak lists, and 10 peaks per region. In analyzing the peak regions to determine the area and position of peak components up to five fits can be carried out with up to ten components.

6. **TIMING** - Typical spectra take 5 to 15 seconds of CPU time for 150 peaks. The sample problem executed by NESC on a CDC CYBER175 took less than 80 CPU seconds, including compilation time.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - GAUSS7 supersedes GAUSS5. GAUSS7 assumes that the user has placed the spectra and efficiency and peak shape data on the computer system via other programs. GAUSS7S defines the parameters of non-Gaussian peak shapes. BINLIB converts the spectral library from card-image to binary format for use by GAUSS7 and GAUSS7S. GAUSS6 (NESC 622) is used for analysis of groups of spectra which require isotopic identification of the gamma rays and isotopic activity calculations from individual lines.

9. **STATUS** - Abstract first distributed January 1974.
   CDC CYBER176 version of GAUSS7 submitted January 1983, sample problem executed by NESC February 1983 on a CDC CYBER175.
   IBM360 version of GAUSS5 submitted September 1973, replaced by GAUSS7 June 1983.

10. **REFERENCES** - C. M. McCullagh and R. G. Helmer, GAUSS VII, A Computer Program for the Analysis of Gamma-Ray Spectra from Ge Semiconductor Spectrometers, EGG-PHYS-5890, October 1982.

GAUSS7, NESC No. 605, GAUSS7 Tape Description and Implementation Information, National Energy Software Center Note 83-69, February 17, 1983.

R. G. Helmer and C. M. McCullagh, GAUSS VII, A Computer Program for the Analysis of Gamma-Ray Spectra from Ge Semiconductor Spectrometers, Nuclear Instruments and Methods, Vol. 206, pp. 477-488, 1983.

11. **HARDWARE REQUIREMENTS** - 144,000 (octal) words of memory

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS/BE level 538 (CDC CYBER176), NOS 1.4 level 543 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program uses the FORTRAN multiple statement feature. For interpolation of the detector efficiency function, two spline routines, ICSEVU and ICSICU, from the proprietary IMSL library are used; these routines are not included with the material distributed.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. G. Helmer and C. M. McCullagh
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
Source (GAUSS7 3478 lines)
Sample problems (GAUSS7 12 lines, SPECTRAL LIBRARY 2487 lines, EFFICIENCY TABLE 18 lines, GAUSS7S 14 lines),
Auxiliary source (GAUSS7S 1821 lines, BINLIB 21 lines)
Sample problem output (GAUSS7 2093 records*, GAUSS7S 2914 records*)
Reference report, EGG-PHYS-5890, and NESC Note
* 133-character records

17. **CATEGORY** - U
KEYWORDS - gamma spectra, Gauss function, Ge semiconductor detectors, spectra unfolding, spectrometers, GAUSS5 codes, GAUSS7S codes, BINLIB codes

18. **SPONSOR** - DOE Office of Safeguards and Security,
Technology Development and Implementation Branch

1. **IDENTIFICATION AND KWIC TITLE** - GAPCON-THERMAL2 Rev. 1
   GAPCON-THERMAL2, fuel rod thermal performance

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC6600,7600,CYBER74

3. **DESCRIPTION** - GAPCON-THERMAL2 Rev. 1 calculates the thermal behavior of a nuclear fuel rod during normal steady-state operation. The program was developed as a tool for estimating fuel-cladding gap conductances and fuel-stored energy. Models used include power history, fission gas generation and release, fuel relocation and densification, and fuel-cladding gap conductance. The gas release and relocation models can be used to make either best-estimate or conservative predictions.

4. **METHOD OF SOLUTION** - The fuel to cladding gap conductance for each equal-length, user-designated axial region is determined by an iterative scheme. Radial temperatures are calculated using a finite difference procedure. The solution procedure consists of iterative convergence for each axial fuel region, followed by iterative convergence on the fuel rod gas release for each time-power step. A mixture of empirical, theoretical, and physical models is used.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   15 axial nodes
   35 time-steps
   No mechanical plastic strain is considered. The thermal model is axisymmetric. The first time-step must be zero time and the second cannot be at zero power.

6. **TIMING** - Typical run time on the CDC CYBER74 is approximately 30 seconds per time-step; the sample problem runs in less than 20 CP seconds on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Most models have been compared individually with experimental data; however, the code as a whole has not been adjusted to conform to any set of data.

8. **RELATED AND AUXILIARY SOFTWARE** - GAPCON-THERMAL2 is a modification of GAPCON-THERMAL1 to reduce the uncertainties associated with the calculation of power history and burnup. GAPCON-THERMAL3 (NESC 770) is a related program which calculates detailed fuel rod mechanical conditions.

9. **STATUS** - Abstract first distributed March 1974.
   UNIVAC1108 version of GAPCON-THERMAL1 submitted October 1973, replaced October 1975 by revised Edition B, deleted January 1976.
   CDC6600 version of GAPCON-THERMAL2 submitted January 1976, replaced December 1980 by revised Edition B submitted March 1980, sample problem executed by NESC April 1980 on a CDC7600.

10. **REFERENCES** - C. E. Beyer, C. R. Hann, D. D. Lanning, F. E. Panisko and L. J. Parchen, GAPCON-THERMAL-2: A Computer Program for Calculating the Thermal Behavior of an Oxide Fuel Rod, BNWL-1898, November 1975.
    C. E. Beyer, C. R. Hann, D. D. Lanning, F. E. Panisko and L. J. Parchen, User's Guide for GAPCON-THERMAL-2: A Computer Program for Calculating the Thermal Behavior of an Oxide Fuel Rod, BNWL-1897, November 1975.
    GAPCON-THERMAL2, NESC No. 618.6600B, GAPCON-THERMAL2 Tape Description, National Energy Software Center Note 81-07, December 28, 1980.

11. **HARDWARE REQUIREMENTS** - About 54K words of main memory is needed for compilation and execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.4 (CDC6600), NOS/BE (CDC CYBER74), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**
C. E. Beyer, C. R. Hann, D. D. Lanning,
F. E. Panisko, and L. J. Parchen
Pacific Northwest Laboratory

16. **MATERIAL AVAILABLE –**
Source (5124 lines)
Sample problem (15 lines)
Sample problem output (27 selected pages)
Reference reports and NESC Note

17. **CATEGORY** – I
KEYWORDS – fuel rods, steady-state conditions, thermal conductivity, performance, cl
water cooled reactors, GAPCON-THERMAL1 codes, GAPCON-THERMAL3 codes

18. **SPONSOR** – NRC Office of Nuclear Reactor Regulation,
Division of Systems Safety,
Core Performance Branch

1. **IDENTIFICATION AND KWIC TITLE** - SETS
   SETS, set equation transformation system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER76,175,180

3. **DESCRIPTION** - SETS is used for symbolic manipulation of Boolean equations, particularly the reduction of equations by the application of Boolean identities. It is a flexible and efficient tool for performing probabilistic risk analysis (PRA), vital area analysis, and common cause analysis. The equation manipulation capabilities of SETS can also be used to analyze noncoherent fault trees and determine prime implicants of Boolean functions, to verify circuit design implementation, to determine minimum cost fire protection requirements for nuclear reactor plants, to obtain solutions to combinatorial optimization problems with Boolean constraints, and to determine the susceptibility of a facility to unauthorized access through nullification of sensors in its protection system.

4. **METHOD OF SOLUTION** - The SETS program is used to read, interpret, and execute the statements of a SETS user program which is an algorithm that specifies the particular manipulations to be performed and the order in which they are to occur.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Any properly formed Boolean equation involving the operations of AND, OR, and NOT is acceptable for processing by the SETS program. Restrictions on the size of an equation that can be processed are not absolute but rather are related to the number of terms in the disjunctive normal form of the equation, the number of literals in the equation, etc. Nevertheless, equations involving thousands and even hundreds of thousands of terms can be processed successfully.

6. **TIMING** - Running time varies with respect to the particular equations being processed and the symbolic manipulations being performed. Although no general rule for predicting run time is known, the reduction (expansion, simplification, and factorization) of an equation usually requires more run time than other manipulations, and this time tends to increase as the number of terms in the disjunctive normal form of the equation increases. NESC executed the SETS sample problem in 20 CP seconds on a CDC CYBER175. The SEP and FTD sample problems required 4 CP seconds and 1 CP second, respectively. The FTD sample problem was executed without plotting.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The SETS program is an interpretive program used to execute the statements of a SETS user program. The SETS user program provides the user with a flexible capability for achieving the symbolic manipulation of Boolean equations.

8. **RELATED AND AUXILIARY SOFTWARE** - Two auxiliary programs, SEP and FTD, are included. SEP performs the quantitative analysis of reduced Boolean equations (minimal cut sets) produced by SETS. The user can manipulate and evaluate the equations to find the probability of occurrence of any desired event and to produce an importance ranking of the terms and events in an equation. FTD is a fault tree drawing program which uses the proprietary ISSCO DISSPLA graphics software to produce an annotated drawing of a fault tree processed by SETS. The DISSPLA routines are not included.

9. **STATUS** - Abstract first distributed March 1974.
   CDC6600 restricted distribution version submitted October 1973, replaced by CDC6600B unrestricted version December 1974, replaced by CDC CYBER76 version May 1985, sample problems executed by NESC May 1985 on a CDC CYBER175.

10. **REFERENCES** - R. B. Worrell, SETS Reference Manual, NUREG/CR-4213 (SAND83-2675), May 1985.
    M. D. Olman, Quantitative Fault Tree Analysis Using the Set Evaluation Program (SEP), NUREG/CR-1935 (SAND80-2712), September 1982.
    Ann W. Shiver, Notes on Using the Fault Tree Drawing Program, Sandia National Laboratories Memorandum, June 25, 1981.
    D. A. Oliver, Fault Tree Drawing Program Users Instructions, SLA-73-0409, April 1973.

SETS, NESC No. 623, SETS Tape Description and Implementation Informatic National Energy Software Center Note 85-68, May 7, 1985.

D. W. Stack, A SETS User's Manual for Accident Sequence Analysi NUREG/CR-3547 (SAND83-2238), January 1984.

G. B. Varnado, W. H. Horton, and P. R. Lobner, Modular Fault Tree Analys Procedures Guide, Volume 1 - Main Report, NUREG/CR-3268/1 (SAND83-0963/1), August 1983.

G. B. Varnado, W. H. Horton, and P. R. Lobner, Modular Fault Tree Analys Procedures Guide, Volume 2 - Appendices A, B, and C, NUREG/CR-3268/2 (SAND83-0963/2 August 1983.

G. B. Varnado, W. H. Horton, and P. R. Lobner, Modular Fault Tree Analys Procedures Guide, Volume 3 - Appendices D, E, F, G, and H, NUREG/CR-3268/3 (SAND83-0963/3 August 1983.

G. B. Varnado, W. H. Horton, and P. R. Lobner, Modular Fault Tree Analys Procedures Guide, Volume 4 - Appendix I, NUREG/CR-3268/4 (SAND83-0963/4), August 1983.

11. **HARDWARE REQUIREMENTS** - SETS requires 155,000 (octal) words of SCM and a minimum of 12,0 (octal) words of LCM for execution. SEP requires 147,000 (octal) words of SCM and 230,0 (octal) words of LCM; FTD requires 70,000 (octal) words of SCM and 350,000 (octal) words LCM.

12. **PROGRAMMING LANGUAGE** - FORTRAN Extended Version 4

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC CYBER76), NOS 2.2 (CDC CYBER175), NOS 2.3 (CDC CYBER180

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - SETS must be compiled wi optimization level of 0 or 1. Full optimization (OPT=2) produces compiler table overflow

A substantial reprogramming effort would be required to convert the SETS program to machine that is not compatible with the CDC systems 60-bit word structure due to t extensive use of masking instructions and the packing of data within a word.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

R. B. Worrell
Reactor Systems Safety Analysis Division 6412
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -

Source (8087 lines)
Sample problem (167 lines)
Auxiliary information (SEP FORTRAN 2285 lines, data 18 lines, output 166 132-charact records, FTD FORTRAN 2255 lines, data 63 lines, output 305 132-character records)
Control information (45 lines)
Sample problem output (259 132-character records)
Reference reports, NUREG/CR-4213, NUREG/CR-1935, and SLA-73-0409, SNLA Memorandum, a NESC Note

17. **CATEGORY** - P
KEYWORDS - network analysis, fault tree analysis, probabilistic estimation, failure mo analysis, reactor safety, mathematical logic, SEP codes, FTD codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Risk Analysis,
Division of Systems and Reliability Research

1. **IDENTIFICATION AND KWIC TITLE -** LANL-J501
   LANL-J501, SC-4020 emulation graphics library

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC6600,7600, Cray1, DEC VAX11/780

3. **DESCRIPTION -** LANL-J501 is a library of graphics subroutines developed to emulate graphics routines originally written for use with the Stromberg Carlson Model 4020 film recorder (SC-4020). The SC-4020 has been superseded and output may be directed to various newer output devices; however, these subroutines ensure compatibility for applications programs.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -** Since the subroutines in LANL-J501 form an SC-4020 emulation library, graphics output will not necessarily look the same on all output devices. In particular, limitations in screen resolution and hardware character size are implied in the context of newer output devices.

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Abstract first distributed May 1974.
   CDC6600 version of Los Alamos Subroutine Library submitted August 1973, replaced by Edition B March 1975, replaced by Edition C May 1976, replaced January 1982 by the LANL-J501 SC-4020 emulation library subset submitted August 1981, source compiled by NESC November 1981 on a CDC CYBER175.
   CDC7600 version of LANL-J501 for the FTN compiler submitted August 1981, source compiled by NESC November 1981 on a CDC CYBER175.
   CDC7600B edition version of LANL-J501 for the CHAT compiler submitted August 1981.
   Cray1 version of LANL-J501 submitted August 1981, source compiled by NESC November 1981 on a Cray1.
   DEC VAX11/780 version of LANL-J501 submitted August 1981, source compiled by NESC November 1981 on a DEC VAX11/780.

10. **REFERENCES -** Gail Rein, J501 SC-4020 Emulation User Manual, LANL PIM-2 Program Library Write-Up, May 1981.

B. Buzbee, G. Carter, D. Kahaner, and J. Norton, N112 Error Handling Package, LANL PIM-2 Program Library Write-Up, July 1979.

Ted Reed, J701 CGS: Common Graphics System, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J702 CGS Metafile Initialization, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J703 Terminate Plotting, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J704 Window, Viewport, and Screen, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J706 Move, Draw, and Mark, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J707 New Page, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J708 Plot Characters, LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J743 Easy Color Call (Hollerith), LANL PIM-2 Program Library Write-Up, April 1981.

Ted Reed, J744 Set Intensity Attribute, LANL PIM-2 Program Library Write-Up, April 1981.

G. Rein, M202 Alphanumeric Format, LANL PIM-2 Program Library Write-Up, September 1980.

G. Rein, M203 Exponential Format, LANL PIM-2 Program Library Write-
September 1980.
G. Rein, M204 Fixed Field Format, LANL PIM-2 Program Library Write-
September 1980.
G. Rein, M205 General Format, LANL PIM-2 Program Library Write-Up, Septem
1980.
G. Rein, M206 Integer Format, LANL PIM-2 Program Library Write-Up, Septem
1980.
G. Rein, M208 Exponential Format with Scale Factor, LANL PIM-2 Program Libr
Write-Up, September 1980.
G. Rein, M416 Move Characters, LANL PIM-2 Program Library Write-Up, Septem
1980.
LANL-J501, NESC No. 633.VX11, LANL-J501 DEC VAX11/780 Version Implementat
Information, National Energy Software Center Note 82-13, November 13, 1981.

11. **HARDWARE REQUIREMENTS** - The CDC6600 and CDC7600 versions of LANL-J501 require 120,0
(octal) words of memory; the DEC VAX11/780 version requires 130K bytes.

12. **PROGRAMMING LANGUAGE** - FORTRAN. The compilers used are - FTN (CDC6600,7600), CH
(CDC7600B), CFT (Cray1), FOR (DEC VAX11/780)

13. **OPERATING SYSTEM** - NOS (CDC6600), LTSS (CDC7600,7600B), CTSS (Cray1), VMS (DEC VAX11/780)

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The Cray1 version can
compiled only with the CFT compiler. Subroutines GCOLOR, GDONE, GINTEN, GLINA2, GMOVA
GMOVR2, GMRKA2, GPAGE, GPLOT, GTEXT, GVIEW2, and GWIND2 are part of the LANL Comm
Graphics System (CGS) which is designed to be a device-independent, system-independe
graphics system available on all LANL computer software systems for all LANL-support
graphics devices. Subroutine GCP2 returns the current (X,Y) position of the pen in t
plotting area. Subroutines BCHARM, BCONVA, BCONVE, BCONVF, BCONVG, BCONVI, and BCONVP a
LANL routines for character manipulation, and subroutines XERROR, XGETF, and XSETF are pa
of the LANL error-handling package. Suitable alternatives for these routines must
provided for the computer environment in which the package is to be used.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

G. L. Rein, T. Reed, B. Buzbee, G. Carter,
D. Kahaner, and J. Norton
C Division
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -

Source (6600-7320 lines, 7600-7381 lines, 7600B-7398 lines, CRA1-7021 lines, VX11-72
lines)
Sample drivers (6600-516 lines, 7600-517 lines, 7600B-507 lines, CRA1-504 line
VX11-506 lines)
Sample output (36 plots)
LANL PIM-2 Program Library Write-Ups and for VAX11/780 version only, NESC Note

17. **CATEGORY** - P
KEYWORDS - computer graphics, utility routines, plotters, display devices

18. **SPONSOR** - Los Alamos National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - REBUS2
   REBUS2, fuel cycle analysis for fast reactors

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - REBUS2 is a system of codes designed for the analysis of fast reactor fuel cycles. Two basic types of analysis problems are solved--the infinite-time, or equilibrium, conditions of a reactor operating under a fixed fuel management scheme, and the explicit cycle-by-cycle, or nonequilibrium, operation of a reactor under a specified periodic fuel management program. For the equilibrium type problems, the code uses specified external fuel supplies to load the reactor. Optionally, reprocessing may be included in the specification of the external fuel cycle and discharged fuel may be recycled back into the reactor. For non-equilibrium cases, the initial composition of the reactor core may be explicitly specified or the core may be loaded from external feeds as in equilibrium problems.
   Three types of search procedures may be carried out in order to satisfy user-supplied constraints -
   (a) adjustment of the reactor burn cycle time to achieve a specified discharge burnup,
   (b) adjustment of the fresh fuel enrichment to achieve a specified multiplication constant at a specified point during the burn cycle, and
   (c) adjustment of the control poison density to maintain a specified value of the multiplication constant throughout the reactor burn cycle.

4. **METHOD OF SOLUTION** - The total reactor burn cycle time is divided into one or more subintervals, the number of which is specified by the user. An explicit burnup is performed in each region of the reactor over each of these subintervals using the average reaction rates over the subinterval. These average reaction rates are based on fluxes obtained from an explicit, two-dimensional, diffusion theory neutronics solution computed at both the beginning and end of the subinterval. The transmutation equations are solved by the matrix-exponential technique. The isotopes to be considered in the burnup equations, as well as their transmutation reactions, are specified by the user.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Recycle of discharged fuel is not allowed in non-equilibrium type problems. Only two-dimensional problems are handled.

6. **TIMING** - Three to 30 minutes are required on the IBM370/195 depending on the size and complexity of the problem.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - REBUS2 will handle both equilibrium and non-equilibrium problems using a number of core geometries including hexagonal mesh. The program has an automatic restart capability. No restrictions are imposed on the number of neutron energy groups, external feeds, or reprocessing plants.

8. **RELATED AND AUXILIARY SOFTWARE** - This is a stand-alone version of the ARC System (reference 7) fuel cycle analysis code REBUS2. It utilizes the ARC System's two-dimensional, diffusion theory capability (reference 6), an improved version of the cross section homogenization code NUC001 (reference 8), the neutronic input processor NUI002 (reference 9), and the hexagonal mesh input processor NUI004.

9. **STATUS** - Abstract first distributed December 1974.
   IBM360 version submitted April 1974, revised November 1974, replaced October 1976 by revised Edition B submitted April 1976, modified August 1976, replaced December 1979 by revised Edition C submitted December 1978, modified March 1979, modified May 1979, sample problem executed by NESC June 1979 on an IBM370/195.

10. **REFERENCES** - R. P. Hosteny, The ARC System Fuel Cycle Analysis Capability, REBUS-
ANL-7721, October 1978.
REBUS2, NESC No. 634.360C,D, ANL-7721 Errata, National Energy Software Cent
Note 80-19, December 28, 1979.
R. P. Hosteny, Instructions for Implementation of an IBM Standalone Version
the REBUS-2 Fuel Cycle Analysis Code, ANL-Applied Physics Note, November 1978.
R. P. Hosteny, Description and Edit of Cross Section Libraries Used by REBUS
ANL-Applied Physics Note, March 1979.
REBUS2, NESC No. 634.360D, List of Source Members and Subroutines in Ea
Member, National Energy Software Center Note 80-20, December 28, 1979.
T. A. Daly, G. K. Leaf, and A. S. Kennedy, The ARC System Two-dimension
Diffusion Theory Capability, DARC2D, ANL-7716, May 1972.
L. C. Just, H. Henryson, II, A. S. Kennedy, S. D. Sparck, B. J. Toppel, a
P. M. Walker, The System Aspects and Interface Data Sets of the Argonne Reactor Computati
(ARC) System, ANL-7711, April 1971.
E. A. Kovalsky, J. Zapatka, H. Henryson, II, J. Hoover, and P. M. Walker, T
ARC System Cross-section Homogenization and Modification Capabilities, ANL-7714, June 197
E. A. Kovalsky and D. E. Neal, The ARC System Neutronics Input Processo
ANL-7713, January 1971.

11. **HARDWARE REQUIREMENTS** - At least 400K bytes of memory are required (530K and 418K for t
two sample problems, respectively). Creation of a load module requires a total
approximately 9.3 million bytes of direct-access storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (99%) and Assembly language (1%)

13. **OPERATING SYSTEM** - OS/360,370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
B. J. Toppel
Applied Physics Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
For 360 users:
Source (PDS REBUS2.SOURCE 5686 blocks)
Object module (PDS REBUS2.OBJECT 3263 blocks)
Load module (PDS REBUS2.LOAD.MOD 1615 blocks)
Sample problems (1463 lines)
Control information (146 lines)
Libraries* (XSISO1 1 block, XSISO2 9 blocks)
Sample problems output (114 pages)
Reference report, ANL-7721 and Errata, and Implementation Note
For non-360 users:
Source (55,295 lines)
Sample problems (1463 lines)
Control information (146 lines)
Sample problems output (114 pages)
Reference report, ANL-7721 and Errata, and Notes
* Maximum blocksize 7294 bytes

17. **CATEGORY** - D
KEYWORDS - two-dimensional, breeding, criticality, burnup, LMFBR reactors, fuel cycle

18. **SPONSOR** - DOE Division of Reactor Research and Technology

1. **IDENTIFICATION AND KWIC TITLE** - GAMTAB
   GAMTAB, radioactive-decay gamma-ray catalog

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - This package contains a two-part catalog of gamma rays emitted by nuclides in radioactive decay and a list of corresponding references. The first part lists the gamma rays in order of ascending energy. This listing consists of gamma-ray energy and uncertainty, abundance, half-life, production mode, and the energies of two of the more abundant associated gamma rays. The second part of the catalog lists up to 50 of the more abundant gamma rays for each nuclide. The listing for each nuclide includes half-life, production mode, possible genetic relationships, and references. This listing is followed by the energy, uncertainty in energy, and abundance of each gamma ray. References available through May 1973 corresponding to the reference keys listed for each nuclide in part 2 are listed as the third file.

4. **METHOD OF SOLUTION** - The gamma ray data is arranged in increasing energy in part 1 and in ascending mass number of the nuclide in part 2.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed June 1974.
   IBM360 version submitted May 1974, corrected to version B January 1975.

10. **REFERENCES** - W. W. Bowman and K. W. MacMurdo, Radioactive Decay Gammas Ordered by Energy and Nuclide, Atomic Data and Nuclear Data Tables, Vol. 13, No. 2-3, February 1974.
    W. W. Bowman and K. W. MacMurdo, Radioactive-Decay Gammas, Savannah River Laboratory Memorandum, May 1974.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** -

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    W. W. Bowman and K. W. MacMurdo
    Savannah River Laboratory

16. **MATERIAL AVAILABLE** -
    Energy data (19,416 lines)
    Nuclide data (6905 lines)
    References (550 lines)
    Reference memorandum

17. **CATEGORY** - Z
    KEYWORDS - gamma radiation, radioactivity, isotopes

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - POLLA
   POLLA, converts r-matrix resonance parameters

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360,370/195

3. **DESCRIPTION** - The program transforms a set of R-matrix nuclear resonance parameters into a set of equivalent S-matrix (or Kapur-Peierls) resonance parameters.

4. **METHOD OF SOLUTION** - The program utilizes the multilevel formalism of Reich and Moore and avoids diagonalization of the level matrix. The parameters are obtained by a direct partial fraction expansion of the Reich-Moore expression of the collision matrix. This approach appears simpler and faster when the number of fission channels is known and small. The method is particularly useful when a large number of levels must be considered because it does not require diagonalization of a large level matrix.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - By DIMENSION statements, the program is limited to maxima of 100 levels and 5 channels.

6. **TIMING** - The sample problem requires less than one minute on the IBM360/91.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed November 1974.
   IBM360 version submitted August 1974, sample problem executed by NESC October 1974 on an IBM370/195.

10. **REFERENCES** - G. de Saussure and R. B. Perez, POLLA, A FORTRAN Program to Convert R-Matrix-Type Multilevel Resonance Parameters for Fissile Nuclei into Equivalent Kapur-Peierls-Type Parameters, ORNL-TM-2599, June 1969.

11. **HARDWARE REQUIREMENTS** - The program requires 240K bytes to compile, 62K bytes to execute.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The running time increases as the ratio of average width to spacing increases.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   G. de Saussure and R. B. Perez
   Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
   Source (232 lines)
   Sample problem (107 lines)
   Sample problem output (4 pages)
   Reference report

17. **CATEGORY** - A
   KEYWORDS - R matrix, S matrix, multilevel analysis, Reich-Moore formula, resonance

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE -** SLOP, CROSS
   SLOP,CROSS, IBM360 Fortran H program checker

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   IBM360,370,303x

3. **DESCRIPTION -** The package contains two PL/I codes, SLOP (Structural Layout Of Programs) and CROSS, designed to check IBM FORTRAN H source programs. SLOP examines the SYSPRINT file produced by a FORTRAN H compilation for local errors and sends its observations to CROSS which detects potential global errors. SLOP summarizes variables, labels, common blocks, and other items in a subroutine, showing which symbols are being improperly used. Optionally, the SLOP program can list the output from the original FORTRAN subroutine compilation, can list and save a 'corrected' and resequenced FORTRAN file, and save and list the information intended for the CROSS routine.
   For each subroutine CROSS tabulates:
   the subroutine name and size,
   entry points,
   listed but unused symbols,
   uninitialized variables,
   unreferenced statement numbers,
   internal statement numbers of input-output statements,
   symbols which appear in input-output statements,
   called subroutines, and
   the active variables in common and/or equivalence blocks,
   together with block names and addresses.
   CROSS lists common and/or equivalenced variables in alphabetic order with addresses and corresponding block names, along with the names of routines in which these variables are actively used. Any suspicious-looking or inconsistent items are flagged. The same information will also be sequenced and listed according to block names and addresses within each block. CROSS also produces a table designed to show instantly which routines need attention because SLOP found errors in them, which are missing or defined more than once, which routines are calling each routine, and how many times each routine is being called by the other. Finally, if any cycles of subroutine calls are detected, a second table indicating these recursive calls will be produced.
   The test case supplied with this package is designed to be self-explanatory, removing the need for separate documentation.

4. **METHOD OF SOLUTION -** The SLOP code processes the results of the IBM FORTRAN H compilation using the XREF option. This compilation produces records of varying length, allowing SLOP to isolate useful information without examining these records directly. Compilation results normally contain FORTRAN source code if the record length is 105, the 'SYMBOL INTERNAL STATEMENT NUMBERS' data if the record length is 133, the 'NAME TAG TYPE ADD.' information if the record length is 128, the 'LABEL DEFINED REFERENCES' information if the record length is 133, and the error messages if the record length is 155. The final record for each subroutine block is indicated by a record length of 100. If an input FORTRAN line is not a comment or continuation line, then the first few non-blank characters after column 6 are examined and used to set a one-character classification tag: A(dimension), C(common), D(data), E(equivalence), G(integer), H(logical), I(if), L(loop), N(entry), R(read), S(store), V(real), W(write or punch or print), X(subroutine or function call), or Z(namelist).
   If a READ, WRITE, PUNCH, or PRINT occurs in an IF statement, the tag 'I' is replaced by a corresponding 'W' or 'R'. When the 'NAME TAG TYPE ADD.' information is encountered, the corresponding data are placed into another type of internal tag. These internal tags and the one-character classification tags are used for each tabulated symbol to identify entries, errors, etc. Errors in the FORTRAN code are corrected whenever possible.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** A program containing up to 300 routines can be processed.

6. **TIMING -** This varies according to size and complexity of the tested FORTRAN program and the options which are exercised. The sample test deck took 19 seconds of CPU time on both an

IBM3033 and IBM370/195 for execution of the three-step procedure, including compilations of the FORTRAN data and the SLOP and CROSS source.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Both PL/I and FORTRAN are used.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed November 1975.
IBM360 version submitted October 1975, replaced by Edition B May 1977, replaced June 1981 by Edition C submitted October 1980, sample problem executed by NESC October 1980 on an IBM3033.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** - 600K bytes of storage are required.

12. **PROGRAMMING LANGUAGE** - PL/I

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - SLOP was designed to examine only the output produced by the IBM FORTRAN H compiler using the XREF option.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
A. J. Strecok
National Energy Software Center
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
Source (SLOP 809 lines, CROSS 364 lines)
Sample problems (SLOP FORTRAN test 292 lines, option control input 1 line)
Control information (JCL 42 lines)
Sample problems output (SLOP 71 lines, 33 pages, CROSS 13 pages)

17. **CATEGORY** - P
KEYWORDS - FORTRAN, errors, testing, programming

18. **SPONSOR** - DOE Technical Information Center

1. **IDENTIFICATION AND KWIC TITLE** - MOCUS
   MOCUS, minimal sets from fault trees

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - From a description of the Boolean failure logic of a system, called a fault tree, and control parameters specifying the minimal cut set length to be obtained MOCUS determines the system failure modes, or minimal cut sets, and the system success modes, or minimal path sets.

4. **METHOD OF SOLUTION** - MOCUS uses direct resolution of the fault tree into the cut and path sets. The algorithm used starts with the main failure of interest, the top event, and proceeds to basic independent component failures, called primary events, to resolve the fault tree to obtain the minimal sets. A key point of the algorithm is that an and gate alone always increases the number of path sets; an or gate alone always increases the number of cut sets and increases the size of path sets. Other types of logic gates must be described in terms of and and or logic gates.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Output from MOCUS can include minimal cut and path sets for up to 20 gates.

6. **TIMING** - Running time is problem dependent. The sample test case requires 2 seconds on the Model 195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - MOCUS guarantees that all the minimal sets requested have been found.

8. **RELATED AND AUXILIARY SOFTWARE** - PREP/KITT (NESC 528). The fault tree description input to MOCUS is identical to the fault tree description input to TREBIL in the PREP package. The output from MOCUS is compatible with KITT input requirements for quantitative reliability evaluation.

9. **STATUS** - Abstract first distributed March 1975.
   IBM360 version submitted February 1975, sample problem executed by NESC March 1975.

10. **REFERENCES** - J. B. Fussell, E. B. Henry, and N. H. Marshall, Minimal Sets from Fault Tree, ANCR-1156, August 1974.
    W. E. Vesely and R. E. Narum, PREP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree, IN-1349, August 1970.
    J. B. Fussell, Synthetic Tree Model--A Formal Methodology for Fault Tree Construction, ANCR-1098, March 1973.

11. **HARDWARE REQUIREMENTS** - 222K bytes for execution and 7 I/O units

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The sample problem uses more storage than that given in the reference report, ANCR-1156. Sample problem execution at Argonne used 222K bytes.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. B. Fussell, E. B. Henry, and N. H. Marshall
    EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
    Source (1739 lines)
    Object (928 lines)
    Sample problem (20 lines)

Control information (JCL 29 lines)
Sample problem output (19 lines, 15 pages)
Reference report, ANCR-1156

17. **CATEGORY** - G
KEYWORDS - reliability, fault tree analysis, system failure analysis, PREP,KITT codes

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE -** FRAP-T6/MOD1
   FRAP-T6/MOD1, transient analysis of fuel rods

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC CYBER176

3. **DESCRIPTION -** FRAP-T6 is the most recent in the FRAP-T (Fuel Rod Analysis Program - Transient) series of programs for calculating the transient behavior of light water reactor fuel rods during reactor transients and hypothetical accidents, such as loss-of-coolant and reactivity-initiated accidents. The program calculates the temperature and deformation histories of fuel rods as functions of time-dependent fuel rod power and coolant boundary conditions. FRAP-T6 can be used as a "stand-alone" code or, using steady state fuel rod conditions supplied by FRAPCON2 (NESC 694), can perform a transient analysis. In either case, the phenomena modeled by FRAP-T6 include: heat conduction, heat transfer from cladding to coolant, elastic-plastic fuel and cladding deformation, cladding oxidation, fission gas release, fuel rod gas pressure, and pellet cladding mechanical interaction. Licensing audit models have been added, also. The program includes a user's option that automatically provides a detailed uncertainty analysis of the calculated fuel rod variables due to uncertainties in fuel rod fabrication, material properties, power and cooling.

4. **METHOD OF SOLUTION -** The models in FRAP-T6 use finite difference techniques to calculate the variables which influence fuel rod performance. The variables are calculated at user-specified slices of the fuel rod. Each slice is at a different elevation and is defined to be an axial node. At each axial node, the variables are calculated at user-specified locations. Each location is at a different radius and is defined to be a radial node. The variables at any given axial node are assumed to be independent of the variables at all other axial nodes. The solution for the fuel rod variables begins with the calculation of the fuel and cladding temperatures. Then, the temperature of the gases in the plenum of the fuel rod is calculated. Next, the stresses and strains in the fuel and cladding and the pressure of the gas inside the rod are computed. This calculation sequence is repeated until essentially the same temperature distribution is calculated for two successive cycles. The cladding oxidation and fission gas release are then calculated, and the time is advanced, after which the complete sequence of calculation is repeated to obtain the fuel rod variables at the advanced time.

   The models interact in several ways. The fuel temperature calculated by the thermal model is dependent upon the size of the fuel-cladding gap calculated by the deformation model, and the diameter of the fuel pellet depends upon the temperature distribution in the pellet. Mechanical properties of the cladding vary significantly with temperature. The internal pressure varies with the temperature of the fuel rod gases and the strains of fuel and cladding. The stresses and strains in the cladding are dependent upon internal gas pressure. Variables calculated in one model are treated as independent variables by the other models. Two nested calculational loops are cycled until convergence occurs. Convergence is accelerated by the Newton method. The optional uncertainty analysis is based on the response surface method.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** Since FRAP-T6 is dynamically-dimensioned, the only constraint on the number of axial and radial nodes is the size of the available computer memory. The amount of memory required is a function of the number of axial and radial nodes and the selected models given by the equation: S = LB + 1710 + 11NR + 257NZ + 8NR•NZ + I2D (7NA•NZA•NR + 24NA•NZA) + IB (6NCH•NZCH + NCH + 2) + IF2 (4 + 117NR + 2NZ + 20NR•NZ) + IG (7 + 4NRF + 8NZ + 26NRF•NZ) + IBAL (10,000) where S is the required number of words of central memory; LB is the memory required to load FRAP-T6 exclusive of array storage (98,000 words); NR is the number of radial nodes and NZ, the number of axial nodes. I2D=1, if two-dimensional r-theta heat conduction is modeled, 0 otherwise; NA is the number of azimuthal sectors and NZA, the number of axial nodes at which two-dimensional r-theta heat conduction is modeled. IB=1, if the fuel rod is in contact with more than one coolant channel, 0 otherwise; NCH is the number of coolant channels surrounding the fuel rod, and NZCH, the number of vertically-stacked zones in a coolant channel. IF2=1, if the FRACAS2 subcode (deformable pellet deformation model) is used, 0 otherwise. IG=1, if the FASTGRASS subcode (fission gas production and release model) is used, 0 otherwise; NRF is the number of radial nodes in the fuel. IBAL=1, if the BALON2 subcode (cladding ballooning model) is

used, 0 otherwise. The LB variable can be reduced to a value of about 65,000 by overlaying.

6. **TIMING** - The running time varies with the size of the time-step, the number of nodes specified, and the models chosen.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The FRAP-T series of programs is designed in a modular manner with each type of calculation and analytical model in a separate module, or subcode. This configuration makes substitution of models and algorithms a straightforward procedure.

8. **RELATED AND AUXILIARY SOFTWARE** - The series makes use of the INEL (formerly NRTS) Environmental Subroutines (NESC 613), which are included in the package. The steady-state fuel rod analysis program FRAPCON2 is designed to supply realistic input conditions to FRAP-T6 for transient analysis. The MATPRO11 Rev. 1 materials properties package is linked with FRAP-T6 to provide the necessary materials properties. FRAP-T6 is designed to calculate fuel rod response for reactor system thermal-hydraulic analysis codes, such as TRAC and RELAP4, or, as an alternative, a condensed version of FRAP-T6 can be incorporated in the system's thermal-hydraulic analysis code so that the systems analysis and detailed fuel rod response can be determined in a single computer analysis. A condensed version of FRAP-T6 has been incorporated in the TRAC-PD3 code.

9. **STATUS** - Abstract first distributed October 1975.
   IBM360 version of FRAP-T submitted April 1975, sample problem executed by NESC October 1975 on an IBM370/195, deleted September 1983.
   CDC7600 version of FRAP-T3 submitted June 1977, replaced May 1979 by FRAP-T4 submitted July 1978, revised April 1979, replaced by CDC CYBER176 version of FRAP-T6/MOD1 September 1983, compiled by NESC September 1983 on a CDC CYBER175.

10. **REFERENCES** - Larry J. Siefken, Chris M. Allsion, Michael P. Bohn, and Scott O. Peck, FRAP-T6: A Computer Code for the Transient Analysis of Oxide Fuel Rods, NUREG/CR-2148 (EGG-2104), May 1981.
    L. J. Siefken, V. N. Shaw, G. A. Berna, and J. K. Hohorst, FRAP-T6: A Computer Code for the Transient Analysis of Oxide Fuel Rods, NUREG/CR-2148 (EGG-NSMD-2104) Addendum, June 1983.
    FRAP-T6/MOD1, NESC No. 658, FRAP-T6/MOD1 Tape Description and Implementation Information, National Energy Software Center Note 83-87, September 2, 1983.
    Donald L. Hagrman and Gregory A. Reymann, Ed., Matpro-Version 11 (Revision 1): A Handbook of Materials Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior, NUREG/CR-0497 (TREE-1280) Rev. 1, February 1980.
    G. A. Berna, M. P. Bohn, W. N. Rausch, R. E. Williford, and D. D. Lanning, FRAPCON-2: A Computer Code for the Calculation of Steady State Thermal-Mechanical Behavior of Oxide Fuel Rods, NUREG/CR-1845, January 1981.

11. **HARDWARE REQUIREMENTS** - 260,000 (octal) words of SCM and 63,000 (octal) words of LCM are required for FRAP-T6.

12. **PROGRAMMING LANGUAGE** - FORTRAN (99%) and Assembly language (1%). The Assembly language is used in a few of the INEL Environmental Routines.

13. **OPERATING SYSTEM** - NOS/BE 1.4.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The FRAP-T6 source is available only in CDC UPDATE utility format, not suited for use on other computer systems. The INEL Graphics Library routines: CATGEN, CATID, CATKEY, COMCLS, COMIN, COMOUT, EXTEND, FINDID, FINDKEY, and GFI were not supplied. If the user does not specify the plotting option and removes the *DEFINE CWAF directive from the FRAP-T6 OLDPL the Graphics Library is not required. However, to obtain graphic output, alternative routines suited to the local computing environment should be provided.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. J. Siefken, V. N. Shah, G. A. Berna,

and J. K. Hohorst
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
Source (FRAP-T6 and MATPRO11 45,732 lines, INEL Environmental Routines 1144 lines)
Sample problems (1073 lines)
Sample problems output (2 microfiche)
Auxiliary routines (FCOOL 516 lines, STRIP4 483 lines, PLOT 1026 lines, and ANALYZE 3122 lines)
Control information (H2OTAB 35 lines)
Reference reports, NUREG/CR-2148 and Addendum, and NESC Note

17. **CATEGORY** - G
KEYWORDS - accidents, heat transfer, pressure, fuel rods, flow blockage, failures, fuel-cladding interactions, transients, loss of coolant, power-cooling-mismatch accidents, thermal reactors, FRAPCON2 codes, RELAP codes, TRAC codes, MATPRO11 codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Accident Evaluation

1. **IDENTIFICATION AND KWIC TITLE** - BETTIS ENVIRONMENTAL LIBRARY
   BETTIS PROGRAMMING ENVIRONMENT LIBRARY

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC6600,7600

3. **DESCRIPTION** - The BETTIS ENVIRONMENTAL LIBRARY consists of a large number of subroutines and functions which are available for use in application programs. These routines effectively extend the FORTRAN language in such areas as system communication, decimal input, file management, scratch I/O, storage allocation, and plotting.

4. **METHOD OF SOLUTION** - The intent is to maintain all system-dependent routines in a well-documented central library to minimize system conversion problems. Routines included are:
   CARDS and INPF systems - for conversion and processing of free-field decimal input.
   FTB-4 system - for very high, disk-streaming rates with storage management and allocation capabilities.
   FMG routine - to interface the file management system and the using program.
   RANDIO routines - for reading and writing indexed files which can be moved between the 6600 and 7600 computers.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The BETTIS ENVIRONMENTAL LIBRARY is used by the newer Bettis programs; an earlier edition of the Bettis Environmental Routines appeared as NESC Abstract 478.

9. **STATUS** - Abstract first distributed April 1975.
   CDC6600 (RUN and FTN compiler) versions submitted November 1974 and January 1975, replaced by Edition B January 1982, compiled by NESC on a CDC6600, tested by NESC using RCPL1 and RCP01 (NESC 670 and 671).
   CDC7600 (RUN and FTN compiler) versions submitted November 1974 and January 1975, replaced by Edition B January 1982, compiled by NESC on a CDC7600.

10. **REFERENCES** - W. R. Cadwell, (Ed.), Reference Manual - Bettis Programming Environment, WAPD-TM-1181, September 1974.
    C. J. Pfeifer, CDC-6600 FORTRAN Programming - Bettis Environmental Report, WAPD-TM-668, January 1967.
    BETTIS ENVIRONMENTAL LIBRARY, NESC No. R665.6600B, BETTIS ENVIRONMENTAL LIBRARY Tape Description and Implementation Information, National Energy Software Center Note 82-15, October 1, 1981.
    BETTIS ENVIRONMENTAL LIBRARY, NESC No. R665.7600B, BETTIS ENVIRONMENTAL LIBRARY Tape Description and Implementation Information, National Energy Software Center Note 82-14, October 1, 1981.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - Almost all of the environmental routines are written in FORTRAN IV, the remainder in COMPASS.

13. **OPERATING SYSTEM** - SCOPE 3.1 and 3.2 (CDC6600), SCOPE 1.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - There are two versions of the BETTIS ENVIRONMENTAL LIBRARY available for each machine. The first is for use with the standard RUN compiler. The second consists of a portion of the library (chapters C-F of reference 1) which has been converted for use with the FORTRAN Extended (FTN) compiler. In the conversion all COMPASS routines were modified to conform to the FTN calling sequence conventions. The remainder of the library (chapters G-M) has not been converted but contains so few COMPASS routines that it can be converted easily by a potential user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
W. R. Cadwell
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE -** Restricted Distribution
Source (RUN 7600B-18,788 lines, 6600B-18,271 lines, FTN 7600B-6603 lines, 6600B-6666 lines)
Reference report, WAPD-TM-1181, and NESC Note for appropriate version

17. **CATEGORY -** P
KEYWORDS - data processing, operation, libraries, maintenance

18. **SPONSOR -** DOE Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - RCP01
   RCP01, Monte Carlo neutron & photon transport

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600,6600

3. **DESCRIPTION** - RCP01 is a Monte Carlo program which estimates neutron capture rates and photon heating rates over the energy range important to the fission process, i.e., 10 Mev to 0 ev. There is a neutron eigenvalue capability as well as the usual fixed source capability. The geometry is modular comprising: (a) module zero, a set of concentric cylinders or spheres with axial material boundaries; (b) final modules, each a collection of rectangular or 60 degree parallelogram initial assemblies superimposed on module zero at arbitrary positions and angular orientations; (c) initial assemblies of rectangles and 60 degree parallelograms with internal structure determined by an overlay on a variable mesh; (d) optional use of doubly repetitive "subcells" containing arbitrary collections of non-intersecting elliptical surfaces within initial assemblies. Other geometric features include the geometry variation which provides trapezoidal and equilateral triangular final assemblies and composite final assemblies which are pairs of final assemblies, one arbitrarily positioned and oriented within the other. Edits of absorption, heating, and neutron production are produced, with corresponding uncertainties, for each material (composition) by nuclide by energy group.

4. **METHOD OF SOLUTION** - Neutron or photon histories are processed until each particle is absorbed, escapes, or degrades in energy below some cut-off point. All events are determined using a sequence of pseudo-random numbers. To calculate absorption rates in energy groups above thermal, RCP01 uses a non-terminating sigma(a)/sigma(t) estimator or the binomial estimator; in the thermal group, a terminating sigma(a)/sigma(t), binomial, or a combination of these estimators is used. Variance reduction techniques available include splitting and Russian roulette based on a set of ellipsoids, a trapping surface capability, and a neutron-conserving thermal energy Russian roulette.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   15 nuclides per job including not more than 10 resonance nuclides or 10 non-resonance nuclides
   100 groups over the total energy range (10 Mev to 0 ev)
   500 energy intervals for each of the inelastic scattering groups (10 Mev to 5.53 Kev)
   1000 energy intervals for each of the epithermal groups (5.53 Kev to .625 ev)
   300 energy intervals for the thermal group
   Programmed variable storage allocation procedures restrict other problem size limits based only on the amount of memory available.

6. **TIMING** - Execution time varies widely depending upon problem complexity. The sample problem requires approximately 35 minutes of CP time for 8 iterations on a CDC6600 and 10 minutes for 21 iterations on the CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Features include -
   (a) inclusion of hydrogen binding effects in the low epithermal energy range through an effective source temperature.
   (b) availability of an exact perturbation capability for one composition in addition to the usual correlated sampling techniques.
   (c) optional region edits available through the use of a collision file.
   (d) use of link files to provide neutron absorption sites as a source file for photon problems, or as a source guess for an eigenvalue calculation. A neutron-photon-neutron subcritical calculation can be performed in a similar manner.

8. **RELATED AND AUXILIARY SOFTWARE** - A library generated by RCPL1 (NESC 671), in File Manager form (see Reference 3), is required as the source of nuclide cross sections. RCP01 uses the Bettis Environmental Library (NESC 665).

9. **STATUS** - Abstract first distributed May 1975.
CDC7600 version of RECAP-12 submitted December 1974, sample problem added June 1975, replaced August 1981 by RCP01 submitted April 1980, sample problem executed by NESC July 1981 on a CDC6600.

10. **REFERENCES** - N. R. Candelore, R. C. Gast, and L. A. Ondis II, RCP01 - A Monte Carlo Program for Solving Neutron and Photon Transport Problems in Three-Dimensional Geometry with Detailed Energy Description, WAPD-TM-1267, August 1978.
A. V. Dralle, N. R. Candelore, and R. C. Gast, RCPL1 - A Program to Prepare Neutron and Photon Cross Section Libraries for RCP01, WAPD-TM-1268, August 1978.
W. R. Cadwell, Editor, Reference Manual - Bettis Programming Environment, WAPD-TM-1181, September 1974.
RCP01, NESC No. R670.7600, RCP01 Tape Description and Implementation Information, National Energy Software Center Note 81-79, July 27, 1981.

11. **HARDWARE REQUIREMENTS** - CDC7600 or CDC6600 with variable requirement of Large Core Memory (LCM) or Extended Core Storage (ECS). The sample problem requires approximately 106K (octal) words of central memory and 46K (octal) words of ECS on the CDC6600.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV with COMPASS equivalent routines for a selected few key subroutines.

13. **OPERATING SYSTEM** - SCOPE 1.1, SCOPE 2.1.5 (CDC7600), SCOPE 3.3, 3.4 (CDC6600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Certain files used externally with RCP01, including RCPL1 and other RCP01 jobs, are in the Bettis File Manager form (see Reference 3). Several routines - LKDATE, BKPF, and BLKIO, which are part of the Bettis computing environment are not provided. RCP01 is written almost entirely in FORTRAN and the authors have attempted to adhere to ANS FORTRAN X3.9-1966 except for the use of a few octal constants, ENCODE/DECODE statements, octal output FORMATs, DATA statements containing implied DO's, PUNCH statements, and calls to NEXT, the Bettis environmental routine used in conjunction with overlay loading, which have a varying number of parameters. The RCP01 file management and graphics routines will have to be modified by the user or replaced with others appropriate to the local computing environment. Results may differ depending on the compiler and mathematical function libraries used. The RUN compiler with three different RUN-compatible libraries on the CDC6600 and FTN on the CDC7600 all produced slightly different results. The output included in the package is from the FTN execution on the CDC7600 at Bettis.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
N. R. Candelore, R. C. Gast, and L. A. Ondis II
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (RCP01 FORTRAN 25,363 lines, COMPASS replacement routines 1776 lines)
Sample problem (73 lines)
Sample problem output (48 selected pages)
Reference report, WAPD-TM-1267, and NESC Note

17. **CATEGORY** - C
KEYWORDS - Monte Carlo method, neutron transport, photon transport, three-dimensional, reaction kinetics, criticality, RCPL1 codes, RECAP codes

18. **SPONSOR** - DOE Division of Naval Reactors

IDENTIFICATION AND KWIC TITLE - RCPL1
RCPL1, prepares RCP01 cross section libraries

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - CDC7600,6600

DESCRIPTION - RCPL1 calculates detailed Doppler-broadened neutron resonance cross sections from unresolved and either single-level or multilevel resolved resonance parameters, for any number of nuclides, within an arbitrary energy structure consisting of up to 99 epithermal groups and one thermal group. The highest energy groups are divided into as many as 500 energy intervals for resonance cross section detail. These groups also allow inelastic scattering, expressed through group-wise transfer matrices, for the resonance nuclides and for any number of additional nuclides without detailed resonance descriptions. Subsequent epithermal groups may be subdivided into 1000 intervals, and the thermal group may contain 299 intervals. Elastic scattering for each nuclide is described by the first four components of the differential scattering cross section in the CM system, and the thermal group will treat two P3 scattering kernels through thermal subgroup transfer matrices.

RCPL1 also calculates Compton, photoelectric, and pair production cross sections for photon interactions with any number of nuclides, and the gamma emission spectra from these nuclides are tabulated. The arbitrary energy group structure consists of up to 100 groups, each divided into as many as 400 intervals.

METHOD OF SOLUTION - Point-wise unresolved neutron cross sections are tabulated by RCPL1 using an approximate sampling scheme and resonance parameters which obey the Porter-Thomas chi-square distribution functions. Single-level resolved resonance calculations are based on the Breit-Wigner representation with Doppler broadening, using the psi and chi functions evaluated in accordance with the methods outlined by Amster. Both the Reich-Moore and Adler-Adler formulations are available in RCPL1 for treatment of multilevel resonance nuclides; Doppler broadening is performed using the exact kernel treatment described by Solbrig.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Resonance nuclides may be described by up to 500 single-level s- and/or p-wave resonances, and by up to 20 sets of unresolved resonance parameters. Multilevel representations permit 100 Reich-Moore resonances in each of four spin states, or 320 Adler-Adler resonances. Multi-isotope nuclides may contain as many as 25 components.

TIMING - On the CDC7600, RCPL1 requires about 1 second to calculate cross sections over a 1000-point energy group for a nuclide with 40 single-level resolved resonances. Other types of resonance treatment require about 1 minute per nuclide. Resonance calculations account for approximately 90 percent of library generation time. RCPL1 runs about eight times slower on the CDC6600 than on the CDC7600. NESC execution of the RCPL1 sample problem required approximately 13 minutes of CP time on a CDC6600.

UNUSUAL FEATURES OF THE SOFTWARE - A merge feature in RCPL1 permits the user to modify, replace, or add to data in an existing library.

RELATED AND AUXILIARY SOFTWARE - All data used for construction of neutron and photon job libraries are extracted by RCPL1 from the on-line multigroup cross section library system XAP (Appendix A, WAPD-TM-1268).

RCPL1 prepares the cross section libraries for the Monte Carlo neutron and photon transport program RCP01. RCPL1 uses the Bettis Environmental Library (NESC 665).

STATUS - Abstract first distributed December 1980.
CDC7600 version submitted December 1978, replaced August 1981 by revised edition submitted April 1980, sample problems executed by NESC July 1980 on a CDC6600.

REFERENCES - A. V. Dralle, N. R. Candelore, and R. C. Gast, RCPL1 - A Program to Prepare Neutron and Photon Cross Section Libraries for RCP01, WAPD-TM-1268, August 1978.

N. R. Candelore, R. C. Gast, and L. A. Ondis II, RCP01 – A Monte Carlo Program for Solving Neutron and Photon Transport Problems in Three-Dimensional Geometry with Detailed Energy Descriptions, WAPD-TM-1267, August 1978.

W. R. Cadwell, Editor, Reference Manual – Bettis Programming Environment, WAPD-TM-1181, September 1974.

RCPL1, NESC No. R901.6600, RCPL1 Tape Description and Implementation Information, NESC Note 81-12, December 23, 1980.

11. **HARDWARE REQUIREMENTS** – CDC7600 or CDC6600 with variable requirement of large core memory (LCM) or extended core storage (ECS)

12. **PROGRAMMING LANGUAGE** – FORTRAN IV (99%) and COMPASS (1%)

13. **OPERATING SYSTEM** – SCOPE 1.1 (CDC7600), SCOPE 3.3, 3.4 (CDC6600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – All files used externally with RCP01 and other RCPL1 jobs are in the Bettis File Manager form (WAPD-TM-1181). Several routines which are part of the Bettis computing environment are not provided. RCPL1 is written almost entirely in FORTRAN and the authors have attempted to adhere to ANSI Standard FORTRAN with the exception of several octal constants, and a few occurrences of ENCODE/DECODE and calls to NEXT, the Bettis environmental routine for overlay loading with a varying number of parameters. Any organization implementing RCPL1 will have to adapt the package to the file management and graphics routines of their local computing environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
A. V. Dralle, N. R. Candelore, and R. C. Gast
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (10,178 lines)
Sample problems (RCPL1 11 lines, XAPLB 117 lines, TEXAP Epithermal library 1509 lines, TEXAP Thermal library 612 lines)
Auxiliary routines (TEXAP 352 lines, XAP retrieval subroutines 739 lines, XAPRM 1532 lines)
Sample problems output (38 selected pages)
Reference report, WAPD-TM-1268 and NESC Note

17. **CATEGORY** – B
KEYWORDS – multigroup theory, cross sections, resonance, Doppler broadening, libraries, multilevel analysis, Porter-Thomas distribution, Breit-Wigner formula, Reich-Moore formula

18. **SPONSOR** – DOE Division of Naval Reactors

IDENTIFICATION AND KWIC TITLE - DEMO4
DEMO4, CRBR reactor & plant transient analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600, IBM370,303x

DESCRIPTION - DEMO4 is a simulation model used to generate thermal-hydraulic transients for the Clinch River LMFBR demonstration plant. The three heat transport loops of the plant are simulated by a two-loop model. One loop, the L-loop, represents two of the actual plant loops, and the second loop, the S-loop, represents a single plant loop.

Thermal power is generated by point neutron kinetics and decay heat tables. The vessel internals are represented by a lower plenum, lower axial blanket, active core, upper axial blanket, radial blanket, bypass channel and an upper plenum with a variable sodium level and a cover gas. Plenum stratification on reduced flow can be modelled. The heated sodium leaves the vessel upper plenum to the primary heat transport system and returns to the vessel lower plenum. The overflow nozzle of the sodium purification system effects the vessel upper plenum level, as well as a user-input return flow from this system.

Each primary heat transport system is represented by piping, valves, the primary pump tank with a free surface and cover gas, and the shell side of the IHX. Each intermediate heat transport system is represented by piping, the tube side of the IHX, the shell side of the superheater and evaporator, and the intermediate pump.

Each water-steam system is represented by piping, recirculation pumps, the tube side of the superheater and evaporator, and a steam drum. The steam leaving all superheaters enters a common steam header, flows through piping to the turbine throttle valve and a steam dump valve. Limited modelling is provided for the feedwater system.

METHOD OF SOLUTION - The DEMO4 code contains sufficient detail in both model and time resolution to handle CRBR plant operational transients and failure events. The reactor model provides both average and hot channel calculations in core in sufficient detail to accommodate most sub-prompt critical excursions. DEMO4 also provides two optional special-case calculations - the primary sodium pipe rupture (RUPTURE) and the steam break and blowdown (SUSOD). DEMO4 uses two integration methods. The SUSOD model, a specialized steam generator program for blowdown and steam/feed pipe break analyses, runs semi-independently on its own variable time-steps, which are set by an internal time-step criterion. These time-steps are typically much shorter than the time-steps of the main program. The simplified steam generator model, STGEN, will call SUSOD at each time-step, and subsequently SUSOD will run using its own time-steps until it reaches the time of the next STGEN step, at which time it will return to the calling program. This cycle will be repeated at each time-step.

The remaining program uses Euler integration. Under normal transient conditions the reactor and protection system integrate on a 0.01 second time-step (H fast) and the remainder of the program integrates on a 0.05 second time-step (H). However, to accommodate slow thermal-hydraulic transients, there is a time-step control to allow for large time-steps (H=0.1 second).

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The reactor core model in DEMO4 provides only for single-phase liquid sodium flow. The steam generator model represents the mixing zone as if it is a small mixed volume at the drum bottom. The remainder of the drum is assumed homogeneous.

TIMING - The sample problem requires about 15 minutes on a CDC7600 and more than 30 minutes on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - DEMO4 is revision 4 of the DEMO program.

STATUS - Abstract first distributed October 1975.
CDC7600 version of DEMO submitted May 1975, revised July 1975, replaced by DEMO4 February 1976, sample problem executed by NESC August 1976 on a CDC7600.

IBM370 version of DEMO4 submitted July 1981, sample problem executed by NESC June 1983 on an IBM3033.

10. **REFERENCES** - Clinch River Breeder Reactor Plant Nuclear Island, LMFBR Demonstration Plant Simulation Model (DEMO), WARD-D-0005, Revision 0, November 15, 1973, Revision 1, February 5, 1974, Revision 2, July 30, 1974, Revision 3, February 15, 1975, and April 15, 1975, Revision 4, January 23, 1976.
DEMO4, NESC No. R676, Erratum to DEMO4 Report, WARD-D-0005, Rev. 4, National Energy Software Center Note 83-77, June 22, 1983.

11. **HARDWARE REQUIREMENTS** - 1 user-defined tape or disk is required for optional plotting in addition to the standard input/output devices.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.0 (CDC7600), OS/370 (IBM370), MVS (IBM303x).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - In routine USERMAN of the CDC version, the user sets a time limit, CPTLIM, which is then compared to the elapsed time to determine when the problem should be terminated.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600
W. H. Alliston
Advanced Energy Systems Division
Westinghouse Electric Corporation

370
E. E. Feldman
EBR-II Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (7600-8866 lines, 370-9332 lines)
Sample problems (640 lines)
Reference report, Revisions, and NESC Note

17. **CATEGORY** - K
KEYWORDS - simulation, nuclear power plants, transients, pipes, blowdown, steam generators, LMFBR reactors, DEMO codes

18. **SPONSOR** - ERDA Division of Reactor Research and Development

1. **IDENTIFICATION AND KWIC TITLE -** ACCEL/MOD2
   ACCEL(MOD2), design of printed-circuit boards

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   UNIVAC1108, CDC6600

3. **DESCRIPTION -** ACCEL is a set of computer programs designed to aid in the construction of electronic printed circuit boards. The ACCEL system performs the following tasks -
   (1) edits the engineers' data, resolves the schematic into a node component-list, looks up physical and electrical data for the parts used in the circuit, and notes any errors in the data;
   (2) locates the components on the board by an iterative process;
   (3) lays out the interconnection pattern between components; and
   (4) generates the output plots.

4. **METHOD OF SOLUTION -** Input information is furnished by the circuit designer in the form of a circuit schematic drawing and information on the parts used in the circuit. This information is then transcribed onto punched cards. The computer output is graphical in the form of several plots. These include (1) a schematic drawing, (2) a parts list, (3) an assembly drawing showing the location of parts on the printed circuit board, (4) a hole-drilling coordinate list, and (5) masks to be used in etching the circuit board layers.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -** This program is the ALO-00199 and ALO-00200 programs transferred from the ALO-COSMIC collection.

9. **STATUS -** Abstract first distributed October 1975.
   UNIVAC1108 version submitted October 1973.
   CDC6600 version submitted October 1973, re-submitted December 1974.

10. **REFERENCES -** C. J. Fisk and D. L. Caskey, User's Manual for ACCEL System (Mod 2), SC-M-69-601, November 1969.
    C. J. Fisk and D. L. Caskey, Program Documentation for ACCEL MOD 2, SC-M-69-602, December 1969.

11. **HARDWARE REQUIREMENTS -** 45,000 decimal words of storage, 10 separate files (3 tape, the rest drum or disk), and a machine word length of 36 bits or greater

12. **PROGRAMMING LANGUAGE -** FORTRAN and Assembly language

13. **OPERATING SYSTEM -** EXEC2 (UNIVAC1108) and SCOPE 3.1.5 (CDC6600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -** The primary output format of ACCEL is a series of plots, and the current plotter device is the Stromberg Datagraphix SC-4020. The standard package of routines for this device called SCORS, Stromberg-Carlson Output Recorder System, is contained in the program. SCORS packages for other machines are available through:
    UAIDE Librarian
    c/o Stromberg-Carlson
    P. O. Box 2449
    San Diego, California 92112

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    C. J. Fisk and D. L. Caskey

Advanced Techniques Division
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
Source (6600-16,596 lines, 1108-CUR format 1346 source and relocatable records)
Sample problems (6600-3715 lines, 1108-CUR format 3715 records)
Absolute form (1108-CUR format 278 binary records)
Reference reports

17. **CATEGORY** - T
KEYWORDS - electronic circuits, computer-aided design, computer graphics

18. **SPONSOR** -

1. **IDENTIFICATION AND KWIC TITLE** - VENTURE
   VENTURE, 1, 2, or 3-d multigroup diffusion

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360/91,75,195

3. **DESCRIPTION** - VENTURE solves the usual neutronics eigenvalue, adjoint, fixed source, and criticality search (direct and indirect) problems, treating up to three geometric dimensions, maps power density and does first-order perturbation analysis at the macroscopic cross section level.

4. **METHOD OF SOLUTION** - An inner, outer iteration procedure is used with several different data handling schemes programmed in parallel. Restrained line overrelaxation is used, and succeeding iterate flux sets may be accelerated by the Chebyshev process and asymptotic extrapolation done when distinct error modes establish. Normally the eigenvalue of a problem is estimated at each outer iteration from an over-all neutron balance; however, source ratios are used in some situations. The difference equation is mesh centered point. Advanced capability is incorporated, as to treat direction-dependent diffusion coefficients and zone-dependent fission source distribution functions. Macroscopic nuclear properties are calculated from microscopic cross sections and zone and sub-zone nuclide concentrations.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - Running time is directly related to problem size and inversely proportional to some measure of central processor and data transfer speeds. The basic rate of solution of eigenvalue problems is about 200 space energy points per second of central processor time on an IBM360/91; this rate falls off approximately as (10/n)**0.7 where n is the average number of points in one dimension, less when the amount of data I/O is low, and more when it is high, except for one-dimensional problems. Thermal reactor lattice and cell problems normally require more time by perhaps a factor of two. Problems involving significant upscatter (multi-thermal-group treatment) require additional computer time by a factor of two or three.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Standard interface file specifications adopted in the ERDA Reactor Physics code coordination effort are used for external files. Input data are supplied from a code-dependent external file generated by a separate processor. Other codes meeting interface specifications will couple directly with this one.

9. **STATUS** - Abstract first distributed June 1976.
   IBM360 version submitted July 1975, sample problem executed by NESC May 1976 on an IBM370/195.

10. **REFERENCES** - D. R. Vondy, T. B. Fowler, and G. W. Cunningham, VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-difference Diffusion-theory Approximation to Neutron Transport, ORNL-5062, October 1975.
   B. M. Carmichael, Standard Interface Files and Procedures for Reactor Physics Codes, Version III, LA-5486-MS, February 1974, Revised.
   D. R. Vondy, T. B. Fowler, and G. W. Cunningham, Input Data Descriptions for the Special Processors in the VENTURE Code Package and Implemented Data File Specifications, ORNL Notes, July 10, 1975, Revised February 10, 1976.
   D. R. Vondy, Programming Practices and Computer Code Development, ORNL-TM-5065, Appendix I, December 1975.
   VENTURE Transmittal Tape Description, ACC Programming Note 76-36, June 1976.
   VENTURE, ACC No. 686.360, ACC Programming Note 76-38, June 1976.

11. **HARDWARE REQUIREMENTS** - A 32K word memory is needed, and one much larger is preferable; auxiliary storage of the disk or drum type is essential, preferably several on different data channels. The programming for three-level hierarchy data storage is included to

permit efficient use of an extended slow memory for large three-dimensional problems when such a memory is available. Typically, the code uses 27 logical I/O units.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and Assembly language

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Programming is in the Standard ANSI FORTRAN 1966 language except for extensions as required for unindexed block data transfers and direct access. Arrays are limited to 3 dimensions, subroutines to 60 arguments, and no use is made of subscripted subscripts. Standard routines developed in the ERDA Reactor Physics code coordination effort are employed for processing input data and data file management. Local system environment routines for computing elapsed time, allocating memory, and setting up direct access file specifications dynamically will require replacement.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. R. Vondy and T. B. Fowler
Oak Ridge National Laboratory
G. W. Cunningham
Computer Sciences Division
Union Carbide Corporation, Nuclear Division

16. **MATERIAL AVAILABLE** -

Source (VENTURE 28,550 lines, cross section code 5888 lines, reaction rate code 2862 lines, DVENTR input processor 3146 lines, DCRSPR input processor 417 lines, DUTLIN input processor 110 lines, DCMACR input processor 196 lines, driver source 598 lines, common FORTRAN routines 1493 lines, common BAL routines 1246 lines)
Sample problem (139 lines)
Sample problem output (61 pages)
Control information (JCL 376 lines)
Load modules (2314 VNTRF 77 blocks, VNTRLD 134 blocks, BLDVN 2069 blocks)
Reference report, ORNL-5062, ORNL Note, ORNL-TM-5065 Appendix I, and ACC Programming Notes

17. **CATEGORY** - C
KEYWORDS - perturbation theory, multigroup theory, neutron diffusion equation, one-dimensional, two-dimensional, three-dimensional, CCCC, r-theta, r-theta-z, slabs, cylinders, triangular configuration, hexagonal configuration

18. **SPONSOR** - ERDA

1. **IDENTIFICATION AND KWIC TITLE** - OMCOST
   OMCOST, power plant non-fuel O & M cost study

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370,3033

3. **DESCRIPTION** - OMCOST estimates annual nonfuel operation and maintenance (OR) costs for large steam-electric power plants, specifically light-water-reactor (LWR) and coal-fired plants. Estimates for coal-fired plants include the option of scrubbing for flue-gas desulfurization (FGD). Four basic OR cost-estimating models for steam-electric power plants are available: a coal-fired with wet limestone FGD system, a coal-fired with dry FGD system, a coal-fired without an FGD system, and an LWR.

4. **METHOD OF SOLUTION** - The cost models are based on early 1982 costs. Escalation rates are included for wages, materials, supplies, government and commercial liability insurance, inspection fees, and disposal, sludge disposal, lime and limestone costs, property insurance, and replacement power insurance. Variables are assigned default values within the program to permit the calculation of an example LWR plant. A coal-fired plant can be run with no input except plant type and net electrical output. The options available are: (1) a general escalation rate to replace the separate escalation rates, (2) the number of units per plant (up to four), (3) wage rates, (4) operator fringe benefits, (5) plant supervision expenses, (6) heating value of coal, (7) sulfur content, (8) tons of lime or limestone per ton of sulfur, and (9) unit costs of purchased lime or limestone and ash and sludge disposal. The user may specify one, two, three, or four units per plant with OR costs for all units escalated to a single specified year.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - It is not possible to produce incremental OR cost estimates for individual units in multiple-unit plants, either in constant-year dollars or in current-year dollars, except by multiple computer runs and hand-calculated differences and escalations. This produces incremental OR cost estimates for each additional unit but does not accurately represent the average cost per unit, which can be better approximated by dividing total annual OR costs for the multiple-unit plant by the number of units. Total OR cost estimates, as units are added to multiple-unit plants, can be predicted by specifying, for example, a single-unit plant in the initial year of operation of the first unit or a two-unit plant in the initial year of operation of the second unit.

6. **TIMING** - Execution time for twenty cases is approximately 1 second on the IBM3033. NESC ran the sample problem in less than 1 second on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - An interactive data preparation program, OMIN, may be used to prepare NAMELIST data for OMCOST.

9. **STATUS** - Abstract first distributed June 1976.
   IBM360 version of OMCST submitted May 1976, replaced October 1979 by OMCOST submitted May 1979, replaced November 1982 by IBM3033 version, sample problem executed by NESC November 1982 on an IBM370/195.

10. **REFERENCES** - M. L. Myers, L. C. Fuller, and H. I. Bowers, Nonfuel Operation and Maintenance Costs for Large Steam-Electric Power Plants - 1982, NUREG/CR-2844 (ORNL/TM-8324), September 1982.
    OMCOST, NESC No. 688, OMCOST Tape Description and Implementation Information, National Energy Software Center Note 83-18, November 17, 1982.

11. **HARDWARE REQUIREMENTS** - 142K bytes of storage are needed.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360,370,3033.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - All OMCOST input data are handled through the NAMELIST feature.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
M. L. Myers, L. C. Fuller, and H. I. Bowers
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
Source (1231 lines)
Sample problem (15 lines)
Auxiliary program (OMIN 604 lines)
Reference report, NUREG/CR-2844, and NESC Note

17. **CATEGORY** - D
KEYWORDS - economics, maintenance, operating cost, PWR reactors, BWR reactors, nuclear power plants, fossil-fuel power plants, flue gas, desulfurization, OMIN codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Health, Siting, and Waste Management

1. **IDENTIFICATION AND KWIC TITLE** - FLANGE-ORNL
   FLANGE-ORNL, analysis of flanged joints

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360/91

3. **DESCRIPTION** - FLANGE-ORNL calculates appropriate loads, stresses, and displacements for the flanges, bolts, and gaskets that comprise a flanged piping joint for internal pressure or moment loading on the pipe, temperature difference between the flange hub and ring, and variations in bolt load that result from pressure, hub-ring temperature gradient and/or bolt-ring temperature differences. Flanges considered may be tapered-hub, straight or blind.

4. **METHOD OF SOLUTION** - The solution is based on discontinuity analysis and the theory of plates and shells.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - Program compilation required 19.4 seconds CPU time. Total execution time for six sample flanged joints required 1.15 seconds.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - FLANGE-ORNL has a unique set of user-controlled options which allow for calculating ASME boiler and pressure vessel code design criteria and/or more extensive stress analysis, and also for specifying various different flange design combinations for the joint. In addition, the program calculates values for various ASME code variables that would otherwise have to be extracted manually from curves and used as input.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed June 1976.
   IBM360 version submitted April 1976, replaced by revised Edition B February 1979, sample problem executed by NESC February 1979 on an IBM370/195.

10. **REFERENCES** - E. C. Rodabaugh, F. M. O'Hara, Jr., and S. E. Moore, FLANGE, A Computer Program for the Analysis of Flanged Joints with Ring-type Gaskets, ORNL-5035, January 1976.

11. **HARDWARE REQUIREMENTS** - 80K bytes memory for extraction and 270K bytes for compilation with standard system I/O units

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    E. C. Rodabaugh
    Columbus Laboratories
    Battelle Memorial Institute
    S. E. Moore
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (1586 lines)
    Sample problems (36 lines)
    Reference report

17. **CATEGORY** - I
    KEYWORDS - deformation, design, elasticity, pipe joints, flanges, pressure, shells, stresses

18. SPONSOR - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - F0355
   F0355, shaper cutter contour generator

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC6600,7600, IBM360,370

3. **DESCRIPTION** - Program F0355 produces a plot which shows the geometry of the cutter required to produce a given external circular spur gear or ratchet wheel. It is particularly applicable for non-involute tooth forms. In addition, the program can provide a comparator chart for inspecting cutters, indicate whether a given geometry can be shaped, and be used to determine the effects of changes in pitch diameter and related variables. The output of the program is a magnified drawing of the shaper cutter, the workpiece, and the paths of the cutter teeth. The program does not print a numerical description of the cutter profile.

4. **METHOD OF SOLUTION** - Essentially, the program rolls the workpiece around a round cutter blank. All portions of the cutter blank which fall within the workpiece contour as it is rotated around the cutter are removed. The resulting information is the contour of a cutter which can be used to produce the workpiece.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Only one plot is drawn per computer run. Current dimensioning allows for a maximum of 2000 points to describe the complete profile of the workpiece. These restrictions are not difficult to remove. Only the points for one tooth need to be specified as input.

6. **TIMING** - The sample problem required approximately 500 seconds of CP time on a CDC6600 and 180 seconds on an IBM370/195 CPU. Plotting took 15 minutes on a CalComp 780 plotter.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The output is entirely graphical.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed November 1976.
   CDC6600 version submitted February 1976, sample problem executed by NESC, using dummy plot routines, on a CDC7600.
   IBM360 version converted from the CDC6600 version August 1976, sample problem executed by NESC September 1976 on an IBM370/195 with plotting on a CalComp 780 plotter.

10. **REFERENCES** - L. K. Gillespie, F0355 - A Program for Generating Shaper Cutter Contours, Bendix Corporation, Kansas City Division, May 9, 1974.
    R. W. Stiles, Shaping Ratchet Teeth, BDX-613-973, Bendix Corporation, Kansas City Division, August 1973.
    G. E. Volkland, Computer Designed Shaper Cutters, SME Paper MR74-193, 1974.
    G. E. Volkland, Shaper Cutters Generated by Computers, Tooling & Production, pp. 36-39, February 1976.
    ACC Programming Note 77-2, October 11, 1976.

11. **HARDWARE REQUIREMENTS** - Approximately 55,000 (octal) words (CDC6600) or 126K bytes (IBM370) storage are required and auxiliary plotting equipment is used.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.4 (CDC6600), SCOPE 2.1 (CDC7600), OS/360,370 (IBM360,370).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The revised input deck format is described in NESC Programming Note 77-2. The program uses the CalComp plotting package and subroutine CIRCL from the CalComp functional software. The sample problem, which calls CIRCL with a zero radius, may be executed by use of the dummy CIRCL subroutine supplied with the package.

15. NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -

6600 L. K. Gillespie and D. Wantoch
Kansas City Division
Bendix Corporation

360 H. S. Edwards
National Energy Software Center
Argonne National Laboratory

16. MATERIAL AVAILABLE -
Source (6600-209 lines, 360-212 lines)
Sample problem input (182 lines)
Sample problem output (a single plot)
Reference reports and ACC Programming Note

17. CATEGORY - T
KEYWORDS - cutting, gears, manufacturing, inspection, computer-aided design

18. SPONSOR -

IDENTIFICATION AND KWIC TITLE - ORCENT2
ORCENT2, nuclear steam turbine cycle analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - IBM360,370,303x

DESCRIPTION - ORCENT2 performs heat and mass balance calculations at valves-wide-open design conditions, maximum guaranteed rating conditions, and an approximation of part-load conditions for steam turbine cycles supplied with throttle steam, characteristic of contemporary light-water reactors. The program handles both condensing and back-pressure turbine exhaust arrangements. Turbine performance calculations are based on the General Electric Company method for 1800-rpm large steam turbine-generators operating with light-water-cooled nuclear reactors. Output includes all information normally shown on a turbine-cycle heat balance diagram.

METHOD OF SOLUTION - The turbine performance calculations follow the procedures outlined in General Electric report GET-6020. ORCENT2 utilizes the 1967 American Society of Mechanical Engineers (ASME) formulations and procedures for calculating the properties of steam, adapted for ORNL use by D. W. Altom.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
12 feed-water heaters
5 moisture removal stages in the low-pressure turbine section
ORCENT2 is limited to 1800-rpm tandem-compound turbine-generators with single- or double-flow high pressure sections and one, two, or three double-flow low-pressure turbine sections. Steam supply for LWR cycles should be between 900 and 1100 psia and slightly wet to 100 degrees F of initial superheat. Generator rating should be greater than 100 MVA.

TIMING - Execution time for one valves-wide-open case followed by one maximum guaranteed case is approximately 5 seconds on the IBM360/91. NESC compiled and executed the sample problems in less than 30 CPU seconds on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - The original ORCENT program, prepared by H. I. Bowers of Oak Ridge National Laboratory, for analyzing turbine cycles with large steam turbine-generators operating with saturated or low-superheat throttle steam, utilized steam properties based on the equations of Keenan and Keyes and turbine performance calculations followed the General Electric procedures described in GER-2454A .

STATUS - Abstract first distributed November 1976.
IBM360 version of ORCENT submitted June 1976, replaced by revised Edition B March 1979, replaced November 1979 by IBM360 version of ORCENT2, sample problems executed by NESC July 1979 on an IBM3033.

REFERENCES - L. C. Fuller, User's Instructions for ORCENT II - A Digital Computer Program for the Analysis of Steam Turbine Cycles Supplied by Light-Water-Cooled Reactors, ORNL/TM-6525, February 1979.

F. G. Baily, J. A. Booth, K. C. Cotton, and E. H. Miller, Predicting the Performance of 1800-rpm Large Steam Turbine Generators Operating with Light-Water-Cooled Reactors, General Electric Company report, GET-6020, February 1973.

R. B. McClintock and G. J. Silvestri, Formulations and Iterative Procedures for the Calculation of Properties of Steam, American Society of Mechanical Engineers, New York, 1967.

ORCENT2, NESC No. 703, ORCENT2 Sample Problem Output, National Energy Software Center Note 80-08, December 5, 1979.

HARDWARE REQUIREMENTS - 210K bytes of storage were needed for execution of the sample problems on an IBM3033.

PROGRAMMING LANGUAGE - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360,370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
L. C. Fuller
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
Source (6529 lines)
Sample problem (49 lines)
Sample problem output (18 pages)
Reference report, ORNL/TM-6525, and NESC Note

17. **CATEGORY** - H
KEYWORDS - heat, mass balance, steam turbines, power plants, steam generators, water cooled reactors, PWR reactors, BWR reactors

18. **SPONSOR** - DOE Office of Nuclear Energy Programs

IDENTIFICATION AND KWIC TITLE - COMCAN3, COMCAN
COMCAN, system safety common cause analysis
COMCAN3, system safety common cause analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER176,175, IBM360

DESCRIPTION - The COMCAN fault tree analysis codes are designed to analyze complex systems such as nuclear plants for common causes of failure. A common cause event, or common mode failure, is a secondary cause that could contribute to the failure of more than one component and violates the assumption of independence. Analysis of such events is an integral part of system reliability and safety analysis. A significant common cause event is a secondary cause common to all basic events in one or more minimal cut sets. Minimal cut sets containing events from components sharing a common location or a common link are called common cause candidates. Components share a common location if no barrier insulates any one of them from the secondary cause. A common link is a dependency among components which cannot be removed by a physical barrier (e.g., a common energy source or common maintenance instructions).

METHOD OF SOLUTION - The COMCAN programs search the fault tree minimal cut sets for shared susceptibility to various secondary events (common causes) and common links between components. In the case of common causes, a location check may also be performed to determine whether barriers to the common cause exist between components. The programs can locate common manufacturers of components having events in the same minimal cut set. A relative ranking scheme for secondary event susceptibility is included in the programs.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - COMCAN is limited to the analysis of fault tree minimal cut sets produced by other programs while COMCAN3 is an independent program, utilizing the fault tree code FATRAM, which is incorporated as a program module, for a thorough analysis of the fault tree for sources of common cause failures.

TIMING - Less than 2 seconds is required to execute either the COMCAN sample problem on an IBM370/195 or the COMCAN3 problem on the CDC CYBER176.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - The format used for COMCAN is compatible with the input format of programs for qualitative and quantitative reliability and safety analyses, such as MOCUS (NESC 653) and PREP,KITT (NESC 528). The cut set input deck can be punched by MOCUS. COMCAN3 is based on the earlier EG&G Idaho fault tree analysis codes - COMCAN, RAS (NESC 889), COMCAN2, and COMCAN2A.

STATUS - Abstract first distributed January 1977.
IBM360 version of COMCAN submitted October 1976, sample problem executed by NESC December 1976 on an IBM370/195.
CDC7600 version of COMCAN2 submitted March 1979, replaced April 1982 by CDC CYBER176 version of COMCAN2A, replaced November 1983 by the "As Is" COMCAN3 software (NESC 9989), replaced by revised edition November 1984, sample problem executed by NESC January 1983 on a CDC CYBER175.

REFERENCES - Dale M. Rasmuson, James C. Shepherd, Neldon H. Marshall, and L. Robert Fitch, Use of COMCAN III in System Design and Reliability Analysis, EGG-2187, March 1982.
COMCAN3, NESC No. 704.C176, COMCAN3 Tape Description, Implementation Information, and EGG-2187 Reference Report Erratum, National Energy Software Center Note 85-26, November 2, 1984.
Gary R. Burdick, Neldon H. Marshall, James R. Wilson, COMCAN - A Computer Program for Common Cause Analysis, ANCR-1314, May 1976.
J. B. Fussell, G. R. Burdick, D. M. Rasmuson, J. R. Wilson, J. C. Zipperer, A Collection of Methods for Reliability and Safety Engineering, ANCR-1273, April 1976.
W. E. Vesely and R. E. Narum, PREP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree, IN-1349, August 1970.

J. B. Russell, E. B. Henry, N. H. Marshall, MOCUS: A Computer Program to Obtain Minimal Sets from Fault Trees, ANCR-1156, August 1974.

D. M. Rasmuson and N. H. Marshall, FATRAM - A Core Efficient Cut-Set Algorithm, IEEE Transactions on Reliability, Vol. R-27, No. 4, pp. 250-253, October 1978.

11. **HARDWARE REQUIREMENTS** - 136K (octal) words of memory for COMCAN3 and 140K bytes of memory for COMCAN

12. **PROGRAMMING LANGUAGE** - FORTRAN 77 (CDC CYBER176), FORTRAN IV (30%) and BAL (70%) (IBM360).

13. **OPERATING SYSTEM** - NOS/BE 1.4 (CDC CYBER176), NOS 1.4 (CDC CYBER175), and OS/360 (IBM360).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The four Assembly language routines included in the IBM360 COMCAN package are the FORTRAN input-output and abnormal termination dump routines: FABEND, FIOCS, IBCOM# and INFILQ. These are a part of the NRTS Environmental Routines package (NESC 613).

    COMCAN3 uses CMM (Common Memory Manager) to allocate main memory, but can be modified to eliminate use of CMM.

    COMCAN3 uses GETPARM, the CDC FTN5 library routine, to pass parameters to the program during execution.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    COMCAN — G. R. Burdick, N. H. Marshall and J. R. Wilson

    COMCAN3 — D. M. Rasmuson, J. C. Shepherd, N. H. Marshall, and L. R. Fitch
    EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
    Source (COMCAN3 FORTRAN Compile 11,415 lines, UPDATE 11,312 lines, COMCAN FORTRAN 1882 lines, BAL 4080 lines)
    Sample problems (COMCAN3 81 lines, COMCAN 211 lines)
    Control information (COMCAN3 12 lines)
    Reference report, EGG-2187 or ANCR-1314, and NESC Note, appropriate to version

17. **CATEGORY** - G
    KEYWORDS - reliability, fault tree analysis, system failure analysis, MOCUS codes, PREP,KITT codes

18. **SPONSOR** - DOE Division of Nuclear Power Development
    DOE Interactive Reliability Analysis Project

1. **IDENTIFICATION AND KWIC TITLE** - NIXLIN
   NIXLIN, least squares fit to nonlinear forms

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360

3. **DESCRIPTION** - NIXLIN performs a function minimization by a direct search iterative process that has the advantage of requiring no derivative evaluations. This particular version is well-suited to fitting nonlinear models to experimental data and to the solution of systems of nonlinear simultaneous equations.

4. **METHOD OF SOLUTION** - The program uses the Simplex method for function minimization.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The dimensions may be increased to accommodate larger problems.

6. **TIMING** - Less than 30 seconds is required for a typical problem.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed February 1977.
   IBM360 version submitted November 1976, sample problems executed by NESC January 1977 on an IBM370/195.

10. **REFERENCES** - J. A. Nedler and R. Mead, A Simplex Method for Function Minimization, Computer Journal, Vol. 7, pp. 308-313, 1965.

11. **HARDWARE REQUIREMENTS** - The program requires 240K bytes to compile, 76K bytes to execute.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. M. Arnett
    Savannah River Laboratory

16. **MATERIAL AVAILABLE** -
    Source (400 lines)
    Sample problems (39 lines)
    Sample problems output (2 pages)
    Reference reprint

17. **CATEGORY** - P
    KEYWORDS - data processing, least square fit, nonlinear problems

18. **SPONSOR** - ERDA Office of Waste Management, Production, and Reprocessing

1. **IDENTIFICATION AND KWIC TITLE** - HAMOC
   HAMOC, fluid hammer analysis of piping system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC6600,7600,CYBER74-18

3. **DESCRIPTION** - HAMOC determines the pressure transients in piping systems attached to a reactor vessel which has been perturbed, by a hypothetical core disruptive accident (HCDA) for example. The continuity and momentum equations are solved. The energy equation is not programmed, but simplified column separation logic is included to treat vapor pressures below saturation. This simplified approach has been checked against experimental data. HAMOC was written specifically for problems in which forcing pressures are known as a function of time at certain end boundary conditions, rather than as a general purpose code for the solution of pump coastdown or valve closing problems.

4. **METHOD OF SOLUTION** - The differential equations of continuity and momentum are solved by the method of characteristics. When column separation occurs, special internal boundary conditions are temporarily established which fix the pressure at the saturated vapor pressure during the existence of the cavity. Special equations give the pressure rise when the cavity collapses.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The program currently provides for maxima of:

   56 legs
   50 nodes per leg
   15 three-way junctions
   50 plots
   1000 points per plot
   1 line per plot

The fluid properties are those for sodium, and the pipe properties are those for Type 304 stainless steel. The above restrictions should not be difficult to alter; the following restrictions are more stringent. There may be 1 or 2 pipe ends with prescribed pressure-time history. All pumps have the same set of characteristics. Fluid temperatures must be constant with time, must be the same for all points within a leg, and must be the same for all connecting legs at a pump, at a tee, or at a Y-junction. The minimum leg length must not be smaller than

(time-step)*(pressure-pulse-speed + fluid-velocity).

6. **TIMING** - The 45-leg sample problem requires about 110 seconds (CYBER74-18) or 21 seconds (CDC7600) execution time for a run of 0.1 seconds real time. Typically, execution time on the CYBER74-18 is about 0.00057 second per mesh-point per time plane. Running times can be reduced significantly, with little loss of accuracy, by using a constant friction factor.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - WHAM6 (NESC 278).

9. **STATUS** - Abstract first distributed March 1977.
   CDC6600 version submitted July 1976, sample problem executed with dummy plot routines by NESC February 1977 on a CDC7600.

10. **REFERENCES** - H. G. Johnson, HAMOC - A Computer Program for Fluid Hammer Analysis, HEDL-TME 75-119, December 1975.

11. **HARDWARE REQUIREMENTS** - A 131K machine is required with dummy plot routines; HAMOC requires 101,000 (octal) words of storage. A tape is used to store data for offline plotting.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.4.2 (CYBER74-18), SCOPE 3.4.4 (CDC6600), SCOPE 2.1.3 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – It is assumed that the operating system will zero the memory at load time. Plotting calls are to standard CalComp subroutines. The source file contains COMDECKs. It should be processed by the UPDATE utility before compilation.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
H. G. Johnson
Hanford Engineering Development Laboratory

16. **MATERIAL AVAILABLE** –
Source (HAMOC 2115 lines, dummy plot routines 50 lines)
Sample problem input (70 lines)
Sample problem output (1 microfiche)
Reference report

17. **CATEGORY** – G
KEYWORDS – liquid metals, pressure, reactor safety, transients, WHAM6 codes

18. **SPONSOR** – ERDA Division of Reactor Development and Demonstration

1. **IDENTIFICATION AND KWIC TITLE** - SPRAY3
   SPRAY3, sodium spray release safety analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER74, CDC6600,7600

3. **DESCRIPTION** - SPRAY3 performs the calculations of thermodynamics, heat and mass transfer, and combustion of sodium spray droplets released in an LMFBR cell as a result of postulated piping failure. Droplet motion and large sodium surface area combine to produce rapid heat release and pressure rise within the enclosed volume.

4. **METHOD OF SOLUTION** - The calculation method utilizes gas convection, heat transfer, and droplet combustion theory to compute the pressure and temperature effects within the enclosure. Nodal temperature solutions are obtained from instantaneous heat and mass balances by the explicit forward-difference method.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Present verification of the code against experimental evidence limits the droplet size range to 0.01-0.30 inch with oxygen concentrations ranging from 0 to 21 percent. The number of space increments should be in the range of 1 to 50 for stability and accuracy.

6. **TIMING** - Approximately 200 seconds running time is required for a typical 45 second problem with 50 space increments and 20 seconds running time with 10 increments.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SPRAY3 treats short-term heat and mass transfer and combustion of sodium droplets, differing in this respect from the SOFIRE code which treats sodium pools. The simplified one-dimensional gas convection model in the cell atmosphere differs from the more exact convection model utilized in the SOMIX code. SPRAY3 includes forced or free-convection heat transfer to the cell walls, differing from the NARX code which is adiabatic on the gas space.

8. **RELATED AND AUXILIARY SOFTWARE** - The SPRAY3 code is an advanced version of the original SPRAY code developed at HEDL, but never documented for release to the National Energy Software Center, and the more recent SPRAY2 code.

9. **STATUS** - Abstract first distributed May 1977.
   CDC7600 version of SPRAY2 submitted July 1976, replaced December 1978 by CDC CYBER74 version of SPRAY3 submitted August 1977, sample problem executed by NESC October 1978 on a CDC7600.

10. **REFERENCES** - P. R. Shire, SPRAY Code User's Report, HEDL-TME 76-94, March 1977.
    P. R. Shire, A Combustion Model for Hypothetical Sodium Spray Fire within Containment for an LMFBR, M.S. Thesis, University of Washington, 1972.
    P. R. Shire, et al., A Sodium Droplet Combustion Model for Reactor Accident Analysis, American Nuclear Society Transactions, Vol. 15, No. 2, p. 812, November 1972.
    P. R. Shire, Reactor Sodium Coolant Hypothetical Spray Release for Containment Accident Analysis: Comparison of Theory with Experiment, American Nuclear Society Topical Conference on Fast Reactor Safety, CONF-740401-P1, 1974.

11. **HARDWARE REQUIREMENTS** - An input device to read cards or card-image input data and output devices for paper and microfiche copy of digital information and micrographic for plot output are utilized. These requirements may be easily modified.

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - SCOPE 3.4.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Some initially-undefined variables require that the memory be set to zero before execution. The proprietary ISSCO DISSPLA package is utilized for SPRAY3 plotting. Dummy routines (BGNPL, CURVE, DONEPL, ENDPL, GFR80, GRAPH, HEIGHT, LEGEND, LINES, MESSAG, PAGE, REALNO, TITLE) included in the package will have to be replaced by the appropriate routines for the local environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
P. R. Shire
Hanford Engineering Development Laboratory

16. **MATERIAL AVAILABLE -**
Source (1243 lines)
Sample problem (15 lines)
Sample problem output (51 selected pages, 3 plots)
Reference report, HEDL-TME 76-94

17. **CATEGORY -** G
KEYWORDS - sodium, droplets, sprays, thermodynamics, mass balance, reactor convection, LMFBR reactors, SOFIRE codes, SOMIX codes, NARX codes

18. **SPONSOR -** DOE Division of Reactor Research and Technology

3. **IDENTIFICATION AND KWIC TITLE** - CRAC2
CRAC2, reactor accident consequence model

4. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
IBM360,370, CDC7600

1. **DESCRIPTION** - CRAC2 is a revision of the CRAC (Calculation of Reactor Accident Consequences) program developed in support of the Reactor Safety Study, WASH-1400, to assess the risk from potential accidents at nuclear power plants. The need for more realistic consequence estimation techniques for purposes such as site evaluation, emergency planning and response, and general risk assessment guided the development of CRAC2. Errors were corrected and changes including modification of the atmospheric dispersion model and introduction of a new meteorological sampling technique, a new evacuation model, and additional output capabilites were made. CRAC2 retains the organization, structure, and analytical capabilities of CRAC.

4. **METHOD OF SOLUTION** - The assessment of accident risk entails the coupling of a series of mathematical and statistical models. CRAC2 requires as input the site-specific parameters, the characteristics of the postulated accidents, the emergency protective measures to be taken, the number and types of consequences to be studied, and the options controlling the output to be produced. A reference or base case with a standard set of data is input at the beginning of each execution. The user need only specify the modifications desired for each case to be executed. Any or all modifications may be made permanent for subsequent cases during a single execution. The program (1) models the meteorological dispersion of the cloud of radioactive material; (2) determines the health effects of the material upon the surrounding population; and (3) estimates the costs to the public from the accident. Detailed meteorological, population, economic, and health data are included. Emergency planning procedures, such as evacuation, are modeled, and detailed parametric and sensitivity studies can be performed in a relatively easy manner. Output available includes interdiction, decontamination, chronic dose commitment, and evacuation data for each spatial interval; dispersion data by spatial interval and the sum of the released inventory; doses and health effects by spatial interval; the contribution to the final results from each meteorological trial; the activity of each isotope at the time of release and the air concentration for each isotope within each spatial interval; economic effects data by spatial interval; and where a site data file has been used, population and topographic data from the site data file.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - Compilation and execution of the five sample problem test cases took approximately 4 minutes on an IBM370/195 and less than 3 minutes on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed May 1977.
IBM360 version of CRAC submitted February 1977, replaced May 1983 by CRAC2 submitted May 1982, revised February 1983, replaced by revised Edition B September 1984, sample problems executed by NESC June 1984 on an IBM370/195.
CDC7600 version submitted May 1982, revised February 1983, replaced by revised Edition B September 1984, sample problem executed by NESC August 1984 on a CDC7600.

10. **REFERENCES** - Lynn T. Ritchie, Jay D. Johnson, and Roger M. Blond, Calculations of Reactor Accident Consequences Version 2 CRAC: Computer Code User's Guide, NUREG/CR-2326 (SAND81-1994), February 1983.
L. T. Ritchie, D. J. Alpert, R. P. Burke, J. D. Johnson, R. M. Ostmeyer, D. C. Aldrich, and R. M. Blond, CRAC2 Model Description, NUREG/CR-2552 (SAND82-0342), March 1984.

U. S. Nuclear Regulatory Commission, Reactor Safety Study, WASH-1400, Appendix VI: Calculation of Reactor Accident Consequences, NUREG 75/014, October 1975.

CRAC2, NESC No. 722.370B, CRAC2 Edition B IBM Version Tape Description and Implementation Information, National Energy Software Center Note 84-58, September 24, 1984.

CRAC2, NESC No. 722.7600B CRAC2 Edition B CDC Version Tape Description and Implementation Information, National Energy Software Center Note 84-59, September 24, 1984.

11. **HARDWARE REQUIREMENTS** - The memory requirement of CRAC2 on CDC systems is 160,000 (octal) words of SCM and 151,000 (octal) words of LCM. During testing, NESC used 326,000 (octal) words of memory on the CDC7600 and 840K bytes of memory on the IBM370/195. CRAC2 also requires direct access storage for 3 cataloged files, a minimum of 25 temporary, or scratch, files, and a line printer capable of printing 138-character records.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/MVT (IBM370), SCOPE 2.1.5 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Memory should be preset to zero for execution on CDC systems. CRAC2 uses the local RANF system routine to generate random numbers. In different computing environments where different sequences of random numbers are produced the sample output may vary. The 12 pages of sample output, titled "Accident Sequence BMR1, Evacuation Scheme Summary" will vary depending on the random numbers used.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

L. T. Ritchie and J. D. Johnson
Sandia National Laboratories, Albuquerque
R. M. Blond
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission

16. **MATERIAL AVAILABLE** -

Source (370-8286 lines, 7600-16,150 lines)
Sample problem input (618 lines)
Sample problem output (370-6840 133-character records, 7600-7644 140-character records)
Libraries (Site data 135 lines, Health data 1423 lines, Meteorological data 8762 lines)
Control information (370-JCL 72 lines)
Reference reports, NUREG/CR-2326 and NUREG/CR-2552, and NESC Note appropriate to version

17. **CATEGORY** - G
KEYWORDS - accidents, nuclear power plants, emergency plans, dispersions, radioisotopes, containment, reactor safety, CRAC codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research, Division of Risk Analysis

1. **IDENTIFICATION AND KWIC TITLE** - K-FIX
   K-FIX, transient 2-dimensional 2-fluid flow

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - The transient dynamics of two-dimensional, two-phase flow with interfacial exchange are calculated at all flow speeds. Each phase is described in terms of its own density, velocity, and temperature. Separate sets of field equations govern the gas and liquid phase dynamics. The six field equations for the two phases couple through mass, momentum, and energy exchange.

4. **METHOD OF SOLUTION** - The equations are solved using an Eulerian finite difference technique that implicitly couples the rates of phase transitions, momentum, and energy exchange to determination of the pressure, density, and velocity fields. The implicit solution is accomplished iteratively using a point relaxation technique without linearizing the equations, thus eliminating the need for numerous derivative terms. Solutions can be obtained in one and two space dimensions in plane geometry and in cylindrical geometry with axial symmetry and zero azimuthal velocity. Solutions in spherical geometry can also be obtained in one space dimension. The geometric region of interest is divided into many finite-sized, space-fixed zones called cells which form the computing mesh. In plane geometry the cells are rectangular cylinders, in cylindrical geometry they are toroids with rectangular cross section, and in spherical geometry they are spherical shells.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - The sample test problem took less than 11 seconds to compile and less than 31 seconds to calculate all variables for 140 time cycles.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - K-FIX is written in a highly modular form to be easily adaptable to a variety of problems.

8. **RELATED AND AUXILIARY SOFTWARE** - K-FIX uses the implicit multifield technique developed for the KACHINA program. K-FIX differs from KACHINA in that it implicitly couples phase transitions and interfacial heat transfer to the fluid dynamics in the pressure iteration.

9. **STATUS** - Abstract first distributed November 1977.
   CDC7600 version submitted May 1977, revised May 1978, sample problem executed by NESC July 1978 on a CDC7600.

10. **REFERENCES** - W. C. Rivard, M. D. Torrey, K-FIX: A Computer Program for Transient, Two-dimensional, Two-Fluid Flow, LA-NUREG-6623, April 1977.
    W. C. Rivard and M. D. Torrey, PERM: Corrections to the K-FIX Code, LA-NUREG-6623 Supplement, March 1978.
    FORTRAN Function and System Subroutines in K-FIX, LASL Note, May 1977.

11. **HARDWARE REQUIREMENTS** - The sample problem, excluding plotting routines, took less than 22,000 words of storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - K-FIX makes use of the CDC7600 UPDATE program for variable dimensioning and for code modification for different model applications. These system-dependent features, together with the program's use of environment-dependent plotting routines and job card timing information, will require use of suitable replacement routines and extra programming effort for implementation of K-FIX at other installations or on different machines.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
W. C. Rivard and M. D. Torrey
Los Alamos Scientific Laboratory

16. **MATERIAL AVAILABLE** –
Source (K-FIX 2641 lines, UPDATE for test 195 lines)
Sample problem (18 lines)
Auxiliary program to test Cycle No. 0 of output (240 lines)
Auxiliary program to test Cycle No. 140 of output (240 lines)
Sample problem output (27 selected pages)
Reference reports and Note

17. **CATEGORY** – H
KEYWORDS – interfaces, heat transfer, two-phase flow, finite difference method, simulation, two-dimensional, pressure, velocity, phase transformations

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - DYNDSK
DYNDSK, optimal disk data set reordering

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,370

DESCRIPTION - DYNDSK optimizes the placement of data sets on an IBM 3330/2314 disk pack to reduce seek time (arm travel) and forecast improvement expected after reorganization. Data sets are theoretically reordered based on size and number of references. With known percentages of seeks between data sets the program computes the average number of cylinders traveled per seek. Input data consists of addresses captured by a DYNAPROBE 8000 hardware monitor and specification of the present location of the data sets.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Only one disk pack can be analyzed at a time.

TIMING - The sample test run on the Argonne IBM370/195 took less than ten seconds of CPU time to compile and execute.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - COMRESS 8700 extraction software prepares the DYNAPROBE 8000 data tape.

STATUS - Abstract first distributed November 1977.
IBM360 version submitted March 1976, sample problem executed by NESC October 1977.

REFERENCES - F. C. Fortune, Monitoring Seeks on an IBM 3330, Report DP-MS-74-7, 1974.
F. C. Fortune, Instructions for Running Disk Analysis Program, SRL Technical Division Memorandum, November 7, 1975.
Record Format for DYNAPROBE 8048 Tape Written in 'STORE' Mode, SRL Note, March 1976.

HARDWARE REQUIREMENTS - 58K core storage for execution

PROGRAMMING LANGUAGE - FORTRAN IV and BAL

OPERATING SYSTEM - OS/VS2 Release 3.7A (IBM370), OS/MVT (IBM360).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - This package assumes a data tape produced by the COMRESS DYNAPROBE 8000 hardware monitor. This tape contains a series of cylinder addresses which are used as input.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
F. C. Fortune
Savannah River Laboratory

MATERIAL AVAILABLE -
Source (FORTRAN 570 lines, BAL 179 lines)
DYNAPROBE 8000 hardware monitor data tape to be used as DYNDSK input (56 records of maximum length 413 bytes)
Sample problem (20 lines)
Control information (JCL 19 lines)
Sample problem output (10 pages)
Reference report, Memorandum, and Note

CATEGORY - P
KEYWORDS - computers, optimization, magnetic disks, performance, data

18. **SPONSOR** - DOE Division of Energy Technology

1. **IDENTIFICATION AND KWIC TITLE** - HETRAP
   HETRAP, fuel rod response LOCA experiments

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360/75,360/91

3. **DESCRIPTION** - HETRAP is a heat transfer analysis program developed for use in the evaluation of LOCA experiments. Its major application is calculation of heat flux and heat transfer coefficients at the surface of an electrically-heated rod during a fast transient, using measured temperatures in the rod. In addition, the code can be used to calculate the steady-state and transient temperature fields in fuel rods and electrically-heated rods for given heat transfer coefficients.

4. **METHOD OF SOLUTION** - The code uses a finite element method with an explicit integration scheme to calculate the transient temperature field within the rod. During the transient the following time-dependent variables are measured: rod power or current, sheath temperature, temperature inside the heater element, coolant pressure and temperature. These measured values are then used to calculate the time-dependent heat transfer coefficient, heat flux at the rod surface, surface temperature, and stored energy in the rod. The calculation is divided into two parts--the steady-state temperature profile and the transient calculation.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   10 cross sections
   50 nodes in each cross section
   50 materials in each cross section
   1000 variable pairs in transient calculations

6. **TIMING** - No study has been made as to typical running time. Four sample problems executed by the NESC took less than one minute on an IBM370/195, including compilation.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - THETA1-B (NESC 512).

9. **STATUS** - Abstract first distributed November 1977.
   IBM360 version submitted October 1976, sample problems executed by NESC October 1977 on an IBM370/195.

10. **REFERENCES** - S. Malang, HETRAP: A Heat Transfer Analysis Program, ORNL-TM-4555, September 1974.

11. **HARDWARE REQUIREMENTS** - Approximately 260K bytes storage, a tape unit, card reader, and printer are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - HETRAP assumes the availability of a CalComp plotting package. Since plotting packages are generally installation-dependent, the FORTRAN calls may require modification to the local computer environment.
    It should be noted that the resulting graphs (plots) will not fit an 11 x 11 frame without a reduction factor. One plot is 11 x 15.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
S. Malang
Engineering Technology Division
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
Source (1284 lines)
Sample problem (166 lines)
Reference report

17. **CATEGORY** - H
KEYWORDS - heat transfer, finite element method, fuel elements, loss of coolant, accidents, THETA1-B codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - RELAP3B/MOD110
RELAP3B/MOD110, reactor system transient code

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600

DESCRIPTION - RELAP3B describes the behavior of water-cooled nuclear reactors during postulated accidents or power transients, such as large reactivity excursions, coolant losses or pump failures. The program calculates flows, mass and energy inventories, pressures, temperatures, and steam qualities along with variables associated with reactor power, reactor heat transfer, or control systems. Its versatility allows one to describe simple hydraulic systems as well as complex reactor systems.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - RELAP3B allows a maximum of 75 volumes connected by a maximum of 100 junctions, with no restrictions as to the order of these connections. However, these maxima may be increased to far greater limits on a large computer.

TIMING - NESC executed the sample problem in less than 1 second of CP time on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - RELAP3B/MOD110 is a modification of the RELAP3/MOD62 code developed by the Aerojet Nuclear Company for use on an IBM360. The additions to and/or modifications of RELAP3/MOD62 include -

(1) Doppler feedback dependence on moderator density;
(2) extended restart capability;
(3) capability to trip individual pumps on independent signals;
(4) automatic time-step selection;
(5) improved definition of the average fuel temperature;
(6) option to allow the fuel-rod gap size to vary during a transient;
(7) capability to modify the steam table mesh;
(8) inclusion of realistic steam generator models;
(9) calculation of reactivity weight factors;
(10) option to specify new fill curves at restart; and
(11) option to specify new feedback coefficients at restart.

STATUS - Abstract first distributed November 1977.
CDC7600 version of RELAP3B/MOD101 submitted April 1976, replaced by CDC7600 version of RELAP3B/MOD110 October 1976, replaced April 1981 by revised Edition B received July 1980, sample problem executed by NESC January 1981 on a CDC7600.

REFERENCES - User's Manual for RELAP3B-MOD110, A Reactor System Transient Code, BNL-NUREG-22011, December 1977, revised July 1980.

HARDWARE REQUIREMENTS - 153,000 (octal) words of central memory and 154,000 (octal) words of large core memory are required.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - SCOPE 2.1.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - For best results RELAP3B/MOD110 should be compiled with OPT=2 and ROUND=+-*/.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
A. Aronson
Thermal Reactor Safety Division
Brookhaven National Laboratory

16. **MATERIAL AVAILABLE -**
Source (22,814 lines)
Sample problem (119 lines)
Sample problem output (35 pages)
Reference report

17. **CATEGORY** - G
KEYWORDS - accidents, transients, hydrodynamics, power plants, reactor safety, water cooled reactors, RELAP codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
Division of Systems Safety

1. **IDENTIFICATION AND KWIC TITLE** - MARCH2
   MARCH2, LWR meltdown accident response model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER180-855,180-815,175,176

3. **DESCRIPTION** - MARCH2 describes the response of water cooled reactors to severe accidents, including consideration of the primary coolant system as well as the containment.

4. **METHOD OF SOLUTION** - Models are included to perform calculations from the start of an accident through the stages of blowdown, boiloff, core heat up, core meltdown, pressure vessel bottom head melting and failure, debris-water interaction in the reactor cavity, and the interaction of the molten debris with the concrete containment base pad. The mass and energy additions into the containment building during this accident scenario are continuously evaluated, and the pressure-temperature response of the containment is calculated either with or without the engineered safety features. The analysis accounts for metal-water reactions, combustion of hydrogen, and heat losses to structures in the containment.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Application is limited to typical LWR systems. The containment can be divided into up to 8 interconnected compartment volumes. Engineered safety features which can be modeled include ECCS, containment sprays, containment building coolers, containment fans, PWR ice condensers, BWR pressure suppression pools, and ECC and containment spray recirculation heat exchangers. The reactor core can be modeled by up to 10 radial and up to 50 axial nodes. Containment structures can be modeled by up to 15 slabs consisting of up to 2 materials each.

6. **TIMING** - Computer running time is highly problem dependent. Representative problems may require on the order of 100 seconds of central processor time on the CYBER176; corresponding times on the CYBER180-855 and CYBER180-815 would be 200 and 2000 seconds, respectively. NESC executed the longest running sample problem in approximately 470 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - MARCH2 analyzes severe accident phenomena from initiation through various stages of accident progression.

8. **RELATED AND AUXILIARY SOFTWARE** - MARCH2 is an improvement and replacement of the earlier MARCH1.1 code which incorporated modifications of the Battelle Columbus Laboratories BOIL1 program and INTER, originally written as a separate program at Sandia Laboratories, as modules for primary system response and debris-concrete interaction calculations, respectively. MARCH provides the boundary conditions for the operation of CORRAL2 (NESC 745).

9. **STATUS** - Abstract first distributed November 1977.
   CDC CYBER73 version of BOIL1 submitted November 1976, replaced January 1981 by CDC CYBER74 version of MARCH submitted October 1980, replaced by MARCH1.1 submitted May 1981, replaced by MARCH2 November 1984, sample problem executed by NESC October 1984 on a CDC CYBER175.

10. **REFERENCES** - R. O. Wooton, P. Cybulskis, and S. F. Quayle, MARCH 2 (Meltdown Accident Response CHaracteristics) Code Description and User's Manual, NUREG/CR-3988 (BMI-2115), September 1984 with Errata February 1985.
    MARCH2, NESC No. 734.C180, MARCH2 Tape Description, National Energy Software Center Note 85-30, November 30, 1984.

11. **HARDWARE REQUIREMENTS** - MARCH2 requires approximately 272K (octal) words of memory for execution on a CDC CYBER175.

12. **PROGRAMMING LANGUAGE** - FORTRAN 77, CDC FTN 5.1+587 compiler

13. **OPERATING SYSTEM** - NOS/BE 1.5-577 and NOS 2.2-605/587 (CDC CYBER180) and NOS 2.2-596/587 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - All input data are provided using NAMELIST.

In addition to printed output, MARCH2 produces plot files for graphic programs and data files for input to CORRAL and other fission product transport codes.

The extensions to ANSI FORTRAN 77 are located in the input routine INP and system environment routines CPUSEC, PERROR, and STEPS.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

R. O. Wooton
Columbus Laboratories
Battelle Memorial Institute

16. **MATERIAL AVAILABLE** -

Source (FORTRAN 23,877 lines, UPDATE 19,855 lines)
Sample problems (1838 lines)
Sample problems output (41,488 137-character records)
Error message texts (85 lines)
Control information (15 lines)
Reference report with Errata and NESC Note

17. **CATEGORY** - G
KEYWORDS - reactor cores, meltdown, accidents, blowdown, reactor safety, containment systems, water cooled reactors, BOIL codes, INTER codes, CORRAL codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Risk Analysis

1. **IDENTIFICATION AND KWIC TITLE** - BIOSSIM
   BIOSSIM, biochemical kinetic simulation system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - BIOSSIM determines the time course of chemical reactions in chemical (or biochemical) systems. The user inputs a description of the chemical reactions of the system with initial chemical concentrations and reaction rate constants. The program calculates the concentrations of these chemicals as a function of time.
   While the simulation program is designed for chemical systems, it has features which facilitate the ability to work with distribution equations for enzyme forms. The simulation program may also be applied to other areas where appropriate. It has been applied to compartmental analysis of radioactive tracer data in physiological modeling and interacting animals in ecological systems. In general, this program can be used as a differential equation solver for any set of simultaneous linear or nonlinear differential equations of first and higher orders.

4. **METHOD OF SOLUTION** - The computation involved in chemical simulation is the integration of the set of differential equations describing the time rate of change of the chemical concentrations, as formulated by the mass action law. The task of writing the differential equations is performed by a section of the simulation program called the "generator". The reminder of the simulation program, called the "simulator", numerically integrates these differential equations using the predictor-corrector method of C. W. Gear.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The generator and simulator programs are set up for:
   200 chemicals
   200 reactions
   50 stoichiometries
   12 chemicals per reaction
   50 enzyme forms
   If the user wants to simulate larger systems, the appropriate array dimensions must be modified in the generator program.

6. **TIMING** - The sample input provided with the program took 7 seconds of CPU time on an IBM370/195 computer.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The methodology of program control restructuring is used in BIOSSIM. A programmer's guide which describes the basic philosophy of this programming technique is included with this package.

8. **RELATED AND AUXILIARY SOFTWARE** - There are a number of programs for solving systems of stiff differential equations in the NESC collection - LSODE (NESC 592), EPISODE (NESC 675), and EPISODEB (NESC 705).

9. **STATUS** - Abstract first distributed December 1977.
   IBM370 version received August 1976, sample problem executed by NESC October 1977 on an IBM370/195.

10. **REFERENCES** - Dr. David Garfinkel, BIOSSIM: A Biochemical Simulation Structure System, Moore School of Electrical Engineering report, August 1976.
    G. C. Roman, David Garfinkel, and Carl B. Marbach, "Memory Concerning Efficient Methods for Solving Large Sets of Stiff Differential Equations", AFIPS Conference Proceeding, National Computer Conference, Vol. 45, pp. 973-978, 1976.
    David Garfinkel, A Machine-Independent Language for the Simulation of Complex Chemical and Biochemical Systems, Computers and Biomedical Research, Vol. 2, pp. 31-44, 1968.
    G. C. Roman and David Garfinkel, BIOSSIM: A Structured Machine-Independent Biological Simulation Language, Computers and Biomedical Research, (in press).

11. **HARDWARE REQUIREMENTS** - 155K of memory for execution

12. **PROGRAMMING LANGUAGE** - FORTRAN (99%) and Assembler (1%)

13. **OPERATING SYSTEM** - OS/360 (IBM360), OS/370 (IBM370).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. Garfinkel
Moore School of Electrical Engineering
University of Pennsylvania

16. **MATERIAL AVAILABLE** -
Source (10,920 lines)
Sample problem (27 lines)
Control information (JCL 442 lines)
Sample problem output (9 pages)
Reference report, MSEE report

17. **CATEGORY** - U
KEYWORDS - differential equations, numerical solution, chemical reactions, biochemistry, simulation

18. **SPONSOR** - NIH

1. **IDENTIFICATION AND KWIC TITLE** - PRP4
   PRP4, determination of product production cost

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360,370,303x

3. **DESCRIPTION** - PRP4 calculates the production cost (product price) when the investments, operating costs, interest rate on debt, rate of return on equity, tax rates, by-product values, and similar related data are supplied. The program can also be used to calculate the annual rate of return on equity when the selling price of the product is supplied. Options incorporated in the program to increase its utility are: use of escalation or inflation rates for costs and product prices, debt retirement by constant annual principal reduction, use of product price ratios when a plant produces several products, and provision for user-specification of annual tax depreciation percentages. Investment tax credits are taken in the year in which the investment is made rather than in the year of plant startup.

4. **METHOD OF SOLUTION** - PRP4 uses the discounted cash flow method in a trial-and-error mode, calculating a year-by-year cash flow history of the project. Provisions are made for handling any desired debt-equity ratio and for choosing various options in the calculation of income taxes. The program can be used in a parametric mode where the cost of the feedstock (e.g. coal) and the rate of return are varied over any desired range of values.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   400 years of project life (NYRS)
   24 products listed (NPRODS)
   24 feedstocks for which the price and rate are given (NFEEDS)
   24 depreciation classes (NCLS)
   24 years of construction period (NCNSTR)
   20 rates of return on equity (NEQMAX)

6. **TIMING** - Execution time for a single case is approximately one second. NESC executed the sample problem in 1 CPU second on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed January 1978.
   IBM360 version of PRP submitted April 1977, replaced by PRP4 June 1984, sample problem executed by NESC November 1983 on an IBM370/195.

10. **REFERENCES** - Royes Salmon, PRP-4: An Updated Version of the Discounted Cash Flow Program PRP, ORNL-5723, May 1983.
    Royes Salmon, PRP: A Discounted Cash Flow Program for Calculating the Production Cost (Product Price) of the Product from a Process Plant, ORNL-5251, March 1977.

11. **HARDWARE REQUIREMENTS** - 110K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. Salmon
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (1152 lines)
    Sample problem (33 lines)

Sample problem output (10 pages)
Reference report, ORNL-5723

17. **CATEGORY** - D
KEYWORDS - production, capital, charges, processing, economics

18. **SPONSOR** - DOE Division of Fossil Energy

1. **IDENTIFICATION AND KWIC TITLE** - MATADOR
   MATADOR, radionuclide behavior in containments

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER180,170,73,74

3. **DESCRIPTION** - MATADOR analyzes the transport and deposition of radionuclides as vapor or aerosol through Light Water Reactor (LWR) containments during severe accidents and calculates environmental release fractions of radionuclides as a function of time. It is intended for use in system risk studies. The principal output is information on the timing and magnitude of radionuclide releases to the environment as a result of severely degraded core accidents. MATADOR considers the transport of radionuclides through the containment and their removal by natural deposition and the operation of engineered safety systems such as sprays. Input data on the source term from the primary system, the containment geometry, and thermal-hydraulic conditions are required.

4. **METHOD OF SOLUTION** - The containment is modeled as a series of interconnected control volumes. In each control volume, radionuclides can be in any of four different states: suspended in the atmosphere, deposited on the walls, picked up by spray water droplets, or residing in bulk water in the sump or on the containment floor. If the physical form of the radionuclides is aerosol, these states are further divided into size classes. Radionuclides can also be picked up and collected by engineered safety systems such as filters, ice condensers, and pressure suppression pools. Radionuclides can transfer from one state to another within each compartment as a result of processes such as deposition on the walls or spray water droplet pickup. They can also transfer from one compartment to another through inter-compartmental flows. A linear first-order differential equation is written for each species in each state and control volume to account for the transfer of species between states in a control volume or between control volumes. These equations are assembled into a matrix equation and solved simultaneously using the matrix expansion technique with scaling. The aerosol agglomeration and gravitational settling calculations are done in series over each time-step using the moments approach. The discrete aerosol size distribution is converted to a log-normal distribution for agglomeration calculations. After these calculations, it is converted back into a discrete distribution for transport calculations over the next time-step. Care is taken to conserve the total aerosol mass as well as individual species masses between conversions. The time-step size is regulated so that the two sets of calculations do not unduly affect each other.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of
   10 interconnected control volumes
   10 chemical species
   10 kinetic transport processes
   10 discrete size classes for aerosols
   Application is limited to LWR systems. Noble gases are assumed to simply transfer in phase with the fluid flow and not deposit on the surfaces or be affected by engineered safety systems.

6. **TIMING** - A typical problem covering 1 hour of accident time without or with sprays operating requires 8 or 50 CP seconds, respectively, on a CDC CYBER180/855. Execution time increases by a factor of 1.5 on a CDC CYBER74 and by a factor of 6 on a CDC CYBER73. NESC executed the sample problem in 5 CP seconds on a CDC CYBER170/875.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - MATADOR treats both vapor and aerosol behavior and can be used for both PWR and BWR applications.

8. **RELATED AND AUXILIARY SOFTWARE** - MATADOR was developed to replace the CORRAL2 program. A physical processes program such as MARCH2, NESC Abstract 734, can be used to generate the thermal-hydraulic data required by MATADOR. MATADOR can directly accept source terms calculated by the TRAP-MELT program. The environmental radionuclide release fractions calculated by MATADOR can be used in a radiological consequence program such as CRAC2, NESC Abstract 722, to calculate the health effects of reactor accidents.

9. **STATUS** - Abstract first distributed February 1978.
CDC CYBER73 version of CORRAL2 submitted May 1977, replaced by CDC CYBER180 version of MATADOR May 1985, sample problem executed by NESC April 1985 on a CDC CYBER170/875.

10. **REFERENCES** - P. Baybutt, S. Raghuram, and H. I. Avci, MATADOR: A Computer Code for the Analysis of Radionuclide Behavior During Degraded Core Accidents in Light Water Reactors, NUREG/CR-4210 (BMI-2125), April 1985.
H. I. Avci, S. Raghuram, and P. Baybutt, MATADOR (Methods for the Analysis of Transport and Deposition of Radionuclides) Code Description and User's Manual, NUREG/CR-4211 (BMI-2126), April 1985.
MATADOR, NESC No. 745, MATADOR Tape Description and Implementation Information, National Energy Software Center Note 85-72, April 18, 1985.
H. Jordan, J. A. Gieseke, and P. Baybutt, TRAP-MELT User's Manual, NUREG/CR-0632 (BMI-2017), February 1979.
R. O. Wooton, P. Cybulskis, and S. F. Quayle, MARCH 2 (Meltdown Accident Response CHaracteristics) Code Description and User's Manual, NUREG/CR-3988 (BMI-2115), September 1984.
Lynn T. Ritchie, Jay D. Johnson, and Roger M. Blond, Calculations of Reactor Accident Consequences Version 2 CRAC: Computer Code User's Guide, NUREG/CR-2326 (SAND81-1994), February 1983.

11. **HARDWARE REQUIREMENTS** - MATADOR requires, without segmentation, approximately 335,000 (octal) words of central memory (SCM) and 116,000 (octal) words of extended core storage (ECS). NESC executed the sample problem using only 237,000 (octal) words of central memory by segmenting the program and reducing the dimensions of several arrays as outlined in the user's manual.

12. **PROGRAMMING LANGUAGE** - FORTRAN 5

13. **OPERATING SYSTEM** - NOS 2.3, NOS/BE 2.2, NOS 2.2 (CDC CYBER170).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
H. I. Avci, P. Baybutt, and S. Raghuram
Columbus Laboratories
Battelle Memorial Institute

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 5121 lines, UPDATE 4966 lines)
Sample problem (684 lines)
Control information (51 lines)
Sample problem output (2805 132-character records)
Reference reports, NUREG/CR-4210 and NUREG/CR-4211, and NESC Note

17. **CATEGORY** - G
KEYWORDS - reactor safety, water cooled reactors, accidents, reactor cores, engineered safety systems, aerosols, containment, radioisotopes, CORRAL2 codes, MARCH codes, CRAC2 codes, TRAP-MELT codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Risk Analysis and Operations

1. **IDENTIFICATION AND KWIC TITLE** - CORTES
   CORTES, thermal & mechanical analysis of tees

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - CORTES is a package consisting of five finite element programs developed for the stress analysis of ANSI B16.9 tee joints. The five programs are:
   SA, the stress analysis program which analyzes pipe joints for the effects of internal pressure and arbitrary combinations of bending moment, torsional moment, axial force, and sheer force on the ends of the branch and run pipes. A limited temperature stress analysis capability is provided.
   EP, the elasto-plastic stress analysis program which analyzes pipe joints for the effects of internal pressure and arbitrary combinations of forces, including moments, and displacements, including rotations, imposed on the ends of the run and branch pipes.
   THFA, the transient heat flow analysis program which determines the time history of temperature variations in the pipe joints. The joint is assumed initially to be at a uniform temperature. Temperature changes are then specified at the inner surface, and a heat flow analysis is performed assuming a perfectly insulated outer surface.
   SHFA, the steady-state heat flow analysis program which determines the steady-state temperature distribution in pipe joints. Temperatures are specified on given cross-sections of the branch and run portions of the tee joint, and the temperature distribution throughout the remainder of the joint is calculated assuming the inner and outer surfaces are perfectly insulated.
   TSA, accepts as input, the output data from THFA or SHFA and performs the thermal stress analysis on the pipe joints.

4. **METHOD OF SOLUTION** - The joint is idealized as a system of 8-node hexahedral finite elements. A modified Zienkiewicz-Irons isoparametric element which has superior bending properties compared with the unmodified isoparametric element is used. The transient heat flow (THFA) problem is solved by a step-by-step integration procedure assuming linear variation of temperature with time within a step.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -
   EP - Displacements and strains are assumed to be small and no geometric (initial stress) stiffness effects are considered. The materials are assumed to yield according to the von Mises criterion, and tangent stress-strain relationships after yield are determined according to conventional flow rule procedures for strain hardening materials.
   THFA - The specified temperature variations at the inner surface are assumed to be symmetrical about the x-y plane.
   SHFA - The temperature distribution is assumed to be symmetric about the x-y plane.
   SA and TSA - Any nodes introduced within the wall thickness are assumed to be uniformly spaced through the thickness.

6. **TIMING** - Execution time varies according to the data used. Excluding wait time, it took approximately 140, 190, 40, 30, and 120 seconds to compile and execute each of the five test problems on an IBM370/195. A large amount of wait time is attributable to numerous I/O operations and is inversely proportional to the size of the container array, A.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The program GRFPAK (NESC 760) provides plotting support for the CORTES programs.

9. **STATUS** - Abstract first distributed June 1978.
   IBM360 version submitted September 1975, revised edition submitted November 1977, replaced by revised Edition B November 1978, replaced by revised Edition C May 1981, sample problems executed by NESC April 1978 on an IBM370/195.

10. **REFERENCES** - A. N. Gantayat and G. H. Powell, Stress Analysis of Tee Joints by the Finite Element Method, UC SESM 73-6 (ORNL-3193-1), February 1973.

Graham H. Powell, Finite Element Analysis of Elasto-Plastic Tee Joints, UC SESM 74-14 (ORNL-SUB-3193-2), September 1974.

R. E. Textor, User's Guide for SHFA: Steady-State Heat Flow Analysis of Tee Joints by the Finite Element Method, UCCND/CSD/INF-60, January 1976.

B. R. Bass, J. W. Bryson, and S. E. Moore, Validation of the Finite Element Computer Program CORTES-SA for Analyzing Piping Tees and Pressure Vessel Nozzles, reprint from Joint Energy Technology Conference and Exhibition, Houston, Texas, September 18-22, 1977.

CORTES, NESC No. 759.360, National Energy Software Center Note 78-28, July 11, 1978.

11. **HARDWARE REQUIREMENTS** - All five programs use card input and a line printer. Execution of the SA test problem required 960K bytes of memory and 12 scratch disk units. The EP test problem required 920K bytes of memory and 11 scratch disk units. The THFA sample problem required 460K bytes of memory and 6 scratch disk units. The SHFA sample problem required 350K bytes of memory and 6 scratch disk units. The TSA test case used 880K bytes of memory and 11 scratch disk units.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Four environmental system routines - ITIME, DATE, ICTICK, and PLOT - used by CORTES were not supplied. Dummy routines have been included for completeness. ITIME and ICTICK return the elapsed wall time and elapsed CPU time, respectively, in hundredths of a second since the previous call to these routines. The first call initializes the routines. PLOT refers to proprietary CalComp software and DATE returns the date in the form MM/DD/YY.

Since comment blocks exceeding 30 consecutive lines are truncated during a FORTRAN G compilation, the FORTRAN H compiler should be used to insure that all comments are listed for the EP, THFA, and SHFA programs.

The output written to unit 10 by SHFA during execution of the sample problem is read as input from unit 10 for the TSA sample problem.

It should be noted that some variables in common blocks /GASS/ and /NQUAD/ may not always be stored identically in all routines.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

A. N. Gantayat and G. H. Powell
College of Engineering
University of California, Berkeley
R. E. Textor and B. R. Bass
Computer Sciences Division
Union Carbide Corporation, Nuclear Division
J. W. Bryson and S. E. Moore
Engineering Technology Division
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -

Source (SA 4298 lines, EP 6250 lines, THFA 3126 lines, SHFA 2967 lines, TSA 3600 lines)
Sample problems (SA 10 lines, EP 38 lines, THFA 64 lines, SHFA 15 lines, TSA 6 lines)
Control information (JCL SA 122 lines, EP 70 lines, THFA 41 lines, SHFA 42 lines, TSA 55 lines)
Sample problems output (SA 12 selected pages, EP 25 selected pages, 2 microfiche, THFA 15 selected pages, 1 microfiche, SHFA 11 selected pages, TSA 17 selected pages, 1 microfiche)
Reference report, Reprint, and NESC Note

17. **CATEGORY** - I
KEYWORDS - stress analysis, heat flow, thermal stresses, pipe joints, finite element method, GRFPAK codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - GRFPAK
GRFPAK, plot package for CORTES FEM programs

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,370

DESCRIPTION - GRFPAK is a graphics package written for the CORTES finite-element programs. It includes three plotting routines to assist in analyzing, interpreting, and presenting CORTES results. One plotting routine displays stresses or stress indices by means of contour curves drawn within either the outside or inside surface outline of a quarter section of the tee-joint. Using this routine, one can also obtain plots of the finite-element mesh as viewed from any point in space. A second plotting routine gives a stress versus distance plot along any specified line of nodes. A third routine displays cross-sectional views of the finite-element mesh for both the undeformed (original) and deformed configuration. The deformed configurations are drawn using an exaggerated scale specified by the user.

METHOD OF SOLUTION - All of the plotter software calls are channeled through one of the several multiple entries in subroutine PLTINT. The segment of GRFPAK designed for contour, mesh, and displacement plotting can produce the finite-element mesh for the original geometry and for each load case of the displaced geometry, and contour plots for any surface in any quadrant for any stress (or temperature). These contours may be displayed on the mesh or on the outline of the tee. The node line plot segment produces the plots of the longitudinal (along the node line) stresses and transverse (normal to the node line) stresses along the 0 degree node line (x-y plane) and 90 degree node line (y-z plane) for a given surface. The global (x, y, z) coordinates for the nodes along the 0 degree node line are given a -45 degree rotation to a new x'-y' coordinate system. The abscissa values in the plots represent x' along this line. For the 90 degree node line the abscissa values for the plots represent the y global coordinate values. For THFA, the temperature values along these node lines are plotted. If more than one time-step is being plotted for THFA or TSA, all of the time-steps will appear on one graph. The cross-section segment of GRFPAK produces plots of the x=0 and z=0 planes of the tee for SA and EP. The entire cross section or only a specified number of nodes along the axes from the control node may be represented.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Requests for plots relating to displacements are invalid for the CORTES programs TSA, THFA, and SHFA. The maximum value for the variable MTOT in the MAIN program is 22,000.

TIMING - Execution time is approximately 12 seconds for sample data which produces nine plots. The NESC executed the sample problem in 35 seconds on an IBM370/195.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - GRFPAK reads and processes data from the CORTES finite-element programs (NESC 759).

STATUS - Abstract first distributed July 1978.
IBM360 version submitted August 1977, sample problem executed by NESC June 1978 on an IBM370/195.

REFERENCES - P. G. Fowler and J. W. Bryson, User's Manual for the CORTES Graphics Package GRFPAK, ORNL/NUREG/TM-127, August 1977.

HARDWARE REQUIREMENTS - Card reader, tape unit, line printer, and CalComp plotting equipment are required. The amount of memory needed depends on the number of nodes and elements in the finite element idealization. The sample problem which consists of 675 elements required 290K bytes of memory.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – The program was developed to produce plots on a 925/1036 CalComp plotter. The amount of memory used can be increased or decreased by changing the value of the variable MTOT and dimensioning the A array by MTOT in the MAIN program. GRFPAK requires as input two data sets generated by CORTES. The logical unit 12 data set contains the connectivity of the nodes, coordinates of the nodes, and the stress quantities (temperature quantities for THFA). Logical unit 16 contains the displacements at the nodes for each load case produced by SA and EP. Logical unit 13 is a temporary unit employed when cross section plots are requested. A dummy subroutine IDAY was provided by the NESC. The routine IDAY, which is an ORNL system routine, returns the current date in the form MM/DD/YY.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

P. G. Fowler and J. W. Bryson
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** –

Source (3516 lines)
Sample problems (unit 5 data set 30 lines, unit 12 data set 131 blocks*, unit 16 data set 16 blocks*)
Control information (JCL 100 lines)
Sample problems output (12 pages and 8 plots)
Reference report

* RECFM=VBS,BLKSIZE=3156

17. **CATEGORY** – N
KEYWORDS – finite element method, pipes, stresses, computer graphics, CORTES codes

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research

IDENTIFICATION AND KWIC TITLE - PTA2
PTA2, pressure transients in piping systems

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370

DESCRIPTION - PTA2 performs pressure-transient analysis of large piping networks. The program is particularly oriented toward the analysis of the effects of a sodium/water reaction on the intermediate heat-transport system of a liquid-metal-cooled fast breeder reactor, but may be applied to other pulse sources and piping systems. A variety of junction types are included, and complex piping networks can be treated. The effects on pulse propagation of cavitation, elastic-plastic deformation of piping, pipe friction, nonlinear velocity terms, gravity, and temperature-dependent material properties are included in the formulation. PTA2 has been validated extensively, using available experimental data.

METHOD OF SOLUTION - PTA2 uses the one-dimensional method of characteristics applied to nonlinear fluid-hammer analysis of pressure transients in large piping systems. A column-separation treatment is used to model cavitation, which is allowed to occur anywhere in the system. The dependence of wave speed on elastic-plastic deformation of the piping is included in the formulation of the governing equations. Various types of junctions and fittings may be specified, including area changes, tees, closed ends, nonreflecting boundaries, orifices, valves, constant-pressure boundaries, surge tanks with gas spaces, impedance discontinuities, dummy junctions, pulse sources, and simple models for pumps and rupture disks.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -

65 pipes
66 junctions
75 nodes per pipe
6 pipes connected at multibranched junctions
4 pulse sources
50 data points per pulse source
10 constant-pressure boundaries
10 rupture disks
10 pumps
10 surge tanks
10 orifices
8 valves
15 data points per valve

These limitations may be changed by altering DIMENSION and COMMON statements in the program.

TIMING - PTA2 requires approximately 30 seconds to execute the longest running sample problem on the IBM370/195.

UNUSUAL FEATURES OF THE SOFTWARE - PTA2 differs from conventional fluid-hammer programs primarily in that cavitation and elastic-plastic pipe deformation effects are included. Cavitation is treated by a column-separation formulation, and large cavitated regions are represented by multiple small cavities separated by short fluid columns. Elastic-plastic deformation of the pipe cross-section alters the local wave speed, which varies with deformation history at each computational node. Temperature-dependent material properties for liquid sodium, liquid water, and Types 304 and 316 stainless steels are included, as well as room-temperature properties for other piping materials. The input data and output results can be in either conventional English or SI units. Pipe temperatures can be specified individually so different material properties can be used for cold and hot pipe runs. Different pulses may be specified at various source points in the piping system. Orifice and valve losses, pipe friction factors, node spacings, and wave speeds are computed internally. There are no restrictions on pipe and junction numbering or designation of left and right ends of pipes, and the flow network is assembled by the program. In addition to nonlinear fluid-hammer analysis, PTA2 can optionally perform a linear analysis.

8. **RELATED AND AUXILIARY SOFTWARE** - Related codes include PTA1, WHAM6 (NESC 278), COMPARE (NESC 702), NAHAMMER (NESC 717), NATRAN2 (NESC 719), NATRANSIENT (NESC 718), and HAMOC (NESC 710).

9. **STATUS** - Abstract first distributed April 1978.
IBM370 version of PTA1 submitted January 1978, modified October 1978, replaced February 1983 by PTA2 submitted May 1982, sample problems executed by NESC May 1982 on an IBM370/195.

10. **REFERENCES** - C. K. Youngdahl, C. A. Kot, and Y. W. Shin, Users' Manual for the Pressure Transient Analysis Computer Code PTA2, ANL-82-20, March 1982.
C. K. Youngdahl, C. A. Kot, and R. A. Valentin, Pressure Transient Analysis in Piping Systems Including the Effects of Plastic Deformation and Cavitation, Journal of Pressure Vessel Technology, Vol. 102, pp. 49-55, February 1980.
C. K. Youngdahl, C. A. Kot, and R. A. Valentin, Pressure Transient Analysis of Elbow-Pipe Experiments Using the PTA-2 Computer Code, Journal of Pressure Vessel Technology, Vol. 103, pp. 33-42, February 1981.
C. K. Youngdahl, C. A. Kot, and R. A. Valentin, Experimental Validation of PTA-1 Computer Code for Pressure-Transient Analysis Including the Effect of Pipe Plasticity, ANL-78-38, July 1978.
C. K. Youngdahl and C. A. Kot, PTA-1: A Computer Program for Analysis of Pressure Transients in Hydraulic Networks, Including the Effect of Pipe Elasticity, ANL-76-64, November 1976.
C. A. Kot and C. K. Youngdahl, PTAC: A Computer Program for Pressure-Transient Analysis, Including the Effects of Cavitation, ANL-78-4, September 1978.

11. **HARDWARE REQUIREMENTS** - The program requires approximately 315 bytes of memory for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/MVT.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
C. K. Youngdahl, C. A. Kot, and Y. W. Shin
Components Technology Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2859 lines)
Sample problems (80 lines)
Sample problems output (44 selected pages)
Reference report, ANL-82-20

17. **CATEGORY** - G
KEYWORDS - pressure gradients, hydraulics, LMFBR reactors, deformation, cavitation, water hammer, plasticity, molten metal-water reactions, elasticity, PTA1 codes

18. **SPONSOR** - DOE Office of Reactor Research and Technology,
Engineered Components Division

IDENTIFICATION AND KWIC TITLE - REFLUX
REFLUX, LWR reflood heat transfer prediction

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360

DESCRIPTION - REFLUX calculates the temperature-time history of a representative fuel rod during the reflood stage of a hypothetical loss-of-coolant accident (LOCA). The logic used for selection of the appropriate flow regime for analysis of the cladding temperature transient is based on the axial position with regard to the continuous liquid level (based on a mass balance), a liquid carry-over criterion (derived from a force balance on a drop suspended in a vapor stream), and the local cladding surface temperature. A generalized boiling curve is constructed, and the local flow and clad conditions determine the applicable heat transfer coefficient.

METHOD OF SOLUTION - The coolant thermal-hydraulic calculation of REFLUX is based on a single subchannel, one-dimensional, separated two-phase flow formulation solution of the conservation equations of mass, energy, and momentum. The equations to be solved are written in backward finite-difference form, in space and time. A marching solution from subchannel inlet to exit is performed at each time-step. The code uses the fuel-clad temperature field from the preceding time-step to advance the coolant thermal-hydraulic solution to the present time-step. The void fraction in the flow boiling regimes is defined by the drift flux model. Provision is made for analyzing non-equilibrium situations encountered under reflood conditions, and a complete two-step dispersed flow film boiling model is included. The coupled fuel-clad temperature field is solved by an implicit finite difference technique for radial conduction, including decay heat generation and temperature-dependent material properties.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - REFLUX is expected to provide reasonable results for flooding rates of 0.4 to 10 in/sec, pressures of 15 to 60 psia, peak powers of 0.5 to 1.5 kw/ft, inlet coolant temperatures of 50 degrees F to saturation, and initial temperatures of 250 to 2000 degrees F. Flow reversals cannot be analyzed with the present version.

TIMING - The NESC executed the sample problem in 62 seconds on an IBM370/165.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed July 1978.
IBM360 version submitted February 1978, sample problem executed by NESC June 1978 on an IBM370/165.

REFERENCES - Walter Lee Kirchner, Reflood Heat Transfer in a Light Water Reactor, NUREG-0106, Vols. I and II, August 1976.

HARDWARE REQUIREMENTS - Tape unit, line printer, and 100K bytes of memory

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - OS/360.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The REFLUX program should be compiled with the H-extended or the G1 compiler to duplicate the author's results. Compiling under the H or G compiler leads to differences in conversion of the input data which produces variations in the output.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
W. L. Kirchner
Los Alamos Scientific Laboratory

16. **MATERIAL AVAILABLE** -
    Source (1621 lines)
    Sample problem (47 lines)
    Sample problem output (30 selected pages)
    Reference report

17. **CATEGORY** - H
    KEYWORDS - coolants, cladding, loss of coolant, accidents, heat transfer, core flooding systems, fuel rods, water cooled reactors

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
    Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE -** BEACON/MOD3
   BEACON/MOD3, containment system fluid flow

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC CYBER176, CDC7600

3. **DESCRIPTION -** The BEACON series of programs is designed to perform a best-estimate analysis of the flow of a mixture of air, water, and steam in a nuclear reactor containment system under loss-of-coolant accident conditions. The code can simulate two-component, two-phase fluid flow in complex geometries using a combination of two-dimensional, one-dimensional, and lumped-parameter representations for the various parts of the system. BEACON/MOD3 contains mass and heat transfer models for wall film and for wall conduction, and is suitable for the evaluation of short-term transients in PWR dry containment systems. The capability to examine the details of a two-component, two-phase flow field in one or two dimensions under nonhomogeneous, nonequilibrium conditions (unequal velocities, unequal temperatures between the two phases) allows analysis of such problems as the calculation of jet impact forces of a fluid leaving a pipe break, the motion of a large pressure wave across a compartment, the variation in flow properties as air is displaced from a compartment by steam and water, the water entrainment or deentrainment by a high-speed vapor flow, the flow of a flashing liquid, and many other complex nonequilibrium problems of containment system analyses.

4. **METHOD OF SOLUTION -** The basic Eulerian flow solution procedure is based on the K-FIX two-dimensional two-phase numerical method. Each phase is described by its own density, velocity, and temperature as determined by separate sets of mass, momentum, and energy equations. The two phases are coupled by exchange parameters which model the exchange of mass, momentum, and energy between the two phases. The two sets of field equations are solved with a Eulerian finite-difference technique that implicitly treats the phase transitions and interphasic heat transfer in the pressure iteration. The implicit solution is accomplished iteratively without linearization and allows both phases to be compressible. The coupling between the two phases can be very loose, as occurs with separated flow, or very tight as with finely dispersed flow. Computations for single phase gas flow can also be obtained without special treatment. BEACON can handle air as a second vapor component.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** BEACON/MOD3 does not have pressure suppression containment models. The Eulerian computational equations have been modified for the variable nodalization of a mesh with the spatial dimensions of each cell stored in row-wide and column-wide arrays. Neither dimension should vary between adjacent cells by more than a factor of two. The centers of adjacent cells must align either in the radial (abscissa) or vertical (ordinate) direction, and no mesh may have more than 50 interior cells in either direction. The coupling of the Eulerian regions must be on a cell-to-cell basis. Due to the array sizes in the code, maxima of 20 Eulerian regions and 20 lumped-parameter regions are allowed per problem setup. The total number of cells (nodes) in all Eulerian regions is limited to 2184.

6. **TIMING -** Running time is highly-variable depending on problem complexity. NESC executed the 8 sample problems in 4 CP minutes on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -** The BEACON solution procedure is based on the solution scheme of K-FIX (NESC 727) developed at Los Alamos National Laboratory. The wall heat conduction subcode used in the CONTEMPT programs (NESC 433 and 818) is also used in BEACON. The program uses the INEL Environmental Library and INEL-IGS graphics software for film plotting. An auxiliary program, PLTBCN, is used to plot a time history of BEACON's fundamental output variables.

9. **STATUS -** Abstract first distributed August 1978.
   CDC7600 version of BEACON/MOD2 submitted January 1978, replaced by BEACON/MOD2A submitted January 1979, revised March 1979, replaced January 1982 by CDC

CYBER176 version of BEACON/MOD3 submitted April 1980, sample problems executed, without the plotting option, by NESC October 1981 on a CDC7600.

10. **REFERENCES** - Charles R. Broadus, Richard J. Doyle, Stephen W. James, James F. Lime, Walter J. Mings, Judith A. Ramsthaler, and Manjit S. Sahota, BEACON/MOD3: A Computer Program for Thermal-Hydraulic Analysis of Nuclear Reactor Containments - User's Manual, NUREG/CR-1148 (EGG-2008), April 1980.

INEL-IGS, Idaho National Engineering Laboratory, Integrated Graphics System Programming Guide, Aerojet Nuclear Company Computer Science Center, March 1976.

BEACON/MOD3, NESC No. 767.C176, BEACON/MOD3 Tape Description and Sample Problem Output, National Energy Software Center Note 82-22, November 19, 1981.

W. C. Rivard and M. D. Torrey, K-FIX: A Computer Program for Transient Two-Dimensional, Two-Fluid Flow, LA-NUREG-6623, NRC-4, April 1977.

F. H. Harlow and A. A. Amsden, Numerical Calculation of Multiphase Fluid Flow, Journal of Computational Physics, Vol. 17, pp. 19-52, 1975.

11. **HARDWARE REQUIREMENTS** - 120,000 (octal) words of SCM and 34,000 (octal) words of LCM for the largest of the eight sample problems. The LCM required is a function of the program size (i.e., the number of nodes or computational cells) and is dynamically allocated by the BEACON code.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (98%) and COMPASS (2%)

13. **OPERATING SYSTEM** - NOS/BE (CDC CYBER176), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - A few of the INEL environmental library and the IGS graphics routines are written in COMPASS; the remainder of the package is in FORTRAN.

The BEACON/MOD3 program is in CDC UPDATE source form for use with the NOS/BE operating system. Modification for use with the SCOPE 2 operating system requires use of the CDC UPDATE utility. The INEL Environmental Library is in CDC UPDATE source form. Modification for use with either operating system requires use of the CDC UPDATE utility. Since BEACON stores variables in large core memory (LCM) in a LEVEL 2, word-addressable mode, a major programming effort would be required to implement the package in other computer environments.

The Integrated Software System Corporation's proprietary graphics software system, DISSPLA, is used by the PLTBCN plot file postprocessor auxiliary program.

NESC replaced subroutine JOBID, which at INEL reads the name from the job card, to allow users to bypass a fatal error. Subroutine JOBLOC in the IGS graphics library contains the same statement (MJ 740B) that caused the JOBID error but was not changed because NESC did not test the plotting package. One can choose the plotting option in all the sample problems except sample problems 3A and 3B by changing NOPLOTS to PLOTS on card number 00150 in each problem set.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

C. R. Broadus, R. J. Doyle, S. W. James,
J. F. Lime, W. J. Mings, J. A. Ramsthaler, and
M. S. Sahota
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -

Source (BEACON UPDATE 24,430 lines, INEL environmental library UPDATE 32,861 lines)
Sample problems (314 lines)
Control information (116 lines)
Sample problems output (22,722 133-character records)
Reference reports, NUREG/CR-1148, INEL-IGS Programming Guide, and NESC Note

17. **CATEGORY** - G

KEYWORDS - fluid flow, two-dimensional, two-phase flow, accidents, one-dimensional, transients, thermodynamics, containment systems, loss of coolant, CONTEMPT-LT codes, CONTEMPT4 codes, K-FIX codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - BEHAVE-SST
   BEHAVE-SST, overpower transient fuel mechanics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - BEHAVE-SST calculates the steady-state and overpower transient behavior of cladding, fuel, and voidage in oxide LMFBR fuel rods prior to cladding failure. Cylindrical symmetry is assumed throughout the program. The BEHAVE-SST program calculates the stress, strain, displacement, and temperature fields in the fuel and cladding. Processes simulated include: cracking of fuel, dilation of fuel and cladding due to irradiation effects and thermal expansion, fuel densification by both stress and diffusion-controlled processes, axial slippage or locking at the fuel-cladding interface, axial flow of fuel, and gas pressurization of the central molten fuel region. Cladding failure is predicted utilizing a life-fraction cumulative damage technique.

4. **METHOD OF SOLUTION** - The finite-element method is used in the cladding and outer fuel zones. Displacement compatibility is maintained axially as well as radially between adjacent elements in the same axial section, but radial displacement compatibility is not maintained between adjacent axial sections. Circular cylindrical ring elements with three degrees of freedom are used in the fuel and cladding. No relative shear deformation is permitted between ring elements, but a special shear element at the fuel-cladding interface permits relative slippage or produces friction-induced fuel pellet locking. An interior inviscid fuel zone interacts with the outer, structural fuel zone as a constant-displacement-rate boundary condition, or as a constant-pressure boundary condition, depending on problem conditions. Within the inviscid fuel region, axial relocation of fuel occurs under certain conditions. Swelling of fuel and cladding, and fission gas release, are represented by empirical models.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The program is dimensioned for a maximum grid structure as defined below:
   (a) cladding divided radially into 10 rings,
   (b) outer (structural) fuel zone divided radially into 10 rings,
   (c) middle (nontransport) fuel region divided radially into 10 rings,
   (d) inner (transport) fuel region divided radially into 10 rings (absent during transients),
   (e) fuel and cladding divided axially into 5 sections.

   The internal steady-state and transient temperature routines are limited to single-phase sodium flow.

6. **TIMING** - A steady-state problem employing the maximum grid structure in the fuel and cladding and 24 time-steps required 47 seconds of CDC7600 processor time, or approximately 2.0 seconds per time-step. A transient problem employing the same grid structure and 43 time-steps required 208 seconds of processor time, or approximately 4.8 seconds per time-step.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -
   (a) Axially interactive effects are calculated.
   (b) Cracks are represented as a continuum, producing zero stress normal to the crack plane. Cracking occurs under any tensile stress normal to two possible directions of cracking ((r, theta) and (r,z)) planes.
   (c) Rapid closure of the fuel-cladding gap is assumed, permitted by immediate cracking of the fuel at the first application of power.
   (d) Fuel is divided into two phenomenological zones, the inner zone being made up of two regions. Boundaries between the zones and regions are defined by time-temperature relations and move in space as a function of time. Crack closure is assumed in the inner zone.

(e) The nodal grid is redefined in the radial direction every time-step by averaging conditions from the old grid. A fine grid is imposed in regions of rapidly-changing properties.

8. **RELATED AND AUXILIARY SOFTWARE** - Transient Heat Transfer program, version D and E (THTD, THTE). BEHAVE-SST is the fourth in the BEHAVE series of programs--BEHAVE1, BEHAVE2, BEHAVE3--modeling fuel rod performance. BEHAVE-SST is intended for use in confirming cladding loading and failure predictions made by the simpler models included in whole core accident analysis programs, such as SAS and MELT.

9. **STATUS** - Abstract first distributed July 1978. CDC7600 version submitted August 1977, sample problems executed by NESC June 1978 on a CDC7600.

10. **REFERENCES** - R. R. Sherry and D. B. Atcheson, User's Manual for the BEHAVE-SST (Steady State and Transient) Fuel Rod Mechanics Program, GEFR-00001, February 1977.
D. B. Atcheson, R. R. Sherry, and K. J. Shimane, Cladding Failure in TREAT Overpower Experiments: A Mechanistic Interpretation and Its Implications for LMFBR Safety Analysis, Proceedings of the International Meeting on Fast Reactor Safety and Related Physics, CONF-761001, Vol. III, pp. 1679-1688, October 1976.

11. **HARDWARE REQUIREMENTS** - 150K of small-core memory (SCM) is required. The program is overlayed extensively.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - An H6000 version used at GE-FBRD provides for temperature coupling to the THTD or THTE programs. The program produces slightly different results depending on the compiler used. MNF versions 4.3, 5.1, 5.12, and 5.20 and FTN 4.5 each produced slightly different output for the steady-state (SS) sample problem. The output included in the package is from the FTN run.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. B. Atcheson
Advanced Reactor Systems Department
General Electric Company

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 10,113 lines, UPDATE 7612 lines)
Sample problems (SS 28 lines, TRANSIENT 184 lines)
Sample problems output (SS 34 selected pages, 1 microfiche, TRANSIENT 22 selected pages, 4 microfiche)
Reference report, GEFR-00001

17. **CATEGORY** - H
KEYWORDS - finite element method, two-dimensional, fuel-cladding interactions, stresses, temperature distribution, fuel cans, swelling, thermal expansion, strains, fuel rods, heat transfer, reactor safety, LMFBR reactors, THTD codes, THTE codes

18. **SPONSOR** - ERDA Division of Reactor Development and Technology

1. **IDENTIFICATION AND KWIC TITLE** - GAPCON-THERMAL3
   GAPCON-THERMAL3, fuel ss & transient behavior

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC6600,7600,CYBER74

3. **DESCRIPTION** - GAPCON-THERMAL3 calculates the thermal and mechanical behavior of the fuel and cladding in a nuclear fuel rod during normal operation for both steady-state and operational transients.

4. **METHOD OF SOLUTION** - The radial temperature profile is obtained by orthogonal collocation. Stresses and strains are determined by using chained iterative radial and axial finite element models. Fission gas release and gap conductance are calculated from empirical models. The solution iterates to convergence on the gap conductance for each axial node and subsequently on gas release rate for the fuel rod. Additional iterative loops handle plasticity, creep, and nonlinear structural effects due to gap closure.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Modeling is axisymmetric for the thermal and mechanical calculations. The current model does not compute the strain at pellet-pellet interfaces. As many as 17 variable-length axial regions can be modeled with no limitation on the number of fuel and cladding radial nodes. No more than 49 time-steps greater than or equal to 1- day duration are allowed.

6. **TIMING** - Three to 30 seconds per time-step are required on the CDC6600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The finite element chained radial-axial-radial mechanics modeling yields a good approximation to total two-dimensional finite element calculation results without commensurate large computer storage and long running time. The program includes variable dimensions to limit storage to individual problem requirements. A restart tape and plot tape are produced by the main code as optional output.

8. **RELATED AND AUXILIARY SOFTWARE** - PLOT3 produces high quality off-line plots of GAPCON-THERMAL3 output. GAPCON-THERMAL3 incorporates the thermal calculations of GAPCON-THERMAL2 (NESC 618) with a more detailed nonlinear mechanical analysis to evaluate the interactive effects. Available output includes fuel and cladding stresses and strains in radial, hoop, and axial directions and fuel and cladding axial and radial displacements.

9. **STATUS** - Abstract first distributed December 1978.
   CDC CYBER74 version submitted January 1978, sample problem executed by NESC June 1978 on a CDC7600.

10. **REFERENCES** - D. D. Lanning, C. L. Mohr, F. E. Panisko, and K. B. Stewart, Gapcon-Thermal-3 Code Description, PNL-2434, January 1978.
    D. D. Lanning, F. E. Panisko, and C. L. Mohr, Verification of the GAPCON-THERMAL-3 Computer Code, PNL-2435, September 1978.

11. **HARDWARE REQUIREMENTS** - About 220K of addressable storage is needed for execution of a typical problem.

12. **PROGRAMMING LANGUAGE** - CDC Extended FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.4 (CDC6600), NOS/BE and SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. D. Lanning, C. L. Mohr, F. E. Panisko,
and K. B. Stewart
Pacific Northwest Laboratory

16. **MATERIAL AVAILABLE** –
    Source (7631 lines)
    Sample problem (94 lines)
    Auxiliary routines (PLOT3 571 lines)
    Reference report, PNL-2434

17. **CATEGORY** – I
    KEYWORDS – cladding, fuel rods, steady-state conditions, deformation, transients, stresses, finite element method, plasticity, creep, GAPCON-THERMAL2 codes, PLOT3 codes

18. **SPONSOR** – NRC Office of Nuclear Reactor Regulation,
    Division of Systems Safety

1. **IDENTIFICATION AND KWIC TITLE** - TRUMP
   TRUMP, transient & s-state temperature dist

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370, CDC7600

3. **DESCRIPTION** - TRUMP solves a general nonlinear parabolic partial differential equation describing flow in various kinds of potential fields, such as fields of temperature, pressure, or electricity and magnetism; simultaneously, it will solve two additional equations representing, in thermal problems, heat production by decomposition of two reactants having rate constants with a general Arrhenius temperature dependence. Steady-state and transient flow in one, two, or three dimensions are considered in geometrical configurations having simple or complex shapes and structures. Problem parameters may vary with spatial position, time, or primary dependent variables--temperature, pressure, or field strength. Initial conditions may vary with spatial position, and among the criteria that may be specified for ending a problem are upper and lower limits on the size of the primary dependent variable, upper limits on the problem time or on the number of time-steps or on the computer time, and attainment of steady state.

4. **METHOD OF SOLUTION** - Solutions may be obtained by use of explicit- or implicit-difference equations, or by an optimized combination of both.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The program currently provides for maxima of -
   40 materials
   5 reactants
   150 surface conditions
   20 boundary nodes
   16 entries per tabulated function (table-length)

6. **TIMING** - Running time is strongly dependent on the complexity of the problem. Calculation of all 16 sample problems required approximately 205 CPU seconds on an IBM370/195, or 144 CP seconds on a CDC7600. Execution time averages from 0.3 to 2 milliseconds per time-step for each nodal point and connection between nodal points.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The package includes three materials properties libraries, each of which contains the properties of approximately 1000 materials in the standard TRUMP input format. System units for the libraries are, respectively: centimeter-gram-second-calorie-degree C, meter-kilogram-second-joule-degree C, and meter-kilogram-second-joule-degree K.

8. **RELATED AND AUXILIARY SOFTWARE** - The FED mesh generation program may be used to generate finite difference zoning for TRUMP. The TRUMP/XB2 program processes the TRUMP thermal property data compilation. The original CDC LRLTRAN version of TRUMP was prepared by A. L. Edwards of Lawrence Livermore Laboratory, Livermore, California.

9. **STATUS** - Abstract first distributed August 1978.
   CDC LRLTRAN version submitted 1973.
   IBM360 version submitted August 1977, sample problems executed by NESC July 1978 on an IBM370/195.
   CDC7600 version submitted September 1979, sample problems executed by NESC January 1980.

10. **REFERENCES** - Arthur L. Edwards, TRUMP: A Computer Program for Transient and Steady-State Temperature Distributions in Multidimensional Systems, UCRL-14754 Rev. 3, September 1, 1972.

D. C. Elrod and W. D. Turner, Implementation of the TRUMP Computer Code on the IBM360 Operating System, UCCND Letter to R. H. Odegaarden, NRC, with attachments, May 12, 1977.

A. L. Edwards, A Compilation of Thermal Property Data for Computer Heat-Conduction Calculations, UCRL-50589, February 24, 1969.

Dale A. Schauer, FED: A Computer Program to Generate Geometric Input for the Heat-Transfer Code TRUMP, UCRL-50816 Rev. 1, January 12, 1973.

11. **HARDWARE REQUIREMENTS** - As dimensioned, the program requires 400K bytes of storage on an IBM370 and 145,100 (octal) words on a CDC7600.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (95%) and BAL (5%) (IBM); FORTRAN IV (CDC)

13. **OPERATING SYSTEM** - OS/360 (IBM360), OS/370 (IBM370), SCOPE 2.1.5 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The code restart feature, the time-sharing option, and the graphics capabilities were not implemented in the ORNL versions of TRUMP. During execution of the sample problems of the IBM version several hundred "harmless" underflows occur in subroutines TALLY and FINK.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. C. Elrod and W. D. Turner
Union Carbide Corporation, Nuclear Division

16. **MATERIAL AVAILABLE** -
Source (360-FORTRAN 4536 lines, BAL 288 lines, 7600-4458 lines)
Sample problem input (360-574 lines, 7600-573 lines)
Materials Properties Libraries (9015 lines)
Auxiliary information (Materials Index 1294 lines)
Control information (360-JCL 90 lines)
Sample problem output (360-64 selected pages, 1 microfiche punch - 1 page listing; 7600-66 selected pages, punch - 1 page listing)
Reference reports, UCRL-14754 Rev. 3, UCRL-50589, and UCCND letter with attachments

17. **CATEGORY** - H
KEYWORDS - temperature distribution, three-dimensional, transients, steady-state conditions, heat transfer, partial differential equations, nonlinear problems, potential flow

18. **SPONSOR** - AEC
NRC Office of Nuclear Regulatory Research,
Division of Safeguards, Fuel Cycle and Environmental Research

1. **IDENTIFICATION AND KWIC TITLE** - FORTIO
   FORTIO, Fortran interface to IBM370 macros

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - FORTIO is a set of Assembly language subroutines which allow FORTRAN IV programs to use several OS/360-370 data management and supervisor macro instructions. In particular, the FORTRAN programmer has available BSAM, QSAM, and BPAM access methods; can open, close and position files; position at or point to a block within a file; create and modify DCB's; dynamically LOAD, LINK, CALL, or DELETE other modules; and dynamically obtain and free storage (GETMAIN, FREEMAIN, GETPOOL, FREEPOOL, etc.).

4. **METHOD OF SOLUTION** - The FORTIO Assembly language subroutines provide an interface between FORTRAN programs and selected IBM360-370 Operating System (OS) Supervisor and Data Management input-output macros.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed August 1978.
   IBM360 version submitted May 1977, sample problem executed by NESC May 1978 on an IBM370/195.

10. **REFERENCES** - L. Shalla, FORTIO--A FORTRAN I/O Interface, ANL-76-56, April 1976.
    IBM Corporation, OS Data Management Macro Instructions, GC26-3794-1, June 1973.
    IBM Corporation, IBM System/360 Operating System Supervisor Services and Macro Instructions, GC28-6646-7, September 1974.

11. **HARDWARE REQUIREMENTS** - Less than 10K bytes of storage is required to load all of the FORTIO subroutines.

12. **PROGRAMMING LANGUAGE** - Basic Assembly Language

13. **OPERATING SYSTEM** - OS/360 (IBM360) and OS/370, OS/VS1, OS/VS2 Release 1 (IBM370).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - To use FORTIO effectively, the IBM360,370 programmer must be familiar with the OS Supervisor and Data Management macros. The FORTIO source files are in IEBUPDAT format.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Shalla
    Applied Mathematics Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (Macros 261 lines, FORTIO 1984 lines)
    3330 load module (24 blocks)
    Sample problems (51 lines)
    Control information (JCL 268 lines)
    Sample problems output (2 pages)
    Reference report, ANL-76-56

17. **CATEGORY** - P
    KEYWORDS - data processing, operating systems, utility routines

18. **SPONSOR** - Argonne National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - HEMP
   HEMP, hydrodynamic elasticmagneto plastic

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - The HEMP code solves the conservation equations of two-dimensional elastic-plastic flow, in plane x-y coordinates or in cylindrical symmetry around the x-axis. Provisions for calculation of fixed boundaries, free surfaces, pistons, and boundary slide planes have been included, along with other special conditions.

4. **METHOD OF SOLUTION** - The solution is by the method of finite differences and uses the Lagrangian formulation. The materials within a physical system are divided into quadrilaterals bounded by J and K grid lines. A decoupling of grid lines is allowed along K-lines, and voids may open and close between K-lines.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The maximum number of J's in any K-line is 101. A problem of up to about 10,000 zones may be run.

6. **TIMING** - Basic HEMP calculation speed is about 5 points (or zones) per millisecond. The number of problem cycles necessary depends on the problem termination time and the time-step size. Typical problems run from a few minutes to several hours with time a function of zone size, material composition and activity in the zones.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The input system, described in the HEMP User's Manual is designed so that the least amount of data to describe a particular physical system need be supplied. However, provision is made for describing initial conditions (zonal or nodal) in great detail, if required.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed August 1978.
   CDC7600 version submitted October 1976, sample problem executed by NESC July 1978 on a CDC7600.

10. **REFERENCES** - Mark L. Wilkins, Calculation of Elastic Plastic Flow, UCRL-7322, Rev. 1, January 24, 1969.
    E. D. Giroux, HEMP User's Manual, UCRL-51079, Rev. 1, December 17, 1973.

11. **HARDWARE REQUIREMENTS** - The HEMP main code fills the small core memory (SCM) with the code, working storage, library, and system routines. The large core memory (LCM) utilized is a function of problem size, the amount required is 527,270 (octal) words.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV, LLL CHAT compiler

13. **OPERATING SYSTEM** - SCOPE 2.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Memory must be precleared to zero. The program treats LCM as an input-output storage device. Data is accessed to and from LCM in K-line groups. The dimensions of variables in LCM numbered COMMON blocks must be adjusted for each problem.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    M. L. Wilkins and J. A. Levatin
    Lawrence Livermore Laboratory

16. **MATERIAL AVAILABLE** -
    Source (14,240 lines)
    Sample problem (29 lines)
    Reference reports

17. **CATEGORY** - H
KEYWORDS - hydrodynamics, Navier-Stokes equations, two-dimensional, equations of state, finite difference method, Lagrange equations, elasticity, plasticity, fluid mechanics

18. **SPONSOR** - ERDA Division of Military Application

IDENTIFICATION AND KWIC TITLE - COMPARE-MOD1A
COMPARE-MOD1A, transient flow w/sinks & doors

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175, IBM3033

DESCRIPTION - COMPARE-MOD1A performs transient analysis of the thermodynamic conditions in zero velocity or stagnant volumes connected by flowing junctions with provision for mass and energy addition. Volume thermodynamics and junction flows are for homogeneous mixtures of: steam, two-phase water to its triple point, any three perfect gases, or combinations of the above. Vent flow can be based on the Moody equation, compressible polytropic orifice flow, and an incompressible subelement inertial relationship. Variable area doors and heat sinks can be modeled. Capabilities are incorporated to provide for accounting of loss coefficient detail, calculation of forces and moments, and plotting of results. The program was written to perform transient subcompartment analysis of nuclear power plants, including those with ice condensers.

METHOD OF SOLUTION - Volume thermodynamics and junction flows are determined independently in a quasi-static explicit manner. Mass and energy inflow or outflow accounting for each volume is done first for each time increment, assuming vent flows are constant. Thermodynamic equilibrium is assumed and state points determined. The resulting thermodynamic conditions are assumed constant and used to calculate the new vent flows between volumes for the next time interval.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -

100 volumes
200 junctions
5 mass and energy addition tables (blowdown sets)
10 variable area doors
500 heat sink nodal points
100 force-moment surfaces
100 junctions with detailed loss coefficient information
10,000 points plotted
5 curves per plot

Water temperature is restricted to the range of 273.16 to 620 degrees K (32.018 to 656 degrees F). Quality minimum is about 0.001. Time increment selection is important because too large a value may result in volume mass being less than or equal to zero. Options are available to guide the user in time increment selection.

TIMING - A two-volume, one-flow junction problem requires 0.002 second per time-step on the CDC7600. The sample problem requires 0.002 CP second per time-step on a CDC CYBER175. The sample problem runs in 2 seconds on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE - Ideal-like gas polytropic equations are used to calculate orifice flow, including losses. Two-phase water with air flow is calculated. Inertial effects and compressibility in the one-dimensional momentum equation are taken into account.

RELATED AND AUXILIARY SOFTWARE - COMPARE-MOD1A is an extension of COMPARE-MOD1, which was a later version of COMPARE (NESC 702), containing additional features. COMPARE-MOD1A uses an auxiliary program, GENPLT, to plot key parameters such as pressures, forces, and moments.

STATUS - Abstract first distributed December 1978.
CDC7600 version of COMPARE-MOD1 submitted January 1978, replaced May 1981 by COMPARE-MOD1A submitted August 1980, replaced February 1983 by revised Edition B, replaced April 1984 by revised Edition C, replaced October 1984 by revised Edition D, sample problem executed by NESC August 1984 on a CDC CYBER175.
IBM3033 version of COMPARE-MOD1A submitted November 1981, replaced October 1984 by revised Edition B, sample problem executed by NESC August 1984 on an IBM3033.

10. **REFERENCES** - R. G. Gido, G. J. E. Willcutt, Jr., J. L. Lunsford, and J. S. Gilbert, COMPARE-MOD 1 Code Addendum, NUREG/CR-1185, Addendum 1 (LA-7199-MS, Addendum), June 1980, and Attachment, September 25, 1980, revised August 1984.

COMPARE-MOD1A, NESC No. 776.7600D, COMPARE-MOD1A Tape Description and Implementation Information, National Energy Software Center Note 85-07, October 8, 1984.

R. G. Gido, J. S. Gilbert, R. G. Lawton, and W. L. Jensen, COMPARE-MOD 1: A Code for the Transient Analysis of Volumes with Heat Sinks, Flowing Vents, and Doors, LA-7199-MS (NRC-4), March 1978.

R. G. Gido, R. G. Lawton, C. I. Grimes, and J. A. Kudrick, COMPARE: A Computer Program for the Transient Calculation of a System of Volumes Connected by Flowing Vents, LA-NUREG-6488-MS, September 1976.

COMPARE-MOD1A, NESC No. 776.3033B, COMPARE-MOD1A Tape Description and Implementation Information, National Energy Software Center Note 85-05, October 8, 1984.

11. **HARDWARE REQUIREMENTS** - 157,000 (octal) words on a CDC7600, 153,000 (octal) words on a CDC CYBER175, 712K bytes on an IBM3033.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - LASL FTN operating system (similar to CDC SCOPE) (CDC7600), NOS2.2 (CDC CYBER175), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - NESC added a dummy TIMING routine to the CDC version for completeness. TIMING is a Los Alamos computing environment routine which should be replaced with an alternative suitable for the environment in which the program is implemented. For plotting, the auxiliary GENPLT program makes use of the Integrated Software Systems Corporation (ISSCO) proprietary graphics software product, DISSPLA.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600	R. G. Gido, G. J. E. Willcutt, Jr., J. L. Lunsford, and J. S. Gilbert Los Alamos National Laboratory
3033	K. J. Conrade Gibbs & Hill, Inc.
3033 GENPLT	M. Birgersson and L. Eyberger National Energy Software Center Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    - Source (7600D-5371 lines, 3033B-5990 lines)
    - Sample problem input (120 lines)
    - Sample problem output (3033B-18 pages)
    - Auxiliary program (GENPLT 7600D-381 lines, 3033B-444 lines)
    - Control information (3033B-89 lines)
    - Reference report, LA-7199-MS, Addendum, Attachment, and NESC Note, appropriate to version

17. **CATEGORY** - H
    KEYWORDS - reactor safety, containment systems, pressure gradients, transients, fluid flow, moment of inertia, thermodynamics, heat transfer, pressure, temperature, PWR reactors, COMPARE codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
    Division of Systems Integration

1. **IDENTIFICATION AND KWIC TITLE** - PROSA2
   PROSA2, probabilistic response surface studies

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM370

3. **DESCRIPTION** - PROSA2 is an implementation of the probabilistic response surface technique developed for obtaining probability distributions of the consequences of postulated nuclear reactor accidents. The problem is to find the distribution of a random variable that is a function of many other random variables when this functionality is not known in analytical form and can be obtained only numerically through parametric studies with a deterministic computer code.
   The program performs the following three main functions:
   (a) Selects values for the input parameters of a deterministic computer code from an input-specified region of interest. The regions are defined by probability distributions and confidence intervals. The program arranges the input values into combinations called "knot-points".
   (b) With output values ("consequences") from the deterministic code for each input-parameter combination, determines response surfaces approximating the functionality between the input and output of the deterministic code.
   (c) Calculates the probability distribution of the output (consequence) variable as a histogram using Monte Carlo sampling.

   Step (a) is omitted if the user uses his own design of knot-points. Both steps (a) and (b) can be omitted if a known analytical function is to be sampled.
   PROSA2 has been used mainly in conjunction with accident-analysis codes, but the methods and the programming are completely general and not limited to such applications.

4. **METHOD OF SOLUTION** - As input data, the program needs the probability distributions of the input parameters of a deterministic code (for which a response surface is being searched). The first part of the program calculates knot-point coordinates. These serve as input for the deterministic code that calculates the values of interesting output variables (consequences) at the specified knot-points. The output/consequence values at the knot-points are used in the second part of PROSA2 to determine (1) global or regionwise response-surfaces by using least squares fitting or generalized Lagrange interpolation, (2) the errors of the fitted response-surfaces, (3) the sensitivity/importance of each input parameter, (4) statistical moments of the input parameters and those of the consequences, and (5) the correlation coefficients between the consequences. By using random sampling of the input parameters and simulation with the response-surface the program calculates (6) the probability distributions as histograms, (7) sample moments of the consequence distributions, (8) joint distributions, and (9) the statistical-error estimates for the histograms. The distributions are obtained in forms of histogram tables with 12 categories and plots in 26 categories. The joint distributions have 12 x 12 or 144 categories. The width of each category is a user-specified fraction of the standard deviations of the consequences. The program includes a technique to handle nonindependent, or correlated, input parameters. Conditional distributions can also be calculated. Up to four simultaneous criteria or conditions can be specified for the consequences. By defining one or more input parameters to be consequences as well, PROSA2 can be used for calculating optimal importance distributions for the input parameters.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of 12 variable input parameters and 6 consequence variables that can be analyzed simultaneously. Eight different distributions are available for the input parameters, including uniform, exponential, normal, truncated normal, log normal, and beta distributions. Any correlations between the input parameters are limited to linear correlations.

For fitting second-degree response-surfaces, the number of randomly selected knot-points should be specified to be at least (n+1)(n+2)/2, where n is the number of input parameters. For third-degree surfaces the limit is (n+1)(n+2)(n+3)/6.

6. **TIMING** - Typical running time for six input parameters and six consequence variables is 60 seconds on an IBM370/195 for 40,000 simulations.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The program includes a weighting scheme that generates a smooth global response-surface from regionwise response-surfaces. A family of functional transformations is available for both input and output (consequence) variables so that essentially non-polynomial response-surfaces can be generated and used. Optimal transformations can be searched due to the error estimation routines in the program. Both systematically and randomly selected knot-points can be used. Least squares fitting and generalized Lagrange interpolation can be used to find the coefficients of a response-surface. Conditional distributions with random conditions can be calculated.

8. **RELATED AND AUXILIARY SOFTWARE** - PROSA2 represents an advanced release of the earlier PROSA1 program. The PROSA programs are designed for use in conjunction with a deterministic/mechanistic accident analysis code, such as VENUS, SAS, or RELAP. The first part of PROSA provides input to the accident analysis code, which in turn provides input to the second part of PROSA.

9. **STATUS** - Abstract first distributed August 1978.
IBM370 version of PROSA1 submitted April 1978, replaced by revised Edition B August 1980, replaced August 1982 by PROSA2 submitted December 1980, sample problem executed by NESC February 1981 on an IBM370/195.

10. **REFERENCES** - J. K. Vaurio and J. Fletcher, PROSA-2: A Probabilistic Response-Surface Analysis and Simulation Code, ANL-81-33, May 1981.

PROSA2, NESC No. 778, PROSA2 Sample Problem Output, National Energy Software Center Note 82-113, August 27, 1982.

J. K. Vaurio and C. Mueller, PROSA-1: A Probabilistic Response-Surface Analysis Code, ANL-78-56, June 1978.

L. Mattila, R. Sairanen, and J. Vaurio, Probabilistic Analysis of LWR LOCA: Fuel Damage and Radioactivity Release, Transactions of the American Nuclear Society, Vol. 30, pp. 409-411, 1978.

J. K. Vaurio, Response Surface Techniques Developed for Probabilistic Analysis of Accident Consequences, Proceedings of the American Nuclear Society Topical Meeting on Probabilistic Analysis of Nuclear Reactor Safety, May 8-10, Los Angeles, California, 1978.

11. **HARDWARE REQUIREMENTS** - 370K bytes of storage, system input, output, and punch units are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (95%) and Assembly language (5%)

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program contains a few FORMAT statements using T format as well as ERR= and END= parameters in READ statements (IBM extensions to ANSI FORTRAN).

PROSA obtains random numbers U (uniformly distributed between 0 and 1) using the FLTRNF function subprogram supplied as an Assembly language routine. Other random variates are calculated from U.

Variable dimensioned arrays are used in the program's least squares fitting procedure. Their size is determined by the number of parameters and the number of output (consequence) variables in each job. Routines are included to provide dynamic storage allocation as well as an abnormal termination dump. These routines, ALLOC2, LOCF, and ABEND, are part of the ANL computing environment and should be replaced with suitable alternative routines in the local computing environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. K. Vaurio

Fast Reactor Safety Technology Management Center
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 5768 lines, Assembly language 365 lines)
Sample problem (90 lines)
Reference report, ANL-81-33, and NESC Note

17. **CATEGORY** - G
KEYWORDS - accidents, risk assessment, Monte Carlo method, fast reactors, reactor safety, response functions, sensitivity, simulation, probability

18. **SPONSOR** - DOE Division of Reactor Research and Technology

IDENTIFICATION AND KWIC TITLE - IMPORTANCE
IMPORTANCE, FTA basic event & cut set ranking

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370

DESCRIPTION - IMPORTANCE computes various measures of probabilistic importance of basic events and minimal cut sets to a fault tree or reliability network diagram. The minimal cut sets, the failure rates and the fault duration times (i.e., the repair times) of all basic events contained in the minimal cut sets are supplied as input data. The failure and repair distributions are assumed to be exponential. IMPORTANCE, a quantitative evaluation code, then determines the probability of the top event and computes the importance of minimal cut sets and basic events by a numerical ranking. Two measures are computed. The first describes system behavior at one point in time; the second describes sequences of failures that cause the system to fail in time. All measures are computed assuming statistical independence of basic events. In addition, system unavailability and expected number of system failures are computed by the code.

METHOD OF SOLUTION - Seven measures of basic event importance and two measures of cut set importance can be computed. Birnbaum's measure of importance (i.e., the partial derivative) and the probability of the top event are computed using the min cut upper bound. If there are no replicated events in the minimal cut sets, then the min cut upper bound is exact. If basic events are replicated in the minimal cut sets, then based on experience the min cut upper bound is accurate if the probability of the top event is less than 0.1.

Simpson's rule is used in computing the time-integrated measures of importance. Newton's method for approximating the roots of an equation is employed in the options where the importance measures are computed as a function of the probability of the top event, and a shell sort puts the output in descending order of importance.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING - The test cases executed in about 1 second on the IBM370/195.

UNUSUAL FEATURES OF THE SOFTWARE - For systems where repair is not allowed, the code accepts proportional hazards as input data. In another option, where repair is permitted, failure rate data can also be expressed in relative terms by representing the failure rate and repair rate data for the basic events in terms of a reference time unit.

RELATED AND AUXILIARY SOFTWARE - Other qualitative evaluation programs for system safety and reliability analysis are MOCUS (NESC 653), PREP (NESC 528), COMCAN (NESC 704), SETS (NESC 623), FTA (NESC 666), and FTAP, Department of Operations Research, Berkeley. A discussion of these and others is contained in reference 2.

The IMPORTANCE program was originally developed on the CDC7600 by Howard E. Lambert at Lawrence Livermore Laboratory, and was later converted to the IBM370 by T. Chawla and G. Hauser of the Reactor Analysis and Safety Division at Argonne National Laboratory.

STATUS - Abstract first distributed August 1978.
IBM370 version submitted April 1977, sample problem executed by NESC July 1978 on an IBM370/195.

REFERENCES - H. E. Lambert, Fault Trees for Decision Making in Systems Analysis, UCRL-51829, October 9, 1975 (Ph.D. Thesis).

Howard E. Lambert and Frank M. Gilman, The IMPORTANCE Computer Code, UCRL-79269 (Preprint), March 14, 1977.

H. E. Lambert and B. J. Davis, The Use of the Computer Code IMPORTANCE with SETS Input, NUREG/CR-1965 (SAND81-7068), March 1981.

HARDWARE REQUIREMENTS - Execution of the sample problem required 140K bytes of storage.

PROGRAMMING LANGUAGE - FORTRAN IV

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program uses logical unit 8 as a storage device.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
H. W. Lambert
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (1586 lines)
Sample problem (123 lines)
Reference reports

17. **CATEGORY** - G
KEYWORDS - fault tree analysis, reliability, system failure analysis, probability, MOCUS codes, FTA codes, PREP codes, COMCAN codes, SETS codes

18. **SPONSOR** - Lawrence Livermore Laboratory
NRC Office of Nuclear Regulatory Research

IDENTIFICATION AND KWIC TITLE - NALAP
NALAP, LMFBR transient response to accident

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER76

DESCRIPTION - NALAP is an LMFBR system transient code. This code, adapted from the light water reactor transient code RELAP3B, simulates thermalhydraulic response of sodium-cooled fast breeder reactors when subjected to postulated accidents such as a massive pipe break as well as a variety of other upset conditions that do not disrupt the system geometry.

METHOD OF SOLUTION - Various components of the plant are represented by control volumes. These control volumes are connected by junctions, some of which may be leak or fill junctions. The fluid flow equations are modeled as compressible, single-stream flow with momentum flux in one dimension. The transient response is computed by integrating the thermal-hydraulic conservation equations from user-initialized operating conditions by an implicit numerical scheme. The point-kinetics approximation is used to represent the time-dependent heat generation in the reactor core.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
40 control volumes
50 connecting junctions
6 thermal properties
25 pressures
13 liquid temperatures per pressure
6 gas temperatures per pressure
Pressure table values must be greater than zero and less than or equal to 7000 psia. The pressure table restrictions may be altered by modifying DIMENSION statements.

TIMING - A 27-volume, 32-junction problem took approximately 32 milliseconds per time-step on a CDC7600. Typically, the time-step for a double-ended pipe break case was 0.05 millisecond near the break time. Beyond 0.3 millisecond after the break, the time-step was increased to 0.5 millisecond. The four sample problems were executed in 6 CP minutes on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE - NALAP allows some volumes (typically in a secondary and/or tertiary loop) to contain water or steam. In fact, all volumes may contain water, in which case NALAP can be used as RELAP3B.

RELATED AND AUXILIARY SOFTWARE - Predecessors to this program are the INEL RELAP editions, RELAP2 and RELAP3 (NESC 369), and RELAP3B (NEC Abstract 733).

STATUS - Abstract first distributed September 1978.
CDC7600 version submitted December 1975, sample problem executed by NESC August 1978 on a CDC7600.

REFERENCES - B. A. Martin, A. K. Agrawal, D. C. Albright, L. G. Epel, and G. Maise, NALAP An LMFBR System Transient Code, BNL 50457, July 1975.
K. V. Moore and W. H. Rettig, A Digital Program for Reactor Blowdown and Power Excursion Analysis, IDO-17263, March 1968.
W. H. Rettig, G. A. Jayne, K. V. Moore, C. E. Slater, and M. L. Uptmor, RELAP3--A Computer Program for Reactor Blowdown Analysis, IN-1321, June 1970.

HARDWARE REQUIREMENTS - CDC7600 (or CYBER76) with 142,000 (octal) words of memory. In addition to card input and printer output, a FORTRAN logical unit 1 may be used for the automatic time-step option, and units 2, 3, and 4 may be used under the restart option. These units may be assigned to disk or tape.

PROGRAMMING LANGUAGE - FORTRAN IV (99%) and COMPASS (1%)

OPERATING SYSTEM - SCOPE 2.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – The following non-ANSI language extensions were used:
    OVERLAY statements and calls.
    ENCODE and DECODE statements to prepare output page headings.
    PROGRAM statements to specify file assignments.
    Non-ANSI system routines called:
    EOF--returns nonzero value when end-of-file reached.
    REMARK--places message on DAYFILE.
    DATE--returns calendar date in the form mm/dd/yy.
    TIME--returns time of day in the form hh.mm.ss.
    SECOND--returns CP time used.
    SHIFT--performs a left or right binary shift.
    If all of these are replaced by dummy routines, only the page headings are affected. A COMPASS routine named WHEN is included which may be removed for non-7600 environments. For restart problems, the data is read from TAPE3 and is written to TAPE4.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
    B. A. Martin, A. K. Agrawal, D. C. Albright,
    L. G. Epel, and G. Maise
    Department of Applied Sciences
    Brookhaven National Laboratory

16. **MATERIAL AVAILABLE** –
    Source (23,504 lines)
    Sample problem (438 lines)
    Sample problem output (2 microfiche)
    Reference report, BNL 50457

17. **CATEGORY** – G
    KEYWORDS – transients, accidents, pipes, kinetics, fluid flow, design basis accidents, heat transfer, hydraulics, reactor cooling systems, ruptures, LMFBR reactors, RELAP codes

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research,
    Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - DOE2.1C, DOE2.1B
DOE2.1B, building energy consumption analysis
DOE2.1C, building energy consumption analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,6600,CYBER175, IBM370,303x, DEC10,20, DEC VAX11/780

DESCRIPTION - DOE2 is a set of computer programs for the analysis of energy consumption in buildings. Programs are included to calculate the heating and cooling loads for each space (zone) in the building for each hour of a year (LOADS), to simulate the operation and response of the equipment and systems that control temperature and humidity and distribute heating and cooling to the space (SYSTEMS), to model primary energy conversion equipment that uses fuel (e.g. oil, gas, or sun) to provide the required heating, cooling, and electricity (PLANT), and to compute the life-cycle cost for building operation based on economic parameters (ECONOMICS). A user-oriented building description language (BDL) facilitates the description of the building geometry, its central plant equipment, its HVAC systems, occupancy, equipment, and lighting schedules, and the selection of other problem parameters. In addition to the LSPE programs (LOADS, SYSTEMS, PLANT, and ECONOMICS), the system includes the BDL processor, two report generators, a weather data processor, and UPDATE, a code maintenance program. Standard output reports are produced by the RPTGEN program. Only the weather data for Chicago, which are required for execution of the sample problems, are included.

METHOD OF SOLUTION - The LOADS program computes hourly space loads resulting from transmission gains and losses through walls, roofs, floors, doors, and windows; solar gains through windows; internal gains from occupants, lighting, and equipment; and infiltration gains and losses caused by pressure differences across openings. The LOADS calculations are based on ASHRAE algorithms, including the response factor technique for calculating transient heat flow through walls and roofs and the weighting factor technique for calculating heating and cooling loads. In addition, custom weighting factors can be calculated for the building in question. Interior daylight illuminance levels are determined hourly and the reduction in electric lighting energy from the use of daylighting is calculated. The SYSTEMS program takes the hourly space loads calculated by LOADS, along with characteristics of the secondary HVAC equipment selected by the user from a list of available system types, and component and control features and thermal characteristics of the zone, and determines the actual room temperature and heat extraction or addition rates using ASHRAE algorithms. The PLANT program uses the building thermal energy load data determined by SYSTEMS and data specifying the type, size, control conditions, and operating parameters of the plant equipment provided by the user, to allocate available equipment and simulate their operation. The PLANT program simulates conventional central plants, solar heating and cooling systems, and plants with on-site generation and waste heat recovery. It also permits load management of plant equipment and energy storage as well as optimal allocation of equipment minimizing source-Btu. It calculates the monthly and annual cost and the amount of each type of fuel used, the daily electrical load profile, and the energy consumption at the site and at the source. The life-cycle costing methodology used in the ECONOMICS program is derived from DOE guidelines. Life-cycle costing method investment statistics (i.e. cost savings, savings-to-investment ratio, energy savings, energy savings-to-investment ratio, and discounted payback period) are calculated to provide a measure for comparing the cost effectiveness of each case against a reference case. The DOE2.1C ECONOMICS has additions that allow the modeling of demand charges, time-of-day charges, seasoned charges, ratchet periods, and sell back of electricity to the utility

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The LOADS program allows the user to configure an arbitrary structure composed of walls, roofs, doors, windows, floors, ceilings, and thermal spaces. The user can specify scheduled occupancy, lighting, electric, and equipment loads in each space. Simulations available in SYSTEMS are a single-zone fan system with optional subzone reheat, multizone fan system, dual-duct fan system, ceiling induction system, unit heater, unit ventilator, floor-panel heating system, two-pipe fan-coil system, four-pipe fan-coil system, two-pipe induction unit system, four-pipe induction unit system, variable-volume fan system with optional reheat, constant-volume reheat fan system, unitary hydronic heat pump, heating and ventilating system,

ceiling bypass variable volume system, residential system, packaged single-zone air conditioner with heating and subzone reheating options, packaged multizone fan system, packaged variable air volume system, and packaged terminal air conditioner. Components which can be modeled by the PLANT program include gas and steam turbines, diesel engine, steam, hot water, and electric boilers, one-stage and two-stage absorption chillers, hermetic and open, centrifugal and reciprocating compression chillers, double-bundle chillers, electric and fossil-fuel domestic hot water heaters, electric and fossil-fuel fired furnaces, and hot and cold water storage tanks. CBS, a part of the PLANT program, simulates solar air and liquid, flat-plate and concentrating collectors with associated controls, heat exchangers, hot tanks, pumps, fans, pipes, and duct-work. Four preassembled solar systems, both commercial and residential, are available. Any loads not met because of insufficient capacity are reported.

The number of the different types of BDL instructions allowed in a single run are limited to maxima of -

128 walls and roofs
128 windows
128 interior walls or ceilings
64 underground walls or floors
64 spaces
64 doors
40 air distribution systems
40 schedules
6 different sizes of each type of primary plant equipment
5 different fuel or utility types

These maxima can be changed (without recompilation) by running a utility program.

6. **TIMING** - 3 to 5 CP seconds are required for each thermal zone for a one-year analysis. The sample problems took 21 minutes of CP time on a CDC CYBER175, 814 CPU seconds on an IBM3033, more than 1 hour on a DEC10, and 169 minutes on a DEC VAX11/780.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The Building Description Language (BDL) is designed to assist the user in the effective application of the system. This command-word-structured, free-format language can greatly simplify the definition of a model for a given building and manipulation of the model components to produce an energy-conservative design.

8. **RELATED AND AUXILIARY SOFTWARE** - SOLSYS (NESC 692), SOLTES1 (NESC 841), the NASA-NECAP program (NASA CR-2590), the NBS NBSLD program (NBSIR 74-574), the DOD BLAST3.0 program (NESC 9990), and the University of Wisconsin TRNSYS program. DOECTZDATA (NESC 982) contains the 16 California climate zone CTZ weather data in machine-independent format for use with DOE2. This weather information is required for use with DOE2 to obtain a California building permit.

9. **STATUS** - Abstract first distributed September 1978.
CDC7600 version of DOE1 submitted June 1978, replaced by DOE2.0 April 1979 for special release only, replaced August 1979 by DOE2.0A as revised July 1979, replaced September 1980 by DOE2.1, replaced November 1981 by DOE2.1A submitted June 1981, replaced September 1983 by DOE2.1B, replaced November 1985 by DOE2.1C, sample problems executed by NESC September 1985 on a CDC CYBER170/875.
IBM370 version of DOE2.1 submitted October 1980, revised January 1981, replaced February 1982 by DOE2.1A, replaced January 1984 by DOE2.1B, sample problems executed by NESC December 1983 on an IBM3033.
DEC VAX11 version of DOE2.1A submitted January 1982, replaced September 1983 by DOE2.1B, replaced November 1985 by DOE2.1C, sample problems executed by NESC September 1985 on a DEC VAX11/780.
DEC10 version of DOE2.1A submitted October 1981, sample problems executed by NESC April 1982 on a DEC20, replaced November 1985 by DOE2.1C.

10. **REFERENCES** - Building Energy Analysis Group, Lawrence Berkeley Laboratory, DOE-2 USERS GUIDE Version 2.1A, LBL-8689 Rev. 2, May 1981.
Building Energy Analysis Group, Lawrence Berkeley Laboratory, DOE-2 SAMPLE RUN BOOK Version 2.1A, LBL-8678, Rev. 2, May 1981.

Group Q-11, Los Alamos National Laboratory, and Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 REFERENCE MANUAL, Parts 1 and 2, LBL-8706 Rev. 3, January 1983.

Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 SUPPLEMENT Version 2.1B, LBL-8706, Rev. 3 Suppl., January 1983.

Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 BDL SUMMARY Version 2.1B, LBL-8688, Rev. 3, January 1983.

Group Q-11, Los Alamos National Laboratory, and Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 REFERENCE MANUAL, Parts 1 and 2, LBL-8706 Rev. 4, May 1984.

Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 SUPPLEMENT Version 2.1C, LBL-8706, Rev. 4 Suppl., May 1984.

Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 BDL SUMMARY Version 2.1C, LBL-8688, Rev. 4, May 1984.

Building Energy Simulation Group, Lawrence Berkeley Laboratory, DOE-2 SAMPLE RUN BOOK Version 2.1C, LBL-8678, Rev. 2, May 1984.

NESC No. 782, DOE2.1A Documentation Updates from DOE-2 User News, February 1983, National Energy Software Center Note 83-49, March 14, 1983.

DOE2.1C, NESC No. 782.7600, DOE2.1C CDC Version Tape Description, Implementation Instructions, and Programming Information, National Energy Software Center Note 86-12, November 27, 1985.

DOE2.1B, NESC No. 782.370, DOE2.1B IBM Version Tape Description, Implementation Instructions, and Programming Information, National Energy Software Center Note 84-09, January 13, 1984.

DOE2.1C, NESC No. 782.DE10, DOE2.1C DEC10 Version Tape Description, Implementation Instructions, and Programming Information, National Energy Software Center Note 86-14, November 27, 1985.

DOE2.1C, NESC No. 782.VX11, DOE2.1C DEC VAX11 Version Tape Description, Implementation Instructions, and Programming Information, National Energy Software Center Note 86-13, November 27, 1985.

M. Lokmanhekim, ASHRAE Task Group on Energy Requirements for Heating and Cooling of Buildings, Procedure for Determining Heating and Cooling Loads for Computerizing Energy Calculations, Algorithms for Building Heat Transfer Subroutines, American Society of Heating, Refrigerating, and Air Conditioning Engineers, 1971.

W. F. Stoecker, ASHRAE Task Group on Energy Requirements for Heating and Cooling of Buildings, Procedures for Simulating the Performance of Components and Systems for Energy Calculations, American Society of Heating, Refrigerating, and Air Conditioning Engineers, 1975.

Life Cycle Costing, Emphasizing Energy Conservation, ERDA 76/130, September 1976, Revised May 1977.

1977 ASHRAE Handbook of Fundamentals, American Society of Heating, Refrigerating, and Air Conditioning Engineers.

J. Duffie and W. Beckman, Solar Energy Thermal Processes, John Wiley and Sons, New York, 1974.

J. F. Kerrisk, Weighting Factors in the DOE-2 ENGINEERS MANUAL Version 2.1A, LBL-11353, (LA-8520-M), DE83 004575, November 1, 1981.

Richard B. Curtis, The Theoretical Basis of the DOE-2 Building Energy-Use Analysis Program, LBL-12300, DE81 028896, April 1981.

James J. Hirsch, Simulation of HVAC Equipment in the DOE-2 Program, LBL-14026, DE83 011560, December 1982.

Stephen Selkowitz, Jong-Jin Kim, Mojtaba Novvab, and Frederick Winkelmann, The DOE-2 and Superlite Daylighting Programs, LBL-14569, DE82 018533, June 1982.

F. C. Winkelman, Daylighting Calculations in DOE-2, LBL-11353, May 1983.

Bruce Birdsall, A Comparison of DOE2.1C Prediction with Thermal Mass Test Cell Measurements, LBL-18981, January 1985.

Overview of the DOE-2 Building Energy Analysis Program, LBL-19735, June 1985.

HARDWARE REQUIREMENTS - The CDC version of DOE2.1C requires 200,000 (octal) words of program storage for execution of the sample problems. The IBM version of DOE2.1B requires 1356K bytes of memory. The DEC VAX11 version of DOE2.1C requires 915K bytes of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN (CDC and DEC versions); the IBM version is all FORTRAN with the exception of NESC-supplied TIME and DATE routines.

13. **OPERATING SYSTEM** - NOS 2.2 (CDC CYBER170), OS/370 (IBM3033,370), VMS 3.5, 4.2 (DEC VAX11), and TOPS-10 (DEC10).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

J. J. Hirsch and W. F. Buhl
Building Energy Simulation Group
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -

ALL MACHINE VERSIONS - DOE2.1B RELEASE

Source (BDLSRC 18,186 lines, BDLMOD 95 lines, SIMSRC 1068 lines, SIMMOD 2 lines, LDSSRC 9828 lines, LDSMOD 100 lines, SYSSRC 10,619 lines, SYSMOD 25 lines, PLTSRC 7211 lines, PLTMOD 7 lines, CBSSRC 4046 lines, CBSMOD 2 lines, ECOSRC 655 lines, ECOMOD 2 lines, REPSRC 918 lines, REPMOD 2 lines, HRPSRC 949 lines, HRPMOD 2 lines, CBSSRC7 3937 lines)

Sample problems (SAMPIN 3830 lines, SAMPIN2 3830 lines, TRY Chicago weather file 8760 lines)

Auxiliary routines and information (UPDATE 1878 lines, UPDSRC 1673 lines, UPDMOD 97 lines, KEYSRC 605 lines, KEYMOD 2 lines, KEYCRD 2053 lines, KEYCMOD 2 lines, CLCSRC 1093 lines, CLCMOD 2 lines, CLCCRD 1886 lines, CLCCMOD 2 lines, RLCSRC 189 lines, RLCMOD 2 lines, REPCRD 2363 lines, REPCMOD 12 lines, WTHSRC 4581 lines, WTHMOD 10 lines, EDTSRC 254 lines, EDTMOD 2 lines, EDTCRD 1157 lines, EDTCMOD 2 lines, PRGSRC 251 lines, PRGMOD 2 lines, LIBIN 477 lines, LIBIN2 477 lines, WTHIN 9 lines, WTHIN2 9 lines, UPPDOC 514 lines, KEYCARD 2044 lines, CLCCARD 1881 lines, REPCARD 2357 lines, EDTCARD 1152 lines)

IBM370

Source (IBM4 338 lines, IBM9 165 lines, IBM10 50 lines, IBM11 47 lines, IBM12 37 lines, IBM13 20 lines, IBM14 12 lines, IBM15 42 lines, IBM16 23 lines, IBM17 14 lines, BDLCOMP 20,207 lines, SIMCOMP 984 lines, LDSCOMP 11,132 lines, SYSCOMP 11,794 lines, PLTCOMP 7708 lines, CBSCOMP 4287 lines, ECOCOMP 679 lines, REPCOMP 914 lines, HRPCOMP 999 lines)

Sample problems (SAMPIN2 3830 lines, WTHIN60 479 lines)

Auxiliary routines and information (INDEX 649 lines, UPDATE 1883 lines, IBM3 73 lines, IBM5 16 lines, DKEY.IBM 1 line, IBM7 40 lines, DCLC.IBM 1 line, IBMFILE18 1 line, IBM19 19 lines, DRLC.IBM 1 line, IBM21 187 lines, IBM22 58 lines, DEPT.IBM 1 line, IBM24 67 lines, LIBIN2 477 lines, WTHIN2 9 lines, KEYCOMP 601 lines, CLCCOMP 1327 lines, RLCCOMP 160 lines, WTHCOMP 4633 lines, EDTCOMP 251 lines, PRGCOMP 255 lines)

Sample problems output (tape-compatible output of sample problems)

Reference reports, LBL-8706 Rev. 3 and Suppl., LBL-8678 V2.1A Rev. 2, LBL-8688 Rev. 3, LBL-8689 Rev. 2, and NESC Notes 83-49 and 84-09

ALL MACHINE VERSIONS - DOE2.1C RELEASE

Source (BDLSRC 21,984 lines, SIMSRC 1420 lines, LDSSRC 12,441 lines, SYSSRC 14,534 lines, PLTSRC 8213 lines, CBSSRC 4046 lines, ECOSRC 2217 lines, ECOMOD 1 line, REPSRC 924 lines, HRPSRC 1047 lines, HRPMOD 1 line)

Sample problems (SAMPIN 3827 lines, TRY Chicago weather file 8760 lines)

Auxiliary routines and information (UPDATE 1878 lines, UPDSRC 1673 lines, KEYSRC 766 lines, KEYMOD 1 line, DKEY 3921 lines, DKEYMOD 1 line, CLCSRC 1093 lines, CLCMOD 1 line, DCLC 1886 lines, DCLCMOD 1 line, LDSDOC 10,500 lines, RLCSRC 189 lines, RLCMOD 1 line, DRLCSRC 2451 lines, DRLCMOD 13 lines, WTHSRC 4718 lines, WTHMOD 1 line, EDTSRC 254 lines, EDTMOD 1 line, DEDT 1411 lines, DEDTMOD 1 line, PRGSRC 253 lines, PRGMOD 1 line, UPDDOC 514 lines, INDEXMOD 241 lines, LIBIN 477 lines, WTHIN 9 lines)

CDC7600

Source (BDLMOD 40 lines, SIMMOD 12 lines, LDSMOD 92 lines, SYSMOD 87 lines, PLTMOD 6 lines, REPMOD 8 lines, BDLCOMP 24,384 lines, SIMCOMP 1409 lines, LDSCOMP 13,950 lines, SYSCOMP 16,192 lines, PLTCOMP 8906 lines, CBSCOMP 4289 lines, ECOCOMP 2382 lines, REPCOMP 918 lines, HRPCOMP 1093 lines)

Auxiliary routines and information (KEYCOMP 758 lines, KEYCARD 3908 lines, CLCOMP 1325 lines, CLCCARD 1881 lines, RLCCOMP 181 lines, REPCARD 2445 lines, WTHCOMP 4977 lines, EDTCOMP 245 lines, EDTCARD 1406 lines, PRGCOMP 245 lines)
Sample problems output (tape-SAMPOUT complete output of sample problems)
Reference reports, LBL-8706 Rev. 4 and Suppl., LBL-8678 V2.1C Rev. 2, LBL-8688 Rev. 4, LBL-8689 Rev. 2, and NESC Notes 83-49 and 86-12

DEC VAX11
Source (BDLMOD 37 lines, LDSMOD 85 lines, SYSMOD 79 lines, BDL.VAX 430 lines, SIM.VAX 178 lines, LDS.VAX 41 lines, SYS.VAX 36 lines, PLT.VAX 26 lines, CBS.VAX 34 lines, ECO.VAX 114 lines, REP.VAX 54 lines, HRP.VAX 28 lines, BDLCOMP 24,358 lines, SIMCOMP 1399 lines, LDSCOMP 13,954 lines, SYSCOMP 16,157 lines, PLTCOMP 8901 lines, CBSCOMP 4293 lines, ECOCOMP 2398 lines, REPCOMP 926 lines, HRPCOMP 1097 lines)
Auxiliary routines and information (INDEX.VAX 664 lines, UPDATE 1885 lines, UPD.VAX 111 lines, KEY.VAX 112 lines, CLC.VAX 56 lines, RLC.VAX 22 lines, WTH.VAX 249 lines, EDT.VAX 59 lines, PRG.VAX 1 line, WTHIN.VAX 9 lines, KEYCOMP 787 lines, CLCCOMP 1345 lines, CLCCARD 1881 lines, RLCCOMP 170 lines, REPCARD 2445 lines, WTHCOMP 4821 lines, EDTCOMP 242 lines)
Sample problems output (tape-complete output of sample problems)
Reference reports, LBL-8706 Rev. 4 and Suppl., LBL-8678 V2.1C Rev. 2, LBL-8688 Rev. 4, LBL-8689 Rev. 2, User News, and NESC Notes 83-49 and 86-13

DEC10
Source (BDLMOD 37 lines, LDSMOD 85 lines, SYSMOD 79 lines, BDL.PDP 448 lines, SIM.PDP 194 lines, LDS.PDP 43 lines, SYS.PDP 37 lines, PLT.PDP 27 lines, CBS.PDP 37 lines, ECO.PDP 50 lines, REP.PDP 56 lines, HRP.PDP 28 lines)
Auxiliary routines and information (INDEX.PDP 566 lines, UPDATE 1881 CARDS, UPD.PDP 107 lines, KEY.PDP 113 lines, CLC.PDP 57 lines, RLC.PDP 41 lines, WTH.PDP 255 lines, EDT.PDP 57 lines, PRG.PDP 58 lines, WTHIN.PDP 9 lines)
Sample problems output (tape-complete output of sample problems)
Reference reports, LBL-8706 Rev. 4, LBL-8678 V2.1C Rev. 2, LBL-8688 Rev. 4, LBL-8689 Rev. 2, and NESC Note 83-49 and 86-14

17. **CATEGORY** - T
KEYWORDS - air conditioning, boilers, buildings, construction, control systems, economics, energy analysis, energy consumption, life-cycle cost, lighting systems, daylighting, operation, roofs, site selection, space heating, systems analysis, ventilation, walls, weather, SOLTES1 codes, NASA-NECAP codes, NBSLD codes, BLAST3.0 codes, TRNSYS codes, DOECTZDATA codes

18. **SPONSOR** - DOE Office of Buildings Energy R&D,
Buildings System Division

IDENTIFICATION AND KWIC TITLE - DSNP
DSNP, dynamic simulation nuclear power plants

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370

DESCRIPTION - DSNP (Dynamic Simulator for Nuclear Power-Plants) is a system of programs and data files by which a nuclear power plant, or part thereof, can be simulated. The acronym DSNP is used interchangeably for the DSNP language, the DSNP libraries, the DSNP precompiler, and the DSNP document generator.

The DSNP language is a special-purpose, block-oriented digital-simulation language developed to facilitate the preparation of dynamic simulations of a large variety of nuclear power plants. It is a user-oriented language that permits the user to prepare simulation programs directly from power plant block diagrams and flow charts by recognizing the symbolic DSNP statements for the appropriate physical components and listing these statements in a logical sequence according to the flow of physical properties in the simulated power plant.

Physical components of nuclear power plants are represented by functional blocks, or modules. Many of the more complex components are represented by several modules. The nuclear reactor, for example, has a kinetic module, a power distribution module, a feedback module, a thermodynamic module, a hydraulic module, and a radioactive heat decay module. These modules are stored in DSNP libraries in the form of a DSNP subroutine or function, a block of statements, a macro, or a combination of the above. Basic functional blocks such as integrators, pipes, function generators, connectors, and many auxiliary functions representing properties of materials used in nuclear power plants are also available.

The DSNP precompiler analyzes the DSNP simulation program, performs the appropriate translations, inserts the requested modules from the library, links these modules together, searches necessary data files, and produces a simulation program in FORTRAN. FORTRAN is considered to be a subset of DSNP and can be inserted anywhere in the simulation program without restriction. I/O statements can be located anywhere in the program in arbitrary sequence. No formatting is required and the listed variables are printed at user-defined intervals in an easy-to-read tabular form.

METHOD OF SOLUTION - The mathematical models used vary from one component module to another. Mostly, however, lumped parameter models were used. The differential equations produced by each component module are solved by a centralized integration scheme. The various loops of the power plant can be solved with different integration schemes using different time-step sizes. Any of eight integration schemes including Adams' 2nd-order, Euler, Milne's 5th-order predictor-corrector, Runge-Kutta 4th-order, Simpson 3rd-order, trapezoidal, and the method used in CSMP III can be selected. DSNP is written in double-precision, and all units are SI metric.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Only overall plant transients can be studied since most models are based on the lumped parameter approximation. For detailed transients inside the core, heat exchanger, or any other component, more sophisticated Level-2 or Level-3 libraries will be developed in the future.

TIMING - Running time is a function of the size of the simulation. The precompilation time is approximately 50 seconds per 1000 FORTRAN statements.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - The auxiliary program, MINIEDITOR, included in the DSNP package is used to change precompiler translation tables.

STATUS - Abstract first distributed January 1979.
IBM370 version submitted September 1978, sample problems executed by NESC December 1978 on an IBM370/195.

REFERENCES - D. Saphier, The Simulation Language of DSNP, ANL-CT-77-20 Rev. 02, September 1978.

D. Saphier, The Level One Modules Library for DSNP, ANL-CT-77-21 Rev. 02, September 1978.

D. Saphier, The Precompiler for DSNP, ANL-CT-77-22 Rev. 02, September 1978.

D. Saphier, MINIEDITOR, ANL-CT-77-18 Rev. 02, August 1978.

D. Saphier, A Simulation Language for Nuclear Power Plants, Proceedings of the 1977 Summer Computer Simulation Conference, July 18-20, 1977, pp. 353-358, AFIPS Press, Montvale, New Jersey, 1977.

Waterloo SCRIPT Reference Guide, University of Waterloo, Waterloo, Ontario, 1976.

DSNP, NESC No. 784.370, Description of Transmittal Tape, NESC Note 79-19, January 30, 1979.

11. **HARDWARE REQUIREMENTS** - 240K bytes of storage are required to compile and translate a typical power plant simulation program. Six scratch files require disk or fast magnetic tape storage and a permanent library file unit is used. All sample problems were executed in a 250K byte or smaller region.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and DSNP

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The documentation was prepared and is maintained using the proprietary University of Waterloo SCRIPT text-processing system. Files 7-10 of the transmittal tape are SCRIPT data files.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. Saphier
Department of Applied Mathematics
Soreq Nuclear Research Centre
Israel
G. F. Popper
Components Technology Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -

Source (Precompiler 2644 lines, Library 3313 lines)
Sample problems (1318 lines, Default data 32 lines, PDS DSNP.CNTL)
Auxiliary routine (MINIEDITOR 113 lines)
Auxiliary information (4 SCRIPT text files PDS LIB.TEXT, PDS TEXT.TEXT, DSNP.TEXT*, and COMP.TEXT* of DSNP manuals, 1 printer file+ of DSNP manuals)
Sample problems output (75 selected pages, complete-9 microfiche)

* RECFM=VB,LRECL=255,BLKSIZE=1680
+ RECFM=VBA,LRECL=125,BLKSIZE=1654

17. **CATEGORY** - K
KEYWORDS - simulation, nuclear power plants, programming languages

18. **SPONSOR** - DOE Division of Reactor Research and Technology

1. **IDENTIFICATION AND KWIC TITLE** - TRANSPORT
   TRANSPORT, design of charged particle beams

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM370

3. **DESCRIPTION** - The first- and second-order optical properties of static-magnet charged particle beam transport systems are analyzed. The program can vary some of the physical parameters of the elements comprising the system and impose various constraints on the beam design.

4. **METHOD OF SOLUTION** - The user describes the beam line as a sequence of elements which may be magnets, the intervals between them or special configurations of the magnets, specifications of the input beam, calculations to be done, and printout required. The program steps through the beam line calculating the appropriate transfer matrix for each element and the products of these matrices.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The effects of space charge are assumed to be negligible.

6. **TIMING** - Running time is dependent on the number of elements in the beam line. A typical problem requires 10 CPU seconds on the IBM370/168. The NESC executed the sample problems in 16 seconds on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - TURTLE is a ray tracing program which uses input compatible with TRANSPORT. TURTLE takes into consideration some higher-order effects that TRANSPORT cannot calculate. The original first-order TRANSPORT computer program was written in BALGOL by C. H. Moore at SLAC in collaboration with H. S. Butler and S. K. Howry in 1963.

9. **STATUS** - Abstract first distributed November 1978.
   IBM370 version submitted July 1975, replaced by revised Edition B October 1982, sample problems executed by NESC September 1982 on an IBM370/195.

10. **REFERENCES** - K. L. Brown, F. Rothacker, D. C. Carey, and Ch. Iselin, TRANSPORT A Computer Program for Designing Charged Particle Beam Transport Systems, SLAC-91, Rev. 2, May 1977 (also published as CERN-73-16 and NAL-91), and Appendix, December 1977.
    David C. Carey, New Features in TRANSPORT, Fermi National Accelerator Laboratory Technical Memorandum, TM-1064, September 7, 1981.
    Karl L. Brown, A First- and Second-order Matrix Theory for the Design of Beam Transport Systems and Charged Particle Spectrometers, SLAC-75, Rev. 3, August 1972.
    David C. Carey, TURTLE (Trace Unlimited Rays Through Lumped Elements), A Computer Program for Simulating Charged Particle Beam Transport Systems, NAL-64, May 1978.

11. **HARDWARE REQUIREMENTS** - 310K bytes of memory, a card input unit, and printer and punch output units are used.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Transfer matrices are written on FORTRAN logical unit 4 for punching. The XL option of the FORTRAN IV H or H-Extended compiler is required to access the bit-manipulation functions LAND, LOR, and SHFTR.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. C. Carey
    Fermi National Accelerator Laboratory

16. **MATERIAL AVAILABLE** –
Source (8500 lines)
Sample problems (1063 lines)
Control information (JCL 55 lines)
Sample problem output (27 selected pages, 1 microfiche)
Reference reports, SLAC-91 Rev. 2 and Appendix, SLAC-75 Rev. 3, and FNAL Technical Memorandum

17. **CATEGORY** – V
KEYWORDS – charged-particle transport, magnets, accelerators, beam dynamics, beam transport, phase space, TURTLE codes

18. **SPONSOR** – ERDA Division of Physical Research
DOE Office of High Energy and Nuclear Physics

1. **IDENTIFICATION AND KWIC TITLE** - CHNSED
   CHNSED, sediment & containment transport model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - CHNSED is an expanded model of hydrologic response of a watershed. It includes the simulation of trace contaminant transport through the watershed. Within the stream channel system trace contaminant is transported in dissolved and adsorbed form. CHNSED includes both SEDTRN, a model of sediment transport through a rectangular stream channel system, and the Wisconsin Hydrologic Transport Model, WHTM (NESC 808), a processes model. Processes considered in CHNSED include particulate mobilization (sheet erosion and overland transport) and dissolved contaminant transport (associated with run off, interflow, and base flow inputs to the channel system). An ion exchange submodel simulates the soil-contaminant-water interaction at the land surface, and sediment transport and partitioning of trace contaminant between water and sediment in the channel system are also included. Following its entry into the channel system, dissolved contaminant transport is derived from flow routing algorithms of the WHTM. Routing of the adsorbed fraction is controlled by sediment transport dynamics, which are governed by bedload and suspended load sediment transport.

4. **METHOD OF SOLUTION** - The sediment transport formulation is an extension of that described by R. A. Bagnold in 1966, and includes Manning's equations to determine flow rate and modification to Stokes' law to allow calculation of particulate fall velocity in both the viscous and inertial particle settling regions. Sediment is separated into three components: resident sediment in the stream bed, sediment in transit as bedload, and sediment in transit as suspended load. Each of these components is partitioned into as many as 12 size classes of logarithmically varying ranges. The partitioning of a contaminant between water and sediment is based on the assumption of an equilibrium distribution being attained within each simulation interval.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Current computer storage allocation allows a watershed to be divided into three segments while the channel system is broken down into seven separate reaches.

6. **TIMING** - A test simulation of a one-year real time duration for a two-segment watershed and three-reach channel system required approximately 5 minutes of CPU time on the IBM System 360/91.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - This is primarily a research model, constructed to be as mechanistic as possible; as such, it requires a rather complete parametric description of the watershed, the channel system, and the initial distribution of sediment within the channel system.

8. **RELATED AND AUXILIARY SOFTWARE** - CHNSED is one of a suite of models termed collectively the unified transport model (UTM).

9. **STATUS** - Abstract first distributed November 1978.
   IBM360 version submitted October 1977, sample problem executed by NESC October 1978 on an IBM3033.

10. **REFERENCES** - D. E. Fields, Simulation of Sediment and Trace Contaminant Transport with Sediment-Contaminant Interaction, ORNL/NSF/EATC-19, March 1976.

M. R. Patterson, J. K. Munro, D. E. Fields, R. D. Ellison, A. A. Brooks, and D. D. Huff, A User's Manual for the FORTRAN IV Version of the Wisconsin Hydrologic Transport Model, ORNL/NSF/EATC-7, October 1974.

R. A. Bagnold, An Approach to the Sediment Transport Problem from General Physics, Geological Survey Professional Paper 422-I, U.S. Government Printing Office, 1966.

D. E. Fields, LINSED: A One Dimensional Multireach Sediment Transport Model, ORNL/CSD-15, October 1976.

D. E. Fields and D. M. Hetrick, HOTSED: A Discrete Element for Simulating Hydrodynamic Conditions and Adsorbed and Dissolved Radioisotope Concentrations in Estuaries, NUREG/TM-266 (in press).

11. **HARDWARE REQUIREMENTS** - 350K bytes of storage are required and FORTRAN logical units 1 through 4 are utilized for temporary files during problem execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (96%) and BAL (4%)

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - An overlay structure is used to reduce main storage requirements. CHNSED is compiled with the FORTRAN H compiler using OPT=2 and the XL option.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. E. Fields
Union Carbide Corporation, Nuclear Division

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 5403 lines, BAL 179 lines)
Sample problem (334 lines)
Control information (JCL 114 lines)
Reference report, ORNL/NSF/EATC-19

17. **CATEGORY** - R
KEYWORDS - sediments, ion exchange, water quality, hydrology, particles, water pollution, trace amounts, soils, erosion, WHTM codes

18. **SPONSOR** - NSF Ecology and Analysis of Trace Contaminants Program

1. **IDENTIFICATION AND KWIC TITLE** - OPTRM
   OPTRM, hydrologic transport with optimization

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - OPTRM is utilized to determine an optimal set of model parameters for the Wisconsin Hydrologic Transport Model, WHTM (NESC 808). An optimal set of parameters is defined as that set which gives in a mathematical sense the best simulation; i.e., which provides the best match on either a monthly or daily basis between observed outflows and simulated outflows. The term outflow applies here to either water or trace contaminant values.

4. **METHOD OF SOLUTION** - OPTRM utilizes a pattern search technique to minimize an objective function designed to quantify the dissimilarity between observed and simulated hydrologic flows or contaminant transport values. The method is an unconstrained nonlinear optimization technique not requiring gradients.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - As currently structured, OPTRM optimizes a set of either six hydrologic response parameters or three contaminant transport-related values. OPTRM determines a set of parameters for a single segment of a watershed. A segment may be considered a normally homogeneous region of the watershed.

6. **TIMING** - A test case optimizing six hydrologic parameters for a real-time simulation interval of 31 days required 5 minutes of CPU time excluding wait time on an IBM360/91. Approximately 70 interactions of the WHTM submodel were made within this time. For a simulation period of one year with a set of six parameters being optimized, approximately one minute of execution time is required per iteration and typically 25 iterations are needed to attain an objective function equal to about 90 percent of its minimum value.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The capability to simulate the hydrologic transport of selected radio-aerosols was added to SWM, the Stanford Watershed Model, originally developed at Stanford in 1960, by Huff and associates at the University of Wisconsin. This model, WHTM, was then modified at ORNL to include parameter optimization.

9. **STATUS** - Abstract first distributed November 1978.
   IBM360 version submitted October 1977, sample problem executed by NESC October 1978 on an IBM3033.

10. **REFERENCES** - D. E. Fields and S. B. Watson, OPTRM - A Hydrologic Transport Model with Parameter Optimization, ORNL/NSF/EATC-14, September 1975.

R. K. Linsley and N. H. Crawford, Computation of a Synthetic Streamflow Record on a Digital Computer, International Association of Scientific Hydrology, Pub. No. 51, pp. 526-538, 1960.

D. D. Huff, Simulation of the Hydrologic Transport of Radioactive Aerosols, Ph.D. Thesis, Stanford University, 1968.

M. R. Patterson, J. K. Munro, D. E. Fields, R. D. Ellison, A. A. Brooks, and D. D. Huff, A User's Manual for the FORTRAN IV Version of the Wisconsin Hydrologic Transport Model, ORNL-NSF-EATC-7, October 1974.

11. **HARDWARE REQUIREMENTS** - OPTRM utilizes an overlay structure requiring 290K bytes of storage. FORTRAN logical units 1 through 4, disk storage, are used as temporary files. The LAND and CHANL input are read from disk logical unit 5 with other input data read from unit 10. In addition to the print output on logical unit 15, units 6 and 13 are used for daily observed and simulated flow print and plot output.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (96%) and BAL (4%)

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program should be compiled with the XL option of the FORTRAN H compiler. OPTRM uses a CalComp package to plot observed and simulated watershed responses.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. E. Fields
Union Carbide Corporation, Nuclear Division

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 4900 lines, BAL 179 lines)
Sample problems (LAND and CHANL input 182 lines, other input 539 lines)
Control information (JCL 113 lines)
Reference report, ORNL/NSF/EATC-14

17. **CATEGORY** - R
KEYWORDS - atmospheric precipitations, chemical effluents, environment, ground water, hydrodynamics, surface waters, water pollution, hydrology, land pollution, regional analysis

18. **SPONSOR** - NSF Ecology and Analysis of Trace Contaminants Program

1. **IDENTIFICATION AND KWIC TITLE** - HAARM3
   HAARM3, aerosol behavior log-normal dist model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC6400,7600,CYBER73

3. **DESCRIPTION** - HAARM3, an acronym for Heterogeneous Aerosol Agglomeration Revised Model 3, is the third program in the HAARM series developed to predict the time-dependent behavior of radioactive aerosols under postulated LMFBR accident conditions. HAARM3 was developed to include mechanisms of aerosol growth and removal which had not been accounted for in the earlier models. In addition, experimental measurements obtained on sodium oxide aerosols have been incorporated in the code. As in HAARM2, containment gas temperature, pressure, and temperature gradients normal to interior surfaces are permitted to vary with time.

   The effects of reduced density on sodium oxide agglomerate behavior and of nonspherical shape of particles on aerosol behavior mechanisms are taken into account, and aerosol agglomeration due to turbulent air motion is considered. Also included is a capability to calculate aerosol concentration attenuation factors and to restart problems requiring long computing times.

4. **METHOD OF SOLUTION** - HAARM3 assumes the time-dependent particle size distribution is log-normal and converts the integro-differential equation describing the concentration decay of aerosol into three first-order differential equations which are integrated using a standard library subroutine. The present model allows the method of integration to be specified. The choices are: Adams Moulton with either a fixed or variable step-size and Runge-Kutta with a fixed step-size.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   1000 time-steps
   42 discrete radii for the distribution calculations

6. **TIMING** - The sample problems each take 1 second of CP time on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Various models have been developed to describe aerosol behavior under postulated accident conditions including the TRAP code at Brookhaven National Laboratory (Nuclear Science and Engineering, Vol. 42, pp. 58-63, 1970), the PARDISEKO3 code at Karlsruhe (KFK 2151, May 1975), and the HAA3B code at Atomics International (NESC 443). HAARM3 can be used to provide the input data for dose calculations, such as COMRADEX4 (NESC 663).

9. **STATUS** - Abstract first distributed November 1978.
   CDC CYBER73 version submitted September 1978, replaced July 1980 by revised Edition B submitted January 1980, sample problem executed by NESC March 1980 on a CDC7600.

10. **REFERENCES** - J. A. Gieseke, K. W. Lee, and L. D. Reed, HAARM-3 Users Manual, BMI-NUREG-1991 with Errata, January 5, 1978.

K. W. Lee, J. A. Gieseke, and L. D. Reed, Sensitivity Analysis of the HAARM-3 Code, NUREG/CR-0527 (BMI-2008), November 1978.

J. A. Gieseke, L. D. Reed, H. Jordan, and K. W. Lee, Characteristics of Agglomerates of Sodium Oxide Aerosol Particles, BMI-NUREG-1977, August 1, 1977.

L. D. Reed and J. A. Gieseke, HAARM-1 Users Manual, BMI-X-658, May 15, 1975.

L. D. Reed and J. A. Gieseke, HAARM-2 Users Manual, BMI-X-665, October 31, 1975.

R. S. Hubner, E. U. Vaughan, and L. Baurmash, HAA-3 User Report, AI-AEC-13038, March 1973.

11. **HARDWARE REQUIREMENTS** - 117,000 (octal) words of storage are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV, FTN4.5 (CDC7600)

13. **OPERATING SYSTEM** - NOS/BE 1.0 (CDC CYBER73), SCOPE 2.1.3 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. A. Gieseke, K. W. Lee, and L. D. Reed
Columbus Laboratories
Battelle Memorial Institute

16. **MATERIAL AVAILABLE** -
Source (2958 lines)
Sample problems (25 lines)
Sample problem output (BASE CASE-22 pages, TURBULENCE-22 pages)
Reference report, BMI-NUREG-1991 with Errata

17. **CATEGORY** - G
KEYWORDS - radioactive aerosols, accidents, containment systems, deposition, diffusion, radioactivity transport, LMFBR reactors, HAA3B codes, COMRADEX codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - MSF21, VTE21
   MSF21,VTE21, desalination plant optimization

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM360,370

3. **DESCRIPTION** - MSF21 and VTE21 perform design and costing calculations for multistage flash evaporator (MSF) and multieffect vertical tube evaporator (VTE) desalination plants. An optimization capability is available, if desired.
   The MSF plant consists of a recovery section, reject section, brine heater, and associated buildings and equipment. Operating costs and direct and indirect capital costs for plant, buildings, site, and intakes are calculated. Computations are based on the first and last stages of each section and a typical middle recovery stage. As a result, the program runs rapidly but does not give stage by stage parameters.
   The VTE plant consists of vertical tube effects, multistage flash preheater, condenser, and brfine heater and associated buildings and equipment. Design computations are done for each vertical tube effect, but preheater computations are based on the first and last stages and a typical middle stage.

4. **METHOD OF SOLUTION** - The general method is to solve for a heat and mass balance in each part of the plant.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - In the MSF program the loss of tray brine temperature is the same for each stage in the heat recovery section and in the heat reject section. The temperature and the flow rate of the heat reject stream are always greater than zero, and there is no option to consider a once-through type plant.
   The VTE plant design is limited to 30 effects.

6. **TIMING** - A single MSF computation typically requires 1.5 seconds on the IBM360/65. An optimization requiring 300 iterations is accomplished in about 75 seconds. On the IBM360/91 an optimized case typically runs about 3 seconds. The four trial cases including MSF21 and VTE21 runs, with and without optimization, for a 2.5 Mgd plant using program-defined default parameters, required a total of 6.5 seconds on the IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The programs include default or built-in values for all design parameters. Only those values which are to be changed must be entered as problem input data.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed November 1978.
   IBM360 version submitted October 1976, sample problems executed by NESC October 1978 on an IBM370/195.

10. **REFERENCES** - W. G. S. Fort, Computer Codes for Office of Saline Water Program Analysis Part V: MSF-21: A Fortran Code for the Rapid Calculation or Optimization of Multistage Flash (MSF) Desalination Plants, ORNL-TM-3535 Part V, February 1972.

W. G. S. Fort and J. V. Wilson, Computer Codes for Office of Saline Water Program Analysis Part VI. VTE-21: A FORTRAN Code for the Rapid Calculation or Optimization of Vertical Tube Evaporator (VTE) Desalination Plants, ORNL/TM-3535 Part VI, September 1976.

P. Glueckstern, J. V. Wilson, and S. A. Reed, Modifications of ORNL's Computer Programs MSF-21 and VTE-21 for the Evaluation and Rapid Optimization of Multistage Flash and Vertical Tube Evaporators, ORNL/TM-5230 and Errata, June 1976.

W. G. S. Fort, S. H. Moore, and J. V. Wilson, Computer Codes for Office of Saline Water Program Analysis Part III, Programs and Subprograms Common to Several Desalination Processes, Including Code PROC21, ORNL-TM-3535 Part III, January 1973.

NESC Note 79-17, NESC No. 798.360, Description of MSF21,VTE21 Input Data, October 11, 1978.

U. S. Department of Interior Office of Saline Water and the Bureau of Reclamation, Desalting Handbook for Planners, First Edition, May 1972.

11. **HARDWARE REQUIREMENTS** - MSF21,VTE21 requires 272K bytes of storage for execution. Standard system card-image input and printer output units are needed.

12. **PROGRAMMING LANGUAGE** - FORTRAN (97%) and BAL (3%)

13. **OPERATING SYSTEM** - OS/360,370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Programs MSF21 and VTE21 are packaged together because they have many subprograms in common. The type of plant to be calculated is specified in the input data.

    Subroutines MAINM, PLANTM, SIZEM, COSTM, and RITEM are specific to program MSF21. Subroutines MAINV, PLANTV, SIZEV, COSTV, RITEV, and UVE are specific to program VTE21. If only one type of plant is to be calculated, the amount of storage required by the program can be reduced by omitting unnecessary subroutines. When subroutines MAINM or MAINV are omitted, dummy subroutines should be substituted or the statements calling the missing subroutine deleted.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    J. V. Wilson
    Engineering Technology Division
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** -

    Source (FORTRAN 5345 lines, BAL 155 lines)
    Sample problems (9 lines)
    Sample problem output (30 pages)
    Reference reports, ORNL-TM-3535 Parts V and VI, ORNL/TM-5230 with Errata, NESC Note, and ORNL-TM-3535 Part III (2 microfiche)

17. **CATEGORY** - D
    KEYWORDS - evaporators, desalination, flash heating, design, optimization, seawater, tubes, cost, economics, performance

18. **SPONSOR** - ERDA Division of Nuclear Research and Applications
    DOI Office of Saline Water

1. **IDENTIFICATION AND KWIC TITLE -** LINPACK
   LINPACK, simultaneous linear algebraic equatns

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   IBM360,370 (designed to be machine-independent)

3. **DESCRIPTION -** LINPACK is a collection of FORTRAN subroutines which analyze and solve various classes of systems of simultaneous linear algebraic equations. The collection deals with general, banded, symmetric indefinite, symmetric positive definite, triangular, and tridiagonal square matrices, as well as with least squares problems and the QR and singular value decompositions of rectangular matrices.

   A subroutine-naming convention is employed in which each subroutine name consists of five letters which represent a coded specification (TXXYY) of the computation done by that subroutine. The first letter, T, indicates the matrix data type. Standard FORTRAN allows the use of three such types: S REAL, D DOUBLE PRECISION, and C COMPLEX. In addition, some FORTRAN systems allow a double-precision complex type: Z COMPLEX*16. The second and third letters of the subroutine name, XX, indicate the form of the matrix or its decomposition:

GE	General
GB	General band
PO	Positive definite
PP	Positive definite packed
PB	Positive definite band
SI	Symmetric indefinite
SP	Symmetric indefinite packed
HI	Hermitian indefinite
HP	Hermitian indefinite packed
TR	Triangular
GT	General tridiagonal
PT	Positive definite tridiagonal
CH	Cholesky decomposition
QR	Orthogonal-triangular decomposition
SV	Singular value decomposition

The final two letters, YY, indicate the computation done by the particular subroutine:

FA	Factor
CO	Factor and estimate condition
SL	Solve
DI	Determinant and/or inverse and/or inertia
DC	Decompose
UD	Update
DD	Downdate
EX	Exchange

The following chart shows all the LINPACK subroutines. The initial 'S' in the names may be replaced by D, C or Z and the initial 'C' in the complex-only names may be replaced by a Z.

	FA	CO	SL	DI	DC	UD	DD	EX
SGE	x	x	x	x				
SGB	x	x	x	x				
SPO	x	x	x	x				
SPP	x	x	x	x				
SPB	x	x	x	x				
SSI	x	x	x	x				
SSP	x	x	x	x				
CHI	x	x	x	x				
CHP	x	x	x	x				
STR		x	x					
SGT			x					
SPT			x					
SCH					x	x	x	x
SQR			x		x			
SSV					x			

The LINPACK package also includes a set of routines to perform basic vector operations called the Basic Linear Algebra Subprograms (BLAS).

4. **METHOD OF SOLUTION** - Gaussian elimination, Cholesky decomposition, QR, and singular value decomposition methods are used.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - There are no subroutines for general sparse matrices or for iterative methods for very large problems.

6. **TIMING** - Running time varies with problem size. NESC executed each test case in about 8 seconds on Argonne's IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The LINPACK subroutines contain no machine-dependent constants, input or output statements, character manipulations, COMMON or EQUIVALENCE statements, nor mixed-mode arithmetic. All subroutines except those with names beginning with Z use the portable subset of ANSI FORTRAN.
   The LINPACK project supports this software in the sense that detailed information on the testing procedures is available, and reports of poor or incorrect performance in conventional FORTRAN operating environments will gain immediate attention from the developers.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed February 1979.
   LINPACK submitted January 1979, revised March 1979, sample problems executed by NESC January 1979 on an IBM370/195 and an IBM3033.

10. **REFERENCES** - J. J. Dongarra, J. R. Bunch, C. B. Moler, G. W. Stewart, LINPACK User's Guide, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, 1979.
    J. J. Dongarra and C. B. Moler, LINPACK Working Note #13: Implementation Guide for LINPACK, ANL-80-105, October 1980.
    Chuck L. Lawson, Richard J. Hanson, David R. Kincaid, and Fred T. Krough, Basic Linear Algebra Subprograms for FORTRAN Usage, SAND77-0898, October 1977 (also published in Association for Computing Machinery, Transactions on Mathematical Software, Vol. 5, No. 3, pp. 308-323, September 1979).
    LINPACK, NESC No. 800, Description of "How to Bring up LINPACK on a UNIX Version 7 System", National Energy Software Center Note 79-65, August 6, 1979.

11. **HARDWARE REQUIREMENTS** - The entire coefficient matrix will usually be stored in the computer memory, although there are provisions for band matrices and for row-by-row processing of large rectangular matrices. 240K bytes of storage are required for execution of a typical sample problem on the IBM360,370 system.

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - OS/360,370 on the IBM360,370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The test drivers call a subroutine TRAPS to set the number of underflows permitted. The call is TRAPS(I1,I2,I3,I4,I5) where
    I1 should be set to zero,
    I2 is the number of floating-point overflows permitted,
    I3 is the number of floating-point underflows permitted,
    I4 is the number of fixed-point divides by zero permitted, and
    I5 is the number of floating-point divides by zero permitted.
    Each installation will have to provide a subroutine TRAPS, which in turn, should call the local error handling routine which should be set to permit a large number of underflows (5000). If the error-handling procedures are determined by the operating system control language this will have to be set appropriately and a dummy subroutine TRAPS supplied. TRAPS is the standard routine used in WATFIV. On the IBM360,370 the routine is ERRSET.
    The sample problems, or testing aids, have been run at the computer installations listed below using a variety of compiler and operating systems.

Test Site	Machine

Argonne National Laboratory	IBM370/195
Bell Laboratories at Murray Hill	Honeywell6080
College of William and Mary	IBM370/148
International Mathematical and Statistical Libraries (IMSL)	EclipseC330
Iowa State University	Itel-AS/5
Lawrence Livermore Laboratory	CDC7600
Los Alamos Scientific Laboratory	CDC7600, Cray1
Monash University, Australia	Burroughs6700
NASA Langley Research Center	CDC Cyber175
National Center for Atmospheric Research	CDC7600, Cray1
National Defense Research Institute, Tumba, Sweden	IBM360/75
Naval Weapons Center, China Lake	UNIVAC1110
Northwestern University	CDC6600
Oak Ridge National Laboratory	IBM360/91
Purdue University	CDC6500
Stanford University, SLAC	IBM370/168
University of California, San Diego	Burroughs6700
University of Kentucky	IBM370/158
University of Illinois, Chicago Circle	IBM370/168
University of Illinois at Urbana-Champaign	CDC Cyber175
The University of Michigan	Amdahl 470/V6
The University of Texas at Austin	CDC6600-6400
University of Toronto, Toronto, Canada	IBM370/165
The University of Wisconsin-Madison	UNIVAC1110
Yale University	DEC-KL-20, KA-10

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

J. J. Dongarra
Mathematics and Computer Science Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE -**

Source (LINPACK S 6861 lines, D 6867 lines, C 8771 lines, Z 8935 lines, BLAS S 562 lines, D 560 lines, C 575 lines, Z 580 lines)
Machine-readable documentation (S 2708 lines, D 2714 lines, C 3189 lines, Z 3189 lines)
Reference reports, SAND-77-0898 and ANL-80-105, and NESC Note

17. **CATEGORY** - P
KEYWORDS - numerical solution, matrices, least square fit

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Engineering, Mathematical and Geo-Sciences
NSF Mathematical and Computer Science Division

1. **IDENTIFICATION AND KWIC TITLE -** 2DEPEP
   2DEPEP, elliptic parabolic & eigenvalue solns.

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC6500,7600

3. **DESCRIPTION -** 2DEPEP solves the partial differential equation system:
   C1(X,Y,U,V,T)•DU/DT=D(OXX)/DX+D(OXY)/DY+F1(X,Y,U,V,T)
   C2(X,Y,U,V,T)•DV/DT=D(OYX)/DX+D(OYY)/DY+F2(X,Y,U,V,T) in a general two-dimensional region, R, with
   U=FB1(S)
   V=FB2(S) for S on BR1, and
   OXX•NX+OXY•NY=GB1(S,U,V,T)
   OYX•NX+OYY•NY=GB2(S,U,V,T) for S on BR2, where BR1 and BR2 are distinct parts of the boundary. (NX,NY)= unit outward normal.
   U=U0(X,Y)
   V=V0(X,Y) for T=T0, and
   OXX=OXX(X,Y,DU/DX,DU/DY,DV/DX,DV/DY,T)
   OXY=OXY(X,Y,DU/DX,DU/DY,DV/DX,DV/DY,T)
   OYX=OYX(X,Y,DU/DX,DU/DY,DV/DX,DV/DY,T)
   OYY=OYY(X,Y,DU/DX,DU/DY,DV/DX,DV/DY,T).
   The Jacobian matrices of derivatives of OXX,OXY,OYX,OYY with respect to DU/DX,DU/DY,DV/DX,DV/DY and of F1,F2 with respect to U,V and of GB1,GB2 with respect to U,V must be symmetric.
   The related elliptic and eigenvalue problems are also solved by 2DEPEP and single equations can be handled efficiently. Examples of applications of the program are elasticity, one- or two-component diffusion, heat conduction, minimal surface, potential problems and the time-independent and time-dependent Schrodinger equations.

4. **METHOD OF SOLUTION -** The user supplies an initial triangulation which defines the region R. This triangulation is refined as controlled by a user-supplied function. For singular elliptic problems, optimal order convergence is possible if this function approximates the function D3MAX(UV), which is the maximum of the third derivatives of U and V.
   The problem is discretized by Galerkin's method, using a trial function space of piecewise quadratic polynomials with respect to the triangulation. An approximate solution is calculated, using either the implicit or the Crank-Nicolson method for each time-step. The non-linear equations which must be solved each time-step are solved by Newton's method. One iteration is sufficient since the solution on the previous time-step is used for starting values. In each application of Newton's method the symmetric, banded Jacobian matrix is inverted directly by Gaussian elimination, with the matrix stored out-of-core when necessary, according to the frontal method. For linear time-independent problems the Jacobian is the same each time-step, so the Cholesky factorization done in the first step is used on all following steps. The isoparametric method is used to handle curved boundaries.
   When C1=C2=0 and all functions are independent of T, that is, when the problem is a steady-state (elliptic) problem, each time-step corresponds to one iteration of Newton's method. (One iteration is sufficient for linear problems.) An eigenvalue problem can be converted to a related parabolic problem where each time-step is equivalent to an iteration of the inverse power method for finding the smallest eigenvalue and the corresponding eigenfunction. A single equation can be handled with no loss of efficiency in storage or execution time.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** At most two simultaneous partial differential equations can be solved. The input data set is limited to 200 cards. This can be increased by changing the value of the variable MXCARD and increasing the dimensions of the arrays L, INDX, and LNAM in the preprocessor.

6. **TIMING -** Execution time is problem dependent. NESC executed the sample problems in 30 seconds on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Local mesh refinement capability makes 2DEPEP ideal for singular problems, such as elastic crack problems.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed May 1979.
IBM360 version submitted February 1978, replaced by CDC6500 version submitted December 1978, revised April 1979, sample problems executed by NESC April 1979 on a CDC7600.

10. **REFERENCES** - Granville Sewell, 2DEPEP, 2-D Elliptic, Parabolic and Eigenvalue Problems, User's Manual, Purdue University, October 1978.

11. **HARDWARE REQUIREMENTS** - 120K (octal) words of memory are required together with an auxiliary storage device, such as disk or tape, for temporary use in large problems (unit 2), and another storage device for temporary use to store the preprocessor output (unit 4).

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program is written to process input data for one problem only per execution.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
E. G. Sewell
Computer Science Department
Purdue University

16. **MATERIAL AVAILABLE** -
Source (Preprocessor-538 lines, Subroutines-1061 lines)
Sample problems (171 lines)
Control information (70 lines)
Reference User's Manual

17. **CATEGORY** - P
KEYWORDS - eigenvalues, two-dimensional, iterative methods, finite element method, partial differential equations, banded matrix

18. **SPONSOR** - Purdue University
Oak Ridge National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - DWG100RQ, DWG101RQ
   DWG100RQ,DWG101RQ, convert to or from SI units

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370,303x

3. **DESCRIPTION** - DWG100RQ,DWG101RQ consists of five programs used to convert SI metric units of measurement from engineering drawings to U.S. customary dimensions based on the rounding rules specified in the Mound Laboratory Design/Drafting Standard DWG No. SPA760290 (DWG100RQ), or to convert U.S. customary units of measurement from engineering drawings to SI metric dimensions based on the rounding rules specified in the Mound Laboratory Design/Drafting Standard DWG No. SPA800269 (DWG101RQ). The five programs are MTRC0001, MTRC0002, MTRC0003, MTRC0004, and MTRC1001. MTRC0002 is a preprocessor used to format input data to align decimal points, generating 83-character data records that can be easily sorted. MTRC0003 and MTRC0004 sort numerical data based on the sign of the number and the sign of the exponent. MTRC0003 writes the numerical data to one of four files based on whether the number is positive or negative and whether the exponent is positive or negative. These files are then sorted by the IBM System SORT utility and merged by MTRC0004 for input either to MTRC0001, if metric units are to be converted to U.S. customary units, or to MTRC1001, if U.S. customary units are to be converted to metric units.

4. **METHOD OF SOLUTION** - Standard unit conversion, 25.4 mm per inch, is applied with special rounding procedures as specified in the referenced Mound documents.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The conversion is only concerned with linear units. A maximum of 26 predefined labels to distinguish individual records is allowed.

6. **TIMING** - 10 to 12 minutes wall clock time is typical on the IBM360/65. NESC executed the sample problem in 5 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - METRICATION (NESC 668) also converts to and from SI units and U.S. customary units.

9. **STATUS** - Abstract first distributed January 1979.
   IBM360 version of MTRC0001 submitted May 1978, replaced by revised edition November 1978, replaced June 1981 by DWG100RQ,DWG101RQ submitted October 1980, sample problem executed by NESC December 1980 on an IBM3033.

10. **REFERENCES** - American Society for Testing and Materials, Standard for Metric Practice, ASTM E380-76, IEEE Standard 268-1975.
    American National Standards Institute, American National Standard Representations for U.S. Customary, SI, and Other Units to be Used in Systems with Limited Character Sets, ANSI X3.50-1976.
    C. W. Schlosser, Preparation of Computerized SI Metric to US Customary Conversion Table, DWG No. SPA760290, Issue 7, July 22, 1980.
    C. W. Schlosser, Units Abbreviations for Computerized Engineering Drawings (Limited Character Sets), DWG No. SPA770089, Issue 1, April 15, 1977.
    C. W. Schlosser, Preparation of Computerized US Customary to SI Metric Conversion Table, DWG No. SPA800269, Issue 0, October 13, 1980.
    DWG100RQ,DWG101RQ, NESC No. 812.360, DWG100RQ,DWG101RQ Tape Description, National Energy Software Center Note 81-51, December 23, 1980.

11. **HARDWARE REQUIREMENTS** - 50K bytes of memory are required to execute MTRC0002, MTRC0003, and MTRC0004. MTRC0001 and MTRC1001 require 90K bytes and the IBM SORT utility uses 70K bytes.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (85%) and COBOL Version.4 (15%)

13. **OPERATING SYSTEM** - OS/360.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The IBM SORT utility is used to sort the input to MTRC0001 or MTRC1001.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. T. Scott and D. Branscomb
Mound Laboratory
Monsanto Research Corporation

16. **MATERIAL AVAILABLE** -
Source (MTRC0001 1383 lines, MTRC1001 1381 lines, MTRC0002 34 lines, MTRC0003 247 lines, MTRC0004 260 lines)
Sample problem (22 lines)
Auxiliary information (MTRC0011 unit conversion table 294 lines)
Control information (JCL 239 lines)
Reference documents, DWG Nos. SPA760290, SPA800269, SPA77089, and NESC Note

17. **CATEGORY** - T
KEYWORDS - SI units, metric system, standards, engineering

18. **SPONSOR** - DOE Division of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - CONTEMPT4/MOD5
   CONTEMPT4/MOD5, PWR & BWR containment analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER176,175,170

3. **DESCRIPTION** - CONTEMPT4/MOD5 describes the response of multicompartment containment systems subjected to postulated loss-of-coolant accident (LOCA) conditions. The program can accommodate both pressurized water reactor (PWR) and boiling water reactor (BWR) containment systems. Also, both design basis accident (DBA) and degraded core type LOCA conditions can be analyzed. The program calculates the time variation of compartment pressures, temperatures, and mass and energy inventories due to intercompartment mass and energy exchange taking into account user-supplied descriptions of compartments, intercompartment junction flow areas, LOCA source terms, and user-selected problem features. Analytical models available to describe containment systems include models for containment fans and pumps, cooling sprays, heat conducting structures, sump drains, PWR ice condensers, and BWR pressure suppression systems. To accommodate degraded core type accidents, analytical models for hydrogen combustion within compartments and energy transfer due to gas radiation are also provided.

4. **METHOD OF SOLUTION** - Containment thermodynamic conditions of hydrogen/air/steam/liquid water mixtures are determined by using modularized equation-of-state subroutines and tabulated water properties. The numerics in the code are completely explicit, except for the predictor-corrector technique used to estimate the heat structure effects on compartment conditions, an implicit calculation of junction flow with inertia, and an optional implicit routine for junction flow calculation approaching pressure equilibrium.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   999 lumped parameter compartments
   99 heat conducting structures using a variety of heat transfer options and boundary conditions
   Intercompartment flow junctions may be calculated for either a sharp-edge orifice (single phase homogeneous or two-phase flow) or a nozzle (vapor flow only). Containment cooling spray analytical models are provided for either single or double heat exchangers.

6. **TIMING** - The long-term BWR sample problem with hydrogen burn requires approximately 580 seconds on a CDC CYBER175, and the ice condenser sample problem requires about 9 seconds on a CDC CYBER170/875.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The architecture of CONTEMPT4/MOD5 is completely modular. Dynamic storage allocation coding, optional automatic time-step control, optimal specification of input data, and a restart capability permit flexible use of the available program features.

8. **RELATED AND AUXILIARY SOFTWARE** - The CONTEMPT4/MOD5 code is the most recent in the CONTEMPT series of programs originally developed at EG&G Idaho, Inc. While it does not replace CONTEMPT-LT/028 (NESC 433), CONTEMPT4/MOD5 can perform simplified boiling water reactor (BWR) containment studies. CONTEMPT4/MOD5 is an improvement to CONTEMPT4/MOD4 for ice containment analysis. STH2OG generates the water properties library used by CONTEMPT4, and PLOTCT44 plots the values of variables calculated by CONTEMPT4.

9. **STATUS** - Abstract first distributed May 1979.
   CDC7600 version of CONTEMPT4/MOD2 submitted February 1978, withdrawn by developers June 1980.
   CDC CYBER176 version of CONTEMPT4/MOD3 submitted June 1981, replaced by CONTEMPT4/MOD3/1.0 December 1981, revised March 1982, replaced June 1984 by revised Edition B submitted August 1983, deleted October 1984.
   CDC7600 version of CONTEMPT4/MOD4 submitted June 1984, revised August 1984, revised December 1984, replaced April 1985 by CONTEMPT4/MOD5 submitted January 1985, sample problems executed by NESC February 1985 on a CDC CYBER175 and CDC CYBER170/875.

10. **REFERENCES** - C. C. Lin, C. Economos, J. R. Lehner, G. Maise, and K. K. Ng, CONTEMPT4/MOD4 A Multicompartment Containment System Analysis Program, NUREG/CR-3716 (BNL-NUREG-51754), March 1984.

C. C. Lin, CONTEMPT4/MOD5: An Improvement to CONTEMPT4/MOD4 Multicompartment Containment System Analysis Program for Ice Containment Analysis, NUREG/CR-4001 (BNL-NUREG-51824), September 1984.

CONTEMPT4/MOD5, NESC No. 818.7600, CONTEMPT4/MOD5 Tape Description, Implementation Information, and Replacement Section for CONTEMPT4/MOD4 Report, National Energy Software Center Note 85-53, March 18, 1985.

11. **HARDWARE REQUIREMENTS** - 60,000 (octal) words of small core memory (SCM) and 220,000 (octal) words of large core memory (LCM) are required on a CDC CYBER176. 160,000 (octal) words of SCM are required on a CDC CYBER170/875. CalComp or FR80 plotting devices are needed for graphical output.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (96%) and COMPASS 1.4 (4%)

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS/BE (CDC CYBER176), and NOS 2.2 (CDC CYBER175,170/875).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - CONTEMPT4 cannot be compiled successfully using the FTN5 compiler. CONTEMPT4, STH2OG, and PLOTCT44 will not load with the NOS1.5-564 or 587 loader; NESC used the NOS1.5-552 loader on a CDC CYBER175.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

C. C. Lin, C. Economos, J. R. Lehner, G. Maise,
and K. K. Ng
Department of Nuclear Energy
Brookhaven National Laboratory

16. **MATERIAL AVAILABLE** -

Source (Source-CONTEMPT4 27,960 lines, ENVIRONMENTAL ROUTINES 30,484 lines, UPDATE source-CONTEMPT4 27,616 lines, ENVIRONMENTAL ROUTINES 33,830 lines, UPDATE compile source-CONTEMPT4 27,960 records*, ENVIRONMENTAL ROUTINES 30,484 records*)

Sample problems (CONTEMPT4 Hydrogen Burn-408 lines, Ice Condenser-194 lines, STH2OG 14 lines)

Auxiliary programs (Source-STH20G 333 lines, PLOTCT44 2286 lines, UPDATE source-PLOTCT44 2286 lines)

Control information (460 lines, segload directives-CONTEMPT4 13 lines, STH2OG 10 lines, PLOTCT44 5 lines)

Sample problem output (CONTEMPT4 Hydrogen Burn-10,374 140-character records, Ice Condenser-4313 140-character records)

Reference reports and NESC Note

* 90-character records

17. **CATEGORY** - G
KEYWORDS - accidents, containment, temperature distribution, ice condensers, pressure, reactor safety, mass transfer, energy transfer, PWR reactors, BWR reactors, CONTEMPT codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
Division of Systems Integration

1. **IDENTIFICATION AND KWIC TITLE -** SLATEC2.0
   SLATEC2.0, mathematical subroutine library

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Cray1, CDC CYBER175 (designed to be machine-independent)

3. **DESCRIPTION -** SLATEC is a large collection of FORTRAN mathematical subprograms brought together in a joint effort by the Air Force Weapons Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Magnetic Fusion Energy Computing Center, National Bureau of Standards, Sandia National Laboratories (Albuquerque and Livermore), and the Martin Marietta Energy Systems Incorporated at Oak Ridge National Laboratory.
   SLATEC is characterized by portability, good numerical technology, good documentation, robustness, and quality assurance. The library can be divided into the following subsections following the lines of the NBS classification system: Elementary and Special Functions, Elementary Vector Operations, Solution of Systems of Linear Equations, Eigenanalysis, QR Decomposition, Singular Value Decomposition, Interpolation, Solution of Nonlinear Equations, Optimization, Quadrature, Ordinary Differential Equations, Partial Differential Equations, Fast Fourier Transforms, Approximation, Psuedo-random Number Generation, Sorting, Machine Constants, and Diagnostics and Error Handling.

4. **METHOD OF SOLUTION -** This information is provided by comments within the individual library subroutines.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -** NESC executed all of the SLATEC library's quick checks in less than 30 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** Two interactive documentation programs, one written in FORTRAN66 and the other in FORTRAN77, are included with the package to provide an on-line documentation facility.

8. **RELATED AND AUXILIARY SOFTWARE -** SLATEC2.0 contains EISPACK2 (NESC 534), LINPACK (NESC 800), FC,LSEI,WNNLS (NESC 909), SPLP, QUADPACK, DEPAC, FISHPACK, FFTPACK, and PCHIP (NESC 9917). Special functions were obtained from FNLIB, FUNPACK (NESC 610), and AMOSLIB. SLAT, an interactive auxiliary program which allows the user to extract selected SLATEC subroutines and all the routines called by those subroutines, is included.

9. **STATUS -** Abstract first distributed May 1982.
   Cray1 version of SLATEC1.0 submitted March 1982, replaced by SLATEC2.0 September 1984, library quick checks and documentation program executed by NESC August 1984 on a CDC CYBER175.

10. **REFERENCES -** Karen H. Haskell, An Interactive Portable Documentation Program for a Mathematical Subroutine Library, SAND82-0202, March 1982.
    SLATEC2.0, NESC No. 820, SLATEC2.0 Tape Description and Implementation Information, National Energy Software Center Note 84-54, September 7, 1984.
    Walter H. Vandevender, The SLATEC Mathematical Subprogram Library, Version 2.0, SAND84-0281, April 1984.
    B. L. Buzbee, The SLATEC Common Math Library, Sources and Development of Mathematical Software, Prentice-Hall Series in Computational Mathematics (to be published), also available as LA-UR-80-3631.
    L. Wayne Fullerton, Portable Special Function Routines, Lecture Notes in Computer Science, Vol. 57, Portability of Numerical Software, G. Goos and J. Hartmanis, Springer-Verlag, Berlin, Heidelberg, New York, 1977.
    Donald E. Amos and Sharon L. Daniel, AMOSLIB, A Special Function Library, Version 9/77, SAND77-1390, September 1977.
    P. Swarztrauber and R. Sweet, Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations, NCAR-TX/IA 109, July 1975.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE** - FORTRAN 66 and FORTRAN 77

13. **OPERATING SYSTEM** - NOS 2.2 (CDC CYBER175) (designed to be operating system independent)

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
W. R. Boland or A. B. White, Jr.
Computer Research and Applications
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source (152,905 lines)
Sample problems (16,110 lines)
Auxiliary information (SLATEC - installation note 311 lines, table of contents 2203 lines, subsidiary subroutines 2004 lines, directory 917 lines, tree 992 lines, SLAT source 713 lines, multi-level trees 1667 lines, FORTRAN77 codes 11,815 lines, FORTRAN77 quick checks 1263 lines, submerged subroutines 7326 lines, machine-readable documentation file 61,490 lines, Haskell documentation program - installation guide 339 lines, table of contents 1056 lines, HELP 678 lines, NEWS 42 lines, PROG1A source 502 lines, PROG1B source 93 lines, PROG1B input 11 lines, PROG2 source 2253 lines, machine-dependent support routines - CDC 5111 lines, VAX 5043 lines, IBM 4739 lines, Chow documentation program - installation guide 39 lines, PRG1 source 226 lines, PRG2 source 468 lines, subsidiary subroutines 91 lines, PRG2 input 81 lines)
Reference report, SAND82-0202, and NESC Note

17. **CATEGORY** - P
KEYWORDS - Adams method, Airy functions, banded matrix, Bessel functions, eigenvalues, eigenvectors, elementary functions, error function, Fourier transformation, gamma function, interpolation, least square fit, Legendre polynomials, libraries, log gamma function, matrices, nonlinear programming, optimization, ordinary differential equations, partial differential equations, Poisson equation, polynomials, quadratures, utility routines, EISPACK2 codes, LINPACK codes, FC,LSEI,WNNLS codes, FUNPACK codes, FISHPACK codes, FNLIB codes, AMOSLIB codes, FFTPACK codes, SPLP codes, DEPAC codes, PCHIP codes, QUADPACK codes

18. **SPONSOR** - DOE Office of Fusion Energy
DOD U. S. Air Force,
Systems Command
DOC National Bureau of Standards

1. **IDENTIFICATION AND KWIC TITLE** - SPAR1
   SPAR1, shielding with analytic ray-tracing

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC6600,7600

3. **DESCRIPTION** - SPAR1 calculates exact gamma-ray fluxes from uniform sources with the shapes of slabs, disks, lines, cylinders, truncated cones, toroids, and spheres. Gamma-ray dose rates and energy absorption rates can also be obtained by including in the program input data gamma-ray buildup factors expressed in Taylor Exponential Coefficient form. Furthermore, SPAR1 will calculate fast-neutron dose rates and thermal-neutron fluxes in those cases where the use of neutron-removal cross sections is valid. In general, all three-dimensional sources having curved surfaces (cylinders, spheres, and toroids) may have both curved and slab shields intervening between the source and the detector point. Slab shields are allowed in all cases. Both slab and curved shields are assumed to be laminar. Source self-attenuation is always included in flux calculations, and multiple energy levels may be considered. Both interior and exterior detector points are allowed for cylindrical, slab, and spherical sources, and line sources may be tilted with respect to their slab shields. The detector point associated with a cylindrical volume source may be arbitrarily located, and a finite cylindrical shield may be considered. A cylindrical surface source is also available.

4. **METHOD OF SOLUTION** - Some of the semi-analytic calculation algorithms used in SPAR1 came directly from references 1, 2, and 3. The exact semi-analytic formulas for the fluxes from cylindrical, spherical, and toroidal sources were derived by Wallace, based on the work reported in references 3, 4, and 5. In all cases, uniform source strength, laminar shields, and the validity of the point kernel are assumed. It is always possible, for the source shapes treated in SPAR1, to formally integrate over at least one dimension of a three-dimensional source, leaving a nonsingular integrand to be numerically evaluated over, at most, two dimensions. This numeric integration is done using Gauss-Legendre quadrature. The derivations are given in detail in reference 6, and the program is fully described in reference 7.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - No more than 20 energy levels, 20 slab and 20 curved shield laminas, and one detector point can be considered in one case. Up to 250 cases can be grouped in one run.

6. **TIMING** - The running time varies from 0.33 to 2 seconds per case, depending on the option selected.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SPAR1 is designed to furnish quick answers to simple shielding problems such as those encountered in scoping studies. SPAR1 requires minimal input, and jobs can be submitted via remote terminals. A special output file formatted for display on a terminal is written by the program.

8. **RELATED AND AUXILIARY SOFTWARE** - SPAR1 uses routines from both the Bettis Environmental Routines (NESC 478) and the later Bettis Environment Library (NESC 665). The program was verified by comparison of results with SPAN4 (NESC 462) for the same problems. SPAN4 interpolates tables of gamma-ray buildup factor data while SPAR1 uses Taylor Exponential Coefficients. SPAN4 performs a three-dimensional quadrature over the source volume while SPAR1 performs at most a two-dimensional quadrature over the horizontal and vertical angles subtended by the source volume, area, or line. An explicit ray-tracing algorithm is used in SPAN4 while all SPAR1 ray-tracing is implicit in the flux equations.

9. **STATUS** - Abstract first distributed September 1979.
   CDC6600 version submitted August 1976, sample problems executed by NESC April 1979 on a CDC7600.

10. **REFERENCES** - T. Rockwell, Ed., Reactor Shielding Design Manual, D. Van Nostrand, Princeton, New Jersey, 1956.

R. G. Jaeger, Ed., Engineering Compendium on Radiation Shielding, Vol. 1, "Shielding Fundamentals and Methods," Springer-Verlag, Inc., New York, New York, 1968.

Hironori Ono and Akira Tsuruo, An Approximate Calculation Method of Flux for Spherical and Cylindrical Sources with a Slab Shield, Journal of Nuclear Science and Technology, Vol. 2, No. 6, pp. 229-235, June 1965.

Akira Tsuruo, Unscattered Flux from Spherical and Cylindrical Sources with Shell-Shaped Shields, Journal of Nuclear Science and Technology, Vol. 2, No. 7, pp. 261-269, July 1965.

D. F. Rhodes, R. A. Stallwood, and W. E. Mott, Intensity of Unscattered Gamma Rays inside Cylindrical Self-Absorbing Sources, Nuclear Science and Engineering, Vol. 9, pp. 41-46, 1961.

O. J. Wallace, Semi-Analytic Flux Formulas for Shielding Calculations, WAPD-TM-1197, June 1976.

O. J. Wallace, SPAR1, A Semi-Analytic Point-Kernel Computer Program for Shielding, WAPD-TM-1196, June 1976.

W. R. Cadwell, Ed., Reference Manual--Bettis Programming Environment, WAPD-TM-1181, September 1974.

O. J. Wallace, SPAN-4--A Point-Kernel Computer Program for Shielding, WAPD-TM-809, December 1969.

11. **HARDWARE REQUIREMENTS** - 50K central memory and one system disk (CDC6600)

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.1 (CDC6600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - This program is structured into distinct parts or overlays that are loaded into the central memory as required. The main or root overlay is always in memory; in addition, a particular primary overlay may also be in the central memory. SPAR1 has a root overlay and four primary overlays. The primary overlays are loaded and executed through calls on the NEXT subroutine described in reference 8. The Bettis Environmental Routines used by SPAR1 are not included in the package. These routines would either have to be acquired and modified, or replaced for implementation in another environment. They are heavily dependent on the operating system under which they were developed.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
O. J. Wallace
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (11,126 lines)
Sample problems (863 lines)
Sample problems output (20 selected pages)
Reference reports, WAPD-TM-1196 and WAPD-TM-1197

17. **CATEGORY** - J
KEYWORDS - shielding, gamma radiation, dose rates, buildup, point kernels, neutron flux, SPAN4 codes, BETTIS ENVIRONMENTAL ROUTINES codes, BETTIS ENVIRONMENTAL LIBRARY codes

18. **SPONSOR** - ERDA Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - HAUSER5
   HAUSER5, nuclear reaction cross sections

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   UNIVAC1100, IBM370,4331, CDC7600,CYBER170

3. **DESCRIPTION** - HAUSER5 calculates angle-integrated and, if desired, angle-differential reaction cross sections which can include capture and fission channels. Cross sections for discrete particle channels can be calculated, as well as the total for each reaction pair. Tertiary reactions can be calculated as though the reaction occurs as two sequential binary reactions. There is no restriction on the spins of the particles.

4. **METHOD OF SOLUTION** - HAUSER5 is based on three models of nuclear reactions--the statistical (or Hauser-Feshbach) model, the pre-equilibrium model (exciton formulation), and a statistical model for direct reactions. Transmission coefficients are interpolated from a table of previously-calculated transmission coefficients which can be supplied as input data or calculated by solving the Schroedinger equation with a spherical potential. The real spherical potential is taken to be the Woods-Saxon shape and the derivative can be Woods-Saxon or Gaussian shape. The fission transmission coefficients are based on the Hill-Wheeler equation.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - HAUSER5 can accurately predict nuclear cross sections over most energy ranges less than about 60 MeV. Presently, the only statistical direct reaction included is the (n,alpha) pickup reaction. The Coulomb function may need to be replaced if heavy ions far below the Coulomb barrier are used. A maximum of six reaction pairs can be calculated. Residual nucleii can be described by 100 discrete levels and by the constant temperature level formula and/or the Fermi-gas level description. The maximum number of orbital angular momentum and energies for transmission functions and compound nuclear fractions is 32. The angular distribution expressed at equally-spaced angles from 0 to 90 degrees can be calculated for up to 20 discrete states. The program does not follow gamma ray cascades down a nucleus.

6. **TIMING** - About 30 seconds for calculating cross sections from 14.8 MeV neutrons on CU(63). The sample problem was executed by NESC in less than 94 CP seconds on an UNIVAC1100/44, 23 CPU seconds on an IBM4331, and 2 CP seconds on a CDC CYBER170/875.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - HAUSER5 provides a single fast code covering unresolved resonance regions to beyond 50 MeV.

8. **RELATED AND AUXILIARY SOFTWARE** - An auxiliary program, TISO, is included in the package. TISO calculates gamma ray transmission coefficients to separate states in the final nucleus, allowing isomeric production to be calculated. HAUSER5 relies very heavily on the earlier STATIS code for the statistical model calculation and the PRECO-B code for the pre-equilibrium section. HAUSER5 was preceded by the HAUSER1-HAUSER4 programs and has been tested against the related HELENE, TNG, and GNASH (NESC 757) codes.

9. **STATUS** - Abstract first distributed October 1979.
   UNIVAC1100 version submitted April 1979, replaced February 1983 by revised Edition B, replaced April 1985 by revised Edition C.
   CDC7600 version submitted March 1983, available "As Is" as NESC No. 9953, sample problem executed by NESC December 1984 on a CDC CYBER170/875.
   IBM370 version submitted February 1984, available "As Is" as NESC No. 9953, sample problem executed by NESC December 1984 on an IBM4331.

10. **REFERENCES** - Frederick M. Mann, HAUSER-5, A Computer Code to Calculate Nuclear Cross Sections, HEDL-TME 78-83, July 1979.
    HAUSER5, NESC No. 830.1100C, HAUSER5 UNIVAC Version Tape Description and Sample Problem Output, National Energy Software Center Note 85-61, December 19, 1984.
    HAUSER5, NESC No. 830.370, HAUSER5 IBM Version Tape Description, National Energy Software Center Note 85-59, December 19, 1984.

HAUSER5, NESC No. 830.7600, HAUSER5 CDC Version Tape Description, National Energy Software Center Note 85-60, December 19, 1984.

Frederick M. Mann, HAUSER-4, A Computer Code to Calculate Nuclear Cross Sections, HEDL-TME 76-80, September 1976.

R. G. Stokstad, STATIS - Yale Internal Report #72, Wright Nuclear Structure Laboratory, 1972.

C. Kalbach, PRECO-B, Program for Calculating Pre-Equilibrium Particle Energy Spectra, Triangle Universities Nuclear Laboratory and North Carolina State University Chemistry Department informal report, 1977.

D. L. Hill and J. A. Wheeler, Nuclear Constitution and the Interpretation of Fission Phenomena, Physical Review, Vol. 89, No. 5, pp. 1102-1145, March 1, 1953.

M. Blann, Pre-equilibrium Decay, Annual Review of Nuclear Science, Vol. 25, pp. 123-166, 1975.

P. H. Cowell and A. C. D. Crommelin, Appendix to Greenwich Observations for 1909, in J. Fox and E. T. Goodwin, Proceedings of the Cambridge Philosophical Society, Vol. 45, No. 1, pp. 373-383, January 1949.

11. **HARDWARE REQUIREMENTS** - HAUSER5 requires an input device (logical unit 5) to read card images, output devices for printed copy (units 6, 8, 10, and 11), and output devices for punched cards (units 7 and 9). The auxiliary program, TISO, requires punch units 7 and 8. HAUSER5 uses 58K words of memory on a UNIVAC1100/44, with overlays, 620K bytes on an IBM4331, and 223,000 (octal) words on a CDC CYBER170/875. TISO requires 17K words of memory on a UNIVAC1100/44, 255K bytes on an IBM4331, and 42,000 (octal) words on a CDC CYBER170/875.

12. **PROGRAMMING LANGUAGE** - FORTRAN V (99%) and Assembler (1%) (UNIVAC1100), FORTRAN IV (IBM370, CDC7600)

13. **OPERATING SYSTEM** - EXEC8 (UNIVAC1100), VM/CMS (IBM4331), NOS 2.2 (CDC CYBER170).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Segments of the code are independent, allowing easy segmentation or overlay, and the storage requirements can also be reduced by eliminating undesired options. The HAUSER5 UNIVAC version will have to be modified to execute under the FORTRAN ASCII compiler, as the present edition of the code produces compiler errors. An NTAB$ element written in Assembler language is included to provide carriage control in the alternate print files.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

1100, 7600	F. M. Mann Hanford Engineering Development Laboratory
370	NEA Data Bank
370 TISO	L. R. Eyberger National Energy Software Center Argonne National Laboratory

16. **MATERIAL AVAILABLE** -

Source (1100-6257 lines, 370-4640 lines, 7600-6296 lines)
Sample problems (HAUSER5 697 lines, TISO 8 lines)
Auxiliary program (TISO 1100-630 lines, 370-630 lines, 7600-622 lines)
Control information (HAUSER5 1100-166 lines, 370-58 lines, 7600-13 lines, TISO 1100-42 lines, 370-55 lines, 7600-19 lines)
Sample problems output (HAUSER5 1100-30 pages, 370-1037 132-character records, 7600-1033 132-character records, TISO 1100-13 pages, 370-41 132-character records, 604 lines, 7600-41 132-character records, 604 lines)
Reference report, HEDL-TME 78-83, and NESC Note, appropriate to version

17. **CATEGORY** - A
KEYWORDS - cross sections, neutron reactions, Hauser-Feshbach theory, precompound-nucleus emission, Racah coefficients, Clebsch-Gordan coefficients, TISO codes, GNASH codes, STATIS codes, PRECO-B codes, HELENE codes, TNG codes

18. **SPONSOR** - DOE Office of Fusion Energy,
Division of Reactor Research and Technology

1. **IDENTIFICATION AND KWIC TITLE** - SOLA-DF
   SOLA-DF, transient 2-dimensional 2-phase flow

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - SOLA-DF is a numerical solution algorithm for gas-liquid mixture dynamics in two space dimensions and time. The two-phase system is described by a set of mixture equations plus a relation describing the relative flow of one phase with respect to the other. The algorithm contains models to represent the interphase exchange rates of mass, momentum, and energy for water-steam mixtures.

4. **METHOD OF SOLUTION** - SOLA-DF uses a finite difference technique, which includes the Implicit Continuous-fluid Eulerian (ICE) method as an optional feature, to solve the drift-flux equations of two phase flow in two-dimensional plane or cylindrical coordinates. A wide variety of boundary conditions are possible, including free-slip, no-slip, specified inflow-outflow, continuative out-flow, periodic, and constant pressure boundaries. Implicit pressure gradients are used to eliminate the Courant condition as a stability requirement, making the code useful at all Mach numbers.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Simple equation of state, relative velocity model and phase transition model are assumed. When large phase transition rates are present, because of the decoupled calculation of phase change and the pressure iteration, care must be exercised to make sure the solution is independent of the time-step.

6. **TIMING** - The "grind" time, or time to advance the solution in one cell by one time-step, is typically 0.5 to 1.0 ms on a CDC7600. NESC executed the sample problem in less than 8 CP minutes on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SOLA-DF is designed to be easy to understand and modify so it can serve as a foundation for code development.

8. **RELATED AND AUXILIARY SOFTWARE** - The solution algorithm has evolved from earlier SOLA series programs. The original SOLA was designed for problems involving a single, incompressible fluid in a fixed region. SOLA-SURF (NESC 651) is an extension which allows for the inclusion of free surfaces. SOLA-ICE (NESC 723) was designed to handle single-component, compressible fluids. SOLA-DF is a direct descendant of SOLA-ICE. A variation of SOLA-DF is contained in SOLA-LOOP (NESC (859), a network code, which handles systems of one-dimensional components coupled through junctions. K-FIX (NESC 727) calculates the transient dynamics of two-dimensional, two-phase flow with interfacial exchange.

9. **STATUS** - Abstract first distributed December 1979.
   CDC7600 version submitted February 1979, sample problem executed by NESC July 1979 on a CDC7600.

10. **REFERENCES** - C. W. Hirt and N. C. Romero, Application of a Drift-Flux Model to Flashing in Straight Pipes, LA-6005-MS, July 1975.

C. W. Hirt, N. C. Romero, M. D. Torrey, and J. R. Travis, SOLA-DF: A Solution Algorithm for Nonequilibrium Two-Phase Flow, NUREG/CR-0690 (LA-7725-MS), June 1979.

R. M. Frank, J506 Advance Film Subroutine, LASL Program Library Write-up, January 1979.

R. M. Frank, J563 Contour Plotting with Film Output Subroutine, LASL Program Library Write-up, January 1979.

S. T. Bennion, J526 Convert Coordinate Subroutine, LASL Program Library Write-up, January 1979.

S. T. Bennion, J528 Define Graph Area Subroutine, LASL Program Library Write-up, January 1979.

S. T. Bennion, J517 Draw Vector Subroutine, LASL Program Library Write-up, January 1979.

R. M. Frank, J523 Draw Frame Subroutine, LASL Program Library Write-up, January 1979.

V. Gardiner, J508 Standardized Plot Subroutine, LASL Program Library Write-up, January 1979.

SOLA-DF NESC No. 832.7600, Errata to LA-7725-MS Input Description, National Energy Software Center Note 80-06, July 9, 1979.

11. **HARDWARE REQUIREMENTS** - 124,000 (octal) words of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE and LTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - SOLA-DF calls a number of LASL film plotting subroutines - ADV, CONTRJB, CONVRT, DGA, DRV, FRAME, LINCNT, and SPLOT. NESC supplied dummy routines for completeness. To duplicate the results in the report the ROUND option should be specified for the compiler. If ROUND is not specified, the results are printed at different time intervals.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

C. W. Hirt, N. C. Romero, M. D. Torrey,
and J. R. Travis
Theoretical Division
Los Alamos Scientific Laboratory

16. **MATERIAL AVAILABLE** -
Source (1401 lines)
Sample problem (20 lines)
Reference report, NUREG/CR-0690, LASL Program Library Write-ups, and NESC Note

17. **CATEGORY** - H
KEYWORDS - fluid flow, two-dimensional, ICE method, two-phase flow, phase transformations, SOLA codes, finite difference method

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - TRAC-PF1
TRAC-PF1, best-estimate analysis PWR LOCA

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - CDC7600, IBM370,3033

DESCRIPTION - TRAC-PF1 performs best-estimate analyses of loss-of-coolant accidents and other transients in pressurized light water reactors. The program can also be used to model a wide range of thermal-hydraulic experiments in reduced-scale facilities. Models employed include reflood, multi-dimensional two-phase flow, nonequilibrium thermodynamics, generalized heat transfer, and reactor kinetics. Automatic steady-state and dump/restart capabilities are provided. The changes reported in TRACNEWS issues through Number 7 are incorporated in this release.

METHOD OF SOLUTION - The partial differential equations describing the two-phase flow and heat transfer are solved by finite differences. The heat-transfer equations are treated using a semi-implicit differencing technique. The fluid-dynamics equations in the one-dimensional components use a multistep procedure that allows the material Courant condition to be violated. The three-dimensional vessel option uses semi-implicit differencing. The finite-difference equations for hydrodynamic phenomena form a system of coupled, nonlinear equations that are solved by a Newton-Raphson iteration procedure.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - All storage arrays in TRAC-PF1 can be dynamically allocated; the only limit on the size of a problem is the amount of central memory available. The number of reactor components in the problem and the manner in which they are coupled are arbitrary. Reactor components available include accumulators, pipes, pressurizers, pumps, steam generators, tees, valves, and vessels with associated internals.

TIMING - Running time is highly problem dependent and is a function of the total number of mesh cells, the maximum allowable time-step size, and whether a three-dimensional vessel model is used. If a purely one-dimensional model is used, very large time-steps can be used for slow transients. If a three-dimensional vessel is employed, a material Courant limit in the vessel may reduce the maximum time-step size allowed and increase the running time. Typical computer times for a CDC7600 average 2-3 ms per time-step per mesh cell. Complete analysis of a detailed PWR LOCA (including reflood) will require several CP hours. The longest running sample problem requires about 70 CP seconds on the CDC7600 and about 300 seconds of CPU time on the IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE - TRAC-PF1 can describe most thermal-hydraulic experiments in addition to a wide variety of light-water-reactor (LWR) systems. The program is modular to more easily accommodate geometric descriptions of a problem and more detailed models of physical processes, and to reduce program maintenance costs.

RELATED AND AUXILIARY SOFTWARE - Seven auxiliary programs are included with the CDC version of TRAC-PF1. EXCON is a postprocessor program used to convert the TRCGRF graphics output file into a set of component data files for input to the general-purpose graphics program TRAP. GRED and GRIT also process the TRCGRF output file. CON1 and CON2 convert older TRAC-PD2/MOD1 input decks into the new format required by TRAC-PF1. TRCUPD processes CDC UPDATE statements. These auxiliary programs are dependent upon the computing environment and will need to be replaced or modified for other computing environments. No auxiliary graphics capability is provided with the IBM version of TRAC-PF1.

STATUS - Abstract first distributed December 1979.
CDC7600 version of TRAC-P1A submitted March 1979, replaced by revised edition July 1979, TRAC-PD2 submitted August 1980, revised November 1980, replaced June 1981 by TRAC-PD2/MOD1, replaced November 1982 by TRAC-PF1 submitted August 1981, revised December 1981, March 1982, and July 1982, sample problems executed by NESC September 1982 on a CDC7600.
IBM370 version of TRAC-PF1 submitted August 1984, sample problems executed by NESC September 1984 on an IBM3033.

10. **REFERENCES** - Thad D. Knight, TRAC-PD2 Independent Assessment, NUREG/CR-3866 (LA-10166-MS), December 1984.

Energy Division, Safety Code Development Group, TRAC-PF1: An Advanced Best-Estimate Computer Program for Pressurized Water Reactor Analysis, NUREG/CR-3567 (LA-9944-MS), February 1984.

Energy Division Safety Code Development Group, Transient Reactor Analysis Code Input Specifications TRAC-PF1 7.0/EXTUPD7.6, LA-TIA-TN-82-1, June 1982.

B. E. Boyack, TRAC-PF1 Developmental Assessment, NUREG/CR-3280 (LA-9704-M), July 1983.

TRAC Newsletter, Number 6, Los Alamos National Laboratory, January 1982.

TRAC Newsletter, Number 7, Los Alamos National Laboratory, May 1982.

J. C. Ferguson and M. R. Turner, TRAP: Plotting Package for TRAC, Revision of NUREG/CR-2054 (LA-8709-MS), rough draft, received August 1981.

TRAC-PF1, NESC No. 836.7600, TRAC-PF1 Tape Description and Implementation Information, National Energy Software Center Note 83-09, October 29, 1982.

TRAC-PF1, NESC No. 836.370, TRAC-PF1 IBM Version Tape Description and Implementation Information, National Energy Software Center Note 85-19, October 30, 1984.

Dean Dobranich, Lawrence D. Buxton, and Chung-Nin Channy Wong, TRAC-PF1 LOCA Calculations Using Fine-Node and Coarse-Node Input Models, NUREG/CR-4044 (SAND84-2305), May 1985.

Gregory D. Spriggs, Jan E. Koenig, and Russel C. Smith, TRAC-PF1 Analysis of Potential Pressurized-Thermal-Shock Transients at Calvert Cliffs/Unit 1 A Combustion Engineering PWR, NUREG/CR-4109 (LA-10321-MS), February 1985.

11. **HARDWARE REQUIREMENTS** - The CDC7600 version requires approximately 62K words of small core memory (SCM) and 131K words of large core memory (LCM). The IBM version requires from 4000K to 7000K bytes on an IBM3033.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (FTN 4.5 FORTRAN compiler) (CDC7600); FORTRAN IV (99.8%) and BAL (0.2%) IBM3033

13. **OPERATING SYSTEM** - SCOPE 2.1.5 (CDC7600), OS/MVT (IBM370), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - COMPASS replacement routines for the TRAC-PF1 linear equation solver are included in the CDC package for more efficient operation. For plotting, TRAP, the CDC version graphics program, makes use of the Integrated Software Systems Corporation's (ISSCO) proprietary software product DISSPLA. The conversion from the CDC to IBM environment was done at Gesellschaft fuer Reaktorsicherheit, West Germany, using an Amdahl 470 V/6 II with IBM MVS operating system and the FORTRAN H Extended Enhanced compiler.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600 J. H. Mahaffy
Energy Division
Los Alamos National Laboratory

370 E. T. Dugan
Department of Nuclear Engineering Sciences
University of Florida

16. **MATERIAL AVAILABLE** -

Source (7600-TRAC-PF1 FORTRAN 49,281 lines, TRAC-PF1 UPDATE 40,749 lines, SOLVE COMPASS 556 lines, 3033-TRAC-PF1 FORTRAN 87,954 lines, BAL 149 lines)
Sample problems (7600-1218 lines, 3033-1216 lines)
Control information (3033-317 lines)
Auxiliary information (7600-TRAP FORTRAN 16,951 lines, TRAP UPDATE 11,637 lines, LBLIST 744 lines, EXCON FORTRAN 1865 lines, EXCON UPDATE 2589 lines, CON1 4197 lines, CON2 810 lines, TRCUPD 568 lines, GRIT 671 lines, GRED 534 lines, 3033-LRECL90,BLOCK DATA,IGVSSL 2,895 lines)
Sample problems output (7600-10,089 132-character records, 3033-12,933 133-character records, 199 80-character records)

Reference reports, Newsletters, and NESC Note, appropriate to version. The rough draft of the NUREG/CR-2054 (LA-8709-MS) revision is distributed with the CDC7600 version only.

17. **CATEGORY** - G
KEYWORDS - accidents, reactor safety, thermodynamics, heat transfer, reactor kinetics, two-phase flow, PWR reactors, loss of coolant, transients, TRAP codes, EXCON codes, GRED codes, GRIT codes, CON1 codes, CON2 codes, TRCUPD codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - FUELS DATA
   FUELS DATA, model verification fuel rod data

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER176,175, CDC7600

3. **DESCRIPTION** - FUELS DATA is a collection of machine-readable fuel behavior data from domestic and foreign water reactor test facilities developed for use in model verification of the Nuclear Regulatory Commission FRAP codes.

4. **METHOD OF SOLUTION** - Measurements have been formatted and stored to facilitate computer application. The storage format for each fuel rod entry provides identification data, design parameters, power history, and corresponding measurement history. The verification data base is expanded prior to evaluating each new version of the model to enable verification runs to have continuing independent benchmark significance because there is always the chance that empiricism in the model based on previous experiments may be misdirected.

   The storage structure is made up of 11 separate file types, 10 of these corresponding to different card types and associated card formats. The identification and design block includes the first four card types: types 1, 2, and 3 appear for each entry. Card type 1 provides the rod designation and run number and experiment and reference report designation. Type 2 contains data availability flags for the 15 measurement parameters which follow and specifies the number of measurement locations. Type 3 represents the main design, fabrication, and system condition data. If local measurements are available, card type 4 gives the instrument location. Card types 5 and 6 describe the rod operating history. Type 5 specifies the heat rating and cumulative irradiation time at the end of an operating step and the associated step power and burnup condition measurements. Type 6 describes normalized axial power distributions during different operating history periods. The rod measurement history is defined by card types 7 through 11. Types 7 and 8 contain instrumented rod measurements corresponding to operating steps defined by card type 5 (e.g., integral measurements for fuel and cladding length change, rod internal pressure, fuel and cladding temperature, cladding circumferential strain, and gap conductance at specified instrument locations). Card types 9, 10, and 11 are used for post-irradiation exam (PIE) measurements. Types 9 and 10 contain integral measurements related to gas, void, pressure, and axial deformation conditions. Card type 11 represents PIE measurements for melt radius, corrosion thickness, permanent hoop strain, and gap conductance from grain growth determination.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   70 operating steps
   5 axial power distribution profiles
   FUELS DATA contains only steady-state fuel behavior data.

6. **TIMING** - A formatted listing of the fuels data file can be produced using the editing program in about 20 CP seconds on a CDC CYBER176 and 9 CP seconds on a CDC CYBER175. Approximately 6.5 CP seconds are required for a typical categorical processing run on a CDC CYBER176 and 17 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The FUELS DATA package contains an editing program to read and print a formatted listing of the fuels data file containing measured data and design parameters for each data category. This fuel rod behavior data file was developed for model verification for the FRAPCON1 (NESC 694) and FRAP-T (NESC 658) programs.

9. **STATUS** - Abstract first distributed January 1980.
   CDC CYBER76 version submitted September 1979, replaced December 1980 by revised CDC CYBER176 version submitted May 1980, replaced January 1982 by Edition B submitted October 1981, replaced June 1984 by Edition C submitted January 1983, edited by NESC February 1983 on a CDC CYBER175.

10. **REFERENCES** – N. L. Hampton, INEL Fuel Code Assessment Data Base Access and Description, EGG-NTAP-6056, Revision 1, March 1983.

N. L. Hampton, INEL Fuel Code Assessment Data Bank Description and Users Manual, EGG-CAAD-5486, July 1981.

R. Chambers, N. L. Hampton, and E. T. Laats, Fuel Code Assessment Data Sample Report, EGG-CAAP-5114, February 1980.

D. R. Coleman and N. R. Scofield, Fuel Code Assessment Data Report Number III – Description of Data Processing Software, CAAP-TR-039, January 1979.

FUELS DATA, NESC No. 844.C176C, FUELS DATA Tape Description, National Energy Software Center Note 84-40, June 25, 1983.

11. **HARDWARE REQUIREMENTS** – 37,000 (octal) words of memory are used by the auxiliary editing program on a CDC CYBER175; 44,000 (octal) words of memory are required on a CDC CYBER176.

12. **PROGRAMMING LANGUAGE** – FORTRAN IV for the auxiliary edit program, data are recorded as EBCDIC characters.

13. **OPERATING SYSTEM** – NOS/BE 1.4 (CDC CYBER176), NOS 1.4 (CDC CYBER175), SCOPE 2.1 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – Each edit subprogram is executed independently; a single input card is used to select the data category to be processed. Subroutine DUMPX produces a formatted listing for all data categories for approximately 700 experiments.

A CDC UPDATE source file is also available for use by installations having the CDC UPDATE utility. The file contains both program and data and provides greater selection capabilities (i.e., specific runs may be compiled separately rather than the entire data set.)

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

E. T. Laats and N. L. Hampton
EG&G Idaho, Inc.
N. R. Scofield
Water and Power Resource Service
Engineering and Research Center
Denver Federal Center
D. R. Coleman
Nuclear Associates International Corporation

16. **MATERIAL AVAILABLE** –

Fuel rod behavior data (28,981 lines, UPDATE 31,088 lines)
Auxiliary edit program (FORTRAN 1515 lines, data 2 lines)
Fuels data sample edits (28 selected pages, 7 microfiche)
Reference reports, EGG-NTAP-6056, EGG-CAAP-5114 and EGG-CAAD-5486, and NESC Note

17. **CATEGORY** – Z
KEYWORDS – data processing, fuel elements, performance, mathematical models, reactor safety, steady-state conditions

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research

1. **IDENTIFICATION AND KWIC TITLE** - TIDY3,TIDY4.63
   TIDY3, utility to edit Fortran source programs
   TIDY4.63, utility to edit Fortran source code

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER74,175, UNIVAC1100

3. **DESCRIPTION** - TIDY is a utility program for processing FORTRAN source programs into a standard form which is easy to read and modify. In processing FORTRAN software it renumbers statement labels so that they appear in increasing order, removes statement labels from unreferenced statements and deletes unreferenced FORMAT and CONTINUE statements, indents DO loops and IF levels (IF level by TIDY4.63 only), and collects and groups TYPE, DATA, and EQUIVALENCE statements (TIDY3 collects only TYPE statements). Each group is alphabetized and rewritten in a column-aligned manner. FORMAT statements are either inserted following the first reference or, optionally, collected at the end of the code. Blanks are inserted and removed to improve readability.

4. **METHOD OF SOLUTION** - TIDY4.63 will accept as input an ASCII or FORTRAN V source code element or a FORTRAN PROC. The utility identifies each individual statement by type and class. Each FORTRAN keyword implies a different statement type, of which there are 63. These are grouped into eight statement classes, which are treated independently by the program. A seven-word header record placed before each statement is used to store the information about the statement for TIDY4.63 processing which is done in three passes.
   TIDY3 will accept as input FORTRAN source, COMPASS source, or CDC UPDATE utility source. The utility identifies each statement by type and class. Each FORTRAN keyword implies a different statement type, of which there are 45. These are grouped into six statement classes, which are treated independently by the program. A six-word header record placed before each statement is used to store the information about the statement for TIDY3 processing which is done in four passes.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -

50 different tabular, non-executable statements	(TIDY4.63)
20 characters in a single array name including DIMENSION specifications	(TIDY4.63)
500 distinct statement labels excluding FORMAT statements	
250 distinct FORMAT statement labels	
20 nested DO LOOPS	
19 TYPE statements	(TIDY3)

6. **TIMING** - Execution time varies with the size of the element that is being processed. As a general rule, TIDY4.63 takes two and one-half times the compilation time without optimization. NESC compiled TIDY4.63 and processed the sample program with several different options in under 2 minutes on an UNIVAC1100/44. NESC processed the TIDY3 sample programs in less than 8 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Users may select various options for processing or "tidying" their programs. TIDY is capable of both batch and interactive processing. TIDY3 recognizes CDC COMPASS routines and copies them 'as is'.

8. **RELATED AND AUXILIARY SOFTWARE** - The original TIDY was developed by Harry M. Murphy, Jr., Air Force Weapons Laboratory, Kirtland Air Force Base, New Mexico, in 1966. TIDY4 was prepared by J. Jackson of BCS Richland, Inc. TIDY-J (NESC 896) processes IBM FORTRAN source programs.

9. **STATUS** - Abstract first distributed January 1980.
   UNIVAC1100 version of TIDY4 submitted January 1979, replaced February 1983 by TIDY4.63 submitted November 1982, sample problem executed by NESC November 1982 on a UNIVAC1100/44.
   CDC CYBER74 version of TIDY3 submitted June 1981, sample problems executed by NESC October 1981 on a CDC CYBER175.

10. **REFERENCES** - J. Diven, TIDY4 User's Guide, BCS Richland document BCSR-91, January 1981, Revised December 1982.
Joseph N. Diven, TIDY Users Guide for RL Users, Computer Sciences Corporation document, September 1974, Revised October 1981.
TIDY3, NESC No. 857.CY74, TIDY3 Tape Description, National Energy Software Center Note 82-20, January 18, 1982.

11. **HARDWARE REQUIREMENTS** - Four mass-storage units are used for storage. 23K words of memory are required for TIDY4.63 execution. TIDY3 requires 46,000 (octal) words of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (TIDY3), FORTRAN ASCII (98%), Meta-Assembler (1%), and Assembler (1%) (TIDY4.63)

13. **OPERATING SYSTEM** - SCOPE 3.4 (CDC CYBER74), NOS 1.3 (CDC CYBER175), EXEC8 (UNIVAC1100).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - In TIDY4.63 the ASM element is written in Meta-Assembler language (MASM) and the F2FRT element in Assembler language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. N. Diven
BCS Richland, Incorporated

16. **MATERIAL AVAILABLE** -
Source (TIDY4.63 FORTRAN 2438 lines, MASM 361 lines, Assembler 6 lines, TIDY3 FORTRAN 2360 lines, UPDATE 1717 lines)
Sample problems (TIDY4.63 61 lines, TIDY3 371 lines)
Sample problems output (TIDY4.63 4 pages, TIDY3 6 pages)
Reference documents and NESC Note, BCSR-91 for TIDY4.63, TIDY Users Guide and NESC Note for TIDY3

17. **CATEGORY** - P
KEYWORDS - data processing, FORTRAN, utility routines

18. **SPONSOR** - DOE Richland Operations Office (TIDY4.63)
Computer Sciences Corporation (TIDY3)

1. **IDENTIFICATION AND KWIC TITLE** - APACHE
   APACHE, 2d chemically reactive fluid flow code

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - APACHE is a time-marching finite-difference code developed to solve the equations of transient viscous multicomponent chemically reactive fluid dynamics in two space dimensions. A steady-state solution is obtained as the asymptotic limit of a transient calculation.

4. **METHOD OF SOLUTION** - APACHE utilizes an Eulerian mesh with cells that are arbitrary trapezoids. It can be run in a purely explicit mode or a partially implicit mode. The explicit mode is an explicit difference scheme with primary stability limitation the Courant-Friedrichs-Lewy condition that an acoustic signal cannot traverse more than one spatial increment per cycle. The partially implicit mode is a variant of the ICE method with primary stability limitation that the fluid cannot traverse more than one spatial increment per cycle. It is primarily useful for flow at low Mach number. The difference approximation to the convective terms is obtained by the tensor viscosity method to achieve numerical stability without excessive damping. Multicomponent diffusion in APACHE is calculated by a self-consistent effective binary diffusion algorithm.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The fluid is assumed to be an ideal-gas mixture with temperature-independent specific heats. Chemical reactions are assumed to be elementary. Current dimensioning in the program allows only one rotational and vibration level of the lasing species to be considered and a maxima of -
   1 chemical reaction
   10 chemical species
   32 cells in the horizontal direction
   22 cells in the vertical direction
   These restrictions may be increased by increasing the values of the appropriate parameter variables and the corresponding DIMENSION statements.

6. **TIMING** - The running time varies from several minutes for very simple problems to two hours for complex ones. NESC executed the sample problem in less than 2 CP minutes on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Geometrical specifications, initial conditions, and boundary conditions are localized in user-input subroutines. The governing equations are written in two-dimensional variable-depth form, which allows the calculation of flow confined between two free-slip walls of variable spacing. Planar and cylindrical geometries are special cases of the variable-depth description. A spatial marching option reduces the computer time needed for steady-state supersonic flow calculations. For applications to CW chemical lasers, a subroutine calculates radiation intensities and laser power in the Fabry-Perot cavity approximation. The partially-generalized spatial mesh allows the convenient representation of curved boundaries and also provides variable zoning.

8. **RELATED AND AUXILIARY SOFTWARE** - APACHE is applicable to problems similar to those solved by RICE (NESC 720), but provides greater geometrical flexibility.

9. **STATUS** - Abstract first distributed April 1980.
   CDC7600 version submitted April 1979, sample problem executed by NESC November 1979 on a CDC7600.

10. **REFERENCES** - J. D. Ramshaw and J. K. Dukowicz, APACHE: A Generalized-Mesh Eulerian Computer Code for Multicomponent Chemically Reactive Fluid Flow, LA-7427, January 1979.
    J. D. Ramshaw and J. K. Dukowicz, APACHE: A Two-Dimensional Reactive Fluid Dynamics Code for Chemical Laser Applications, LA-UR-78-2765, November 1978.
    Otis A. Farmer and John D. Ramshaw, A Method for Rapid Attainment of the Steady State in Two-Dimensional Time-Marching Supersonic Flow Calculations, Journal of Computational Physics, Vol. 24, No. 1, pp. 23-28, May 1977, (Appendix A of LA-7427).

John D. Ramshaw, Raymond C. Mjolsness, and Otis A. Farmer, Numerical Method for Two-Dimensional Steady-State Chemical Laser Calculations, Journal of Quantitative Spectroscopy and Radiative Transfer, Vol. 17, No. 2, pp. 149-164, February 1977, (Appendix B of LA-7427).

J. K. Dukowicz and J. D. Ramshaw, Tensor Viscosity Method for Convection in Numerical Fluid Dynamics, Journal of Computational Physics, Vol. 32, No. 1, pp. 71-79, July 1979.

R. M. Frank, J506 Advance Film Subroutine, LASL Program Library Write-up, January 1979.

S. T. Bennion, J526 Convert Coordinate Subroutine, LASL Program Library Write-up, January 1979.

R. Elliot, J516 Plot a Point Subroutine, LASL Program Library Write-up, January 1979.

Gene Willbanks, J520 Type Specific Point Subroutine, LASL Program Library Write-up, January 1979.

R. Elliot, J522 Type Specified Point Vertically Subroutine, LASL Program Library Write-up, January 1979.

APACHE, NESC No. 858.7600, Modification of LA-7427 Input Description, NESC Note 80-30, December 17, 1979.

11. **HARDWARE REQUIREMENTS** - APACHE requires 33,000 (octal) words of small core memory and 56,000 (octal) words of large core memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - NESC included dummy routines for the Stromberg-Carlson plotter routines: ADV, CONVRT, DRV, LINCNT, PLT, SPLOT, TSP, and TSPV, and for the following LANL graphics initialization and buffering routines: GRF80, GRPHFTN, GRPHLUN, LIB4020, and SETFLSH. Alternative routines for the computer environment in which the program is being executed are required to obtain graphical output.

    Subroutines GEOM, INITIAL, and BNDARY in APACHE are user-input routines specific to the sample problem. Changes will be required for other problems.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    J. D. Ramshaw and J. K. Dukowicz
    Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -

    Source (FORTRAN 4670 lines, CDC UPDATE 3310 lines)
    Sample problem (11 lines)
    Sample problem output (1 microfiche)
    Reference report, LA-7427, Program Library Write-ups, and NESC Note

17. **CATEGORY** - H
    KEYWORDS - fluid flow, two-dimensional, ICE method, finite difference method, chemical lasers, radiation effects, reaction kinetics, space-time, x-y, r-z, RICE codes

18. **SPONSOR** - DOD Air Force Weapons Laboratory,
    Chemical Laser Branch

IDENTIFICATION AND KWIC TITLE - SOLA-LOOP
SOLA-LOOP, two-phase flow network analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,6600

DESCRIPTION - SOLA-LOOP is designed for the solution of transient two-phase flow in networks composed of one-dimensional components. The fluid dynamics is described by a nonequilibrium, drift-flux formulation of the fluid conservation laws. Although developed for nuclear reactor safety analysis, SOLA-LOOP may be used as the basis for other types of special-purpose network codes. The program can accommodate almost any set of constitutive relations, property tables, or other special features required for different applications.

METHOD OF SOLUTION - The drift-flux equations are formulated as continuity equations, the momentum equation, and the internal energy equation. The mixture density, the macroscopic vapor density, the center of mass velocity, and the mixture specific internal energy are chosen as dependent variables, and time and axial position are the independent variables. Constitutive relations and exchange rates are determined by the intended use of the code. The calculation cycle used to solve by point relaxation methods the finite difference formulation of the flow equations in a single one-dimensional component is made up of four tasks. First, the momentum equation is advanced explicitly using the values from the previous cycle for all contributions. Next, an iteration is made to replace the pressure with advanced time values. This pressure iteration scheme is a variant of the Implicit Continuous fluid Eulerian (ICE) technique. Then, all other dependent variables are updated, and in the fourth task data output, time-step control, and housekeeping operations are performed. Various boundary conditions may be applied at the ends of the one-dimensional component meshes to represent inlet and exit conditions including prescribed velocities or pressures, uniform or gradient-free outflow, and periodic boundaries in which the bottom and top of a component are joined. Where two or more components are coupled, special coupling equations are solved to obtain the appropriate boundary conditions for each. Different time-steps can be used in various components. The time-steps are determined by numerical stability requirements and other user-specified conditions.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Conservation of momentum is not required by the finite difference approximations used for the momentum equation. Current dimensioning in the SOLA-LOOP program allows maxima of -

10 components
8 segments per component
200 junctions
6 time levels, pressure groups, and vapor production rates per cell
5 boundary data sets

These restrictions may be adjusted by changing the values of the variables NP, NS, NJ, NK, and NM, respectively, and all appropriate DIMENSION statements.

TIMING - The time required is highly problem-dependent. NESC executed the sample problem in less than 3 CP minutes on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE - Network systems often contain low-speed flow with slowly-varying properties in one region and high-speed flow or flow that requires a finely-detailed description in another. The variable time-steps and subcycling provisions in SOLA-LOOP are designed specifically for such systems.

RELATED AND AUXILIARY SOFTWARE - The solution algorithm has evolved from earlier SOLA series programs. The original SOLA was designed for problems involving a single incompressible fluid in a fixed region. SOLA-LOOP is an advanced network code derived from the SOLA-DF (NESC 832) code, which is based on a drift-flux approximation for the dynamics of a two-phase mixture.

K-FIX (NESC 727) and K-TIF (NESC 876) are detailed models for transient, two-phase flows in two and three dimensions.

9. **STATUS** - Abstract first distributed April 1980.
CDC7600 version submitted February 1979, sample problem executed by NESC November 1979 on a CDC7600.

10. **REFERENCES** - C. W. Hirt, T. A. Oliphant, W. C. Rivard, N. C. Romero, and M. D. Torrey, SOLA-LOOP: A Nonequilibrium, Drift-Flux Code for Two-Phase Flow in Networks, NUREG/CR-0626 (LA-7659), June 1979.
C. W. Hirt, N. C. Romero, M. D. Torrey, and J. R. Travis, SOLA-DF: A Solution Algorithm for Nonequilibrium Two-Phase Flow, NUREG/CR-0690 (LA-7725-MS), June 1979.
C. W. Hirt, B. D. Nichols, and N. C. Romero, SOLA - A Numerical Solution Algorithm for Transient Fluid Flow, LA-5852, April 1975.
SOLA-LOOP, NESC No. 859.7600, SOLA-LOOP Title Input, NESC Note 80-29, December 17, 1979.

11. **HARDWARE REQUIREMENTS** - 34,000 (octal) words of memory are needed to execute the program.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Because of computing environment differences the time-step/subcycle sequence used by SOLA-LOOP is likely to produce slightly varying results on different computer systems.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
C. W. Hirt, T. A. Oliphant, W. C. Rivard,
N. C. Romero, and M. D. Torrey
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source (3994 lines)
Sample problem (22 lines)
Sample problem output (20 pages)
Reference report, NUREG/CR-0626 (LA-7659), and NESC Note

17. **CATEGORY** - H
KEYWORDS - fluid flow, network analysis, two-dimensional, ICE method, two-phase flow, phase transformations, finite difference method, SOLA codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - FESH
FESH, x-y multi-gp neutron transport PL method

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC6600,7600

DESCRIPTION - FESH solves the spherical harmonics approximation to the second-order multigroup neutron transport equation in two dimensions. A three-dimensional spherical harmonics approximation of user-specified order is applied to the angular variable and two-dimensional spatial finite elements to the spatial variable. Scattering is assumed to be isotropic. Either multiplication eigenvalue problems or subcritical inhomogeneous source problems can be solved with several combinations of vacuum and reflective boundary conditions possible.

METHOD OF SOLUTION - FESH solves the multigroup transport equations (outer iterations) using a power iteration technique on the fission source with coarse mesh rebalance acceleration. The within-group (inner iteration) equation is solved by a block successive overrelaxation method with coarse mesh rebalance acceleration available as an option. Each block represents coupling and source information for each spatial mesh point.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Sources and scattering are assumed to be isotropic; up-scattering is not allowed. Flexible dimensioning permits combinations of problem parameters to occupy an array of 50,000 words. Most group-dependent data is stored in extended core storage (ECS).

TIMING - The time required for execution is problem-dependent. NESC executed the sample problem in 80 CP seconds on a CDC6600 and 20 CP seconds on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE - The unique feature is a rigorous application of transverse buckling which incorporates transverse flux anisotropy into the buckled leakage.

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed January 1980.
CDC6600 version submitted November 1979, sample problem executed by NESC December 1979 on a CDC6600 and a CDC7600.

REFERENCES - R. Blomquist and E. E. Lewis, A Rigorous Treatment of Transverse Buckling Effects in Two-Dimensional Neutron Transport Computations, Nuclear Science and Engineering, Vol. 73, pp. 125-139, 1980.

R. N. Blomquist and E. E. Lewis, Complex Trial Functions in the Even-Parity Transport Equation, Transactions of the American Nuclear Society, 1978 Annual Meeting, San Diego, California, June 18-22, 1978, Vol. 28, pp. 256-257.

R. N. Blomquist and E. E. Lewis, Instruction Manual for the Computer Code FESH: Finite Element Spherical Harmonics, Northwestern University memorandum, March 1978.

HARDWARE REQUIREMENTS - 200,000 (octal) words of central memory and 142,000 (octal) words of ECS are needed to execute the program. Central memory requirements for single precision arithmetic may be estimated as (45M+10) * (L(L+1)/2)**2 + NSP*((L(L+1)/2)+2) words, where M is the number of material regions, L is the order of the spherical harmonics approximation, and NSP is the number of spatial mesh points.

PROGRAMMING LANGUAGE - FORTRAN IV (MNF, University of Minnesota FORTRAN)

OPERATING SYSTEM - SCOPE.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - Because of the central memory required to load the program, the dimension of the Q array must be decreased before FESH can be loaded onto a CDC7600. NESC reduced the dimension of the Q array to 20,000 to execute the sample problem on a CDC7600. The dimensions of the Q and XLARG arrays should be altered to fit the user's specific problem.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

R. N. Blomquist
Applied Physics Division
Argonne National Laboratory
E. E. Lewis
Department of Mechanical and Nuclear Engineering
Northwestern University

16. **MATERIAL AVAILABLE –**

Source (2014 lines)
Sample problem (69 lines)
Reference memorandum

17. **CATEGORY** – C
KEYWORDS – two-dimensional, three-dimensional, buckling, multigroup theory, PL method, spherical harmonics, x-y, neutron transport theory

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research
Northwestern University,
Nuclear Engineering Program

IDENTIFICATION AND KWIC TITLE - INTEROP
INTEROP, nonlinear optimization algorithms

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER173, CDC6600,7600

DESCRIPTION - The INTERactive OPtimization system (INTEROP) is a collection of search direction algorithms for constrained and unconstrained nonlinear optimization problems. The search direction algorithms available in INTEROP include: modified Fletcher-Powell, modified Fletcher-Reeves, steepest-descent Newton, homogeneous predictor, and modified Powell.

METHOD OF SOLUTION - The optimization model is defined in terms of parameters (optimization variables), and states which are linear and nonlinear functions of the parameters. The bounds, if any, are determined for the states and the parameters. The objective function is formulated as a linear combination of the states and the parameters. Subroutine MODEL is a user-supplied subroutine that defines the states in terms of the parameters. The optimization routines use conjugate gradient search direction algorithms and penalty functions.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The program is dimensioned for a maximum of 20 parameters and 20 states.

TIMING - NESC required less than 1.5 seconds of CP time on a CDC6600 and less than 0.5 seconds of CP time on a CDC7600 to complete the sample problem.

UNUSUAL FEATURES OF THE SOFTWARE - The user can interactively define the optimization model, select the optimization algorithm, and change the optimization model as desired.

RELATED AND AUXILIARY SOFTWARE - INTEROP was developed as an interactive counterpart of MOM (Utah State University). OPTIMIZERS (NESC 829) is a collection of routines addressed to the unconstrained nonlinear optimization problem. Programs GPM (University of Minnesota) and GRG (Case Western Reserve University) were developed for constrained optimization problems.

STATUS - Abstract first distributed August 1980.
CYBER173 version submitted September 1979, sample problem executed by NESC October 1979 on a CDC6600 and CDC7600.

REFERENCES - D. M. Rasmuson and R. L. Thurgood, User's Guide for the Interactive Optimization System (INTEROP), TREE-1292, September 1978.

R. L. Thurgood, Computer Algorithms for Solution of Nonlinear Optimization Problems, PhD Dissertation, Department of ELectrical Engineering, Utah State University, Logan, Utah, 1969.

William C. Shaw, MOM-A Computer Program for Modern Optimization Methods, MS Thesis, Department of Electrical Engineering, Utah State University, Logan, Utah, 1972.

J. B. Rosen and S. Wagner, GPM-Nonlinear Programming Subroutine Package: Description and User Instructions, University of Minnesota Technical Report 75-9, Department of Computer Information and Control Sciences, 1975.

L. Lasdon, et al., Design and Testing a Generalized Reduced Gradient Code for Nonlinear Optimization, Case Western Reserve University, Technical Memo 353, Operation Research Department, March 1975.

HARDWARE REQUIREMENTS - INTEROP requires approximately 130K (octal) words for execution on a CDC6600 and 76K (octal) words on a CDC7600.

PROGRAMMING LANGUAGE - FORTRAN IV (90%) and COMPASS (10%)

OPERATING SYSTEM - SCOPE 3.4.4 (CDC6600), SCOPE 2.1.3 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - CVI, a subroutine used to convert free-format input data, is written in CDC COMPASS assembly language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. M. Rasmuson and R. L. Thurgood
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 5420 lines, COMPASS 585 lines)
Sample problem (41 lines, MODEL 9 lines)
Reference report, TREE-1292

17. **CATEGORY** - P
KEYWORDS - nonlinear problems, optimization, algorithms

18. **SPONSOR** - DOE Division of Nuclear Power Development

1. **IDENTIFICATION AND KWIC TITLE** - BNWIGL, UNIWIGL
   BNWIGL, 2-group time-dependent 1-d diffusion
   UNIWIGL, 2-group time-dependent 1-d diffusion

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - UNIVAC1108,1100, CDC6600

3. **DESCRIPTION** - BNWIGL and UNIWIGL solve the one-dimensional, two-energy group, time-dependent diffusion theory equation with thermal feedback. The stand-alone, one-dimensional, steady-state diffusion theory code, HFN, is incorporated to perform critical searches and to determine the initial direct and adjoint fluxes for input to the time-dependent calculation. Problems in slab, cylindrical, and spherical geometries with up to six delayed neutron groups can be solved. Thermal feedback is introduced through the solution of the non-boiling heat transfer equations. Transients can be initiated either from changes in the thermal-hydraulic parameters or by simulated control rod movement in either of the two independent pseudo-rod models. Effects of two and three dimensions can be simulated through the use of interpolation tables for control rod worths and Doppler weighting factors.

4. **METHOD OF SOLUTION** - The numerical techniques used for solving the time-dependent diffusion theory equation are taken from WIGL2 (see reference 2). Principal improvements have been the introduction of Doppler weighting factors and control rod worth functions which allow nonlinear changes in control region cross sections as functions of rod position. Values of the Doppler weighting factors and rod worth functions are entered in tabular form. Lagrangian interpolation is used to arrive at intermediate values of the argument required during execution.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The total storage set aside for all parameters is 16,000 words for the CDC6600 version and 12,000 for the UNIVAC1108 version. Storage is dynamically allocated permitting the user to establish trade-offs in use of spatial detail, numbers of materials, and delayed neutron groups.

6. **TIMING** - A CDC6600 version problem with 111 mesh points, 6 delayed neutron groups, and 13 materials takes less than 1 CP second per time-step. NESC compiled the UNIWIGL program and executed the sample problem in less than 1.5 minutes of CP time on a CDC6600. A UNIVAC1108 version problem with 141 space points, 6 delayed neutron groups, and 4 materials takes approximately 1.17 seconds per time-step. NESC compiled the BNWIGL program and executed the sample problem in 4 CP minutes on a UNIVAC1100/44.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - BNWIGL and UNIWIGL are enhanced versions of the WIGL2 program (NESC 274). The time-dependent, two-energy group, diffusion theory WIGL2 subroutines have been retained without major modification. The steady-state diffusion theory code HFN (NESC 241) has been added.

9. **STATUS** - Abstract first distributed August 1981.
   CDC6600 version of UNIWIGL submitted November 1974, sample problem executed by NESC February 1980 on a CDC6600.
   UNIVAC1108 version of BNWIGL submitted November 1974, sample problem executed by NESC May 1980 on a UNIVAC1100/44.

10. **REFERENCES** - C. M. Heeb, W. W. Porath, and H. Toffer, NEWIGL - A Two-Group Time-Dependent One-Dimensional Neutron Diffusion Theory Code, BNWL-1833 (UNI-203), May 1974.

11. **HARDWARE REQUIREMENTS** - If the programs are segmented, 154,000 (octal) words of memory are required for execution of UNIWIGL (CDC6600), and 51,000 words of memory are required for BNWIGL (UNIVAC1108).

12. **PROGRAMMING LANGUAGE** - FORTRAN (99%) and COMPASS (1%) (CDC6600), FORTRAN V (UNIVAC1108)

13. **OPERATING SYSTEM** - SCOPE 3.4.4 (CDC6600), EXEC8 (UNIVAC1108).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutine DVCHK is the only subroutine in UNIWIGL that is written in CDC COMPASS assembly language. The program assumes that memory has been preset to zero prior to execution. Because of calls to routines contained in the 6600 record manager, UNIWIGL will not run on a CDC7600.

NESC provided a dummy SECOND routine in the BNWIGL package for completeness. This computing environment routine is expected to return the elapsed CP time for the job. A suitable alternative should be provided for the computing environment in which the program is implemented. Users implementing BNWIGL on a system other than an 1108 may expect slight differences from the results shown in the reference report, BNWL-1833.

The two versions are identical except for the following features:

(a) BNWIGL contains a provision for Doppler weighting factors not contained in UNIWIGL.

(b) BNWIGL has the ability to decrease the time-step after a user-selected reactivity limit is reached; UNIWIGL does not.

(c) BNWIGL calculates the time integral of the power to produce a final deposited enthalpy edit. UNIWIGL does not contain this edit.

(d) UNIWIGL produces printer plots of fluxes, adjoint fluxes, and normalized power distributions for each spatial mesh point at various time-steps; BNWIGL does not.

(e) UNIWIGL's thermal hydraulic section has been modified to allow for separate moderator and coolant regions.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

C. M. Heeb
Pacific Northwest Laboratory
W. W. Porath
Exxon Nuclear Company
H. Toffer
United Nuclear Industries, Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution

Source (1108-9172 lines, 6600-FORTRAN 10,192 lines, CDC UPDATE 8761 lines)
Sample problem (1108-88 lines, 6600-221 lines)
Materials library (1108-15 lines)
Control information (1108-165 lines, 6600-91 lines)
Reference report

17. **CATEGORY** - F

KEYWORDS - space-time, one-dimensional, neutron diffusion equation, two-group, slabs, cylinders, spheres, heat transfer, feedback, WIGL2 codes, HFN codes

18. **SPONSOR** - United Nuclear Industries, Inc.
Exxon Nuclear Company

1. **IDENTIFICATION AND KWIC TITLE** - ICARUS
   ICARUS, redundant system unavailability model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM370,303x

3. **DESCRIPTION** - ICARUS calculates the unavailability characteristics of a periodically tested standby system with m-out-of-n redundancy (1.LE.m.LE.n.LE.4). The main functions of the program are to calculate the average unavailability, the optimum test interval, and fractional unavailabilities due to testing, repair, and random failures for three different testing strategies. The program will also calculate the average unavailability as a function of the test interval at each point in the range 0.2T(optimum) to 1.8T(optimum) at intervals of 0.2T(optimum). ICARUS can be used to evaluate sensitivities to different failure modes and data, as well as current testing or repair strategies, to determine if changes to these strategies will optimize the system availability.

4. **METHOD OF SOLUTION** - The system configuration (m and n), testing scheme, testing and repair times, and values for the testing, repair, and standby failure parameters are specified as input data. Using these data and analytical equations, the program calculates the average unavailability for the system and solves for the optimum test interval of the system using the unavailability equation. The program then calculates the contributions (number and percentage) that testing, repair, and random failures make to the average unavailability.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The system configuration is limited to m/n with 1.LE.m.LE.n.LE.4. The three testing strategies allowed are random, uniformly staggered, and nearly simultaneous. In the random scheme, the components are tested at randomly shifted times throughout the test interval. The uniformly staggered scheme performs the component tests at equally-spaced times throughout the test interval. In the nearly simultaneous schemes, all components are tested consecutively at the beginning of the interval.
   The equations assume only one component per redundancy. However, redundancies with several components in series can be analyzed by properly defining the failure data for a series system in terms of the data for individual components.

6. **TIMING** - Typical running time for all m/n systems and all three testing schemes is less than 1 second of CPU time on an IBM370/195. NESC compiled the program and executed the sample problems in 5 seconds of CPU time on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The analytical unavailability equations for all possible systems and each testing strategy are included. For each system, the equations (divided into coefficient equations) are polynomials with both positive and negative powers of the test interval. This allows for the calculation of the optimum test interval by taking the derivative of the average unavailability equation with respect to the test interval, setting that equal to zero, and solving for the optimum test interval. When a numerical solution is required, the Newton-Raphson method is used. Direct analytical equations are available for the random testing scheme.

8. **RELATED AND AUXILIARY SOFTWARE** - ICARUS results were compared to results produced by the FRANTIC-NRC computer code (NESC 766), which calculates time-dependent and average unavailabilities due to the effects of test downtime, repair time, test-caused failures, and test staggering. ICARUS can be used with the PROSA1 (NESC 778) response surface analysis code to determine the sensitivities and probability distributions of the unavailabilities and optimum test intervals.

9. **STATUS** - Abstract first distributed June 1981.
   IBM370 version submitted February 1980, sample problems executed by NESC February 1980 on an IBM3033.

0. **REFERENCES** - Jussi K. Vaurio and Dominic Sciaudone, Unavailability Modeling and Analysis of Redundant Safety Systems, ANL-79-87, October 1979.

ICARUS, NESC No. R871.370, ICARUS Sample Problem Output, National Energy Software Center Note 81-57, June 17, 1981.

11. **HARDWARE REQUIREMENTS** - 60K bytes of memory are required for execution of the program.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

J. K. Vaurio
Reactor Analysis and Safety Division
Argonne National Laboratory
D. Sciaudone
Knolls Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (922 lines)
Sample problems (8 lines)
Reference report and NESC Note

17. **CATEGORY** - G
KEYWORDS - availability, reliability, systems analysis, testing, failures, reactor safety, maintenance

18. **SPONSOR** - DOE Division of Reactor Research and Technology

1. **IDENTIFICATION AND KWIC TITLE** - K-FIX/3D
   K-FIX(3D), 3d extension 2-phase flow dynamics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - This package consists of two programs K-FIX(3D) and K-FIX(3D,FLX) which extend the transient, two-dimensional, two-fluid program K-FIX (NESC 727) to perform three-dimensional calculations. The transient dynamics of three-dimensional, two-phase flow with interfacial exchange are calculated at all flow speeds. Each phase is described in terms of its own density, velocity, and temperature. The application is to flow in the annulus between two cylinders where the inner cylinder moves periodically perpendicular to its axis.
   K-FIX(3D) is easily adaptable to a variety of two phase flow problems while K-FIX(3D,FLX) combines KFIX(3D), the three-dimensional version of the KFIX code, with the three-dimensional, elastic shell code FLX for application to a very specific class of problems. KFIX(3D,FLX) was developed specifically to calculate the coupled fluid-structure dynamics of a light water reactor core support barrel under accident conditions. Motion may be induced by blowdown, prescribed displacement, or seismic action.

4. **METHOD OF SOLUTION** - In K-FIX(3D), the six field equations for the two phases couple through mass, momentum, and energy exchange. The equations are solved using an Eulerian finite-difference technique that implicitly couples the rates of phase transitions, momentum, and energy exchange to determination of the pressure, density, and velocity fields. The implicit solution is accomplished iteratively without linearizing the equations, thus eliminating the need for numerous derivative terms. With the three-dimensional K-FIX code calculations in Cartesian and cylindrical geometries can be performed. Obstacles built from the computing cells can be specified within the computing volume. In cylindrical geometry, calculations can be performed in the full 360 degrees or any angular segment. To enhance computing efficiency a new cell indexing scheme has been introduced, and computing time is reduced further by deletion of the viscous stress and heat conduction terms from the momentum and energy equations. FLX, which uses an explicit finite-difference solution algorithm to solve the shell equations, is explicitly coupled to the K-FIX(3D) fluid-dynamics program. A finite-difference numerical model is used for describing the dynamics of a core barrel.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - The sample test problem for K-FIX(3D) requires 14 seconds to compile and less than one minute to execute on a CDC7600. The sample test problem for K-FIX(3D,FLX) requires 18 seconds to compile and less than 14 minutes to execute on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - The transient two-dimensional, two-fluid K-FIX program was extended to develop KFIX(3D). The FLX code has also been coupled to the two-dimensional SOLA-DF code in the SOLA-FLX program for reactor safety applications.

9. **STATUS** - Abstract first distributed October 1981.
   CDC7600 version of K-FIX(3D,FLX) submitted July 1979, revised February 1980, sample problem executed by NESC March 1980 on a CDC7600.
   CDC7600 version of K-FIX(3D) submitted April 1981, sample problem executed by NESC August 1981 on a CDC7600.

10. **REFERENCES** - W. C. Rivard, M. D. Torrey, K-FIX: A Computer Program for Transient, Two-Dimensional, Two-Fluid Flow, THREED: An Extension of the K-FIX Code for Three-Dimensional Calculations, LA-NUREG-6623, Supplement II, January 1979, and Addendum.
   J. K. Dienes, C. W. Hirt, W. C. Rivard, L. R. Stein, and M. D. Torrey, FLX: A Shell Code for Coupled Fluid-Structure Analysis of Core Barrel Dynamics, NUREG/CR-0959, (LA-7927), November 1979.

W. C. Rivard and M. D. Torrey, K-FIX: A Computer Program for Transient, Two-Dimensional, Two-Fluid Flow, LA-NUREG-6623, April 1977.

K-FIX(3D), NESC No. 877, K-FIX(3D) Tape Description, Implementation Information, and Miscellaneous Subroutine Descriptions, National Energy Software Center Note 82-01, October 9, 1981.

11. **HARDWARE REQUIREMENTS** - The K-FIX(3D) sample problem, excluding plotting and timing routines, took about 50,000 (octal) words of small core memory (SCM) and 65,000 (octal) words of large core memory (LCM) storage. The K-FIX(3D,FLX) sample problem, excluding plotting and timing routines, took about 71,300 (octal) words of SCM and 570,000 (octal) words of LCM storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Memory must be preset to zero when loading the programs and the parameter LCM=1 must be added to the FTN card of K-FIX(3D,FLX) to allow proper indexing of very large arrays. Dependence on CDC system features and the local plotting and timing routines requires modification and incorporation of suitable replacement routines for implementation on different systems and in other computing environments.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
W. C. Rivard and M. D. Torrey
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source ((3D) FORTRAN 8342 lines, UPDATE 3980 lines, (3D,FLX) 9826 lines)
Sample problems ((3D) 40 lines, (3D,FLX) 48 lines)
Reference reports and NESC Note

17. **CATEGORY** - H
KEYWORDS - interfaces, shells, two-phase flow, reactor safety, simulation, three-dimensional, pressure, velocity, water cooled reactors, K-FIX codes, FLX codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - ELEFUNT
   ELEFUNT, tests of Fortran elementary functions

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
IBM360,370,303x, CDC6600,7600, UNIVAC1108,1100

3. **DESCRIPTION** - ELEFUNT is a FORTRAN test package for the elementary functions. Each program is an aggressive test of one or more of the elementary function subroutines generally supplied with the support library accompanying a FORTRAN compiler. Functions tested are ALOG/ALOG10, ASIN/ACOS, ATAN, EXP, POWER, SIN/COS, SINH/COSH, SQRT, TAN/COTAN, and TANH.

4. **METHOD OF SOLUTION** - The programs check the accuracy of the functions by using purified random arguments from appropriate intervals in carefully selected identities. They also check special properties of each function, test for the handling of special arguments, and exercise the error returns.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The package contains one subroutine (MACHAR) for dynamic determination of parameters describing the floating-point arithmetic system of the host machine. Should this hardware-sensitive subprogram malfunction, the test programs must be modified to insert the necessary machine-dependent parameters in DATA statements, or otherwise make them available. This computing environment inquiry routine is known to malfunction when the arithmetic registers are wider than the storage registers.

6. **TIMING** - Running time is generally short and varies with the host machine and the function being tested. NESC executed all of the drivers in 5 seconds of CPU time on an IBM3033, 17 seconds of CP time on a CDC6600, 2 seconds of CP time on a CDC7600, and 20 seconds of CP time on a UNIVAC1100/44.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - At this time there are no other diagnostic/test packages available for the elementary functions. The package is aggressive in detecting specific problems in the functions being tested, is highly portable, and contains a unique computing environment inquiry package.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed September 1980.
   IBM370, CDC7600, and UNIVAC1100 version submitted November 1979, programs executed by NESC March 1980 on an IBM3033, a CDC6600, a CDC7600, and a UNIVAC1100/44.

10. **REFERENCES** - William J. Cody, Jr. and William M. Waite, Software Manual for the Elementary Functions, Prentice Hall Inc., Englewood Cliffs, New Jersey, 1980.
    ELEFUNT, NESC No. 881, ELEFUNT Tape Description and Implementation Information, National Energy Software Center Note 80-65, April 14, 1980.
    ELEFUNT, NESC No. 881, Comments on ELEFUNT Test Output, National Energy Software Center Note 80-66, April 14, 1980.

11. **HARDWARE REQUIREMENTS** - The maximum space required by any one test driver is 50K bytes on an IBM3033, 16,000 (octal) words on a CDC6600, 5700 (octal) words on a CDC7600, and 3600 words on a UNIVAC1100/44.

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - OS/370 (IBM3033), SCOPE 3.4.4 (CDC6600), SCOPE 2.1.5 (CDC7600), and EXEC8 (UNIVAC1100).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Test output produced by other host machines may differ from the test output supplied on microfiche by NESC for the CDC, IBM, and UNIVAC.
    Elements of the package have been tested successfully by the author on the following additional machines: BESM-6, Burroughs 6700, Cray1, PDP10, PDP11, Varian V76, and Z80 (using Microsoft FORTRAN). Modifications are required to execute the package on Honeywell

equipment. On the CDC6000/7000 series hardware the PROGRAM card must be inserted at the beginning of each driver.

Because the 1966 FORTRAN standard did not specify some of the functions usually found in a support library, and the ANSI X3.9-1978 standard fails to mention a COTANgent program, some libraries may not have all of the functions being tested or may use names other than those used in this package. Drivers for the ASIN/ACOS and TAN/COTAN tests may have to be modified for this reason. All drivers may also require modification if the MACHAR subprogram malfunctions or if a local random number generator is to be used. MACHAR deliberately causes two floating-point underflows; it is assumed that program execution will continue each time.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

W. J. Cody
Mathematics and Computer Science Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE -**

Source (ALOG/ALOG10 223 lines, ASIN/ACOS 227 lines, ATAN 242 lines, EXP 199 lines, POWER 241 lines, SIN/COS 222 lines, SINH/COSH 244 lines, SQRT 170 lines, TAN/COTAN 208 lines, TANH 189 lines, auxiliary subroutines 266 lines)
Test output (3 microfiche, 370-66 pages*, 7600-51 pages*, 1100-59 pages*)
NESC Notes

* Hard-copy output for a specific machine available upon request.

17. **CATEGORY** - P
KEYWORDS - elementary functions, testing, FORTRAN, libraries

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Engineering, Mathematical and Geo-Sciences

IDENTIFICATION AND KWIC TITLE - EQ3/6
EQ3/6, geochemical modeling of aqueous systems

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600, Cray1

DESCRIPTION - The EQ3/6 release 3230B software package is a set of computer programs and supporting data files, used in modeling aqueous geochemical systems. The two main programs are EQ3NR and EQ6. EQ3NR is a geochemical aqueous speciation-solubility program which models the thermodynamic state of an aqueous solution by calculating the distribution of aqueous species, such as simple ions, ion-pairs, and aqueous complexes. The EQ6 program, which must be initialized by an EQ3NR calculation, computes either reaction paths of reacting aqueous systems or heterogeneous equilibrium with fixed masses of chemical elements. Two auxiliary programs, MCRT and EQTL, are included in the package. MCRT is a database building program used to process thermodynamic input data files into a form suitable for the EQ3/6 thermodynamic database and to perform temperature extrapolation of 25 degree C data. The primary data file that supports EQ3/6 contains thermodynamic data corresponding to the temperatures 0, 25, 60, 100, 150, 200, 250, and 300 degrees C, a pressure of 1.013 bar (1 atmosphere) up to 100 degrees C, the steam/liquid water equilibrium pressure at higher temperatures, and other necessary supporting data. EQTL, a database preprocessor, reads this primary data file, checks each reaction for mass and charge balance, fits interpolating polynomials to all data on temperature grids, and reformats the data into suitable form in three secondary data files read directly by EQ3NR or EQ6.

METHOD OF SOLUTION - EQ3NR uses a modified Newton-Raphson algorithm to calculate the distribution of aqueous species. Input primarily consists of data derived from total analytical concentrations of dissolved components and can also include pH, alkalinity, electrical balance, phase equilibrium (solubility) constraints, and a default value for Eh, pe, or the logarithm of oxygen fugacity. The program evaluates the degree of disequilibrium for various reactions and computes either the saturation index or thermodynamic affinity for minerals. Individual values of Eh, pe, equilibrium oxygen fugacity, and Ah (redox affinity) are computed for aqueous redox couples. EQ3NR can be used alone. It is required to initialize reaction-path calculations performed by EQ6, its companion program.

EQ6 first checks that the input system is in homogeneous equilibrium. If not, the system is "equilibrated" according to the specified mass balance constraints. This will yield a single Eh for the solution and alter to some extent all the other solution parameters, including the pH. If there are any supersaturated phases, EQ6 then "precipitates" a set so that no supersaturations remain. This may result in still different values for the pH and other solution parameters. Any such initial precipitates may be retained in the system or deleted before the reaction progresses. Calculations may then be performed to model simple titration or irreversible reaction with "reactants" in systems that are either closed to solids or open (flow-through) systems. EQ6 solves at each point of reaction progress the algebraic equations describing mass and charge balance, mass action, and non-ideality. Finite-difference expressions of high order are used to estimate derivatives with respect to reaction progress and predict the values of a basis set of unknowns at a subsequent point. The predicted values are then corrected by using the Newton-Raphson method. Convergence is aided by optimizing starting estimates and by under-relaxation techniques.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The temperature range of the thermodynamic data in the primary data file is 0 to 300 degrees C. The activity coefficient approximations for aqueous solutes are not dependable at ionic strengths of greater than roughly one molal.

TIMING - On a CDC7600 the EQ3NR test case requires about 2 seconds to run and the EQ6 test case about 10 seconds.

UNUSUAL FEATURES OF THE SOFTWARE - The programs were developed for the FTN and CFT FORTRAN compiler language on the CDC7600 and Cray1 computers with specific conventions adopted to facilitate transportability to UNIVAC, IBM, DEC VAX, and other systems.

8. **RELATED AND AUXILIARY SOFTWARE** - Other well-known geochemical codes for the EQ3 distribution-of-species problem are SOLSAT (Helgeson), SOLMNEQ (Kharaka and Barnes), the WATEQ series (Ruesdell, Plummer, Ball), REDEQL (Morel and Morgan), and MINEQL (Westall). Similar in modeling function to EQ6 are Helgeson's PATH1 and PATHCALC programs.

9. **STATUS** - Abstract first distributed August 1980.
CDC7600 version submitted March 1979, replaced by revised version November 1979, revised December 1980, revised April 1981, revised July 1981, revised December 1981, revised March 1982, revised September 1982, revised March 1983, revised February 1984, replaced November 1984 by Edition B submitted April 1984 and revised July 1984, sample problem executed by NESC October 1984 on a CDC7600.

10. **REFERENCES** - T. J. Wolery, Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: The EQ3/6 Software Package, UCRL-52658, February 1979.

Thomas J. Wolery, EQ3NR A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: User's Guide and Documentation, UCRL-53414, April 18, 1983.

EQ3/6, NESC No. 886.7600B, EQ3/6 Tape Description and Implementation Information, National Energy Software Center Note 85-28, November 27, 1984.

T. J. Wolery and L. J. Walters, Jr., Calculation of Equilibrium Distributions of Chemical Species by Means of Monotone Sequences, Mathematical Geology, Vol. 7, pp. 99-115, 1975.

H. C. Helgeson, Evaluation of Irreversible Reactions in Geochemical Processes Involving Minerals and Aqueous Solutions-I. Thermodynamic Relations, Geochimica et Cosmochimica Acta, Vol. 32, pp. 853-877, 1968.

11. **HARDWARE REQUIREMENTS** - About 136,000 (octal) words of SCM and 157,000 (octal) words of LCM are required on a CDC7600 for EQ3NR, about 124,000 (octal) words of SCM and 165,000 (octal) words of LCM for EQ6. Three units in addition to the standard input/output units are used by EQ3NR, 11 units in addition to the standard I/O units by EQ6.

12. **PROGRAMMING LANGUAGE** - FORTRAN Extended 4.8 (CDC7600) and CFT (Cray1)

13. **OPERATING SYSTEM** - SCOPE 2.1.5 (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The program is written in FORTRAN 66, but FORTRAN 77 compatible. Central memory must be preset to zero when running EQ6.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
T. J. Wolery
Earth Sciences Division
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (EQ3NR 7325 lines, EQ6 13,146 lines, EQLIB 1434 lines)
Sample problems (EQ3NR 52 lines, EQ6 297 lines)
Library data (21,303 lines)
Auxiliary source (EQTL 1971 lines, MCRT 3507 lines)
Sample problems output (EQTL 268 lines, MCRT 664 lines and 4308 120-character records, EQ6 1922 and 133 120-character records, EQ3NR 62 lines and 547 120-character records)
Reference reports, UCRL-52658 and UCRL-53414, and NESC Note

17. **CATEGORY** - R
KEYWORDS - thermodynamic properties, chemical reactions, aqueous solutions, geochemistry, thermal equilibrium, minerals, EQTL codes, MCRT codes

18. **SPONSOR** - DOE-NV Nuclear Waste Storage Investigations
DOE-CH Salt Repository Project Office

IDENTIFICATION AND KWIC TITLE - GETOUT
GETOUT, radionuclide transport geologic media

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - UNIVAC1100

DESCRIPTION - GETOUT is a set of four FORTRAN programs and associated subroutines developed as an aid to investigate the migration of radionuclide chains from an underground source. The model to be analyzed is an underground nuclear waste disposal site and a uniform one-dimensional soil column that connects the site with a surface water body. At an arbitrary time after the waste is deposited, the radioactive material is released to an underground aquifer which flows at constant velocity directly through the soil column into the surface water body. The program takes into account the complications introduced by the radioactive decay of first-order chains to produce other species which have different absorption characteristics and, in turn, decay at different rates.

METHOD OF SOLUTION - GETOUT's programs ONE, TWO, and THREE solve analytical expressions describing the migration of single nuclides, and 2- and 3-member chains, respectively. Program FOUR solves more complex chains described by empirical combinations of simpler chains. The equations used were developed by Lester, Burkholder, Jansen, and Cloninger. Solutions are computed for impulse release without dispersion, impulse release with dispersion, band release without dispersion, and band release with dispersion. Time/inventory profiles are calculated.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
88 discharge profiles
51 single chains
26 two-member chains
11 three-member chains

TIMING - NESC executed the four programs in 320, 225, 280, and 150 CP seconds, respectively, on an UNIVACII00/44.

UNUSUAL FEATURES OF THE SOFTWARE - GETOUT can be executed in either batch or interactive mode.

RELATED AND AUXILIARY SOFTWARE - Data for the inventory library, MINV, are typically derived from the output of a program such as ORIGEN (NESC 874).

STATUS - Abstract first distributed April 1981.
UNIVAC1100 version submitted February 1980, sample problems executed by NESC May 1980 on an UNIVAC1100/44.

REFERENCES - W. V. DeMier, M. O. Cloninger, H. C. Burkholder, and P. J. Liddel, GETOUT - A Computer Program for Predicting Radionuclide Decay Chain Transport Through Geologic Media, PNL-2970, August 1979.

GETOUT, NESC No. 887.1100, Errata to PNL-2970, National Energy Software Center Note 81-23, April 14, 1981.

M. J. Bell, ORIGEN - The ORNL Isotope Generation and Depletion Code, ORNL-4628, May 1973.

D. A. Baker, G. R. Hoenes, and J. K. Soldat, FOOD - An Interactive Code to Calculate Internal Radiation Doses from Contaminated Food Products, BNWL-SA-5523, 1976.

Harry C. Burkholder and Michael O. Cloninger, "The Reconcentration Phenomenon of Radionuclide Chain Migration", Adsorption and Ion Exchange Separations, American Institute of Chemical Engineers Symposium Series 179, Vol. 74, pp. 83-90, 1978, also published as BNWL-SA-5786, 1976.

D. H. Denham, D. A. Baker, J. K. Soldat, and J. P. Corley, Radiological Evaluations for Advanced Waste Management Studies, BNWL-1764, September 1973.

H. C. Burkholder, M. O. Cloninger, D. A. Baker, and G. Jansen, Incentives for Partitioning High-Level Waste, Nuclear Technology, Vol. 31, pp. 202-217, November 1976, also published as BNWL-1927, November 1975.

D. H. Lester, George Jansen, and H. C. Burkholder, "Migration of Radionuclide Chains Through an Adsorbing Medium", Adsorption and Ion Exchange, American Institute of Chemical Engineers Symposium Series 152, Vol. 71, pp. 202-213, 1975.

11. **HARDWARE REQUIREMENTS** - Program ONE requires 29,000 words of main memory and 205,000 words of direct access storage for execution. Programs TWO and THREE require 31,000 words of main memory and 86,000 and 47,000 words of direct access storage, respectively, and program FOUR requires 44,000 words of main memory and an additional 475,000 words of direct access storage for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - EXEC8.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Programs ONE, TWO, THREE, and FOUR must be executed in sequence. The intermediate output for each of the 1-, 2-, and 3-member chains is written to separate files on a disk. These files may be examined and, if desired, edited before program FOUR is executed. Each program makes use of the UNIVAC system routine FACSF for interpretation and processing of an Executive control statement within the program.

    These programs should be compiled under the ASCII (FTN) compiler. Modifications are necessary to compile the programs under the older FORTRAN V E3 and T3 compilers.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    M. O. Cloninger, W. V. DeMier,
    and P. J. Liddell
    Pacific Northwest Laboratory
    H. C. Burkholder
    Columbus Laboratories
    Battelle Memorial Institute

16. **MATERIAL AVAILABLE** -

    Source (6449 lines)
    Sample problem (135 lines)
    Nuclide inventory library (59 108-character records)
    Control information (189 lines)
    Reference report, PNL-2970, and NESC Note

17. **CATEGORY** - R
    KEYWORDS - radionuclide migration, underground storage, fission products, ground water, radioactive waste storage

18. **SPONSOR** - DOE Office of Nuclear Waste Isolation

IDENTIFICATION AND KWIC TITLE - MINPACK1
MINPACK1, nonlinear equations & least squares

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,370 (designed to be machine-independent)

DESCRIPTION - MINPACK1 is a package of FORTRAN subprograms for the numerical solution of systems of nonlinear equations and nonlinear least squares problems. The individual subprograms are:

IDENTIFICATION	DESCRIPTION
CHKDER	Check gradients for consistency with functions
DOGLEG	Determine combination of Gauss-Newton and gradient directions
DPMPAR	Provide double precision machine parameters
ENORM	Calculate Euclidean norm of vector
FDJAC1	Calculate difference approximation to Jacobian (nonlinear equations)
FDJAC2	Calculate difference approximation to Jacobian (least squares)
HYBRD	Solve system of nonlinear equations (approximate Jacobian)
HYBRD1	Easy-to-use driver for HYBRD
HYBRJ	Solve system of nonlinear equations (analytic Jacobian)
HYBRJ1	Easy-to-use driver for HYBRJ
LMDER	Solve nonlinear least squares problem (analytic Jacobian)
LMDER1	Easy-to-use driver for LMDER
LMDIF	Solve nonlinear least squares problem (approximate Jacobian)
LMDIF1	Easy-to-use driver for LMDIF
LMPAR	Determine Levenberg-Marquardt parameter
LMSTR	Solve nonlinear least squares problem (analytic Jacobian, storage conserving)
LMSTR1	Easy-to-use driver for LMSTR
QFORM	Accumulate orthogonal matrix from QR factorization
QRFAC	Compute QR factorization of rectangular matrix
QRSOLV	Complete solution of least squares problem
RWUPDT	Update QR factorization after row addition
R1MPYQ	Apply orthogonal transformations from QR factorization
R1UPDT	Update QR factorization after rank-1 addition
SPMPAR	Provide single precision machine parameters

METHOD OF SOLUTION - MINPACK1 uses the modified Powell hybrid method and the Levenberg-Marquardt algorithm.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING - Running time depends on the number of functions and variables, the behavior of the functions, the requested accuracy, and the starting point. On the IBM3033, the CPU time measured for compilation, link edit, and execution of a test driver ranges from four to 26 seconds.

UNUSUAL FEATURES OF THE SOFTWARE - These routines have been extensively tested on many machines and have performed well on a large number of test problems.

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed October 1980.

MINPACK1 submitted June 1980, sample problems executed by NESC June 1980 on an IBM3033, replaced by Edition B April 1982.

10. **REFERENCES** - M. J. D. Powell, "A Hybrid Method for Nonlinear Equations", in Numerical Methods for Nonlinear Algebraic Equations, P. Rabinowitz, Editor, Gordon and Breach, 1970.

J. J. More, "The Levenberg-Marquardt Algorithm, Implementation and Theory", in Numerical Analysis, G. A. Watson, Editor, Lecture Notes in Mathematics 630, Springer-Verlag, 1977.

B. S. Garbow, K. E. Hillstrom, and J. J. More, Implementation Guide for MINPACK-1, ANL-80-68, July 1980.

J. J. More, B. S. Garbow, and K. E. Hillstrom, User Guide for MINPACK-1, ANL-80-74, August 1980.

MINPACK1, NESC No. 888.370B, Edition B Changes to the MINPACK1 Program and Errata for ANL-80-68, Implementation Guide for MINPACK1, National Energy Software Center Note 82-45, April 30, 1982.

11. **HARDWARE REQUIREMENTS** - The test executions require from 92K to 158K bytes of storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/360 (IBM360), OS/370 (IBM370).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Three machine-dependent parameters are set by calls to subroutine SPMPAR (single precision) or DPMPAR (double precision). For non-IBM machines, this presumes prior user activation (removal of 'C' from column 1) of appropriate constants embedded in the program.

The testing aids include drivers, parameter initialization subroutines, function evaluation subroutines, Jacobian evaluation subroutines, and test data. Small changes may be required to the drivers, for example, to renumber the logical input and output units or to include a program card.

Machines and locations used for MINPACK1 testing were -

MACHINE	LOCATION
IBM360,370	Massachusetts Institute of Technology
	Argonne National Laboratory
	Federal Reserve Board
	Oak Ridge National Laboratory
	David Sarnoff Research Center
	University of Illinois at Chicago Circle
	University of Kentucky
CDC6000-7000	University of Illinois at Urbana-Champaign
	Kirtland Air Force Base
	Lawrence Livermore National Laboratory
	Sandia National Laboratories, Albuquerque
	Sandia National Laboratories, Livermore
	Oak Ridge National Laboratory
UNIVAC 1100	University of Wisconsin
	Naval Weapons Center, China Lake
DEC-PDP 10	Oak Ridge National Laboratory
Honeywell 6000	University of Waterloo
Burroughs 6700	Data Resources Inc.
	International Bank for Reconstruction and Development
Cray-1	Oak Ridge National Laboratory
	Lawrence Livermore National Laboratory
Prime 400	Management Decision Systems Inc.
Itel AS/6	Rice University
ICL 2980	Numerical Algorithms Group, Ltd.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

B. S. Garbow
Mathematics and Computer Science Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
Source (S 4916 lines, D 4970 lines)
Test drivers (S 5299 lines, D 5313 lines)
Machine-readable documentation (S 3526 lines, D 3528 lines)
Reference reports, ANL-80-68 and ANL-80-74, and NESC Note

17. **CATEGORY** - P
KEYWORDS - least square fit, nonlinear problems, nonlinear programming, numerical solution

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Engineering, Mathematical and Geo-Sciences

IDENTIFICATION AND KWIC TITLE - RAS
RAS, reliability analysis for phased missions

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER176, CDC7600,6600

DESCRIPTION - The Reliability Analysis System, RAS, is an integrated package of computer programs for the quantification of fault trees. In particular, RAS has the capability of performing phased mission analysis. A phased mission is a task to be performed by a system during which the logic model and/or the component failure mode characteristics change at predetermined times. RAS is capable of finding minimal cut sets from fault trees and of calculating reliability characteristics for the basic events, the minimal cut sets, and the top event of a fault tree. In addition, mission cut set cancellation and four methods of bounding mission unreliability have been incorporated into RAS.

METHOD OF SOLUTION - RAS is based upon the MOCUS, POCUS, KITT1, SRTPRN, and COMCAN programs. A new FATRAM algorithm for determining minimal cut sets is included in RAS. MOCUS is used to determine the minimal cut sets from a fault tree. POCUS and KITT1 are used to calculate reliability characteristics for the basic events, the cut sets, and the top event of a fault tree. SRTPRN sorts minimal cut sets into groups according to the importance of the cut sets. COMCAN is used, in common cause failure analysis, to search basic events in minimal cut sets for shared secondary failure event susceptibilities or common linking conditions among components.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maximum of -
5 distinct phases per mission

TIMING - NESC executed the sample problem in less than 1 second of CP time on a CDC7600 and less than 3 seconds of CP time on a CDC6600.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - RAS contains the POCUS, SRTPRN, MOCUS (NESC 653), KITT1 (NESC 528), and COMCAN (NESC 704) computer programs.

STATUS - Abstract first distributed August 1980.
CDC CYBER76 version submitted March 1980, replaced July 1981 by CYBER176 version.
CDC CYBER176 version submitted April 1981, sample problem executed by NESC May 1981 on a CDC7600 and CDC6600.

REFERENCES - Dale M. Rasmuson, Neldon H. Marshall, and Gary R. Burdick, User's Guide for the Reliability Analysis System (RAS), TREE-1168, September 1977.

RAS, NESC No. 889.C176, RAS Tape Description and Implementation Information, National Energy Software Center Note 81-62, June 8, 1981.

J. B. Fussell, E. B. Henry, and N. H. Marshall, MOCUS: A Computer Program to Obtain Minimal Sets from Fault Trees, ANCR-1156, August 1974.

W. E. Vesley and R. E. Narum, PREP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree, IN-1349, August 1970.

C. A. Dolan, SRTPRN: A Program to Sort and Prune Fault Tree Cut Sets, TREE-1012, December 1976.

G. R. Burdick, N. H. Marshall, and J. R. Wilson, COMCAN - A Computer Program for Common Cause Analysis, ANCR-1314, June 1976.

HARDWARE REQUIREMENTS - If the program is segmented, 42,000 (octal) words of small core memory (SCM) and 10 (octal) words of large core memory (LCM) are required for execution on a CDC7600. For the CDC6600, 135,000 (octal) words of central memory and 10 (octal) words of Extended Core Storage (ECS) are required. Without segmentation, additional memory will be required.

PROGRAMMING LANGUAGE - FORTRAN IV (96%) and COMPASS (4%)

13. **OPERATING SYSTEM -** SCOPE 2.1 (CDC7600), NOS/BE (CDC CYBER176, CDC6600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -** Subroutines FAPFIM, FABEND, FTBIN, FTBMXJ and FTBMEM are written in COMPASS assembly language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
D. M. Rasmuson, N. H. Marshall,
and G. R. Burdick
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE -**
Source (RAS 11,233 lines, SCOPE environmental routines 535 lines, NOS/BE environmental routines 566 lines)
Sample problem (91 lines)
Susceptibility tables (28 lines)
Control information (97 lines)
Reference report, TREE-1168, and NESC Note

17. **CATEGORY -** G
KEYWORDS - reliability, fault tree analysis, safety, failures, system failure analysis, LMFBR reactors, COMCAN codes, MOCUS codes, POCUS codes, PREP,KITT codes, SRTPRN codes

18. **SPONSOR -** ERDA Division of Reactor Development and Demonstration

1. **IDENTIFICATION AND KWIC TITLE** - QLN1
   QLN1, quantitative gamma-ray spectra analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - UNIVAC1108,1100

3. **DESCRIPTION** - QLN1 identifies gamma-ray emitters contributing to Ge(Li) detector spectra, and computes quantitative amounts of isotopes contributing to the data.

4. **METHOD OF SOLUTION** - A calibration spectrum is searched for peaks and a table of peak shape parameters as a function of energy is compiled. Sample spectra are searched for peaks and fitted peak areas, energies, and computed centroids, including complex peaks. A library of peak energies and intensities is compared to the observed peaks to identify contributing isotopes. Energies and intensities of candidate isotopes are also compared to the observed peaks to establish probabilities that candidates, in fact, contribute to spectra. Quantitative results are computed using a digital method and a fitting method which fits the data with one or more modified Gaussian peaks together with a parabolic baseline.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maximum of -
   100 peaks per spectrum

6. **TIMING** - Running time is roughly proportional to the number of peaks analyzed. On a UNIVAC1108, one should allow 2 seconds for each peak. NESC compiled QLN1 and executed the sample problem in less than 5 CP minutes on a UNIVAC1100/44.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - QLN1 automatically analyzes Ge(Li) detector gamma-ray spectra for all peaks, including peaks not even partially resolved by the spectrometer, and for isotopes making contributions to the spectra. QLN1 also flags peaks having interferences to warn the user to accept only the fitted results.

8. **RELATED AND AUXILIARY SOFTWARE** - An auxiliary program, LISTER, prepares a data file containing lists of candidate isotope gamma-ray energies and intensities. LISTER can process up to 1000 gamma-ray lines; inclusion of lines is left to the user's discretion. QLN1 is based on the earlier SAMPO, ALLSPICE, and GAMANAL computer programs. SAMPO was used because of its ability to resolve complex peaks. ALLSPICE was used to compute input parameters for SAMPO and for its ability to locate peaks and compute peak areas. Many ideas in the GAMANAL program were used in the component identification part of QLN1.

9. **STATUS** - Abstract first distributed August 1982.
   UNIVAC1108 version submitted October 1976, replaced August 1982 by revised edition submitted May 1980, sample problem executed by NESC September 1980 on a UNIVAC1100/44.

10. **REFERENCES** - Herbert P. Yule, "A Computer Code for Qualitative Analysis of Gamma-Ray Spectra" in Computers in Activation Analysis and Gamma-Ray Spectroscopy, Proceedings of the American Nuclear Society Topical Conference at Mayaguez, Puerto Rico, April 30-May 4, 1978, CONF-780421, pp. 278-296, 1979.

H. P. Yule, Computer Program QLN1 for Complete and Automatic Analysis of Gamma-ray Spectra, NUS Corporation report, October 1976.

QLN1, NESC No. 902, QLN1 Tape Description and Implementation Information, National Energy Software Center Note 82-79, August 10, 1982.

J. T. Routti and S. G. Prussin, Photopeak Method for the Computer Analysis of Gamma-Ray Spectra from Semiconductor Detectors, Nuclear Instruments and Methods, Vol. 72, pp. 125-142, 1969.

H. P. Yule, Activation Analysis Section: Summary of Activities, July 1969 to June 1970, Chapter 6: Application of Computers to Activation Analysis, NBS Technical Note 548, pp. 124-139, December 1970.

J. J. Steyn and M. Reier, A Method for Systematically Analyzing Ge(Li) Photopeaks, Journal of Radioanalytical Chemistry, Vol. 15, pp. 669-673, 1973.

11. **HARDWARE REQUIREMENTS** - The LISTER program requires 35,000 words of memory and 5 direct-access devices (logical units 10, 14, 28, 29, and 31) for execution. QLN1 requires 47,000 words of memory and 5 direct-access devices (logical units 14, 20, 21, 22, and 23) for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN V

13. **OPERATING SYSTEM** - EXEC8.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The iterative technique employed in the SAMPO part of QLN1 generates frequent overflow conditions. NESC commented out the call to the NBS routine, DIVOFL, which suppresses premature run termination caused by overflows and divide checks. The algorithm used by the SAMPO program has also proved to be compiler dependent; QLN1, run on the same machine but using different compilers, may generate slightly different results.

    The author has developed a FORTRAN 77 PRIME750 version of QLN1 for use with the PRIMOS 17 or PRIMOS 18 operating system which is expected to become available shortly.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    H. P. Yule
    NUS Corporation

16. **MATERIAL AVAILABLE** -

    Source (4266 lines)
    Sample problem (3320 lines)
    Auxiliary program (LISTER - 328 lines, data - 1138 lines)
    Control information (116 lines)
    Sample problem output (24 pages)
    Reference conference paper, NUS report, and NESC Note

17. **CATEGORY** - O
    KEYWORDS - activation analysis, Li-drifted Ge detectors, experimental data, data processing, gamma radiation, isotopes, libraries, radioactivity, spectra, SAMPO codes, ALLSPICE codes, GAMANAL codes

18. **SPONSOR** - EPA
    DOC National Bureau of Standards

1. **IDENTIFICATION AND KWIC TITLE** - GWCORE
   GWCORE, GSPC 79 core graphics routines package

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - This package of FORTRAN callable subroutines is an implementation of the 1979 ACM SIGGRAPH core graphics specification. It is a machine-independent, device-independent graphics language. It provides the primitives - lines, markers, polylines, polymarkers, polygons, moves, and text, as well as segmentation capabilities which permit many control functions such as visibility, highlighting, new frames, detectability, and image transformation. A number of attributes can be set for the primitives. Raster extensions, including color index table loading and filled polygons, are provided. Input capability for six logical devices is provided.

4. **METHOD OF SOLUTION** - The user enters parameters to the primitives in real-world coordinates. The viewing transformation routines apply matrix multiplication to these coordinates to provide user-specified projections and clipping. The results of these transformations are normalized device coordinates between 0.0 and 1.0. These normalized device coordinates are sent to the various device drivers (Tektronix, plotter, line printer-plotter, etc.) and converted by the device driver into device-specific commands and device coordinates.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - World coordinates can be any real number. Segment names can be any integer. A polygon is limited to 1500 vertices. The internal storage of output primitives is limited to 30,000 integer*4 words but can be easily enlarged. A maximum of 1000 segments is permitted, and only one output view surface may be selected at a time.

6. **TIMING** - The running time is application dependent.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - GWCORE features include -
   (a) standard graphics capabilities based on the 1979 core specification,
   (b) device independence eliminating the need to learn the manufacturer's graphics programming language once a new device driver is written for that device,
   (c) program portability such that a program running on one core specification system should run on another with only minor changes, and
   (d) well-documented modular subroutines with comments making up approximately one-third of the source program.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed July 1981.
   DEC VAX11/780 version of GWCORE submitted September 1980, replacement submitted April 1981, revised June 1981, replaced September 1983 by Edition C, submitted July 1982, and Edition D, sample problems executed by NESC December 1982 on a DEC VAX11/780.

10. **REFERENCES** - James Hanlon, Design Document for GWCORE Input Implementation, excerpted from, "Implementation and Evaluation of Input Functions for the 1979 CORE Graphics Systems", Masters Thesis, Department of Electrical Engineering and Computer Science, School of Engineering and Applied Science, The George Washington University, Washington, D. C., December 1981.

GWCORE, NESC No. 905.VX11 Edition C, GWCORE VAX11 Tape Description and Implementation Information for Use on DEC VAX11 VMS Systems, National Energy Software Center Note 84-19, March 14, 1983.

GWCORE, NESC No. 905.VX11 Edition D, GWCORE VAX11 Tape Description and Implementation Information for Use on Other Than DEC VAX11 VMS Systems, National Energy Software Center Note 84-20, May 25, 1983.

GWCORE, NESC No. 905, Supplementary Material to Computer-readable SIGGRAPH Document, National Energy Software Center Note 84-21, May 25, 1983.

Status Report of the Graphics Standard Planning Committee (GSPC), Computer Graphics, Volume 13, Number 3, August 1979.

James Foley and Andries VanDam, Interactive Computer Graphics, Addison-Wesley, Reading, Massachusetts, 1982.

11. **HARDWARE REQUIREMENTS** - GWCORE was written for a virtual machine environment, the VAX11/780. Overlaying will undoubtedly be needed in environments where the program size is limited. A rough estimate of the working virtual size of application programs written with GWCORE is one-half million bytes. Integer*4 and real variables are equivalenced.

12. **PROGRAMMING LANGUAGE** - The device-independent part of GWCORE is written solely in VAX11/780 FORTRAN IV-Plus. There is very limited use of FORTRAN 77 IF-THEN-ELSE control structures and CHARACTER data types.

    The Tektronix 4012 driver is written in FORTRAN.

    The Ramtek 9400 output driver is written in C.

    The Ramtek 9400 input driver is written in FORTRAN.

13. **OPERATING SYSTEM** - VMS 1.6, 2.3, and 3.0 with VAX level Ramtek device driver developed by Ramtek.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Every effort was made to keep the machine dependencies to a minimum. When necessary, they appear isolated in special subroutines. Module specifications are provided for each subroutine and known system dependencies are listed there. The device-independent part of GWCORE is intended to be machine independent. No similar claim is made for device drivers. Communication to the devices from the device-independent core is accomplished according to well-defined, strict specifications.

    The package consists of about 300 subroutines in the device-dependent GWCORE, about 15 in the Tektronix driver, and about 100 in the Ramtek driver. The routines, when organized in an object module library, occupy about 200K bytes.

    To use GWCORE effectively, a copy of the Status Report of the GSPC (see reference) is required. A machine-readable copy of this document with GWCORE subroutine names and other information added is included in the package.

    Edition C is the standard DEC VAX11/780 edition readable on DEC VAX11 VMS systems. Edition C has a maximum block size of 2048 bytes. Edition D was prepared from Edition C to be readable on other than DEC VAX11 VMS systems.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    P. Wenner
    EE/CS Department, SEAS
    George Washington University

16. **MATERIAL AVAILABLE** -

    Source (ATTRIB1.FOR VX11C 53 blocks, VX11D 2288 lines, ATTRIB2.FOR VX11C 55 blocks, VX11D 2522 lines, CORERROR.FOR VX11C 13 blocks, VX11D 683 lines, CORINT.FOR VX11C 21 blocks, VX11D 1260 lines, CORTEXT1.FOR VX11C 46 blocks, VX11D 2259 lines, CORTEXT2.FOR VX11C 76 blocks, VX11D 2414 lines, DUM.FOR VX11C 1 block, VX11D 6 lines, DUMP.FOR VX11C 4 blocks, VX11D 233 lines, INPUT1.FOR VX11C 49 blocks, VX11D 5624 lines, INPUT2.FOR VX11C 14 blocks, VX11D 2482 lines, PDFILE.FOR VX11C 40 blocks, VX11D 2409 lines, PRIMITIVE.FOR VX11C 75 blocks, VX11D 3405 lines, RASTER1.FOR VX11C 35 blocks, VX11D 1686 lines, RASTER2.FOR VX11C 43 blocks, VX11D 2329 lines, SCANCON.FOR VX11C 13 blocks, VX11D 848 lines, SURF.FOR VX11C 10 blocks, VX11D 593 lines, VIEWPARM.FOR VX11C 53 blocks, VX11D 3184 lines, VIEWTRAN.FOR VX11C 60 blocks, VX11D 3014 lines)

    Sample problems (TEST1.FOR VX11C 2 blocks, VX11D 91 lines, TEST2.FOR VX11C 1 block, VX11D 47 lines, TEST3.FOR VX11C 4 blocks, VX11D 275 lines, TEST4.FOR VX11C 1 block, VX11D 32 lines)

    Auxiliary machine-readable documentation (README.1ST VX11C 6 blocks, VX11D 281 lines, DESIGN.MAN VX11C 77 blocks, VX11D 4697 lines, CH1.MAN VX11C 26 blocks, VX11D 1025 lines, CH2.MAN VX11C 21 blocks, VX11D 897 lines, CH3.MAN VX11C 13 blocks, VX11D 513

lines, CH4.MAN VX11C 19 blocks, VX11D 946 lines, CH5.MAN VX11C 33 blocks, VX11D 1409 lines, CH6.MAN VX11C 39 blocks, VX11D 1665 lines, CH7.MAN VX11C 38 blocks, VX11D 1665 lines, CH8.MAN VX11C 3 blocks, VX11D 129 lines, CH9.MAN VX11C 3 blocks, VX11D 129 lines, APPA.MAN VX11C 7 blocks, VX11D 449 lines, APPB.MAN VX11C 11 blocks, VX11D 577 lines, APPC.MAN VX11C 2 blocks, VX11D 129 lines, APPD.MAN VX11C 10 blocks, VX11D 321 lines, APPE.MAN VX11C 12 blocks, VX11D 577 lines, APPF.MAN VX11C 3 blocks, VX11D 257 lines, CON.MAN VX11C 16 blocks, VX11D 641 lines, REFER.MAN VX11C 3 blocks, VX11D 129 lines, SPECS1D.MAN VX11C 64 blocks, VX11D 5488 lines, SPECS2D.MAN VX11C 60 blocks, VX11D 5370 lines, SPECS3D.MAN VX11C 57 blocks, VX11D 5665 lines, SPECS4D.MAN VX11C 97 blocks, VX11D 6904 lines, SPECS5D.MAN VX11C 77 blocks, VX11D 6432 lines, SPECS6D.MAN VX11C 64 blocks, VX11D 4721 lines, INSPEC1.MAN VX11C 26 blocks, VX11D 2753 lines, INSPEC2.MAN VX11C 26 blocks, VX11D 3265 lines, RAMCALL.MAN VX11C 3 blocks, VX11D 248 lines, RAMINPUT.MAN VX11C 39 blocks, VX11D 4056 lines, RAMUSER.MAN VX11C 6 blocks, VX11D 473 lines)

Auxiliary routines and information (DDTX.FOR VX11C 5 blocks, VX11D 384 lines, TXDD.FOR VX11C 6 blocks, VX11D 370 lines, WRITL.FOR VX11C 1 block, VX11D 50 lines, BROWN.C VX11C 1 block, VX11D 49 lines, DDRM.C VX11C 7 blocks, VX11D 541 lines, RAMDEF.C VX11C 2 blocks, VX11D 34 lines, RM.C VX11C 6 blocks, VX11D 426 lines, RMINSTR.C VX11C 6 blocks, VX11D 388 lines, RMSEG.C VX11C 6 blocks, VX11D 455 lines, RTKBUFFER.C VX11C 20 blocks, VX11D 1304 lines, CGP.H VX11C 4 blocks, VX11D 234 lines, DIDD.H VX11C 2 blocks, VX11D 119 lines, RAMDEF.H VX11C 1 block, VX11D 19 lines, RAMOP.H VX11C 3 blocks, VX11D 148 lines, RAMTEK.H VX11C 3 blocks, VX11D 124 lines, INSV.MAR VX11C 1 block, VX11D 7 lines, INSV.S VX11C 1 block, VX11D 13 lines, RAMOUT.FOR VX11C 1 block, VX11D 71 lines, RAMINPUT.FOR VX11C 46 blocks, VX11D 3906 lines)

Data library (ERRORS.DAT VX11C 10 blocks, VX11D 253 lines)

Control information (COMPILE.COM VX11C 1 block, VX11D 33 lines)

Sample problem output (6 pages)

Reference Thesis excerpt and NESC Notes, appropriate to version

17. **CATEGORY** - N
KEYWORDS - computer graphics, computer output devices, plotters, display devices

18. **SPONSOR** - DOE Office of Basic Energy Sciences
NASA Langley Research Center

1. **IDENTIFICATION AND KWIC TITLE -** SOLCOST3.0
   SOLCOST3.0, solar heating & cooling design

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
CDC CYBER172,175

3. **DESCRIPTION -** The SOLCOST solar energy design program is intended for sizing and evaluating several types of solar systems for residential and single-zone commercial buildings including service hot water and space heating systems using liquid or air collectors. Other systems incorporating heat pumps and absorption cooling are also available but are still being validated. The SOLCOST program computes an optimum solar collector area and tilt angle from an analysis of life cycle cost differences for a solar system versus a reference (conventional) HVAC system. This computation utilizes historical solar radiation and weather data for 336 cities to perform one day long computation for each month of the year. The program predicts the annual fraction of heating or cooling load provided by the solar system, the optimum collector area and tilt angle for the installation, and a detailed cash flow summary including payback and rate of return for the optimum collector area.

4. **METHOD OF SOLUTION -** SOLCOST analysis consists of two parts - a solar collector system performance analysis and a life-cycle cost analysis. SOLCOST computes hourly solar fluxes incident on the tilted collector at mid-month points for average clear and average cloudy day conditions for each month of the year. The insolation model is based on the method in Chapter 59 of the ASHRAE Applications Handbook. The hourly insolation values are passed to the solar collector performance segment where they are used with time-varying ambient temperatures and inlet temperatures to predict instantaneous solar energy collection rates. The collector's performance is modeled with an efficiency curve. Usable solar energy is estimated by applying a system transport efficiency to the collected energy values. Having the usable solar energy defined on a per square foot basis, SOLCOST then computes the annual fraction of the load supplied by collector areas sized to provide from 10 percent to 100 percent of the total load. This calculation is repeated for all specified tilt angles and the results passed to the life cycle cost routine where the fuel requirements are estimated for the solar system as a function of collector area and for the reference HVAC system.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -** NESC executed each of the sample problems in less than 2 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** SOLCOST can be used to evaluate energy conservation features as part of a solar space heating system.

8. **RELATED AND AUXILIARY SOFTWARE -** The package contains an interactive program which prepares input files for SOLCOST. The interactive program can create new files or edit old ones. The original version of SOLCOST was developed at Martin Marietta, Denver, Colorado.

9. **STATUS -** Abstract first distributed April 1981.
   CDC CYBER172 version submitted April 1980, sample problems executed by NESC December 1980 on a CDC CYBER175.

10. **REFERENCES -** SOLCOST, Solar Energy Design Program for Non-Thermal Specialists, ANSI Standard FORTRAN Version 3.0, USER'S GUIDE for Batch Processing, Interactive Input, Solar Environmental Engineering Company, January 1980.
   SOLCOST3.0, NESC No. 907.C172, SOLCOST3.0 Transmittal Tape Description, Implementation Information, and User's Guide Errata, National Energy Software Center Note 81-22, December 10, 1980.
   M. Connolly, R. Giellis, C. Jensen, and R. McMordie, "Solar Heating and Cooling Computer Analysis - A Simplified Sizing Design Method for Non-Thermal Specialists", Proceedings of the International Solar Energy Society Joint Conference August 15-20, 1976, Winnipeg, Canada, Vol. 10, pp. 220-234, 1976.

Sue B. Weir and Russ R. Holder, Commercial Energy Costs for SOLCOST Data Bank Cities, Winter 1982-1983, UAH-345, received November 23, 1983.

11. **HARDWARE REQUIREMENTS** - 74,000 (octal) words of memory are needed to execute SOLCOST. The interactive input program requires 115,000 (octal) words of memory. However, by using the auxiliary subroutines included in the package, the interactive input program can be reduced to 65,000 (octal) words of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS 1.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
L. J. Lantz
Solar Environmental Engineering Company

16. **MATERIAL AVAILABLE** -
Source (8992 lines)
Sample problem (599 lines)
Weather data library (2016 lines)
Auxiliary information (interactive input program-8810 lines, interactive input sample problem-80 lines, COMNT-46 lines, PROMPT-49 lines, DFALT-43 lines, COMTAB-506 lines, PRMTAB-957 lines, DFLTAB-1523 lines)
Reference report, SEEC User's Guide, and NESC Note

17. **CATEGORY** - T
KEYWORDS - life-cycle cost, solar space heating, solar energy, buildings, optimization, weather, heating load, cooling load, design, energy analysis

18. **SPONSOR** - DOE Office of Solar Applications,
Education and Communications Branch

IDENTIFICATION AND KWIC TITLE - MOCARS
MOCARS, MC distribution & simulation limits

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER76, CDC7600

DESCRIPTION - MOCARS uses Monte Carlo techniques to determine the distribution and simulation limits for a function. MOCARS randomly samples data from any of 12 different probability distributions and either evaluates a user-specified function or cut set system unavailability using the sample data. After ordering the data, the values at various quantities and associated confidence bounds are calculated. The available distributions are uniform, exponential, normal, binomial, Poisson, lognormal, Weibull, gamma, beta, Cauchy, Pearson Type IV, and empirical. If the cut set unavailability function is evaluated, MOCARS can determine the importance ranking for components in the unavailability calculation. Frequency and cumulative distribution histograms are also calculated from the sample data.

METHOD OF SOLUTION - The unavailability of each cut set is approximated by the failure rate and fault duration time for each event in the cut set. The system unavailability is merely the sum of the minimal cut set unavailabilities. MOCARS uses two measures to assess component importance. The first ranks components by their contribution to system unavailability, and the second ranks the uncertainty contribution of each component to the uncertainty in system unavailability.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maximum of -
20 quantile values
When calculating component importance, sampling distributions are assumed to be normal, lognormal, or exponential.

TIMING - NESC executed each sample problem in less than 2 seconds of CP time on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - The MOCARS package contains a preprocessor program which builds the sample function from the data and passes dimensioning information to MOCARS to be used in the dynamic allocation of storage. MOCARS evaluates system unavailability using the minimal fault tree cut sets from the RAS program (NESC 889), or other fault tree codes such as PREP (NESC 528) and MOCUS (NESC 653).

STATUS - Abstract first distributed May 1981.
CDC CYBER76 version submitted February 1978, replaced by revised edition submitted December 1980, sample problems executed by NESC January 1981 on a CDC7600.

REFERENCES - Scott D. Matthews and John P. Poloski, MOCARS: A Monte Carlo Code for Determining Distribution and Simulation Limits and Ranking System Components by Importance, TREE-1138 (Revision 1), August 1978.

Excerpts from INEL-IGS, Idaho National Engineering Laboratory Integrated Graphics System Programming Guide, Aerojet Nuclear Company, Computer Science Center, March 1976.

MOCARS, NESC No. 912.CY76, MOCARS Tape Description, National Energy Software Center Note 81-50, January 12, 1981.

MOCARS, NESC No. 912.CY76, Modifications Required for MOCARS Use on NOS and NOS/BE Systems, National Energy Software Center Note 84-37, June 15, 1984.

HARDWARE REQUIREMENTS - If a segmented load is performed, 15,000 (octal) words of memory are required for execution. Without segment loading additional memory will be needed.

PROGRAMMING LANGUAGE - FORTRAN IV (76%) and COMPASS (24%)

OPERATING SYSTEM - SCOPE 2.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS –** The INEL Environmental Routines CVI, FABEND, FAPFIM, FTBMEM, and FTBIN are written in CDC COMPASS assembly language; the remainder of the package is in FORTRAN. NESC provided dummy routines for the Integrated Graphics System (IGS) library routines EXITG, GRIDG, LABELG, LINESG, MODESG, OBJCTG, PAGEG, SETUPG, SUBJEG, TITLEG, XNORMZ, and YNORMZ. These IGS routines should be replaced with suitable alternatives for the local computing environment, if graphical output is desired.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**
S. D. Matthews and J. P. Poloski
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE –**
Source (MOCARS 2434 lines, Preprocessor 367 lines, Environmental routines 1450 lines)
Sample problems (155 lines)
Control information (88 lines)
Reference report, Excerpts from Guide, and NESC Notes

17. **CATEGORY –** G
KEYWORDS – Monte Carlo method, systems analysis, reliability, failures, system failure analysis, statistical models, simulation, RAS codes, MOCUS codes, PREP,KITT codes

18. **SPONSOR –** EG&G Idaho, Incorporated

IDENTIFICATION AND KWIC TITLE - RELAP5/MOD1/029, RELAP5/MOD1/008
RELAP5/MOD1/029, LWR loss of coolant analysis
RELAP5/MOD1/008, LWR loss of coolant analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER176,175, CDC7600, IBM3033,370

DESCRIPTION - RELAP5 was developed to describe the behavior of a light water reactor (LWR) subjected to postulated transients such as loss of coolant from large or small pipe breaks, pump failures, etc. RELAP5 calculates fluid conditions such as velocities, pressures, densities, qualities, temperatures; thermal conditions such as surface temperatures, temperature distributions, heat fluxes; pump conditions; trip conditions; reactor power and reactivity from point reactor kinetics; and control system variables. In addition to reactor applications, the program can be applied to transient analysis of other thermal-hydraulic systems with water as the fluid.

RELAP5/MOD1 uses a five equation two-phase flow hydrodynamic model consisting of the two phasic continuity equations, the two phasic momentum equations, and an overall energy equation augmented by the requirement that one of the phases be saturated. In this model only two interphase constitutive relations are required, those for interphase drag and interphase mass exchange. Models are included for abrupt area changes, choking, mass transfer, interphase drag, wall friction, and branching.

METHOD OF SOLUTION - For hydrodynamics, the space approximation uses a staggered mesh, where integral forms of the continuity and energy equations are approximated over control volumes, and line integral forms of the momentum equations are applied from the midpoint of one control volume to the midpoint of the adjoining control volume. Hydrodynamic equations are advanced in time using a semi-implicit, linearized method. Heat conduction is approximated by finite differences and advanced by the Crank-Nicolson scheme. A modified Runge-Kutta technique for stiff equations is used to solve the reactor kinetics equations. The interaction among hydrodynamics, heat conduction, trips, reactor kinetics, and the control system is explicit.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The limitations on the number of hydrodynamic volumes, heat structures, trips, minor edits, etc. are primarily dictated by the available memory of the computer. Dynamic allocation of storage is used for all problem-dependent data. Design of the fields used for input data can also impose limits. Problems with over 150 hydrodynamic volumes and over 100 heat structures have been run on a CDC CYBER176 using 270K of SCM and 200K of LCM storage for input processing and less during transient analysis.

TIMING - The computer time depends on the number of volumes, heat structures, and the type of transient. Simulation of a postulated small break loss-of-coolant accident for the LOFT reactor using 87 volumes, 96 junctions, and 32 heat structures required 3152 seconds of CYBER176 time for 3600 seconds of reactor transient analysis. EDHTRK sample problem execution time is approximately 20 CP seconds on a CDC CYBER176 and 39 CP seconds on a CDC CYBER175; WORKSHOP PROBLEM 2, 40 CP seconds on a CDC CYBER176 and 71 CP seconds on a CDC CYBER175; WORKSHOP PROBLEM 3, 118 CP seconds on a CDC CYBER176 and 215 CP seconds on a CDC CYBER175. Execution of the sample problems on the IBM3033 and IBM370/195 requires from 1 second to 3 minutes of CPU time.

UNUSUAL FEATURES OF THE SOFTWARE - Automatic time-step control is used for hydrodynamic advancement.

RELATED AND AUXILIARY SOFTWARE - The primary improvement in RELAP5 compared to the earlier RELAP4 series (NESC 369) is the use of an advanced hydrodynamic model for two-phase flow which allows different velocities and different temperatures for the phases. RELAP5/MOD1 extends the earlier RELAP5/MOD0 capability to include models unique to small break situations, and provides added capability for modeling accumulators, noncondensible gas, nucleonics, control systems, separators, and boron concentrations. MOD1 also contains improvements in the flow regime maps, choked flow models, general running time, and output edits.

9. **STATUS** - Abstract first distributed March 1981.
CDC7600 version of RELAP5/MOD0 submitted May 1979, replaced by revised edition February 1980, replaced by CDC CYBER176 version of RELAP5/MOD1 December 1980, replaced by CDC CYBER176 version of RELAP5/MOD1/006 April 1981, replaced by CDC CYBER176 version of RELAP5/MOD1/014 August 1981, replaced by CDC CYBER176 version of RELAP5/MOD1/018 July 1982, replaced December 1984 by RELAP5/MOD1/029, sample problems executed by NESC November 1984 on a CDC CYBER175.
IBM3033 version of RELAP5/MOD1/008 submitted May 1983, sample problems executed by NESC May 1983 on an IBM3033 and an IBM370/195.

10. **REFERENCES** - Victor H. Ransom, Richard J. Wagner, John A. Trapp, Kenneth E. Carlson, Dennis M. Kiser, Han-Hsiung Kuo, Hueiming Chow, Ralph A. Nelson, and Stephen W. James, RELAP5/MOD1 Code Manual Volume 1: System Models and Numerical Methods, NUREG/CR-1826(EGG-2070), Revision 2, September 1981.
Richard J. Wagner, Kenneth E. Carlson, Dennis M. Kiser, Victor H. Ransom, Han-Hsiung Kuo, Hueiming Chow, John A. Trapp, Stephen W. James, and Douglas G. Hall, RELAP5/MOD1 Code Manual Volume 2: Users Guide and Input Requirements, NUREG/CR-1826(EGG-2070), Revision 2, September 1981.
R. A. Riemke, H. Chow, and V. H. Ransom, RELAP5/MOD1 Code Manual Volume 3: Checkout Problems Summary, EGG-NSMD-6182, February 1983.
EG&G Idaho, NRTS Environmental Subroutine Manual, December 9, 1980.
D. G. Hall and E. C. Johnson, RELAP5/MOD1 Quick Reference Manual, EGG-CDD-6027, October 1982.
Environmental Library Installation Procedures, EG&G Note, September 1983.
RELAP5/MOD1/029, NESC No. 917.C176, Description of RELAP5/MOD1/029 CDC UPDATE Format Tape and Implementation Information, National Energy Software Center Note 85-36, December 24, 1984.
RELAP5/MOD1/029, NESC No. 917.C176B, Description of RELAP5/MOD1/029 Edition B Tape for Reading on Non-CDC Systems and Implementation Information, National Energy Software Center Note 85-37, December 24, 1984.
RELAP5/MOD1/008, NESC No. 917.3033, RELAP5/MOD1/008 Tape Description and Implementation Information, National Energy Software Center Note 84-11, February 17, 1984.
P. Saha, J. H. Jo, L. Neymotin, U. S. Rohatgi, and G. Slovik, Independent Assessment of TRAC-PD2 and RELAP5/MOD1 Codes at BNL in FY 1981, NUREG/CR-3148 (BNL-NUREG-51645), December 1982.
J. M. McGlaun and L. N. Kmetyk, RELAP5 Assessment: Semiscale Natural Circulation Tests S-NC-2 and S-NC-7, NUREG/CR-3258 (SAND83-0833), May 1983.

11. **HARDWARE REQUIREMENTS** - RELAP5 has run on a 64K CDC7600, a 132K CDC CYBER176 both with and without use of LCM storage, and a 256K CDC CYBER175 without use of ECS storage. The CDC RELAP5 package contains options (implemented through the CDC UPDATE utility program) intended to allow RELAP5 implementation on a CYBER76 operating under SCOPE2, a CYBER175 under NOS or NOS2, and a CYBER170 or similar CYBER series hardware under NOS/BE.
RELAP5 on an IBM3033 or IBM370/195 requires from 980K to 1500K bytes.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (90%) and COMPASS (10%) (CDC CYBER176), FORTRAN IV (99%) and BAL (1%) (IBM3033)

13. **OPERATING SYSTEM** - NOS/BE (CDC CYBER176), SCOPE2.1.5 (CDC7600), NOS2.2 (CDC CYBER175), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - RELAP5/MOD1 contains a limited plotting capability. It has been interfaced to the local INEL system and proprietary graphics software to plot and compare simulation results with experiment. A number of the NRTS Environmental Subroutines are written in the CDC assembly language, COMPASS, including those for input and output processing, and packing and unpacking. RELAP5 is written exclusively in FORTRAN but uses MASK, SHIFT, and Boolean AND and OR operations to pack and unpack integer data. Several of the routines which are CDC operating system or INEL computing environment dependent will require modification or replacement in other environments. The RELAP5 Edition B package is the same as the C176 edition except that it is written in a format that can be read on non-CDC machines.

The IBM version of RELAP5 contains an assembly language subroutine JTIME which only runs on VM systems. Users with other operating systems must replace this routine, which requests the remaining CPU time of a job, with an alternative routine suited to their computing environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

CYBER176, CYBER176B — V. H. Ransom, R. J. Wagner, K. E. Carlson, J. A. Trapp, D. M. Kiser, H. H. Kuo, H. M. Chow, R. A. Nelson, D. G. Hall, S. W. James, and E. C. Johnson
EG&G Idaho, Inc.

3033 — NEA Data Bank

16. **MATERIAL AVAILABLE -**

Source (C176-RELAP5 390 records*, Environmental subroutines 387 records*, C176B-RELAP5 40,717 lines, Environmental subroutines 36,983 lines, 3033-RELAP5 and Environmental subroutines FORTRAN source 51,322 lines, Environmental subroutines assembler 1507 lines)
Load module RELAP5.LOADMOD (3033-1204 blocks**)
Sample problem input (C176-210 records*, C176B-22,781 lines, EDHTRK C176-3 records*, C176B-159 lines, WORKSHOP PROBLEM 2 C176-11 records*, C176B-1002 lines, WORKSHOP PROBLEM 3 C176-5 records*, C176B-230 lines, 3033-3655 lines)
Binary steam tables (3033-97 blocks***)
Control information (C176-11 records*, C176B-444 lines, 3933-JCL 174 lines, overlay lines 63 lines)
Auxiliary information (RELAP5 source UPDATE input C176-24 records*, C176B-1788 lines)
Sample problem output (EDHTRK C176-109 records*, C176B-5576 140-character records, WORKSHOP PROBLEM 2 C176-172 records*, C176B-8584 140-character records, WORKSHOP PROBLEM 3 C176-70 records*, C176B-3407 140-character records, 3033-48,855 132-character records)
Reference reports, NUREG/CR-1826, Vols. 1 and 2, Rev. 2, EGG-NSMD-6182, EGG-CDD-6027, NRTS Environmental Subroutine Manual, EG&G Note, and NESC Note, appropriate to version

* 512-word maximum length
** RECFM=FB,LRECL=80,BLKSIZE=800
*** RECFM=VS,LRECL=796,BLKSIZE=800

17. **CATEGORY** - G
KEYWORDS - hydrodynamics, two-phase flow, loss of coolant, thermal conduction, heat transfer, blowdown, reactor safety, transients, accidents, control systems, reactor kinetics, simulation, RELAP codes, water cooled reactors

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - SALE
SALE, analytical chemistry quality control

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,3033

DESCRIPTION - The Safeguards Analytical Laboratory Evaluation (SALE) program is a statistical analysis program written to analyze the data received from laboratories participating in the SALE quality control and evaluation program. The system is aimed at identifying and reducing analytical chemical measurement errors. Samples of well-characterized materials are distributed to laboratory participants at periodic intervals for determination of uranium or plutonium concentration and isotropic distributions. The results of these determinations are statistically evaluated and participants are informed of the accuracy and precision of their results.

METHOD OF SOLUTION - Various statistical techniques produce the SALE output. Assuming an unbalanced nested design, an analysis of variance is performed, resulting in a test of significance for time and analyst effects. A trend test is performed. Both within-laboratory and between-laboratory standard deviations are calculated.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Up to 1500 pieces of data for each nuclear material sampled by a maximum of 75 laboratories may be analyzed.

TIMING - Seven seconds of IBM3033 CPU time were required to execute the sample problem.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed August 1982.
IBM360 version submitted November 1980, sample problem executed by NESC March 1981 on an IBM3033.

REFERENCES - Darla J. Carroll, William J. Bush, and Cynthia A. Dolan, SALE: Safegaurds Analytical Laboratory Evaluation Computer Code, ANCR-1316, September 1976.
SALE, NESC No. 919.360, SALE Tape Description, National Energy Software Center Note 82-72, August 3, 1982.

HARDWARE REQUIREMENTS - 380K bytes of memory are required for execution.

PROGRAMMING LANGUAGE - FORTRAN IV (97%) and Assembly language (3%)

OPERATING SYSTEM - OS/360.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The plot option requires graphics routines not included in the SALE package. The INEL library and IGS (Integrated Graphics System) routines SYMBL4, MODESG, SUBJEG, OBJCTG, SETSMG, GETMSG, PAGEG, EXITG, LEGNDG, MLTPLG, NUMBRG, GRIDG, LABELG, and TITLEG will have to be replaced with suitable alternatives for the local environment.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
C. D. Gentillon
EG&G Idaho, Inc.

MATERIAL AVAILABLE -
Source (FORTRAN 2924 lines, BAL 79 lines)
Sample problem (program controls 84 lines, data 1485 lines)
Sample problem output (complete on tape, 3715 133-character records)
Reference report, ANCR-1316, and NESC Note

CATEGORY - U

KEYWORDS - chemical analysis, data analysis, quality control, evaluation, performance testing, statistics, sampling, uranium, plutonium

18. **SPONSOR** - ERDA Office of Safeguards and Security

1. **IDENTIFICATION AND KWIC TITLE** - DEVOG
   DEVOG, coupled molecular scattering equations

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - DEVOG solves the coupled, second-order differential equations of atomic and molecular quantum scattering theory. The program is independent of the chemical system or the method (close coupling, coupled states, etc.). The physical problem is defined by user-supplied subroutines, POT and LIST.

4. **METHOD OF SOLUTION** - DeVogeleare's algorithm for the numerical integration of second-order differential equations without explicit first derivatives is used. The S-matrix is computed by matching the wave function and its derivatives to spherical Bessel functions.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The number of coupled equations which can be solved depends on the amount of main memory available.

6. **TIMING** - DEVOG requires 0.8 seconds of CP time for a 2-channel problem and 151 seconds of CP time for a 28-channel problem on a CDC7600. NESC executed the sample problem in less than 1 second of CP time on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Step-size changes of arbitrary value are easily introduced into the program.

8. **RELATED AND AUXILIARY SOFTWARE** - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. An auxiliary program, COEF, is included which defines the list of quantum numbers and evaluates the R-independent F-coefficients. Other general integration programs used to solve the coupled equations of molecular scattering theory are PC (NESC 921) and MNN (NESC 942).

9. **STATUS** - Abstract first distributed May 1981.
   CDC7600 version submitted February 1981, sample problem executed by NESC March 1981 on a CDC CYBER175.

10. **REFERENCES** - Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980.

Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980.

DEVOG, NESC No. 920.7600, DEVOG Tape Description, National Energy Software Center Note 81-36, May 21, 1981.

William A. Lester, Jr., DeVogeleare's Method for the Numerical Integration of Second-Order Differential Equations without Explicit First Derivatives: Applications to Coupled Equations Arising from the Schroedinger Equation, Journal of Computational Physics, Vol. 3, pp. 322-326, 1968.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest, and R. B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

A. C. Allison, The Numerical Solution of Coupled Differential Equations Arising from the Schroedinger Equation, Journal of Computational Physics, Vol. 6, pp. 378-391, 1970.

11. **HARDWARE REQUIREMENTS** - 144,000 (octal) words of memory are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutines POT and LIST, which define the physical problem, must be supplied by the user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

L. D. Thomas
National Resource for Computation in Chemistry
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -

Source (1400 lines)
Sample problem (FORTRAN 1060 lines, data 5 lines)
Auxiliary information (COEF 324 lines, data 27 lines, machine-readable documentation 157 lines)
Control information (47 lines)
Sample problem output (11 pages)
Excerpts from reference reports, LBL-9501 Vols. I and II, and NESC Note

17. **CATEGORY** - W
KEYWORDS - S matrix, inelastic scattering, Schroedinger equation, Bessel functions, wave functions, PC codes, MNN codes

18. **SPONSOR** - DOE Office of Basic Energy Sciences
NSF

1. **IDENTIFICATION AND KWIC TITLE** - PC
   PC, coupled molecular scattering equations

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - PC solves the coupled, second-order differential equations of atomic and molecular quantum scattering theory. The program is independent of the chemical system or the method (close coupling, coupled states, etc.). The physical problem is defined by user-supplied subroutines, POT and LIST.

4. **METHOD OF SOLUTION** - The variable-order, variable-step, predictor-corrector algorithms developed by Shampine and Gordon are used. The S-matrix is computed by matching the wave function and its derivatives to spherical Bessel functions.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The number of coupled equations which can be solved depends on the amount of main memory available.

6. **TIMING** - PC requires 1.5 seconds of CP time for a 2 channel problem and 256 seconds of CP time for a 28-channel problem on a CDC7600. NESC executed the sample problem in less than 22 seconds of CP time on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - PC contains only one error parameter which maintains a fixed level of accuracy throughout the calculation. PC performs best at low energy where the wavelength is long.

8. **RELATED AND AUXILIARY SOFTWARE** - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. An auxiliary program, COEF, is included which defines the list of quantum numbers and evaluates the R-independent F-coefficients. Other general integration programs used to solve the coupled equations of molecular scattering theory are DEVOG (NESC 920) and MNN (NESC 942).
   The Shampine-Gordon algorithms which perform the solution of an initial-value problem for a system of first-order ordinary differential equations are DE/STEP,INTRP and DEROOT/STEP,INTRP (NESC 640).

9. **STATUS** - Abstract first distributed May 1981.
   CDC7600 version submitted February 1981, sample problem executed by NESC March 1981 on a CDC CYBER175.

10. **REFERENCES** - Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980.

Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980.

PC, NESC No. 921.7600, PC Tape Description, National Energy Software Center Note 81-38, May 21, 1981.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest, and R. B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

L. F. Shampine and M. K. Gordon, Computer Solution of Ordinary Differential Equations, The Initial Value Problem, W. H. Freeman, San Francisco, 1975.

11. **HARDWARE REQUIREMENTS** - 143,000 (octal) words of memory are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutines POT and LIST, which define the physical problem, must be supplied by the user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

L. D. Thomas
National Resource for Computation in Chemistry
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -

Source (1828 lines)
Sample problem (FORTRAN 1060 lines, data 5 lines)
Auxiliary information (COEF 324 lines, data 27 lines, machine-readable documentation 157 lines)
Control information (39 lines)
Sample problem output (15 pages)
Excerpts from reference reports, LBL-9501 Vols. I and II, and NESC Note

17. **CATEGORY** - W
KEYWORDS - S matrix, inelastic scattering, Schroedinger equation, wave functions, Bessel functions, DEVOG codes, MNN codes

18. **SPONSOR** - DOE Office of Basic Energy Sciences
NSF

1. **IDENTIFICATION AND KWIC TITLE** - SCORE-EVET
   SCORE-EVET, 3d hydraulic reactor core analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - SCORE-EVET was developed to study multidimensional transient fluid flow in nuclear reactor fuel rod arrays. The conservation equations used were derived by volume averaging the transient compressible three-dimensional local continuum equations in Cartesian coordinates. No assumptions associated with subchannel flow have been incorporated into the derivation of the conservation equations. In addition to the three-dimensional fluid flow equations, the SCORE-EVET code contains a one-dimensional steady state solution scheme to initialize the flow field, steady state and transient fuel rod conduction models, and comprehensive correlation packages to describe fluid-to-fuel rod interfacial energy and momentum exchange. Velocity and pressure boundary conditions can be specified as a function of time and space to model reactor transient conditions, such as a hypothesized loss-of-coolant accident (LOCA) or flow blockage.

   The basic volume-averaged transient three-dimensional equations for flow in porous media are solved in their general form with constitutive relationships and boundary conditions tailored to define the porous medium as a matrix of fuel rods. By retaining generality in the form of the conservation equations, a wide range of fluid flow problem configurations, from computational regions representing a single fuel rod subchannel to multichannels, or even regions without a fuel rod, can be modeled without restrictive assumptions. The completeness of the conservation equations has allowed SCORE-EVET to be used, with modification to the constitutive relationships, to calculate three-dimensional laminar boundary layer development, flow fields in large bodies of water, and, with the addition of a turbulence model, turbulent flow in pipe expansions and tees.

4. **METHOD OF SOLUTION** - The numerical technique used to solve the volume-averaged three-dimensional equations is based on the marker and cell (MAC) method for incompressible flow, as modified by Hirt and Cook, and the implicit continuous fluid Eulerian (ICE) method for compressible flow. The one-dimensional transient heat conduction equation used in the fuel rod thermal transport model is solved by dividing the fuel and cladding into a finite number of nodes and applying a Crank-Nicolson implicit finite difference formulation.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   64 flow channels
   40 cells in any one direction (boundary plus real cells)
   40 possible loss coefficients
   For the fuel rod thermal transport model, five nodes are allowed in the fuel and two nodes in the cladding.

6. **TIMING** - NESC executed the three sample problems in 12, 15, and 2 CP minutes, respectively, on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - An auxiliary program to convert the formatted water properties data to a binary data file for use by SCORE-EVET is included in the package. If the fuel rod thermal model is used, the fluid-solid interfacial heat transfer is calculated by a slightly modified version of the heat transfer and critical heat flux correlations developed for RELAP4/MOD5 (NESC 369).

9. **STATUS** - Abstract first distributed August 1982.
   CDC7600 version submitted April 1977, replaced by revised edition April 1978, sample problems executed by NESC April 1981 on a CDC CYBER175.

10. **REFERENCES** - Robert L. Benedetti, Lee V. Lords, and Dennis M. Kiser, SCORE-EVET: A Computer Code for the Multidimensional Transient Thermal-Hydraulic Analysis of Nuclear Fuel Rod Arrays, TREE-NUREG-1133, February 1978.

SCORE-EVET, NESC No. 931, SCORE-EVET Tape Description and Implementation Information, National Energy Software Center Note 82-89, August 14, 1982.

Walter J. Wnek, John D. Ramshaw, John A. Trapp, E. Daniel Hughes, and Charles W. Solbrig, Transient Three-Dimensional Thermal-Hydraulic Analysis of Nuclear Reactor Fuel Rod Arrays: General Equations and Numerical Scheme, ANCR-1207, November 1975.

C. W. Hirt and J. L. Cook, Calculating Three-Dimensional Flows around Structures and over Rough Terrain, Journal of Computational Physics, Vol. 10, pp. 324-340, 1972.

11. **HARDWARE REQUIREMENTS** - 200,000 (octal) words of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. L. Benedetti, L. V. Lords, and D. M. Kiser
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
Source (12,848 lines)
Sample problems (295 lines)
Water properties library (2544 lines)
Auxiliary conversion program (17 lines)
Control information (30 lines)
Sample problems output (3 microfiche)
Reference report, TREE-NUREG-1133, and NESC Note

17. **CATEGORY** - G
KEYWORDS - three-dimensional, fluid flow, water reactors, fuel rods, loss of coolant, accidents, flow blockage, incompressible flow, hydraulics, thermodynamic properties, RELAP4 codes

18. **SPONSOR** - AEC
NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

1. **IDENTIFICATION AND KWIC TITLE** - WECS
   WECS, wind energy value to electric utilities

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - WECS is a package of five computer models developed by the Solar Energy Research Institute to implement a method for determining the value of Wind Energy Conversion Systems (WECS) to electric utilities. These models, WTP, WEIBUL, ROSEW, ULMOD, and FINAM, may be used with most utility planning models. The value determination procedure begins with the processing of weather data by either the WTP or WEIBUL program to produce hourly wind speed data or wind probability distributions for each hour of a monthly typical day, respectively. The function of WTP is to convert a single year of standard weather data into a format acceptable to the ROSEW program. WEIBUL is preferable to WTP if two or more years of weather data are available because its probabilistic representation of hourly wind speeds is more likely to represent the long-term wind speeds than WTP's hourly average wind speeds. Both programs use the same four types of input weather data - SOLMET, TMY, and TDF from the National Climatic Center in Asheville, North Carolina, and Aerospace from Aerospace Corporation.

   ROSEW calculates the wind energy system hourly power output using weather data supplied and wind machine characteristics. For WTP-supplied weather data, a single hourly wind power is calculated. For WEIBUL-supplied weather data, a group of wind powers with associated probabilities for each hour is calculated.

   ULMOD uses the electricity production estimate calculated by ROSEW to reduce a user-supplied utility hourly-load forecast. This reduced load profile is then put into a variety of forms suitable for use with electric utility planning models (e.g. LOLP, PRODUCTION COSTING, GENERATION EXPANSION PLANNING). Utility load forecasting uncertainty can be reflected.

   FINAM is designed to determine the value (in $/kW) and marginal value of alternative electric utility investment options, such as Wind Energy Conservation Systems, by using base case utility operating data with up to ten change cases. Each change case contains operating data for a hypothesized amount of alternative investment. Sensitivity studies may be performed by changing a specific cost component, such as the cost of any fuel type.

4. **METHOD OF SOLUTION** - WTP reads the necessary data, makes the proper unit conversions, and uses interpolation to replace bad data. WEIBUL calculates the Weibull shape and scale parameters by fitting the observed wind frequency distribution by either a least squares or maximum likelihood method. Only points above a user-specified wind-speed are included in the fit. ROSEW uses two methods to calculate the hourly wind power. The first uses the standard equation to determine the power in an airstream with a given velocity calculating the air density from the other hourly weather parameters. The second uses an input velocity-power output table where the appropriate output power is derived directly from a given wind velocity. In ULMOD utility load forecasting uncertainty is handled by the application of up to five different amounts of megawatt variability and their associated probabilities. FINAM uses present worth economics to determine the breakeven cost ($/kW) for the alternative investment. Operating cost estimates for up to 20 years may be considered. Marginal value is determined by fitting a curve to the change case values and differentiating.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - On the CDC7600 typical CP times are 25 seconds for WTP, approximately 10 seconds per year of weather data for WEIBUL, 5 seconds for ROSEW, 5 seconds to 2 minutes for ULMOD dependent on whether it is a simple hour-by-hour calculation or the Weibull distribution calculation and the inclusion of load forecasting uncertainty, and 1 second for FINAM. NESC CP times observed during execution on the CYBER175 were 16 seconds for WTP, 26 seconds for WEIBUL, 5 seconds for ROSEW, 6 minutes for ULMOD, and 1 second for FINAM.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - WTP hourly output data include dry bulb temperature (degrees C), barometric pressure (bars), relative humidity, wind speed (meters/sec), opaque sky cover (fractional), and direct and total insolation (Kw/m**2). A summary of missing

data is provided also. In WEIBUL the maximum expected wind speed and number of wind speed intervals to be used can be specified. ROSEW accounts for vertical height extrapolation of the wind. The ULMOD ability to handle a distribution of WECS output per hour and utility load forecasting uncertainty is unique.

8. **RELATED AND AUXILIARY SOFTWARE** - The WECS programs are intended for use with the two traditional utility planning models - an expansion planning model and a detailed electric utility-production cost model. An electric utility trying to determine the value of WECS penetration may prefer to use their corporate financial model instead of FINAM.

9. **STATUS** - Abstract first distributed May 1981.
CDC7600 version of WECS submitted March 1981, replaced by Edition B submitted September 1981, sample problems executed by NESC March 1982 on a CDC CYBER175.

10. **REFERENCES** - David Percival and James Harper, Electric Utility Value Determination for Wind Energy, Volume I: Methodology, Volume II: A User's Guide, SERI/TR-732-604, February 1981.
WECS, NESC No. 932.7600B, WECS Tape Description, Implementation Information and Errata to SERI/TR-732-604 Volume II, National Energy Software Center Note 82-47, May 31, 1982.

11. **HARDWARE REQUIREMENTS** - CDC7600 storage requirements are 50,000 (octal) words SCM for WTP, 100,000 (octal) words SCM for WEIBUL, 50,000 (octal) words SCM for ROSEW, 53,000 (octal) words SCM and 61,000 (octal) words LCM for ULMOD, and 31,100 (octal) words SCM and 32,000 (octal) words LCM for FINAM. On the CYBER175 NESC used 46,000 (octal) words of CM storage for WTP, 144,000 (octal) words for WEIBUL, 108,000 (octal) words for ROSEW, 200,000 (octal) words for ULMOD, and 112,000 (octal) words for FINAM.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.2 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The programs rely on the contents of memory being preset to zero. ULMOD calls the CDC Sort/Merge package for the development of all load duration curves. If different sort/merge routines are substituted, differences in output may result. FINAM uses the RLDOPM, RLFOTH, UERTST, and UGETIO routines from the proprietary International Mathematical and Statistical Library (IMSL). These are not included in the WECS package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. R. Harper and C. D. Percival
Utility Applications and Policy Branch
Solar Energy Research Institute

16. **MATERIAL AVAILABLE** -
Source (WTP 970 lines, WEIBUL 1078 lines, ROSEW 2231 lines, ULMOD 2354 lines, FINAM 2004 lines)
Sample problems (WTP 5 lines, WEIBUL 6 lines, ROSEW 33 lines, ULMOD 50 lines, FINAM 368 lines)
Library data (weather data Albuquerque TMY 8760 132-character records, utility-load data 732 lines)
Reference reports and NESC Note

17. **CATEGORY** - D
KEYWORDS - wind power, electric utilities, economic analysis, forecasting, weather, simulation, wind power plants, energy models, energy management, WTP codes, WEIBUL codes, ROSEW codes, ULMOD codes, FINAM codes

18. **SPONSOR** - DOE Wind Energy Systems Division

IDENTIFICATION AND KWIC TITLE - SCAP
SCAP, point kernel single or albedo scatter

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175

DESCRIPTION - SCAP solves for radiation transport in complex geometries using the single- or albedo-scatter point kernel method. The program is designed to calculate the neutron or gamma-ray radiation level at detector points located within or outside a complex radiation scatter source geometry or a user-specified discrete scattering volume. The geometry is described by zones bounded by intersecting quadratic surfaces with an arbitrary maximum number of boundary surfaces per zone. The anisotropic point sources are described as point-wise energy dependent distributions of polar angles on a meridian; isotropic point sources may be specified also. The attenuation function for gamma rays is an exponential function on the primary source leg and the scatter leg with a buildup factor approximation to account for multiple scatter on the scatter leg. The neutron attenuation function is an exponential function using neutron removal cross sections on the primary source leg and scatter leg. Line or volumetric sources can be represented as distributions of isotropic point sources, with uncollided line-of-sight attenuation and buildup calculated between each source point and the detector point.

METHOD OF SOLUTION - A point kernel method using an anisotropic or isotropic point source representation is used. Line-of-sight material attenuation and inverse square spatial attenuation between the source point and scatter points and the scatter points and detector point are employed. A direct summation of individual point source results is obtained.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The geometric zone description is restricted to zones defined by boundary surfaces defined by the general quadratic equation or one of its degenerate forms. Due to flexible dimensioning in SCAP, there are no restrictions on the number of energy groups or geometric zones.

TIMING - SCAP computes approximately 200 source point to scatter point to detector point calculations per CP second on the CDC7600. Execution time is independent of the number of energy groups and is dependent only on the calculation of geometry-dependent data. NESC executed the ten sample problems in less than 5 minutes of CP time on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE - The use of a generalized method of determining scatter point densities (general geometry) based on the electron density of the media encountered on a line-of-sight as well as the use of a generalized spherical geometry integration technique over scatter zones defined in a complex geometry are unique features of the program.

All input data are read by a routine which allows free field input of data.

RELATED AND AUXILIARY SOFTWARE - An auxiliary program, GAMLIB, is included which prepares the gamma-ray absorption coefficient library for use by SCAP. Neutron and gamma-ray point source distribution data can be supplied on punched cards from the MAP program as anisotropic energy-dependent source data.

STATUS - Abstract first distributed August 1982.
CDC7600 version submitted June 1977, replaced by revised edition submitted April 1980, revisions received February and May 1981, sample problems executed by NESC June 1981 on a CDC CYBER175.

REFERENCES - R. K. Disney, A. R. McIlvaine, and S. E. Bevan, SCAP Computer Program Description, Single Scatter, Albedo Scatter, or Point Kernel Analysis Program in Complex Geometry, ARD Computer Program Abstract: SH-24, April 1980, revised February 13, 1981.

SCAP, NESC No. R933.7600, SCAP Tape Description and Implementation Information, National Energy Software Center Note 82-75, August 5, 1982.

R. K. Disney and S. L. Zeigler, Point Kernel Techniques, WANL-PR(LL)-034, Vol. 6, August 1970.

R. G. Soltesz, R. K. Disney, and S. L. Zeigler, Cross Section Generation and Data Processing Techniques, WANL-PR(LL)-034, Vol. 3, August 1970.

11. **HARDWARE REQUIREMENTS** - 55,000 (octal) words of memory are needed to execute the SCAP program on the CDC CYBER175.

12. **PROGRAMMING LANGUAGE** - FORTRAN (99%) and COMPASS (1%)

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutine RFLS, which allocates the requested small core memory (SCM), is written in CDC COMPASS assembly language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. K. Disney and S. E. Bevan
Advanced Reactors Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (FORTRAN 2547 lines, COMPASS 12 lines)
Sample problems (355 lines)
Gamma-ray cross section library (907 lines)
Auxiliary program (GAMLIB 41 lines)
Control information (35 lines)
Sample problems output (2 microfiche)
Reference report, ARD Program Abstract SH-24, and NESC Note

17. **CATEGORY** - J
KEYWORDS - radiation transport, point kernels, shielding, albedo, gamma radiation, anisotropic scattering, point sources, Clinch River Breeder Reactor, MAP codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Project

IDENTIFICATION AND KWIC TITLE - MAPPER
MAPPER, report quality graphics on command

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,370,303x, CDC6600,7600, Cray1, DEC10,DEC VAX11/780

DESCRIPTION - MAPPER is designed to provide a command language whereby non-programmers can produce report quality visual aids. The user can produce presentation and report quality slides, graphs, charts, tables, and maps in both color and black and white on 35mm film, Tektronix terminals, and Versatec and CalComp plotters. Several versions of MAPPER can also be used to make 35mm and 16mm color or black and white movies.

MAPPER can draw boxes, circles, ellipses, and complex line segments in a wide variety of line formats. There are six types of label commands and 12 to 15 lettering styles available to meet labeling requirements. Label options include manual sizing and location, two forms of automatic sizing and location, flexible string control, rotation, justification control, and multiple line capability. The user has the choice of color control and selective shading of specific areas. Symbols may be defined, positioned, scaled, distorted, and shaded as specified. Axes, curves, and error bars may be drawn. Additional features include user-defined logos, skipping, multilevel projection ports, contouring, three types of file subroutine usage, movie generating commands, and FORTRAN support capabilities.

METHOD OF SOLUTION - MAPPER reads English language type command files that the user has generated executing each command as it is read. MAPPER acts as a FORTRAN front-end to the DISSPLA proprietary graphics software product of Integrated Software Systems Corporation (ISSCO). In some machine versions, an interactive editor allows Tektronix users to create new features on the scope and to have these automatically added to the command file. A Tektronix Graphics Tablet can be used to generate MAPPER command files directly.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Three-dimensional surfaces and mapping data bases are not included.

TIMING - A test case of 89 Versatec plots took 50 seconds on an IBM3033. A test case of 5 Tektronix plots was completed in less than 9 seconds on a DEC KL10. A test case of 16 35mm color film plots took 15 minutes on a DEC VAX11/780.

UNUSUAL FEATURES OF THE SOFTWARE - Symbols may be rotated, scaled, distorted, and reflected. Automatic shape connection is provided for flow diagram presentation.

RELATED AND AUXILIARY SOFTWARE - The original MAPPER release 1.0 was developed at LANL by D. A. Dahl for their CDC6000,7000 systems. The CDC version of MAPPER release 2.0 was converted at Oak Ridge to both the IBM and DEC10 computer systems. The MAPPER master source and ESP, an auxiliary program which processes MAPPER master source into machine-specific FORTRAN source are included with the MAPPER3.0 and MAPPER4.0 releases.

STATUS - Abstract first distributed September 1981.
IBM360 version of MAPPER2.0 submitted June 1981.
DEC10 version of MAPPER2.0 submitted June 1981.
DEC VAX11/780 versions of MAPPER3.0 and MAPPER4.0 submitted October 1981, replaced by revised editions December 1982 and May 1983, sample problem executed by NESC August 1983 on a DEC VAX11/780.
CDC6600 versions of MAPPER3.0 and MAPPER4.0 submitted October 1981, replaced by revised editions December 1982 and May 1983, compiled by NESC August 1983 on a CDC CYBER175.
CDC7600 versions of MAPPER3.0 and MAPPER4.0 submitted October 1981, replaced by revised editions December 1982 and May 1983, compiled by NESC August 1983 on a CDC CYBER175.
Cray1 versions of MAPPER3.0 and MAPPER4.0 submitted October 1981, replaced by revised editions December 1982 and May 1983.

10. **REFERENCES** - B. A. Clark, K. N. Fischer, C. W. Nestor, S. K. Penny, and D. A. Dahl, MAPPER User's Manual, ORNL/CSD/TM-163, November 1983.

MAPPER, NESC No. 939, Author's Installation Notes, National Energy Software Center Note 81-82, June 19, 1981.

Jeanne M. Hurford, GR830.1 MAPPER - Version 4.0 Summary, LANL PIM-8 Program Library Write-Up, January 1983.

Patrick Hodson, GR897 MAPPER - Version 3.0, LANL PIM-8 Program Library Write-Up, September 1982.

Patrick Hodson, J5AJ1 MAPPER - Version 3.0, LANL PIM-2 Program Library Write-Up, July 1981.

R. Elliott, J5AJ1 MAPPER on LTSS, LANL PIM-2 Program Library Write-Up, July 1980.

David A. Dahl, J5AJ MAPPER Version 2, LANL PIM-2 Program Library Write-Up, March 1979.

Ted Reed, GR800 CGS Device Control User Manual, LANL PIM-8 Program Library Write-Up, May 1982.

Ted Reed, GR801 CGS Graphics User Manual, LANL PIM-8 Program Library Write-Up, May 1982.

David Dahl, Kenneth Rea, and Patrick Hodson, U2AE ESP: Easy Structured Programming, LANL PIM-2 Program Library Write-Up, May 1981.

Patrick Hodson, GR891 MAPEDIT: An Additive Graphics Editor for MAPPER, LANL PIM-8 Program Library Write-Up, September 1982.

MAPPER, NESC No. 939.VX11, MAPPER DEC VAX Version Tape Description and Implementation Information, National Energy Software Center Note 84-13, February 17, 1984.

MAPPER, NESC No. 939.6600, MAPPER CDC6600 Version Tape Description and Implementation Information, National Energy Software Center Note 84-15, February 17, 1984.

MAPPER, NESC No. 939.7600, MAPPER CDC7600 Version Tape Description, National Energy Software Center Note 84-14, February 17, 1984.

MAPPER, NESC No. 939.CRA1, MAPPER CRAY1 Version Tape Description, National Energy Software Center Note 84-16, February 17, 1984.

MAPPER, NESC No. 939, CDC6600,7600, CRAY1, and DEC VAX11 Versions, Self-Teaching MAPPER Course Available, National Energy Software Center Note 84-12, October 1, 1983.

11. **HARDWARE REQUIREMENTS** - DISSPLA software is required along with the appropriate film, plotter, and graphics input devices (e.g. CalComp 1036 and 1055 plotters, Versatec and Gould 5005 plotters, FR-80 film recorder, AED 512-compatible terminals, and Tektronix 4010-compatible terminals and Graphics Tablet), and 470K bytes of storage (IBM), 178 plus 15 pages of virtual memory (DEC10), 152,000 (octal) words of memory (CDC7600), or 439K bytes of memory (DEC VAX).

12. **PROGRAMMING LANGUAGE** - FORTRAN (99%) and COMPASS (1%) (CDC6600), FORTRAN IV (all other versions)

13. **OPERATING SYSTEM** - MVS (IBM), TOPS 10 (DEC10), NOS,NOS/BE (CDC6600), LTSS (CDC7600), CTSS (Cray1), VMS 3.2 (DEC VAX).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The MAPPER2.0 and MAPPER3.0 releases require release 8.2 of the proprietary DISSPLA graphics software system. In addition, the IBM and DEC10 versions require the DISSPOP option. The MAPPER4.0 releases require DISSPLA 9.0. Extraction labels for the ESP program must be entered as upper-case characters. The REPLAC character-manipulation subroutine, which is a part of the Oak Ridge computing environment, is not included in the IBM and DEC10 versions. A suitable alternative, appropriate to the local computing environment, will have to be supplied.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

360, DEC10 B. A. Clark, K. N. Fisher, C. W. Nestor, and
S. K. Penny
Computer Sciences Division
Union Carbide Corporation, Nuclear Division
D. A. Dahl
EG&G Idaho, Inc.

6600, 7600, P. Hodson
Cray1, VAX11 Computing Division
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source (360-4078 lines, DEC10-BACKUP format 75 2720-character records, VX11-MAPPER3.0 12,809 lines, MAPPER4.0 12,551 lines, 6600-MAPPER3.0 11,899 lines, MAPPER4.0 12,418 lines, 7600-MAPPER3.0 13,602 lines, CRA1-MAPPER3.0 12,762, MAPPER4.0 12,507 lines)
Device drivers (360-261 lines)
Sample problems (360-2763 lines, VX11-15,467 lines, 6600-15,467 lines, 7600-15,467 lines, CRA1-15,467 lines)
Auxiliary information (MAPEDIT 6600-401 lines, ANIMATE 6600-2175 lines, 7600-1126 lines, ANIPLT 7600-282 lines, TABLET 7600-309 lines, MAPPER master source 18,345 lines, ESP VX11-6969 lines, 6600-7127 lines, 7600-7124 lines, CRA1-7120 lines, HP3000-7788 lines, PRIME-6930 lines, DEC10-6856 lines, IBM-6835 lines)
Control information (360-262 lines, 6600-95 lines, 295 90-character records, 7600-47 90-character records)
Sample problem output (MAPPER3.0 and MAPPER4.0 17 plots)
Reference ORNL User's Manual or LANL Program Library Write-Ups and NESC Notes, as appropriate to version

17. **CATEGORY** - N
KEYWORDS - computer graphics, interactive display devices, plotters, diagrams, photographic films, maps, computer output devices

18. **SPONSOR** - Union Carbide Corporation Nuclear Division
Los Alamos National Laboratory

IDENTIFICATION AND KWIC TITLE - MNN
MNN, solution of close coupling equations

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175,74

DESCRIPTION - MNN solves the coupled differential equations of the coupled-channel method for the quantum mechanical treatment of inelastic collisions of electrons, atoms, and molecules.

METHOD OF SOLUTION - The program uses the Numerov method with automatic step-size selection. Scattering boundary conditions are applied in a standard way.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The number of coupled equations which can be solved depends on the amount of main memory available.

TIMING - Execution time is dependent on the number of channels, but will typically range from 0.4 to 700 CP seconds on the CDC7600. NESC executed the sample problem in 2 CP seconds on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - This program, Version 79-6 of MNN, was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. COEF, an auxiliary program, defines the list of quantum numbers and determines the R-independent F-coefficients. Other programs used to solve the coupled equations of molecular scattering theory are DEVOG (NESC 920) and PC (NESC 921). The DCS2 program (reference 6) can be used to compute differential cross sections from MNN output.

STATUS - Abstract first distributed August 1982.
CDC7600 version submitted February 1981, sample problem executed by NESC July 1981 on a CDC CYBER175.

REFERENCES - Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980.

Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980.

MNN, NESC No. 942, MNN Tape Description, National Energy Software Center Note 82-87, August 13, 1982.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest, and R. B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

Maynard A. Brandt, Donald G. Truhlar, and F. A. Van-Catledge, Electron scattering by nitrogen molecules: Theory and application to elastic scattering and rotational excitation at 30-75 eV, Journal of Chemical Physics, Vol. 64, No. 12, pp. 4957-4967, 1976.

Kunzio Onda, Donald G. Truhlar and Maynard A. Brandt, New Version of Program for Calculating Differential and Integral Cross Sections for Quantum Mechanical Scattering Problems from Reactance or Transition Matrices, Computer Physics Communications, Vol. 21, pp. 97-108, 1980.

HARDWARE REQUIREMENTS - 134,000 (octal) words of memory are required to execute the sample problem.

PROGRAMMING LANGUAGE - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175,74).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutines POT, PREPOT, POTCAL, and LIST, and a driver program, which define the physical problem, must be supplied by the user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. G. Truhlar and D. Thirumalai
Department of Chemistry
University of Minnesota
M. A. Brandt
Facility Code RSMO2N
Control Data Corporation
K. Onda
Laboratory for Astronomy and Solar Physics
NASA Goddard Space Flight Center

16. **MATERIAL AVAILABLE** -

Source (3631 lines)
Sample problem (FORTRAN 1173 lines, data 20 lines)
Auxiliary information (COEF FORTRAN 324 lines, data 27 lines, machine-readable documentation 465 lines)
Control information (46 lines)
Sample problem output (14 pages)
Excerpts from reference report LBL-9501 Vols. I and II and NESC Note

17. **CATEGORY** - W
KEYWORDS - quantum mechanics, potentials, collisions, Schroedinger equation, wave functions, inelastic scattering, DEVOG codes, PC codes, DCS2 codes, POT codes, LIST codes, COEF codes

18. **SPONSOR** - NSF
University of Minnesota

1. **IDENTIFICATION AND KWIC TITLE** - RIO
   RIO, power plant reliability characteristics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - RIO, which consists of two FORTRAN programs, determines reliability importance and allocates optimal reliability goals for nuclear power plant safety systems. The first program, PHASE1, determines the importance of each safety system's contribution to overall plant risk and ranks the systems accordingly. The second program, PHASE2, is a nonlinear optimization code that determines optimal values of systems' reliability characteristics subject to the risk constraints imposed on the plant.

4. **METHOD OF SOLUTION** - In PHASE1, RIO calculates the importance of each safety system by taking into account the magnitude of each system's reliability value and how often the particular system appears in the accident sequences.
   PHASE2 has the capability of solving linear, nonlinear, constrained, or unconstrained optimization problems. Each nuclear power plant has an associated risk, usually a release of radioactive materials to the environment. Release of radioactive materials is categorized according to the magnitude and isotopic content. The risk can be defined in terms of the accident sequences that contribute to the probability of occurrence for each level of release. To formulate an objective function that can be optimized by RIO, the sum of all the accident sequences in the various release categories is considered. Thus, the objective function to be minimized (or maximized) is defined in terms of all the safety systems that are involved in the various release categories.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -

150 accident sequences per release category	(PHASE1)
25 events per accident sequence	(PHASE1)
25 sets of data for describing the safety systems, initiators, and containment failure modes	(PHASE1)
40 constraint equations	(PHASE2)
20 independent variables	(PHASE2)

6. **TIMING** - NESC executed the sample problem in less than 1 CP second for PHASE1 and less than 2 CP seconds for PHASE2 on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The CDC UPDATE program is used to define the input for PHASE2 of RIO.

8. **RELATED AND AUXILIARY SOFTWARE** - PREP,KITT (NESC 528) obtains system reliability information from a system fault tree.

9. **STATUS** - Abstract first distributed August 1982.
   CDC7600 version submitted February 1980, replaced by revised edition June 1981, sample problems executed by NESC July 1981 on a CDC CYBER175.

10. **REFERENCES** - John P. Poloski, RIO: A Program to Determine Reliability Importance and Allocate Optimal Reliability Goals, TREE-1287, September 1978.
    RIO, NESC No. 943, RIO Tape Description, National Energy Software Center Note 82-88, August 13, 1982.

11. **HARDWARE REQUIREMENTS** - 30,000 (octal) words of memory are required by the PHASE1 program; PHASE2 requires 40,000 (octal) words.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (86%) and COMPASS (14%)

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutine CVI in PHASE1, which reads free-form input, is written in COMPASS assembly language. PHASE2 makes use of

the CDC UPDATE program to supply the control variables, define the objective function, and describe the constraints to be imposed on the model. Significant effort would be required to implement PHASE2 in computing environments without CDC UPDATE or a similar facility.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

J. P. Poloski
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE -**

Source (PHASE1 FORTRAN 473 lines, PHASE1 UPDATE 1062 lines, PHASE1 COMPASS 576 lines, PHASE2 FORTRAN 2613 lines, PHASE2 UPDATE 2482 lines)
Sample problems (PHASE1 129 lines, PHASE2 143 lines)
Control information (72 lines)
Reference report and NESC Note

17. **CATEGORY** - G
KEYWORDS - reliability, nuclear power plants, safety, risk assessment, system failure analysis, optimization, nonlinear programming, PREP,KITT codes

18. **SPONSOR** - DOE Division of Nuclear Research Applications

1. **IDENTIFICATION AND KWIC TITLE** - PUBG
   PUBG, Purex solvent extraction process model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM3033, CDC CYBER175

3. **DESCRIPTION** - PUBG is a chemical model of the Purex solvent extraction system, by which plutonium and uranium are recovered from spent nuclear fuel rods. The system comprises a number of mixer-settler banks. This discrete stage structure is the basis of the algorithms used in PUBG. The stages are connected to provide for countercurrent flow of the aqueous and organic phases. PUBG uses the common convention that has the aqueous phase enter at the lowest numbered stage and exit at the highest one; the organic phase flows oppositely. The volumes of the mixers are smaller than those of the settlers. The mixers generate a fine dispersion of one phase in the other. The high interfacial area is intended to provide for rapid mass transfer of the plutonium and uranium from one phase to the other. The separation of this dispersion back into the two phases occurs in the settlers.

   The species considered by PUBG are Hydrogen (1+), Plutonium (4+), Uranyl Oxide (2+), Plutonium (3+), Nitrate Anion, and reductant in the aqueous phase and Hydrogen (1+), Uranyl Oxide (2+), Plutonium (4+), and TBP (tri-n-butylphosphate) in the organic phase. The reductant used in the Purex process is either Uranium (4+) or HAN (hydroxylamine nitrate).

4. **METHOD OF SOLUTION** - The discrete stage structure is modeled and solved in PUBG as follows. The differential equations for the time rate of change of concentrations are written in terms of the flows, mass transfer rates, and reaction rates. Because the residence times in the mixers are small, the steady-state approximation is used, and the resulting mass balance equations are solved by Newton's method. The differential equations for the settlers are solved by fourth-order Runge-Kutta integration.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maximum of -
   100 mixer-settler stages
   All feed streams enter the contactor through the mixers, with only one feed stream of each phase able to enter a mixer. All product streams exit the contactor from the settlers, with only one product stream of each phase able to exit a settler. A product stream may reenter the system through only one mixer, in addition to any feed streams entering that mixer.

6. **TIMING** - The twenty stage partitioning contactor (the 1B contactor) runs in less than 2.5 CPU minutes on an IBM3033 and less than 2.5 CP minutes on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - PUBG contains three features not available in other computer simulations of the Purex process: (a) the user can vary the rate of mass transfer of uranium and plutonium across the phase boundaries; (b) the user can cause continual random fluctuations in the feed stream concentrations as they enter the system; and (c) PUBG takes account of the oxidation of Uranium (4+) to Uranyl Oxide (2+) by nitrate ion, thus simulating realistically the 1B partitioning contactors.

8. **RELATED AND AUXILIARY SOFTWARE** - TRANSIENTS, SEPHIS/MOD4 (NESC 690), and SOLVEX (NESC 662) are other solvent extraction programs.

9. **STATUS** - Abstract first distributed August 1982.
   IBM3033 version submitted September 1981, sample problems executed by NESC October 1981 on an IBM3033.
   CDC CYBER175 version derived October 1981, sample problems executed by NESC November 1981 on a CDC CYBER175.

10. **REFERENCES** - John F. Geldard and Adolph L. Beyerlein, A User's Manual for PUBG. A New Chemical Model of the Purex Solvent Extraction Process, Clemson University report, September 1981.
   PUBG, NESC NO. 959, PUBG Sample Problem Output, National Energy Software Center Note 82-90, August 17, 1982.

A. L. Beyerlein, J. F. Geldard, H. F. Chung, and J. E. Bennett, Deviations from Mass Transfer Equilibrium and Mathematical Modeling of Mixer-Settler Contactors, Transactions of the American Nuclear Society, Vol. 33, Supplement 1, pp. 56-58, 1979.

A. L. Beyerlein, J. F. Geldard, H. F. Chung, and J. E. Bennett, Deviations from Mass Transfer Equilibrium and Mathematical Modeling of Mixer-Settler Contactors, National Bureau of Standards Special Publication NBS-SP 582, pp. 702-711, June 1980.

J. T. Lowe, Calculation of the Transient Behavior of Solvent Extraction Processes, Industrial and Engineering Chemistry, Process Design and Development, Vol. 7, pp. 362-366, 1968.

11. **HARDWARE REQUIREMENTS** - The IBM3033 version requires 150K bytes of memory for execution; 62,000 (octal) words are required by the CDC CYBER175 version.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/MVS or OS/MVT (IBM3033), NOS 1.3 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

3033 J. F. Geldard and A. L. Beyerlein
Department of Chemistry and Geology
Clemson University

CYBER175 L. R. Eyberger
National Energy Software Center
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
Source (3033-1657 lines, C175-1658 lines)
Sample problems (39 lines)
Control information (JCL 3033-60 lines)
Reference User's Manual and NESC Note

17. **CATEGORY** - U
KEYWORDS - reprocessing, solvent extraction, mixer-settlers, Purex process, plutonium, uranium, SOLVEX codes, SEPHIS/MOD4 codes, TRANSIENTS codes

18. **SPONSOR** - Los Alamos National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - GASPAR
   GASPAR, evaluation of atmospheric releases

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM370,303x

3. **DESCRIPTION** - GASPAR implements the air released dose models of the NRC Regulatory Guide 1.109 for noble gases (semi-infinite plume only) and the radioiodine and particulate emissions (specifically 1.109-10 through 1.109-13 and a portion of 1.109-14). GASPAR computes both population (ALARA-As Low As Reasonably Achievable and NEPA-National Environmental Policy Act) and individual doses. Site data, meteorological data, radionuclide release source terms, and location meteorological data for selected individuals are specified as input data. The site data include population data and milk, meat, and vegetation production. The meteorological data include dispersion X/Q, X/Q decayed, X/Q decayed and depleted, and deposition. Population doses, individual doses, and cost benefit tables are calculated.

4. **METHOD OF SOLUTION** - There are two basic types of calculations, the population dose calculation and the individual dose calculation; however, both may be combined in a single GASPAR execution. There are usually several source terms corresponding to several release points. As the dose is computed for each source term it is accumulated so that the dose printed for the first source term is the actual dose for that term. For all subsequent source terms the dose printed is the accumulated dose with the dose printed for the last source term, the grand total for the problem. For the cost benefit table, individual source term doses are generated. Seven pathways by which the nuclides travel to man are considered. These are plume, ground, inhalation, vegetation, cows' milk, goats' milk, and meat. For the individual dose calculations, man is subdivided into the four age groups of infant (0 to 1 year), child (1-11 years), teenager (12-18 years), and adult (over 18 years). Each of these calculations take into account eight body organs - T. body, G.I. tract, bone, liver, kidney, thyroid, lung, and skin.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   99 source terms
   10 source terms in Cost Benefit Table
   33 nuclides
   5 individuals

6. **TIMING** - Execution of the 4 sample problems takes approximately 10 CPU seconds on the IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - Other programs which calculate organ dose include: AERIN (NESC 908), which calculates organ and tissue burdens resulting from acute exposure to a radioactive aerosol, DACRIN (NESC 923), which calculates organ dose from acute or chronic radionuclide inhalation, SUBDOSA (NESC 924), which calculates external doses from atmospheric releases of radionuclides, and ARRRG,FOOD (NESC 925), and PABLM (NESC 926), which calculate radiation doses to humans from radionuclides in the environment.

9. **STATUS** - Abstract first distributed January 1982.
   IBM370 version submitted February 1981, sample problems executed by NESC June 1981 on an IBM3033.

10. **REFERENCES** - K. F. Eckerman and D. G. Lash, GASPAR Evaluation of Atmospheric Releases, NRC Radiological Assessment Branch memorandum, Revised August 19, 1977.

11. **HARDWARE REQUIREMENTS** - 270K bytes of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (98%) and Assembly language (2%)

13. **OPERATING SYSTEM** - OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS –**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

K. F. Eckerman
Oak Ridge National Laboratory
D. G. Lash
Radiological Assessment Branch
J. A. Shields
Division of Automatic Data Processing
U.S. Nuclear Regulatory Commission

16. **MATERIAL AVAILABLE –**

Source (FORTRAN 2519 lines, Assembly language 63 lines)
Sample problems (662 lines)
Sample problems output (57 selected pages)
Reference memorandum

17. **CATEGORY** – G
KEYWORDS – radiation doses, organs, inhalation, ingestion, radioisotopes, AERIN codes, DACRIN codes, SUBDOSA codes, ARRRG,FOOD codes, PABLM codes

18. **SPONSOR** – NRC Office of Nuclear Reactor Regulation

DENTIFICATION AND KWIC TITLE - XOQDOQ
XOQDOQ, nuclear power plant effluent releases

OMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
3M370,303x, CDC CYBER175

ESCRIPTION - XOQDOQ was designed for meteorological evaluation of routine releases from ommercial nuclear power reactors. It calculates average relative effluent concentrations nd average relative deposition values at locations specified by the user and at standard adial distances and segments for downwind sectors. It also calculates these values at the pecified locations for intermittent releases.

ETHOD OF SOLUTION - XOQDOQ uses a Gaussian "straight-line" equation to implement the ssumptions outlined in Section C of the U. S. Nuclear Regulatory Commission's Regulatory uide 1.111. Long-term average values of relative effluent concentration are calculated by ssuming a long-term continuous release with effluent distributed evenly across a 22-1/2 egree sector.

ESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
30 receptor locations
14 velocity categories
7 stability categories
5 release exit points
5 receptor types

IMING - NESC executed the sample problem in less than 10 CPU seconds on an IBM3033, 8 CP econds on a CDC CYBER175.

NUSUAL FEATURES OF THE SOFTWARE -

ELATED AND AUXILIARY SOFTWARE -

TATUS - Abstract first distributed August 1982.
IBM370 version submitted January 1981, revised November 1982, sample problem executed by NESC December 1982 on an IBM3033.
CDC CYBER175 version submitted October 1982, sample problem executed by NESC December 1982 on a CDC CYBER175.

EFERENCES - J. F. Sagendorf and J. T. Goll, XOQDOQ, Program for the Meteorological valuation of Routine Effluent Releases at Nuclear Power Stations, NUREG-0324 Draft, eptember 1977, with Errata.
U. S. Nuclear Regulatory Commission, Office of Standards Development, egulatory Guide 1.111, Methods for Estimating Atmospheric Transport and Dispersion of aseous Effluents from Light-Water-Cooled Power Reactors, March 1976, with Errata, January 977.

ARDWARE REQUIREMENTS - The IBM version requires 240K bytes of memory to execute the sample oblem; the CDC version requires 137,000 (octal) words of memory.

OGRAMMING LANGUAGE - FORTRAN IV (IBM370), FORTRAN 77 (CYBER175)

ERATING SYSTEM - OS/370 (IBM370), NOS 1.3 (CYBER175).

THER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

ME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
370 J. Shields
Division of Automatic Data Processing
U.S. Nuclear Regulatory Commission

CYBER175 G. C. Almon

Electricity Supply Commission
South Africa

16. **MATERIAL AVAILABLE** -
Source (370-2326 lines, C175-2361 lines)
Sample problem (54 lines)
Reference report, NUREG-0324

17. **CATEGORY** - R
KEYWORDS - radioactive effluents, plumes, stack disposal, meteorology, nuclear power plants

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation,
Division of Site Safety and Environmental Analysis

IDENTIFICATION AND KWIC TITLE - BICYCLE
BICYCLE, levelized life cycle cost calculation

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC6600,CYBER175

DESCRIPTION - BICYCLE calculates levelized life-cycle costs for plants that produce electricity, heat, gaseous fuels, or liquid fuels. BICYCLE also gives a detailed breakdown of the various life-cycle components making up the total and yearly cash flows in current dollars during each year of the project's lifetime.

METHOD OF SOLUTION - Life-cycle costs are calculated using two basic methods that reflect two modes of debt capital repayment. One method (proportional) assumes that the ratio of outstanding debt capital to outstanding equity capital remains constant, and the other (fixed-payment) assumes that the debt capital repayment schedule is fixed in advance, and all expenses other than the initial capital investment come from equity capital.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - With current program dimensioning, 12(the number of years a plant operates)+(the number of years for capital construction) must be less than 1000.

TIMING - NESC executed the sample problems in less than 1 CP second on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - POWERCO (NESC 340) calculates the cost of electricity produced by nuclear power stations, assuming all cash expenses are known.

STATUS - Abstract first distributed August 1982.
CDC6600 version submitted July 1981, sample problems executed by NESC January 1982 on a CDC6600.

REFERENCES - R. W. Hardie, BICYCLE II: A Computer Code for Calculating Levelized Life-Cycle Costs, LA-8909, November 1981.

HARDWARE REQUIREMENTS - 23,000 (octal) words are required to execute the sample problems.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - NOS 1.4 (CDC CYBER175).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
R. W. Hardie
Los Alamos National Laboratory

MATERIAL AVAILABLE -
Source (775 lines)
Sample problems (23 lines)
Reference report

CATEGORY - D
KEYWORDS - life-cycle cost, power plants, electricity, process heat, gas fuels, liquid fuels, economics, capital, POWERCO codes

SPONSOR - DOE Office of Solar Energy

IDENTIFICATION AND KWIC TITLE - SOFTWARE TOOLS
SOFTWARE TOOLS, program development interface
SOFTWARE TOOLS, program development environmnt

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
Base, DEC VAX11/780 (The Base version is not tailored to any one machine but serves as a portable base for the user who can add "primitives" or modify the Base source to tailor SOFTWARE TOOLS to the local computing environment.)

DESCRIPTION - One of the problems encountered by computer users is the lack of common utility routines for different computer systems. The software which was initially presented in Kernighan and Plauger's SOFTWARE TOOLS represented a first step toward a solution to this problem. A common editor, text formatter, sort, and other program development tools were presented through two mechanisms:

(a) all source was written in RATFOR, a FORTRAN preprocessor language directly translatable into FORTRAN, and
(b) system-dependent routines were pushed down either into macro replacements or primitive function calls, to be implemented by the individual charged with bringing up the utilities in the local computing environment.

These mechanisms, together with adoption of certain conventions pertaining to data types, permit many sites running different operating systems to implement these tools. If the shell, or command line interpreter, is implemented, this software can essentially define a portable "virtual operating system" providing inter-system uniformity at the three levels of user interface--virtual machine (the primitives), utilities, and command language.

The SOFTWARE TOOLS package consists of a set of program development utilities and a program library modeled after the Bell Laboratories' proprietary UNIX operating system.

METHOD OF SOLUTION - Many of the utilities originated in the Kernighan-Plauger book; enhancements and new tools have been contributed by various other sites world-wide. Considerable effort has gone into identifying and specifying the primitives (machine-specific functions) needed to support the complete package. Implementing these routines on a new system can take anywhere from one week to six months, depending on the friendliness of the local operating system. Once these primitives are available, the remainder of the package comes up with few problems.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed March 1982.
Base version submitted July 1981, RATFOR bootstrap executed by NESC January 1982 on an IBM3033.
DEC VAXi1/780 version submitted July 1981, revised November 1981 and August 1982, selected tools executed by NESC September 1982 on a DEC VAX11/780.

REFERENCES - B. W. Kernighan and P. J. Plauger, Software Tools, Addison-Wesley, Reading, Massachusetts, 1976.

Dennis E. Hall, Deborah K. Scherrer, and Joseph S. Sventek, A Virtual Operating System, Communications of the Association for Computing Machinery, Vol. 23, No. 9, September 1980.

SOFTWARE TOOLS, NESC No. 967, SOFTWARE TOOLS Base Version Tape Description, National Energy Software Center Note 82-36, March 30, 1982.

SOFTWARE TOOLS, NESC No. 967.VX11, SOFTWARE TOOLS VAX/VMS Version Tape Description and Implementation Information, National Energy Software Center Note 83-22, September 29, 1982.

11. **HARDWARE REQUIREMENTS** - On the VAX, the entire system requires approximately 22,000 blocks of disk storage if no files are deleted, or approximately 16,000 blocks if both source and object files are deleted during the building process.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and RATFOR. In the DEC VAX11/780 version some of the primitives are written in the MACRO-11 assembly language.

13. **OPERATING SYSTEM** - VMS3.0 (DEC VAX11/780)

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Most of the files on the transmittal tape contain both upper- and lower-case characters.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

    Base — D. K. Scherrer

    VAX11 — J. S. Sventek
    Computer Science and Mathematics Department
    Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
    Source (Base-RATFOR bootstrap 3407 lines, RATFOR preprocessor 3324 lines, other 36,554 lines, VX11-DISTN.BCK 2209 blocks*, SRC.BCK 946 blocks*, VMS.BCK 244 blocks*)
    Machine-readable documentation (Base-implementation instructions 4156 lines, programmer's manual 14,595 lines, spelling dictionary 42,697 lines, VX11-DOC.BCK 132 blocks*)
    Auxiliary information (VX11-MSGSYS.BCK 3 blocks*)
    NESC Note, appropriate to version
    * Maximum block size = 2064 bytes

17. **CATEGORY** - P
    KEYWORDS - FORTRAN, programming, libraries, utility routines, operating systems

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
    Division of Engineering, Mathematical and Geo-Sciences

IDENTIFICATION AND KWIC TITLE - NJE3.00
NJE3.00, VAX VMS IBM NJE protocol emulator

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC VAX11/780

DESCRIPTION - NJE3.00 is communications software developed to enable a VAX VMS system to participate as an end-node in a standard IBM network by emulating the Network Job Entry (NJE) protocol. NJE3.00 supports job networking for the operating systems used on most large IBM-compatible computers (e.g., VM/370, MVS with JES2 or JES3, SVS, MVT with ASP or HASP). Files received from the network can be printed or directed to a user-designated directory. Files sent to the network can be routed to any network node for printing, punching, or job submission, or to a CMS user's virtual reader. The system will also send commands and messages to other nodes on the network. Commands are provided to transmit general sequential files, to display the status of the communications line, or to list the queue of files being sent. VAX NJE operators may also display internal VAX NJE system status information. The communications software does ASCII-EBCDIC character representation translation.

METHOD OF SOLUTION - Reliability is provided by transmitting cyclic-redundancy-check bytes computed by the sender with each logical network record. The receiver calculates the same quantity from the data received and does a comparison. If the comparison fails, the receiver asks for the record to be retransmitted. Each record contains a sequence byte to ensure that out-of-sequence record conditions do not occur. Transmission of a network "file" or collection of records is not considered completed until the receiver acknowledges successful reception. Only at this time does the sender relinquish responsibility for the file. Incomplete files are discarded by the receiver in the event the sender computer goes down during transmission of a file.

Asynchronous transmission permits a user to request a transmission and then go on to other interactive work while the transmission proceeds. In NJE3.00, when the user enters an emulator command a small process places the command parameters in a standard "message" that is passed to a dedicated, detached process via the VMS mailbox mechanism. The detached process reads the message and either takes action or queues the task. The queue scheduling algorithm is first-in first-out.

The automatic routing mechanism is based on entries in the NJE emulator parameter file. When a file is received, its network header records contain the destination information. Each VAX user recipient has an entry in the parameter file. This file maps userids to directory specifications. Incoming messages are directed to the user's terminal if he is logged on; otherwise, the message is discarded. Operator messages cannot be lost; they are directed to the hardcopy console. Messages directed to PRINTER are printed on a system printer.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING - The NJE emulator process runs continuously.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed July 1982.
DEC VAX11/780 version of NJE submitted July 1981, replaced by revised edition submitted February 1982, replaced August 1983 by the "As Is" NJE3.00 software (NESC 9916), replaced by revised edition December 1983.

REFERENCES - NJE User's Guide, ANL-CSD Memorandum, August 1983.
Extension of the IBM Network for DEC VAX Computers, Argonne National Laboratory, Computing Services Division Technical Memorandum TM-383 Revised, September 1983.

NJE3.00, NESC No. 972.VX11, NJE3.00 Tape Description, National Energy Software Center Note 84-07, December 2, 1983.

NJE3.00, NESC No. 972.VX11, Changes Required To Use NJE with the VAX/VMS V4.X Operating System, National Energy Software Center Note 85-74, May 24, 1985.

11. **HARDWARE REQUIREMENTS** - VAX11/780 with DUP-11 UNIBUS interface and synchronous modem or modem eliminator.

12. **PROGRAMMING LANGUAGE** - VAX-11 FORTRAN 77 (99%) and MACRO-11 (1%)

13. **OPERATING SYSTEM** - VMS 3.4.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The IBM-specific FORTRAN and assembly language source decks are not required for NJE to function. They are put into a library on the IBM machine and used with special applications requiring data conversion only.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. E. Engert and R. C. Raffenetti
Computing Services--Support Services Division
Argonne National Laboratory
J. Osudar
Science Applications, Inc.

16. **MATERIAL AVAILABLE** -

Source (FORTRAN 228 blocks*, IBM-specific FORTRAN 121 blocks*, MACRO-11 2 blocks*, IBM-specific assembly language 6 blocks*, Include 3 blocks*, MESSAGE 1 block*)
Object (125 blocks*)
Load modules (78 blocks*)
Control information (command procedures 47 blocks*, NJE3.00 implementation information 21 blocks*)
Library information (2 blocks*)
Auxiliary information (compiler and assembler output listings 463 blocks*, linker output listings 83 blocks*, Help documentation 35 blocks*, machine-readable documentation 509 blocks*, miscellaneous information 2 blocks*)
Reference Memorandum and NESC Note

* maximum block size = 2048 bytes

17. **CATEGORY** - P
KEYWORDS - computer networks, IBM computers, DEC computers, communications

18. **SPONSOR** - Argonne National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - SWIFT
   SWIFT, waste-isolation flow & transport model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - SWIFT solves the coupled or individual equations governing fluid flow, heat transport, brine displacement, and radionuclide displacement in geologic media. Fluid flow may be transient or steady-state. One, two, or three dimensions are available, and transport of radionuclides chains is possible.

4. **METHOD OF SOLUTION** - Finite differencing is used to discretize the partial differential equations in space and time. The user may choose centered or backward spatial differencing, coupled with either central or backward temporal differencing. The matrix equations may be solved iteratively (two line successive-over-relaxation) or directly (special matrix banding and Gaussian elimination).

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - On the CDC7600 in direct solution mode, the maximum number of grid blocks allowed is approximately 1400.

6. **TIMING** - Execution time is dependent on problem characteristics. NESC executed each of the 17 sample problems in less than 35 CP seconds on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SWIFT can be run in one, two, or three dimensions, with constant pressure or fluid flux boundary conditions, with injection and/or withdrawal walls, with the option to solve individually or collectively the equations of fluid flow, heat flow, brine, or containment displacement, with a choice of finite-difference solution techniques, and with a choice of Cartesian or radial coordinates.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed April 1982.
   CDC7600 version submitted November 1981, replaced by revised edition April 1982, sample problems executed by NESC March 1982 on an CDC7600.

10. **REFERENCES** - Mark Reeves and Robert M. Cranwell, User's Manual for the Sandia Waste-Isolation Flow and Transport Model (SWIFT) Release 4.81, NUREG/CR-2324 (SAND81-2516), November 1981.

    SWIFT, NESC No. 973.7600, SWIFT Tape Description, User's Manual (NUREG/CR-2324) Errata, and Availability of Self-Teaching Curriculum Report (NUREG/CR-1968), National Energy Software Center Note 82-37, April 5, 1982.

    Nancy C. Finley and Mark Reeves, SWIFT Self-Teaching Curriculum: Illustrative Problems to Supplement the User's Manual for the Sandia Waste-Isolation Flow and Transport Model (SWIFT), NUREG/CR-1968 (SAND81-0410), November 1981 (in publication).

    R. T. Dillon, R. B. Lantz, and S. B. Pahwa, Risk Methodology for Geologic Disposal of Radioactive Waste: The Sandia Waste Isolation Flow and Transport (SWIFT) Model, SAND78-1267, October 1978.

    INTERCOMP Resource Development and Engineering, Inc., Development of Model for Calculating Disposal in Deep Saline Aquifers, Parts I and II, PB-256903, National Technical Information Service, Washington, D.C., 1976.

    D. S. Ward, M. Reeves, and L. E. Duda, Verification and Field Comparison of the Sandia Waste-Isolation Flow and Transport Model (SWIFT), NUREG/CR-3316 (SAND83-1154), April 1984.

11. **HARDWARE REQUIREMENTS** - 70,000 (octal) words of memory are required to compile the SWIFT source. 130,000 (octal) words of small core memory (SCM) and 400,000 (octal) words of large core memory (LCM) are needed to execute the sample problems. SWIFT is designed to permit the user to adjust the machine requirements to problem complexity.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Object code may be generated when using the FTN compiler with the Level 414 library which causes an abort at load time because of insufficient available LCM. If this happens, redefine the DIMENSION of the G array and the value of the variable, ICORE, as 131061.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

R. M. Cranwell
Division 4413
Sandia National Laboratories, Albuquerque
M. Reeves
INTERA Environmental Consultants, Inc.

16. **MATERIAL AVAILABLE** -

Source (14,412 lines)
Sample problems (SI units 1787 lines, English units 1836 lines)
Sample problems output (SI units 33,449 133-character records, English units 33,499 133-character records)
Reference report, NUREG/CR-2324, and NESC Note

17. **CATEGORY** - H
KEYWORDS - adsorption, anisotropy, charged-particle transport, compressible flow, convection, decay, flow models, ground water, heat flow, hydrology, isotopes, porosity, pressure gradients, temperature gradients, velocity, viscous flow

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Risk Analysis

1. **IDENTIFICATION AND KWIC TITLE** - NONSAP-C
   NONSAP-C, nonlinear stress concrete structures

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - NONSAP-C is a finite element program for determining the static and dynamic response of three-dimensional reinforced concrete structures. Long-term, or creep, behavior of concrete structures can also be analyzed. Nonlinear constitutive relations for concrete under short-term loads are incorporated in two time-independent models, a variable-modulus approach with orthotropic behavior induced in the concrete due to the development of different tangent moduli in different directions and an elastic-plastic model in which the concrete is assumed to be a continuous, isotropic, and linearly elastic-plastic strain-hardening-fracture material. A viscoelastic constitutive model for long-term thermal creep of concrete is included.
   Three-dimensional finite elements available in NONSAP-C include a truss element, a multinode tendon element for prestressed and posttensioned concrete structures, an elastic-plastic membrane element to represent the behavior of cavity liners, and a general isoparametric element with a variable number of nodes for analysis of solids and thick shells.

4. **METHOD OF SOLUTION** - NONSAP-C uses the isoparametric finite element formulation. Dynamic problems are solved by integration of the equations of motion in the time domain using either the Wilson-Theta or Newmark-Beta integration algorithms. Equilibrium iteration or stiffness reformulation schemes can be applied in solving the nonlinear discretized equations.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - An out-of-core equation solver for large systems of linear equations allows practically unlimited problem size. The truss and tendon elements are assumed to have constant area. The tendon element cannot be used in geometrically nonlinear analyses. The membrane element can have from 4 to 8 nodes and the general three-dimensional isoparametric element from 8 to 21.

6. **TIMING** - A problem with 10,569 equations and a half bandwidth of 532 required 2750 CPU seconds on a CDC7600. The longest running sample problem requires about 670 CPU seconds on a CDC7600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Time-independent and time-dependent concrete constitutive relations are available, and a reinforced concrete material model which allows for concrete cracking is included.

8. **RELATED AND AUXILIARY SOFTWARE** - NONSAP-C is based on the NONlinear Stress Analysis Program, NONSAP (reference 2). A companion code, INGEN (NESC 975), which is a general-purpose two- and three-dimensional mesh generator for use with finite element programs, can serve as a preprocessor for NONSAP-C. MOVIE.LASL, which is a LANL interactive graphics program for display of finite element models and results of finite-element analysis programs, can serve as a postprocessor.

9. **STATUS** - Abstract first distributed April 1982.
   CDC7600 version submitted December 1978, revised October 1981, sample problems executed by NESC February 1982 on a CDC7600.

10. **REFERENCES** - C. A. Anderson, P. D. Smith, and L. M. Carruthers, NONSAP-C: A Nonlinear Stress Analysis Program for Concrete Containments Under Static, Dynamic, and Long-Term Loadings, NUREG/CR-0416 (LA-7496-MS Rev. 1), January 1982.
   K. J. Bathe, E. L. Wilson, and R. H. Iding, NONSAP-A Structural Analysis Program for Static and Dynamic Response of Nonlinear Systems, UC-SESM-74-3, February 1974.
   P. D. Smith, W. A. Cook, and C. A. Anderson, Finite Element Analysis of Prestressed Concrete Reactor Vessels, Paper H2/5, 4th International Conference on Structural Mechanics in Reactor Technology, San Francisco, California, August 1977.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Use of the CDC FTN co
options, ROUND and OPT=2 is recommended.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
W. A. Cook
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source (4234 lines)
Sample problems (1191 lines)
Sample problems output (33 selected pages)
Reference report, LA-9402-MS

17. **CATEGORY** - P
KEYWORDS - mesh generation, finite element method, interpolation, QMESH codes, SLIC c
NONSAP codes, ADINA codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research
DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - SLUMB.REV0
   SLUMB.REV0, 1-d Schlumberger inversion program

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - UNIVAC1108,1100

3. **DESCRIPTION** - SLUMB accepts field data from a Schlumberger resistivity array and inverts it in terms of a one-dimensional layered geoelectrical model. Because the inverse problem is nonlinear, an initial guess model is required; this can be obtained by traditional curve matching or by repeated use of the forward algorithm.

4. **METHOD OF SOLUTION** - The inversion of geophysical field data involves two steps. The first step is solving the forward problem, i.e. calculating the response of an assumed model. In this step, the potential integral is approximated by a finite sum using a 61-point filter. If increased accuracy is needed for larger resistivity contrasts, a 436-point filter is provided.
   The second step is the inverse problem, which is the mathematical adjustment of the model so that the response fits the field data. The inversion technique used is ridge regression.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - NESC compiled the program and executed the sample problems in 122 CP seconds on a UNIVAC1100/44.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - SLUMB is interactive and provides graphic displays of the data. SLUMB also provides for including the effects of finite MN spacing by calculating the theoretical apparent resistivity from the two potentials at M and N. This makes the forward problem twice as time-consuming computationally, but allows greater versatility during field measurements. MN may be extended larger than AB/5 in order to take advantage of increased voltage levels.

8. **RELATED AND AUXILIARY SOFTWARE** - SLUMB was originally developed in 1976 by Luiz Rijo.

9. **STATUS** - Abstract first distributed August 1982.
   UNIVAC1108 version submitted December 1980, sample problems executed by NESC March 1982 on an UNIVAC1100/44.

10. **REFERENCES** - Stewart Sandberg, Documentation and Analysis of the Schlumberger Interactive 1-D Inversion Program SLUMB, IDO/DOE/ET27002-2, September 1979.
    L. Rijo, W. H. Pelton, E. C. Feitosa, and S. H. Ward, Interpretation of Apparent Resistivity Data from Apodi Valley, Rio Grande Do Norte, Brazil, Geophysics, Vol. 42, pp. 811-822, 1977.

11. **HARDWARE REQUIREMENTS** - 22,000 words of memory are required for execution. Unit 3 is used as an alternate print file.

12. **PROGRAMMING LANGUAGE** - FORTRAN V (99%) and Assembler (1%)

13. **OPERATING SYSTEM** - EXEC8.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - SLUMB makes use of the FORTRAN V PARAMETER statement. The program frequently calculates floating-point values too small to be represented correctly in a 36-bit UNIVAC word. An EXEC8 option sets the offending values to zero and execution continues. If underflow suppression is not available, DOUBLE PRECISION may be necessary.
    SLUMB may be compiled with either the UNIVAC T3 (FOR) or ASCII (FTN) compiler. Element F2FRT, which is written in assembly language, is included for use with the FTN compiler to define unit 3 as an alternate print file. When using the FOR compiler, an appropriate NTAB$ routine should be provided.

SLUMB calls ICSSCU, a spline curve smoothing routine from the proprietary International Mathematical and Statistical Library (IMSL), and routines from Tektronix's proprietary PLOT10 graphics package to produce graphical output. The NESC provided dummy replacement routines for the missing PLOT10 routines: BELL, CHSYNC, DRAWA, DRAWR, ERASE, FINITT, INITT, MOVEA, SWINDO, TOUTPT, and VWINDO. If PLOT10 and IMSL routines are not available, suitable alternatives for the local environment are required to obtain graphic output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

T. Killpack
Earth Science Laboratory
University of Utah Research Institute

16. **MATERIAL AVAILABLE -**

Source (FORTRAN 988 lines, Assembler 7 lines)
Sample problems (28 lines)
Library data (436-point filter 218 lines)
Reference report, IDO/DOE/ET27002-2

17. **CATEGORY** - R
KEYWORDS - geophysical surveys, geothermal energy, resistivity logging, electric potential, experimental data

18. **SPONSOR** - DOE Division of Geothermal Energy

IDENTIFICATION AND KWIC TITLE - ASPEN
ASPEN, advanced system for process engineering

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370,303x, DEC VAX11/780

DESCRIPTION - ASPEN (Advanced System for Process Engineering) is a state-of-the-art process simulator and economic evaluation package which was designed for use in engineering fossil energy conversion processes. ASPEN can represent multiphase streams including solids, and handle complex substances such as coal. The system can perform steady-state material and energy balances, determine equipment size and cost, and carry out preliminary economic evaluations. It is supported by a comprehensive physical property system for computation of major properties such as enthalpy, entropy, free energy, molar volume, equilibrium ratio, fugacity coefficient, viscosity, thermal conductivity, and diffusion coefficient for specified phase conditions - vapor, liquid, or solid. The properties may be computed for pure components, mixtures, or components in a mixture, as appropriate. The ASPEN Input Language is oriented towards process engineers.

METHOD OF SOLUTION - ASPEN uses a preprocessor type of structure that generates a main calling program from a user input file in the ASPEN Input Language. The major sections and flow of information in the ASPEN program are as follows. The input translator processes the user input file, enters all data regarding the process into a problem data file, and generates the main FORTRAN program containing the necessary model calls. A physical property initialization subprogram, which depends on the property models used in the simulation, is generated also. These programs are then compiled and linked with user program and ASPEN libraries to create a custom simulation program for the problem. The simulation program reads input data from the problem data file and after performing any calculations required writes a new problem data file if necessary. The system report writer can then be used to produce reports from this file. ASPEN is a file-oriented system. Executive programs written in the machine's operating system language control the execution of the various programs and the creation and selection of files used.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING - Execution time is entirely dependent on the simulation to be performed. NESC executed the sample problems in less than 2 CPU minutes on an IBM3033 under VM/CMS and in 200 CPU seconds on an IBM3033 under OS. The longest running sample problem requires approximately 8 CPU minutes on a DEC VAX11/780.

UNUSUAL FEATURES OF THE SOFTWARE - ASPEN utilizes a plex data structure. Information is stored in blocks of contiguous locations. These are created dynamically from a pool of free storage. They may be of any length and may contain integer values, real values, or character strings. The plex-handling capability is provided by a group of subroutines called the Data Management System.

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed August 1982.
IBM3033 CMS version submitted January 1982, replaced May 1983 by revised Edition B, replaced October 1984 by revised Edition C, sample problems executed by NESC July 1984 on an IBM3033 under the VM/CMS operating system.
IBM370 OS version submitted January 1982, replaced October 1984 by revised Edition B, sample problems executed by NESC August 1984 on an IBM3033 under the MVS operating system.
DEC VAX11/780 VMS version submitted February 1982, revised May 1982, replaced by Edition B February 1983, replaced by Edition C February 1985, sample problems executed by NESC December 1984 on a DEC VAX11/780.

REFERENCES - ASPEN User Manual - Volumes 1 and 2, Massachusetts Institute of Technology, DOE/MC/16481-1203, May 1982.

ASPEN System Administrator Manual - Volumes 1 and 2, Massachusetts Institute of Technology, DOE/MC/16481-1201, May 1982.

ASPEN Technical Reference Manual - Volumes 1 and 2, Massachusetts Institute of Technology, DOE/MC/16481-1202, May 1982.

ASPEN/CMS Installation Manual, Massachusetts Institute of Technology, November 1, 1981.

ASPEN IBM/OS Installation Manual, Massachusetts Institute of Technology, November 1, 1981, revised October 1984.

K. E. Williams, VAX/ASPEN Installation Guide, DOE/METC/85-8, November 1984.

K. E. Williams and P. A. Regenhardt, METC VAX/IBM Guide to ASPEN, DOE/METC/85-9, November 1984.

ASPEN, NESC No. 979.3033, ASPEN IBM CMS Version Tape Description and Information on Supplementary Material (NESC EXECs), National Energy Software Center Note 82-94, August 23, 1982.

ASPEN, NESC No. 979.370B, ASPEN IBM OS Version Tape Description and Implementation Information, National Energy Software Center Note 85-09, October 8, 1984.

ASPEN, NESC No. 979.VX11C, ASPEN VAX/VMS Version Tape Description, National Energy Software Center Note 85-49, February 4, 1985.

11. **HARDWARE REQUIREMENTS** - The IBM CMS and OS transmittal tapes are recorded at 6250 bpi. The IBM version CMS edition requires approximately 200 cylinders of IBM3350 or equivalent disk storage for the ASPEN system account, using three minidisks of 115, 30, and 35 cylinders, respectively, on an IBM3350 or equivalent disk drive and 2 megabytes of storage. In addition, 5 cylinders of IBM3350 or equivalent disk storage and 2 megabytes of virtual storage are needed for each user account. The IBM version OS edition requires approximately 150 cylinders of IBM3350 or equivalent disk storage and the ability to execute programs requiring a 1650K byte region.

    The DEC VAX version requires approximately 210K blocks of disk storage and a paging file quota of 16,362 for the system account and 20K blocks of disk storage with an overdraft of 20K blocks, a file open quota of 40, and a paging file quota of 8,192 (4 megabytes virtual machine size) for each user account.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (99%) and Assembly language (1%) for the IBM versions. All of ASPEN except easily replaceable system utilities is written in ANS FORTRAN X3.9-1966. The DEC VAX version is written in FORTRAN 77.

13. **OPERATING SYSTEM** - VM/CMS (IBM303x), VMS 3.0,3.1,3.7 (DEC VAX11/780), OS (IBM370), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Reduced minidisk storage can be utilized after installation of the IBM CMS version of ASPEN. The FORTRAN files occupy 36,160 blocks, or 44% of the space requirements, and the sample problems occupy 1780 blocks, or 2%. There are 2347 CMS files of which 1507 are of type FORTRAN. Three separate TAPE LOAD commands bring in the information to minidisks A, D, and E. The supplementary NESC information can go to any minidisk. The space occupied by the A, D, E, and supplementary information is 12,476, 4536, 2263, and 62 blocks, respectively. The maximum block length is 4101. The IBM CMS version requires 5 cylinders minidisk (3350 storage) and virtual machine size of 2.5 megabytes for each user account.

    The FORTRAN source and sample output files of the IBM version OS edition occupy 29 and 15 megabytes of storage, respectively.

    The DEC VAX version contains 1857 files of which 1679 are of type FOR (FORTRAN). The remainder are of types INP, DAT, COM, DOC, INF, TMP, MSG, MAR, PG, SPL, OUT, SMP, XRF, and HLP. These files are either used during system generation or represent output files generated by the system for use in checking for correct implementation. The command procedures (COM files) are designed for use with VAX/VMS version 3.0 or later. The DEC VAX version contains the ASPEN Graphics System. This system uses calls to subroutines to generate actual terminal control sequences rather than formal meta code. While eliminating the need for a separate device driver for each different device, this necessitates editing of some of the code for addition of new devices. The devices currently supported are: Tektronix 401x, 411x, 410x, and 4027; AED767; SELANAR adapted VT-100; ZETA11 and 34 plotters, and the Varian printer-plotter.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
R. A. Bajura
Process Technology and Engineering Branch
Morgantown Energy Technology Center

16. **MATERIAL AVAILABLE -**
Source (IBM CMS 354,802 lines in CMS format, IBM OS 361,067 lines, DEC VAX 445,599 lines)
Reference reports, Manuals, Guide, Handbook, and NESC Note, appropriate to version

17. **CATEGORY -** U
KEYWORDS - processing, computerized simulation, flowsheets, engineering, economic analysis, multiphase flow, chemical reactions

18. **SPONSOR -** DOE Office of Fossil Energy

IDENTIFICATION AND KWIC TITLE - BENDPAC
BENDPAC, stress analysis of flanged pipe bends

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM303x,370

DESCRIPTION - BENDPAC is a package of seven programs designed to calculate the following:

(a) stresses and deflections in pipe bends terminated by flanges, infinitely long tangent pipes, or short equal length flange-ended tangents when under pressure (PRESEF) or pure in-plane bending (BENDEF);

(b) stresses in flange-ended pipe bends from in-plane end loading other than pure bending (SHEREF), coil spring type out-of-plane loading (COILEF), or any other type of out-of-plane loading (TURNEF); and

(c) flexibility matrices for flange-ended pipe bends for any in-plane end loading (FLEXIN) or out-of-plane end loading (FLEXOT).

METHOD OF SOLUTION - Linear thin shell theory is used, and eigenloads diffuse along the tangent and curved pipes from the flange and the curve-straight junction. The interaction of junction effects from opposite ends of the curved pipe and the interaction of junction and flange effects from opposite ends of each tangent are accommodated.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Wall thickness should not exceed 0.3 of the pipe radius. All variables are expressed as truncated trigonometric series with a maximum of 16 terms.

TIMING - Executing BENDEF on an IBM3033, the running time may vary from 6 CPU seconds when using 4 trigonometric series terms to almost 3 CPU minutes for 16 terms. Typical running time for 8 terms is 22 seconds. NESC executed the sample problem, which exercises all seven programs, using 4 series terms, in 21 CPU seconds on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed August 1982.
IBM3033 version of BENDEF,PRESEF submitted March 1982, replaced August 1982 by BENDPAC, replaced May 1983 by revised Edition B, sample problem executed by NESC April 1983 on an IBM3033.

REFERENCES -
J. F. Whatham, The Use of Computer Codes BENDEF and PRESEF, AAEC/M98, July 1981, amended June 1982.

J. F. Whatham, The Use of Computer Codes FLEXIN and FLEXOT, AAEC/M99, January 1982, amended June 1982.

J. F. Whatham, The Use of Computer Codes SHEREF, COILEF, and TURNEF, AAEC/M100, March 1982, amended June 1982.

BENDPAC, NESC No. 980.3033B, BENDPAC Tape Description, National Energy Software Center Note 83-55, April 14, 1983.

J. F. Whatham and J. J. Thompson, The Bending and Pressurizing of Pipe Bends with Flanged Tangents, Nuclear Engineering and Design, Vol. 54, pp. 17-28, 1979.

M. J. Hopper, Harwell Subroutine Library Report, AERE-R7477, 1973.

HARDWARE REQUIREMENTS - 380K bytes of memory are required to compile and execute the programs.

PROGRAMMING LANGUAGE - FORTRAN IV (93%) and Assembly language (7%)

OPERATING SYSTEM - MVS and OS/MVT.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS –** BENDPAC uses subroutines EB06AD, EB08AD, FM02AD, MC03AD, MC14AD, and MC15AD from the U.K.A.E.A. Harwell Subroutine Library. These routines, included as part of the package with Harwell's permission, are not in the public domain and extraction for other use is not permitted. Subroutines FM02AD, MC03AD, SIDCOM, DSID, and DARRAY are written in Basic Assembly Language (BAL).

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

J. F. Whatham
Australian Atomic Energy Commission
Australia

16. **MATERIAL AVAILABLE –**
    Source (FORTRAN 6772 lines, BAL 530 lines)
    Sample problem (53 lines)
    Control information (JCL 75 lines)
    Sample problem output (29 pages)
    Reference reports, AAEC/M98, AAEC/M99, AAEC/M100, and NESC Note

17. **CATEGORY –** I
    KEYWORDS – stress analysis, pipes, pipe joints, bending, flanges, strains, flexibility, BENDEF codes, PRESEF codes, SHEREF codes, COILEF codes, TURNEF codes, FLEXIN codes, FLEXOT codes

18. **SPONSOR –** Australian Atomic Energy Commission

IDENTIFICATION AND KWIC TITLE - EGUN
EGUN, calculation of electron trajectories

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370,303x,3081

DESCRIPTION - EGUN, the SLAC Electron Trajectory Program, computes trajectories of charged particles in electrostatic and magnetostatic focusing systems including the effects of space charge and self-magnetic fields. Starting options include Child's Law conditions on cathodes of various shapes, user-specified initial conditions for each ray, and a combination of Child's Law conditions and user specifications. Either rectangular or cylindrically symmetric geometry may be used. Magnetic fields may be specified using arbitrary configuration of coils, or the output of a magnet program, such as Poisson, or by an externally calculated array of the axial fields.

METHOD OF SOLUTION - The program first solves Laplace's equation. Next, the first iteration of electron trajectories is started using one of the four starting options. On the first iteration cycle, space charge forces are calculated from the assumption of paraxial flow. As the rays are traced, space charge is computed and stored. After all the electron trajectories have been calculated, the program begins the second cycle by solving the Poisson equation with the space charge from the first iteration. Subsequent iteration cycles follow this pattern. The Poisson equation is solved by an alternate column relaxation technique known as the semi-iterative Chebyshev method. A fourth-order Runge-Kutta method is used to solve the relativistic differential equations of the trajectory calculations.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
9001 mesh points in a square mesh
300 mesh points in the axial direction
100 mesh points in the radial direction
101 potentials
51 rays
In cylindrical coordinates, the magnetic fields are axially symmetric. In rectangular coordinates, any orientation of a two-dimensional magnetic field is possible.

TIMING - Running times vary greatly with the problem and the computer. A typical problem runs on an IBM370/168 in from 0.5 to 2 minutes of CPU time. NESC executed the sample problem in 12 CPU seconds on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE - EGUN has special options for round beams in rectangular coordinates, heavy ion beams, image tubes, shadow grids, and dielectrics.

RELATED AND AUXILIARY SOFTWARE - An auxiliary plotting program is included with the package. EGUN supersedes the programs described in SLAC-51 and SLAC-166.

STATUS - Abstract first distributed June 1982.
IBM370 version submitted January 1982, sample problem executed by NESC June 1982 on an IBM3033 and IBM370/195.

REFERENCES - William B. Herrmannsfeldt, Electron Trajectory Program, SLAC-226, November 1979.

EGUN, NESC No. 983.370, EGUN Tape Description, National Energy Software Center Note 82-53, June 30, 1982.

W. B. Herrmannsfeldt, Numerical Design of Electron Guns and Space Charge Limited Transport Systems, SLAC-PUB-2631, October 1980.

Wm. B. Herrmannsfeldt, Poisson Equation Solving Program, SLAC-51, September 1965.

William B. Herrmannsfeldt, Electron Trajectory Program, SLAC-166, September 1973.

11. **HARDWARE REQUIREMENTS** - 450K bytes of memory and two direct-access devices (logical units 1 and 8) are required.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (99%) and Assembler (1%)

13. **OPERATING SYSTEM** - OS/MVS, OS/SVS, VM.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - EGUN uses the SLAC system routine, LEFT1, to determine the amount of CPU time remaining for job execution. This was not supplied. Use of LEFT1 is a nonessential option installed at the user's convenience in certain environments. NESC substituted a dummy subroutine LEFT1 and function ICLOCK for testing. Function ICLOCK is a Basic Assembly Language routine which calculates the elapsed CPU time. The sample plotting program included in the package uses the proprietary CalComp graphics library. Users will have to supply alternative timing and plotting routines suited to the local computing environment. Prospective new users of the program may contact the author to determine whether EGUN is appropriate for their intended applications.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

W. B. Herrmannsfeldt
Stanford Linear Accelerator Center
Stanford University

16. **MATERIAL AVAILABLE** -

Source (FORTRAN 3785 lines, BAL 92 lines)
Sample problem (94 lines)
Example plotting program (59 lines)
Control information (JCL 96 lines)
Sample problem output (31 pages, 4 plots)
Reference report, SLAC-226, and NESC Note

17. **CATEGORY** - V
KEYWORDS - accelerators, beam dynamics, beam transport, Dirichlet problem, finite difference method, ion beams, klystrons, Laplace equation, phase space, Poisson equation, r-z, x-y, electron beams

18. **SPONSOR** - DOE Office of High Energy and Nuclear Physics

1. **IDENTIFICATION AND KWIC TITLE** - XERROR
   XERROR, Fortran library error-handling package

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,6600,CYBER175 (designed to be machine-independent)

3. **DESCRIPTION** - XERROR is a collection of portable FORTRAN routines which serves as a central facility for processing error messages associated with errors occurring in libraries of FORTRAN routines. Two releases of XERROR are provided, one written in American National Standard X3.9-1966 FORTRAN and the other in American National Standard X3.9-1978 FORTRAN.

4. **METHOD OF SOLUTION** - An internal table of messages which have been reported is kept in several local arrays in a lower level routine. The performance of the package upon occurrence of an error is dependent on the contents of this internal message table and current values of certain user-adjustable flags (global variables), which are stored as local variables in a bottom level routine. Five routines are provided to set or clear global variables, and there are four routines which may be used to ascertain the current values of the global variables.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The internal message table is normally set to a maximum length of 10 messages.

6. **TIMING** - NESC executed the test programs in less than 1 CP second on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - XERROR has the ability to place a limit on the number of times any one message is printed, to request error messages to be printed on up to 5 logical units, and to provide a summary of the number of times each message has been printed. Four levels of message severity are available.

8. **RELATED AND AUXILIARY SOFTWARE** - XERROR is the error-handling package used with the SLATEC1.0 Mathematical Subroutine Library (NESC 820).

9. **STATUS** - Abstract first distributed August 1982.
   CDC7600 version submitted May 1982, sample problems executed by NESC June 1982 on a CDC CYBER175.

10. **REFERENCES** - Rondall E. Jones and David K. Kahaner, XERROR, The SLATEC Error-Handling Package, SAND82-0800, May 1982 (also published in Software-Practice and Experience, Vol. 13, pp. 251-257, 1983).
    XERROR, NESC No. 988, XERROR Tape Description, National Energy Software Center Note 82-102, August 20, 1982.
    P. A. Fox, A. D. Hall, and N. L. Schryer, The PORT Mathematical Subroutine Library, Association for Computing Machinery Transactions on Mathematical Software, Vol. 4, No. 2, pp. 104-106, June 1978.

11. **HARDWARE REQUIREMENTS** - 26,000 (octal) words of memory are required to execute XERROR with the test programs provided.

12. **PROGRAMMING LANGUAGE** - FORTRAN 66 and FORTRAN 77

13. **OPERATING SYSTEM** - NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Dummy routines are supplied for the missing FDUMP and XERABT utilities, which provide traceback and abort facilities in the Sandia computing environment. Suitable replacements for these routines will be required for the local computing environment.
    Each test program includes a simplified rendition of the Bell Laboratories' I1MACH routine to determine the few particular machine-specific constants needed by the XERROR package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

R. E. Jones
Division 2614
Sandia National Laboratories, Albuquerque
D. K. Kahaner
Scientific Computing Division 713
National Bureau of Standards

16. **MATERIAL AVAILABLE -**

Source (FORTRAN66 708 lines, FORTRAN77 647 lines)
Sample problems (FORTRAN66 101 lines, FORTRAN77 105 lines)
Sample problems output (FORTRAN66 8 pages, FORTRAN77 8pages)
Reference report, SAND82-0800, and NESC Note

17. **CATEGORY -** P
KEYWORDS - utility routines, libraries, data processing, FORTRAN

18. **SPONSOR -** Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - NCAR GRAPHICS
   NCAR GRAPHICS, graphics utilities and plot pkg

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Base, IBM303x,370

3. **DESCRIPTION** - The NCAR GRAPHICS software package includes plotting utilities for generating graphs, labels, contour plots, surface plots, 3-D projections, streamline plots, vector field plots, and maps. Locally implemented support routines (primitives) must be supplied by the user for the portable Base version which requires tailoring to the local computing environment. Several data files are provided in card-image form together with a portable program for converting these into binary files. These include two character font digitizations (Complex and Duplex) for the highest quality characters and continental and U. S. outline data for drawing maps in various projections.

4. **METHOD OF SOLUTION** - High-level utilities call lower-level routines in a system plot package that produces device-independent plotting instructions (metacode) for driving any actual graphics device. This requires that the implementer write a metacode translator. Two portable translators are provided with the package to aid in this task. One produces low resolution character plots for a printer; the other is a 'shell' in which the user sets a number of constants pertaining to the host processor and target graphics device, which provide a minimal interface to the intended graphics device.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The utilities are written with variable-dimensioned arrays, so there are no inherent restrictions on the size of the fields to be plotted. An internal workspace in several of the contouring routines may be exhausted if complex contours with a very large number of levels are attempted.

6. **TIMING** - Running times vary with the utility used.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Several of the utilities have multiple versions that provide a choice between fast, low-quality plots or high-quality plots that require more computer time. In the Base version, the basic system plot package which provides the low-level primitives used by all of the utilities is contained in a file named PLOT.m.n, where m and n are small integers that designate a version for a computer with m characters per default type INTEGER word and n bits per character.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed October 1982.
   Base version submitted January 1981.
   IBM3033 version derived April 1982, sample problems executed by NESC August 1982 on an IBM3033.

10. **REFERENCES** - Gregory R. McArthur, Ed., The Graphics System Implementor's Guide, NCAR Technical Note NCAR/TN-165+IA, February 1981.

Gregory R. McArthur, Ed., An Introduction to the SCD Graphics System, NCAR Technical Note NCAR/TN-161+IA, January 1981.

Gregory R. McArthur, Ed., The SCD Graphics Utilities, NCAR Technical Note NCAR-TN/166+IA, February 1981.

Gregory R. McArthur, Ed., Selected User Reference Papers, NCAR Technical Note NCAR/TN-174+IA, June 1981.

Gregory R. McArthur, Ed., The System Plot Package, NCAR Technical Note NCAR-TN/162+IA, January 1981.

NCAR GRAPHICS, NESC No. 993.BASE, NCAR GRAPHICS BASE Version Tape Description and Implementation Information, National Energy Software Center Note 83-02, October 12, 1982.

NCAR GRAPHICS, NESC No. 993.3033, NCAR GRAPHICS IBM Version Tape Description and Implementation Information, National Energy Software Center Note 83-03, October 12, 1982.

Thomas Wright, A Schizophrenic System Plot Package, Computer Graphics, Volume 9, No. 1, pp. 252-255, Spring 1975.

11. **HARDWARE REQUIREMENTS** - At least 16 bits per INTEGER type word are required to implement the system plot package. Some of the utilities require a relatively large amount of memory. For example, AUTOGRAPH, which contains routines to draw and annotate curves or families of curves, combined with DASHSMTH, which smooths the curves drawn by AUTOGRAPH, along with the routines they call from the system plot package require about 14,000 memory locations on a Cray1. The largest utility in the IBM3033 version required 360K bytes of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (BASE), FORTRAN IV (98%) and Assembler (2%) (IBM3033).

13. **OPERATING SYSTEM** - COS 1.08 (Cray1), OS/MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - To implement the Base version, 14 small support routines (primitives) must be provided. These routines isolate capabilities that cannot be easily provided in FORTRAN.

The basic system plot package and many of the utilities conform to a portable subset of the FORTRAN programming language standard, X3.9-1966, and have been verified by the Bell Laboratories PFORT verifier. A few of the utilities have not reached this stage of portability but are included, since the changes necessary to implement them on different computers are fairly minor.

Some of the utility packages that provide different versions share routine names, so that they cannot all be included in the same object library unless some of the names are changed.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

Base — T. Wright, D. Robertson, L. Henderson, F. Clare, J. Humbrecht, R. Ubelmesser, and D. Kennison
National Center for Atmospheric Research

3033 — L. R. Eyberger
National Energy Software Center
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -

Source (Base-77,752 lines, 3033-50,822 lines)
Sample problems (FORTRAN Base-3909 lines, 3033-3942 lines)
Library data (Base-12,091 lines, 3033-12,091 lines)
Auxiliary programs (Base-7708 lines, 3033-7763 lines)
Reference NCAR Technical Notes and NESC Note, as appropriate to version

17. **CATEGORY** - P
KEYWORDS - computer graphics, computer output devices, plotters, utility routines, maps, display devices

18. **SPONSOR** - National Center for Atmospheric Research,
Scientific Computing Division

IDENTIFICATION AND KWIC TITLE - WOOD4.VER2
WOOD4.VER2, economics of wood energy systems

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER175

DESCRIPTION - WOOD4 is designed as a tool for determining the financial feasibility of a wood energy system. The program makes a financial comparison between a wood energy system and any energy system fired with a conventional fuel, i.e., oil, gas, or coal. This comparison can be made for the replacement of an existing system or between two proposed systems. In either case, a set of input data defining the analysis to be performed, operating specifications for the boiler, fuel characteristics, and financial parameters for use in the calculations is required.

METHOD OF SOLUTION - Economic indicators are generated based on life cycle costs. The data included in the life cycle cost routine are the fixed and variable costs normally associated with this type of industrial investment. These data are initialized at the beginning of the program by 35 user-supplied input parameters. WOOD4.VER2 can handle different types of analysis, editing, and iteration procedures. The selection of these features allows the user to perform sensitivity analyses; to calculate estimated annual fuel consumption and annual fuel costs and produce a cash flow table with the cash payback period of the initial investment, the total investment, net present value, and internal rate of return; and to vary selected parameters for engineering design studies.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING - Less than 1 CPU second is generally required in batch mode; running time is highly user-dependent in interactive mode.

UNUSUAL FEATURES OF THE SOFTWARE - Although designed for interactive use, WOOD4 can also be used in batch mode.

RELATED AND AUXILIARY SOFTWARE - The original version of WOOD4 was developed as a joint project between SJEC, Inc. and the Engineering Experiment Station of the Georgia Institute of Technology, with the participation of Arthur Anderson and Company. It was based on earlier work done by the New England Regional Commission.

STATUS - Abstract first distributed October 1982.
CDC Cybernet Timesharing System version submitted March 1982.

REFERENCES - D. H. Gustashaw, Operations Procedures and User Instructions for Wood 4 Version 2, A Computer Program for Economic Analysis of Industrial Wood Energy Systems, Southern Solar Energy Center SSEC, Inc. Working Paper 044, August 1981.
WOOD4.VER2, NESC No. 994, WOOD4.VER2 Tape Description and Errata to SSEC 044 WP Reference Working Paper, National Energy Software Center Note 83-01, October 4, 1982.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - NOS 1.5 (CYBER175).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
D. H. Gustashaw
Southern Solar Energy Center, Inc.

MATERIAL AVAILABLE -
Source (1768 lines)
Sample problems (146 lines)
Reference working paper and NESC Note

17. **CATEGORY** - D
KEYWORDS - wood fuels, economics, energy systems, investment, life-cycle cost, payback period

18. **SPONSOR** - DOE Office of the Assistant Secretary for Conservation and Renewable Energy

1. **IDENTIFICATION AND KWIC TITLE -** HIDDEN
   HIDDEN, hidden surface processing algorithm

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC7600

3. **DESCRIPTION -** HIDDEN is a general purpose, hidden surface processing algorithm which allows the user to display data as a color grey level picture or as a line drawing. It also provides the facility to display three-dimensional contour plots. Input to the algorithm is in the form of edges linked together as polygons. Output is in the form of vectors for line-drawing displays or as segments of a raster line with intensity information.

4. **METHOD OF SOLUTION -** HIDDEN uses Watkin's visible surface algorithm which accepts convex or concave polygons as input. The coordinates for these polygons are in a left-handed coordinate system. Polygon clipping is performed to a frustrum of vision that opens out along the positive z-axis. The algorithm assumes that the eyepoint is located at the origin of the system. Three-dimensional polygons are projected onto a two-dimensional plane. The projection plane is then divided into horizontal raster lines, and the algorithm computes the visibility of the polygons, a raster line at a time. A segment (the portion of the raster line which intersects the polygon) is sorted and compared with other segments to see which are visible. Shading is accomplished via the Gourard smooth-shading technique.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -** To do contour plots, a current contour value and a delta contour value are included with the segment information. A simple calculation can then be performed to determine the x location of contour bands on the segment. When moving to the next scan line, a different location for the x values may be obtained. When these points are connected, a curved contour band is produced. This is a rather unique technique. Most contour plotting techniques draw straight lines across the face of a polygon. Thus, to approximate curves, they must either increase the number of polygons or apply curve fitting techniques.

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Abstract first distributed January 1983.
   CDC7600 version submitted August 1974, replaced by revised edition submitted December 1978.

10. **REFERENCES -** Michael J. Archuleta, Displaying Complex Three-Dimensional Objects, UCID-30057, Rev. 1, April 15, 1974, with modifications of December 16, 1974 and April 28, 1975.

    M. J. Archuleta, Hidden Surface Line Drawing Algorithm, University of Utah report, UTECH-CSC-72-121, June 1972.

    H. Gourard, Computer Display of Curved Surfaces, University of Utah report, UTECH-CSC-71-113, June 1971.

    G. S. Watkins, A Real Time Visible Surface Algorithm, University of Utah report, UTECH-CSC-70-101, June 1970.

    Edna Carpenter, Stanley V. Solbeck, and Karl Dusenbury, Livermore Timesharing System, Part 4: Library Files, Chapter 304: ORDERLIB Subroutine Library, LCSD-408, Edition 1 Revision 0, October 22, 1980.

    William S. Derby, John T. Engle, and Jeanne T. Martin, LRLTRAN Language Used with the CHAT and CIVIC Compilers, LCSD-302, Rev. 0, March 30, 1981.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** LRLTRAN (76%) and FORTRAN IV (24%)

13. **OPERATING SYSTEM -** LTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – The major portion of HIDDEN is written in the LRLTRAN language for the CHAT compiler. Lawrence Livermore National Library computing environment subroutines FRAME, LINE, SETLCH, FROST, EFBC, FTYPE, and ITYPE are not included in the HIDDEN package; however, documentation is provided for all of these routines except FTYPE and ITYPE. FTYPE converts binary floating-point variables to F-type ASCII data string output, and ITYPE converts binary integers to ASCII output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
M. J. Archuleta
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** –
Source (2514 lines)
Reference, UCID-30057 Rev. 1 with modifications, and Excerpts from LCSD-408

17. **CATEGORY** – P
KEYWORDS – computer graphics, diagrams, algorithms, computer output devices, display devices, three-dimensional, two-dimensional

18. **SPONSOR** – ERDA Division of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - REED
   REED, forecasting rural electric energy demand

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM303x,370

3. **DESCRIPTION** - REED is a nonlinear, simultaneous-equation econometric model developed to forecast annual electricity sales for Rural Electric Cooperatives by state and sector to the year 2000. The model contains submodels for residential, commercial, industrial, and irrigation sectors; is sensitive to economic, demographic, and climatic variables; provides detailed forecasts of electricity demand (kWh consumption) and price for 45 contiguous states; and has been validated over the sample period 1966-1977. The program supplies the forecasts for three scenarios - Mid-Price Case, Low-Price Case, and High-Price Case.

4. **METHOD OF SOLUTION** - Each sector is characterized by a pair of equations in which the quantity of electricity demanded and the average electricity price are endogenous. The irrigation submodel also includes a customer equation. The use of both demand and price equations controls the simultaneity problem which arises from the use of average price, derived from declining-block rate schedules, rather than marginal price. The demand equations and the irrigation-customer equation have a log-linear, Koyck distributed lag specification; the price equations are linear with quadratic terms.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - NESC executed the sample problem in less than 1 CPU second on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - REED is similar in structure to the State-Level Electricity Demand (SLED) forecasting model.

9. **STATUS** - Abstract first distributed January 1983.
   IBM3033 version submitted June 1982, sample problem executed by NESC September 1982 on an IBM370/195.

10. **REFERENCES** - Ruth J. Maddigan, Wen S. Chern, Colleen A. Gallagher, Brady D. Holcomb, and James C. Cobbs, The ORNL Rural Electric Energy Demand Forecasting Model, ORNL/TM-7863, September 1981.

Brady D. Holcomb and Colleen A. Gallagher, Program User's Manual, The ORNL Rural Electric Energy Demand Forecasting Model, ORNL Draft, May 1981.

REED, NESC No. 997, REED Tape Description, National Energy Software Center Note 83-34, October 7, 1982.

W. S. Chern, R. E. Just, B. D. Holcomb, and H. D. Nguyen, Regional Econometric Model for Forecasting Electricity Demand by Sector and by State, NUREG/CR-0250 (ORNL/NUREG-49), October 1978.

11. **HARDWARE REQUIREMENTS** - 230K bytes of memory are required for execution. The model library data is read from logical unit 9.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (94%) and Assembler language (6%)

13. **OPERATING SYSTEM** - OS-MVT and OS-MVS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Subroutine IDAY, which returns the current date, is written in Basic Assembler Language.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    W. S. Chern, C. G. Rizy, B. D. Holcomb, and
    R. J. Maddigan
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE –**
    Source (FORTRAN 964 lines, BAL 63 lines)
    Sample problem (4 lines)
    Model library data (5842 lines)
    Auxiliary data conversion programs (94 lines)
    REA database (200 lines)
    Control information (JCL 89 lines)
    Reference report, ORNL/TM-7863, Draft User's Manual, and NESC Note

17. **CATEGORY** – D
    KEYWORDS – energy demand, forecasting, rural areas, electric power, nonlinear probl
    energy accounting, energy consumption, US REA, SLED codes

18. **SPONSOR** – U. S. Department of Agriculture,
    Rural Electrification Administration

1. **IDENTIFICATION AND KWIC TITLE** - RABFIN,PARTS
   RABFIN,PARTS, gaseous effluent dose parameters

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - RABFIN calculates technical specification dose parameters for the noble gas portion of gaseous effluents from nuclear power plants. Finite noble gas doses from short-term (purge) releases are calculated; the output includes the finite plume air, total body, and skin doses. Corresponding dose quantities computed assuming semi-infinite exposure geometry are also presented for comparison purposes. PARTS calculates technical specification dose parameters for the iodine and particulate portions of gaseous effluents.

4. **METHOD OF SOLUTION** - RABFIN employs the atmospheric dispersion models of the XOQDOQ program and the dose integral routine of the U. S. Nuclear Regulatory Commission Regulatory Guide 1.109.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -

50 nuclides	(PARTS)
20 nuclides	(RABFIN)
14 wind speed classes	(RABFIN)
7 stability classes	(RABFIN)

   No provision is included to evaluate simultaneously multiple releases, e.g., a continuous and purge release. The user must run each case and carry out the addition.

6. **TIMING** - NESC executed the RABFIN and PARTS sample problems in 13 and 1 CP seconds, respectively, on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - RABFIN uses the atmospheric dispersion models incorporated in the XOQDOQ program (NESC 964).

9. **STATUS** - Abstract first distributed February 1983.
   CDC7600 version submitted January 1981, sample problems executed by NESC October 1982 on an CDC CYBER175.

10. **REFERENCES** - J. S. Boegli, R. R. Bellamy, W. L. Britz, and R. L. Waterfield, Preparation of Radiological Effluent Technical Specifications for Nuclear Power Plants, NUREG-0133, October 1978.

U. S. Nuclear Regulatory Commission, Office of Standards Development, Regulatory Guide 1.109, Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I, Revision 1, October 1977.

RABFIN,PARTS, NESC No. 998, RABFIN,PARTS Tape Description, National Energy Software Center Note 83-45, October 7, 1982.

11. **HARDWARE REQUIREMENTS** - RABFIN requires 22,000 (octal) words of memory for execution; PARTS requires 31,000 (octal) words.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

J. A. Shields
Division of Automatic Data Processing
U.S. Nuclear Regulatory Commission

16. **MATERIAL AVAILABLE** –
Source (RABFIN 793 lines, PARTS 394 lines)
Sample problems (RABFIN 59 lines, PARTS 193 lines)
Sample problems output (RABFIN 11 pages, PARTS 17 pages)
Reference reports and NESC Note

17. **CATEGORY** – R
KEYWORDS – radioactive effluents, nuclear power plants, gases, plumes, air, dispersio
body, skin, doses, specifications, XOQDOQ codes

18. **SPONSOR** – NRC Office of Nuclear Reactor Regulation

IDENTIFICATION AND KWIC TITLE - FAMREC
FAMREC, fuel assembly mechanical response code

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600

DESCRIPTION - The Fuel Assembly Mechanical REsponse Code (FAMREC) calculates the lateral mechanical response of a row of fuel assemblies while allowing for two types of nonlinearities. The first type is a geometric nonlinearity in the form of gaps between individual assemblies and between peripheral assemblies and a boundary wall. Impacting is monitored across the gaps. The second nonlinearity is the permanent deformation of the fuel assembly spacer grid to compressive loading.

METHOD OF SOLUTION - The response is calculated in the modal plane. The uncoupled differential equations are solved in closed form using Laplace transformations. The discrete displacements and velocities are then calculated and the gaps in the system monitored at each axial elevation for impacting. These impact forces are then applied statically at a given time-step, and equilibrium is found using a Gaussian elimination technique.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
3601 time-steps and forces
80 modes
30 applied forces
15 fuel assemblies
5 impact grids per assembly

TIMING - Running time is not only problem dependent, but also dependent on which of the three available impact calculation procedures is selected. A problem with 17 assembly rows and 5 grids per assembly for 1000 time-steps required 86 CP seconds and 155 PP seconds on a CDC CYBER173. The problem used the impact calculational procedure which falls in the middle as far as run time is concerned. NESC executed the sample problem in 54 CP seconds on a CDC7600.

UNUSUAL FEATURES OF THE SOFTWARE - FAMREC was generated as an audit tool including three different methods for calculating impact forces to allow three levels of estimation.

RELATED AND AUXILIARY SOFTWARE - Several of the subroutines in FAMREC are taken from the FORTRAN Matrix Analysis library (FORMA) developed at the Martin Marietta Corporation, Denver Division. The program uses the INEL-IGS graphics software for film-recorder plotting.

STATUS - Abstract first distributed February 1983.
CDC7600 version submitted July 1979, made available September 1982 on an "As Is" basis as NESC 9996, sample problem executed by NESC September 1982 on a CDC7600.

REFERENCES - R. L. Grubb, Pressurized Water Reactor Lateral Core Response Routine, FAMREC (Fuel Assembly Mechanical Response Code), NUREG/CR-1019, September 1979.
INEL-IGS, Idaho National Engineering Laboratory, Integrated Graphics System Programming Guide, Aerojet Nuclear Company Computer Science Center, March 1976.
R. L. Wohlen, Synthesis of Dynamic Systems Using FORMA - FORTRAN Matrix Analysis, Martin Marietta Corporation report MCR-71-75, May 1971.

HARDWARE REQUIREMENTS - 134,000 (octal) words of small core memory (SCM) and 166,000 (octal) words of large core memory (LCM) are required to execute the program.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - SCOPE 2.1.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – NESC supplied dummy routi for the missing INEL-IGS routines: EXITG, GRIDG, LABELG, LEGNDG, MODESG, MLTPLG, NUME OBJCTG, PAGEG, SEGMTG, SETSMG, SUBJEG, and TITLEG. Suitable alternative routines should supplied for the computing environment in which the program is to be implemented to obt graphical output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
R. L. Grubb
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** –
Source (2607 lines)
Sample problem (2825 lines)
Sample problem output (36 selected pages)
Reference report, NUREG/CR-1019, and Excerpts from INEL-IGS Programming Guide

17. **CATEGORY** – I
KEYWORDS – fuel elements, loss of coolant, elasticity, accidents, dynamic loads, mechani vibrations, nonlinear problems, impact shock, stresses, PWR reactors, FORMA codes

18. **SPONSOR** – NRC Office of Nuclear Reactor Regulation,
Division of Systems Safety

IDENTIFICATION AND KWIC TITLE - INDCEPT
INDCEPT, industrial boiler plant capital cost

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM303x,360,370

DESCRIPTION - The INDCEPT program provides conceptual, capital investment cost estimates for single- and multiple-unit industrial steam boiler plants. Boiler plant cost models are provided to reflect various types and sources of coal and alternate means of sulfur and particulate removal. Cost models are also included for low-Btu and medium-Btu coal gasification plants. Cost estimates can be made as a function of boiler type, size, location, and dates of construction or operation. The output includes a detailed breakdown of the estimate into direct and indirect costs.

METHOD OF SOLUTION - INDCEPT uses cost indices to adjust a reference cost model to the specific size, time, and location provided by the user.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Size scaling factors have a finite range of applicability off the reference size. An applicable range of 100 to 500 MBtu/h is suggested.

TIMING - The typical running time is less than 1 CPU second per case. NESC executed the sample problem in less than 1 CPU second on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - Two auxiliary programs, INDTAC and CONLAM, which are included in the INDCEPT package, initially process data which will be subsequently used by the INDCEPT program. The program is a spin-off of CONCEPT5 (NESC 498).

STATUS - Abstract first distributed January 1983.
IBM3033 version submitted September 1982, sample problem executed by NESC October 1982 on an IBM3033.

REFERENCES - H. I. Bowers, L. C. Fuller, C. R. Hudson, II, User's Manual for the INDCEPT Code for Estimating Industrial Steam Boiler Plant Capital Investment Costs, ORNL/TM-8146, September 1982.
INDCEPT, NESC No. 1000.3033, INDCEPT Tape Description and JCL for Sample Problem, January 27, 1983.

HARDWARE REQUIREMENTS - INDCEPT requires approximately 220K bytes of storage.

PROGRAMMING LANGUAGE - FORTRAN IV (98%) and assembly language (2%)

OPERATING SYSTEM - OS/MVS (IBM3033), OS/360,370 (IBM360,370).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - INDCEPT and INDTAC use an ORNL assembly language subroutine called IDAY to obtain the date of the run. The ORNL routine is included in the package but should be replaced with the equivalent subroutine for the local computing environment.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
H. I. Bowers and C. R. Hudson, II
Oak Ridge National Laboratory

MATERIAL AVAILABLE -
Source (INDCEPT 2010 lines, IDAY 63 lines)
Sample problem (1 line)
Auxiliary programs and data (INDTAC 679 lines, COMO 13,282 lines, CONLAM 484 lines, LAMA 3473 lines)
Sample problem output (16 pages)

17. **CATEGORY** - D
KEYWORDS - capitalized cost, industrial plants, boilers, coal gasification, investment, economics, CONCEPT codes, INDTAC codes, CONLAM codes

18. **SPONSOR** - DOE Morgantown Energy Technology Center

1. **IDENTIFICATION AND KWIC TITLE** - SCREEN
   SCREEN, identifying effective input variables

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM370,303x

3. **DESCRIPTION** - SCREEN is a statistical sensitivity analysis procedure for ranking input data of large computer codes in the order of sensitivity importance. The problem is to determine a group of the most important input parameters of a computer code when the total number of input variables is large, so large that standard sensitivity evaluations varying each input variable (one or two at a time) would be prohibitively expensive.

4. **METHOD OF SOLUTION** - SCREEN selects values for the input parameters of a deterministic computer program from input-specified regions of interest. The regions are defined by probability distributions and confidence intervals. The program arranges these input values into combinations called 'knot-points' that serve as input for the deterministic code that calculates the values of interesting output variables (consequences) for the specified knot-points.
   The output/consequence values for the knot-points are then used to determine (1) which input variables are most correlated with the output/consequence values, using stagewise correlation analysis, (2) which input variables are most likely to contribute to discontinuities or threshold effects in the output values, using statistical tests for subset characteristics, and (3) which group of input parameters yields the best significant regression model, using quadratic models and successive regression analyses with an increasing number of parameters. The regression part of SCREEN evaluates all regressions of two variables using the principle of stepwise regression analysis for a large number of variables. Both residual errors and special sensitivity/spuriousness indices can be used to select seed input variables for each step of the regression analysis. The significance of each added parameter of a model can be assessed by F-statistics for regression models. Student t-statistics and extreme value statistics are used for testing threshold effects.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   1000 input parameter variables
   6 output/consequence variables
   When selecting the cases to be run (knot-points), eight optional distributions are available for the input parameters, including uniform, exponential, normal, truncated normal, log-normal, and beta distributions.

6. **TIMING** - Running time depends strongly on the size of the problem, i.e., number of input parameters, knot-points, and the number of regression steps needed to complete the screening. For small problems where the number of input parameters and knot-points are both less than 50, the total running time is typically a few CPU seconds on an IBM370/195. Large problems, with approximately 500 input parameters and 50 knot-points, take several minutes of CPU time per consequence on an IBM370/195. NESC executed the sample problem in 2 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - Compared to other screening techniques available, SCREEN has the following somewhat unique features: (a) the values of the input parameters (knot-point coordinates) are selected from a continuous distribution rather than from discrete levels; (b) quadratic regression models rather than linear models are used; (c) the total number of input variables may be much larger than the number of cases and no prior elimination of variables by judgment is necessary; (d) the regression analysis in SCREEN is more extensive than the standard stepwise regression analysis procedure; and (e) extreme value and t-tests are used to identify parameters important to threshold (discontinuity) effects.

8. **RELATED AND AUXILIARY SOFTWARE** - The SCREEN code can be used in conjunction with any separate deterministic code (typically an accident-analysis code such as SAS3D) that provides data for screening. It can also be used to generate input data in the correct format for the response-surface analysis code PROSA2 (NESC 778).

9. **STATUS** - Abstract first distributed February 1983.
IBM370 version submitted December 1981, sample problem executed by NESC October 1982 on an IBM3033.

10. **REFERENCES** - J. K. Vaurio, Statistical Identification of Effective Input Variables, ANL-82-57, September 1982.
SCREEN, NESC No. 1002, SCREEN Tape Description, National Energy Software Center Note 83-48, October 15, 1982, revised April 24, 1984.
J. K. Vaurio, Response Surface Techniques Developed for Probabilistic Analysis of Accident Consequences, Proceedings of the American Nuclear Society Topical Meeting on Probabilistic Analysis of Nuclear Reactor Safety, Los Angeles, California, May 8-10, 1978.
J. K. Vaurio, Methods for Statistical Determination of Effective Input Variables, Transactions of the American Nuclear Society, Vol. 32, pp. 296-297, 1979.
J. K. Vaurio, Statistical Determination of Threshold Variables, Transactions of the American Nuclear Society, Vol. 35, pp. 263-264, 1980.

11. **HARDWARE REQUIREMENTS** - 250K bytes of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (93%) and Assembler language (7%).

13. **OPERATING SYSTEM** - OS/MVT, MVS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - SCREEN contains some FORMAT statements which use the T edit descriptor and READ statements which use the ERR= and END= error and end-of-file specifiers. Subroutines ABEND, ALLOC2, FLTRNF, FREE2, and LOC are written in Basic Assembly Language. FLTRNF, ALLOC2, and FREE2 are Argonne National Laboratory computing environment routines. The FLTRNF function statement U=FLTRNF(0) returns uniform random numbers U, between 0 and 1. Subroutines ALLOC2 and FREE2 dynamically allocate and release space for the arrays used in the regression analysis. Subroutine SASIN, which prepares input for an external deterministic code that calculates consequences, is to be supplied by the user. Versions of SASIN appropriate for the VENUS2 and SAS3D computer programs are included in the package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. K. Vaurio
Reactor Analysis and Safety Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 4570 lines, BAL 344 lines)
Sample problem (179 lines)
Auxiliary routine (SASIN 928 lines)
Reference report, ANL-82-57, and NESC Note

17. **CATEGORY** - G
KEYWORDS - accidents, regression analysis, correlations, probability, least square fit, randomness, risk assessment, safety, statistics, sensitivity analysis, VENUS2 codes, PROSA2 codes, SAS3D codes

18. **SPONSOR** - DOE Office of Breeder Technology Projects

1. **IDENTIFICATION AND KWIC TITLE** - WYLVAX
   WYLVAX, interactive line-oriented text editor

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - WYLVAX is an interactive, line-oriented, text editor which allows the user to create, modify, and correct text, and search and display it by submitting commands from a terminal. WYLVAX features include: an English-like grammar, a simple command syntax, yet complex commands can be formed quickly, and a powerful command language with the facility for conditional command submission.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maximum line length is 133 characters; long lines are truncated. Only positive integer line numbers less than or equal to 65,535 are allowed. The maximum number of lines in the text file is dependent upon the virtual storage available. Each line has an additional overhead of 8 bytes. Machines with very small meory may be impacted somewhat by many concurrent WYLVAX users.

6. **TIMING** - WYLVAX is invoked for an indefinite period. The terminal used is tied up for the length of an editing session. CPU usage depends on the activity of the user.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - In conjunction with the VMS operating system WYLVAX can manipulate very large files at high speed because of the virtual memory storage of the text file being edited.

8. **RELATED AND AUXILIARY SOFTWARE** - WYLVAX is syntactically compatible with the Stanford WYLBUR IBM system text editor.

9. **STATUS** - Abstract first distributed November 1982.
   DEC VAX11/780 version submitted January 1982, replaced by revised edition submitted August 1982, sample session executed by NESC October 1982 on a DEC VAX11/780.

10. **REFERENCES** - WYLVAX, NESC No. 1003, WYLVAX Tape Description and Implementation Information, National Energy Software Center Note 83-15, October 15, 1982.

11. **HARDWARE REQUIREMENTS** - The WYLVAX executable image requires 76,000 bytes of virtual storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN-77 (40%) and MACRO-11 (60%)

13. **OPERATING SYSTEM** - VMS 3.0.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The DISPLAY command, which returns the hexadecimal representation of its argument, lists the representation in reverse order.
    The WYLVAX transmittal tape is written in VMS COPY format for use with the DEC VAX computer and VMS operating system.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. A. Palmer
    Stanford Linear Accelerator Center

16. **MATERIAL AVAILABLE** -
    Source (FORTRAN 6097 lines, MACRO 10,092 lines)
    Libraries (MACRO 64 lines, HELP 2151 lines, TEXT 63 lines, OBJECT 169 blocks•)
    Executable image (43 blocks•)
    NESC Note
    • maximum block size = 2048 bytes

17. **CATEGORY** - P
KEYWORDS - utility routines, text editors, data processing, interactive display devices, WYLBUR codes

18. **SPONSOR** - DOE Office of Energy Research

1. **IDENTIFICATION AND KWIC TITLE** - RATAF
   RATAF, radioactive liquid tank failure study

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM370,303x

3. **DESCRIPTION** - RATAF calculates the consequences of radioactive liquid tank failures. In each of the processing systems considered, RATAF can calculate the tank isotopic concentrations in either the collector tank or the evaporator bottoms tank.

4. **METHOD OF SOLUTION** - The activity of the shim bleed wastes is based on the primary coolant letdown system effluent activity. Input activities are based on the weighted average activity of the composite stream entering the waste collection tanks. The tank factors provide the capability to consider radionuclide removal by demineralizers or other treatment equipment prior to the tank. For evaporator bottoms tanks, the tank factors provide the capability to consider the effects of radionuclide concentration in the evaporator.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maximum of -
   800 nuclides

6. **TIMING** - NESC executed the sample problem in 5 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - RATAF is based on the PWR-GALE and BWR-GALE computer programs.

9. **STATUS** - Abstract first distributed January 1983.
   IBM370 version submitted January 1981, sample problem executed by NESC October 1982 on an IBM3033.

10. **REFERENCES** - J. S. Boegli, R. R. Bellamy, W. L. Britz, and R. L. Waterfield, Preparation of Radiological Effluent Technical Specifications for Nuclear Power Plants, NUREG-0133, October 1978.

RATAF, NESC No. 1004, RATAF Tape Description and Sample Problem Input, National Energy Software Center Note 83-25, January 27, 1983.

F. P. Cardile and R. R. Bellamy, Ed., Calculation of Releases of Radioactive Materials in Gaseous Liquid Effluents from Boiling Water Reactors (BWR-GALE Code), NUREG-0016, Revision 1, January 1979.

Calculation of Releases of Radioactive Materials in Gaseous and Liquid Effluents from Pressurized Water Reactors (PWR-GALE Code), NUREG-0017, April 1976.

M. J. Bell, ORIGEN - The ORNL Isotope Generation and Depletion Code, ORNL-4628, May 1973.

11. **HARDWARE REQUIREMENTS** - 300K bytes of memory are required to execute the program.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS-MVT, OS-MVS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. A. Shields
Division of Automatic Data Processing
U.S. Nuclear Regulatory Commission

16. **MATERIAL AVAILABLE** -
   Source (1818 lines)
   Sample problem (35 lines)
   Nuclear library data (4065 lines)

Control information (JCL 67 lines)
Reference report, NUREG-0133, and NESC Note

17. **CATEGORY** - G
KEYWORDS - tanks, containers, failures, radioactive effluents, nuclear power plants, PWR-GALE codes, BWR-GALE codes

18. **SPONSOR** - NRC Office of Nuclear Reactor Regulation

1. **IDENTIFICATION AND KWIC TITLE** - MT3D.REV2
   MT3D.REV2, 3d magnetotelluric modeling program

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
PRIME400, DEC VAX11/780

3. **DESCRIPTION** - MT3D is a set of three programs for three-dimensional magnetotelluric (MT) modeling. The programs are used for modeling one or a few small bodies in a half space with vertical symmetry planes. The first program, MT3D.1, generates two block matrices which are used by the second program, MT3D.2, to calculate the fields within the body for both source field polarizations. The third program, MT3D.3, integrates over the fields in the body to obtain the scattered fields at the receiver sites.

4. **METHOD OF SOLUTION** - A three-dimensional volume integral equation solution has been adapted to simulate the MT response of a three-dimensional body in the earth. The body is replaced by polarization currents which depend on the difference between the conductivity of the body and that of the surrounding earth. The resulting volume integral equation is reduced to a matrix equation by the method of moments. After the matrix equation is solved for the polarization current, the electric and magnetic fields at the surface of the earth can be calculated using half space dyadic Green's functions.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   110 cells representing the body
   100 receiver positions
   1 half-space resistivity
   1 frequency
The body must have at least two planes of symmetry.

6. **TIMING** - Execution time depends on the size and complexity of the model. For large or complex models large amounts of CPU time are required. A model containing 2 cells at one frequency and one half-space resistivity with 5 surface receiver positions required 69 seconds of CPU time on a PRIME400 and 14 seconds of CPU time on a DEC VAX11/780.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - This release corrects an error in the calculation of horizontal secondary magnetic fields at the receivers for elongated bodies in the previous edition, and includes a more efficient generation of the system matrix.

9. **STATUS** - Abstract first distributed November 1982.
   PRIME400 version of MT3D.REV1 submitted December 1980, replaced by MT3D.REV2 submitted March 1982, made available October 1982 on an "As Is" basis as NESC 9991.
   DEC VAX11/780 version derived October 1982, sample problem executed by NESC October 1982 on a DEC VAX11/780.

10. **REFERENCES** - Carleen Nutter and Phillip E. Wannamaker, MT3D: A 3 Dimensional Magnetotelluric Modeling Program (User's Guide and Documentation for Rev. 1), DOE/ID/12079-20 (ESL 47), November 1980.

Carleen Nutter, UPDATE to MT3D Rev.1 Users Guide (ESL #47), Documentation for Version 2.0, ESL ##, February 1982.

MT3D.REV2, NESC No. 1005.400, MT3D.REV2 Tape Description, Implementation and Sample Problem Output Information, National Energy Software Center Note 83-17, October 28, 1982.

MT3D.REV2, NESC No. 1005.VX11, MT3D.REV2 Tape Description, Implementation and Sample Problem Output Information, National Energy Software Center Note 83-16, October 28, 1982.

G. W. Hohmann, Three-dimensional Induced Polarization and Electromagnetic Modeling, Geophysics, Vol. 40, pp. 309-324, 1975.

11. **HARDWARE REQUIREMENTS** - The largest program, MT3D.2, requires 576K 16-bit words of virtual storage on the PRIME400 and 901K bytes of virtual memory on the DEC VAX11/780. In addition, the programs require 10 sequential access files.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (PRIME400), FORTRAN77 (VAX11/780)

13. **OPERATING SYSTEM** - PRIMOS IV (PRIME400), VMS 3.0 (VAX11/780).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - With the PRIME400 version, the -BIG option on the FORTRAN compiler should be used to allow for large arrays spanning segment boundaries.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

400	G. W. Hohmann and P. E. Wannamaker Department of Geology and Geophysics University of Utah C. Nutter University of Utah Research Institute Earth Science Laboratory
VAX11	L. R. Eyberger National Energy Software Center Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    - Source (400-1761 lines, VX11-2044 lines)
    - Sample problem (400-8 lines, VX11-8 lines)
    - Library data (400-1200 88-character records, VX11-1200 88-character records)
    - Control information (400-80 lines)
    - Reference report, DOE/ID/12079-20 (ESL 47) and UPDATE, and NESC Note, as appropriate to version

17. **CATEGORY** - R
    KEYWORDS - three-dimensional, magnetotelluric surveys, electromagnetic fields, geothermal exploration

18. **SPONSOR** - DOE Division of Geothermal Energy

1. **IDENTIFICATION AND KWIC TITLE** - MAEROS
   MAEROS, multicomponent aerosol time evolution

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - MAEROS calculates aerosol composition and mass concentration as a function of particle size and time. The processes that may be considered are coagulation due to Brownian motion, gravity, and turbulence; particle deposition due to gravitational settling, diffusion, and thermophoresis; particle growth due to condensation of a gas, typically water vapor; and time-varying sources of particles of different sizes and chemical compositions.

4. **METHOD OF SOLUTION** - The numerical technique used is based upon dividing the particle size domain into m sections and imposing the condition of mass conservation for each chemical component for the processes considered. Aerosol mass concentrations are grouped into sections (i.e., size classes) for which an average composition is determined. For m sections, a set of 2m(m+2) sectional coefficients must be calculated before integrating in time. These coefficients are determined from the basic coagulation, condensation, and deposition coefficients. Since the sectional coefficients depend on the physical properties of the containment chamber (e.g., temperature, pressure, chamber volume, and deposition surface area), they will generally need to be recalculated for a particular application. However, for a given containment chamber, the sectional coefficients will probably vary only with temperature and pressure. Consequently, the code has been developed so that sectional coefficients are stored at a user-specified upper and lower bound for both temperature and pressure, and linear interpolation is used to determine the appropriate sectional coefficients for a given temperature and pressure. A Runge-Kutta-Fehlberg method is used to integrate in time.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   20 sections
   8 components
   50 rows for plotting
   101 columns for plotting
   MAEROS is limited to geometrically spaced sections in particle mass (i.e., v(m+1).GE.2v(m), where v(m) is the largest particle mass in section m).
   The code is also restricted to coagulation, deposition, and condensation mechanisms which are dependent only on particle mass, not on chemical composition. The source mechanisms may be both particle size and composition dependent.

6. **TIMING** - NESC ran the sample problem on a CDC CYBER175 in approximately 12 CPU seconds.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The program is set up to execute the sample problem without additional input. To solve other problems, the user is expected to modify the source code as explained in the NUREG/CR-1391 reference report.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed February 1983.
   CDC7600 version submitted October 1982, sample problem executed by NESC November 1982 on a CDC CYBER175.

10. **REFERENCES** - Fred Gelbard, MAEROS User Manual, NUREG/CR-1391, (SAND 80-0822), December 1982.

11. **HARDWARE REQUIREMENTS** - 55,100 (octal) words of memory

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE (CDC7600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**
K. K. Murata
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE –**
Source (2365 lines)
Reference report

17. **CATEGORY** – R
KEYWORDS – aerosols, deposition, flocculation, vapor condensation, chemical composition, diffusion, particle size, time dependence

18. **SPONSOR** – NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - FLOOD4
FLOOD4, PWR core reflood dynamics modeling

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER176,175

DESCRIPTION - FLOOD4 calculates the thermal-hydraulic performance of pressurized water reactors and reactor simulators during the core reflood phase of a postulated loss-of-coolant accident (LOCA). The program calculates the reflood rate and core temperature history, given the user-specified core power and peaking profiles, loop resistances, coolant injection rate, core and downcomer flow areas, and initial pressure.

METHOD OF SOLUTION - FLOOD4 uses a core fluid entrainment correlation which is not an explicit function of the core inlet flow rate. Liquid is entrained based on steam escaping from the boiling region. Vaporization of the liquid results in a pressurization of the core region and causes the liquid level in the downcomer to increase. The momentum equation includes inertial terms whereby the program can model the tendency of the liquid to oscillate back and forth between the downcomer and the core. The Hamming predictor-corrector method is used to solve for the water flow rate as it oscillates. Energy removal from the core is simulated by using heat transfer coefficient correlations which model the boiling curve. The pressure in the steam dome and loops is calculated from steam mass balances and use of the perfect gas approximation. Energy removal from the lower plenum and downcomer walls is considered, as well as entrainment and counter-current flow in the downcomer. Liquid carried from the core to the upper plenum is de-entrained and may fall back into the averaged power assemblies in the core at a rate controlled by counter-current flow relations, or it may be re-entrained and carried into the steam generators where it is vaporized. Emergency core cooling may be injected into the reactor vessel upper plenum, lower plenum, or cold leg pipes. The steam flowing in the pipes is specified to mix completely with any cooling water injected into the pipes. After the cooling water tanks are depleted, nitrogen gas injection may be specified. The effect of steam generator tube ruptures on the core thermal transient may also be calculated. The unsteady thermal energy radial conduction equation is solved by an implicit method, similar to Crank-Nicolson, but more flexible and stable.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
300 heat slabs (conduction regions) in the core
50 downcomer axial nodes
9 rod radial conduction regions
FLOOD4 has rather simple core heat transfer models and is not an accurate model in cases where steam superheating is large because of low liquid entrainment rates. Cross flow in the core is not considered for either up-flow or down-flow.

TIMING - Computer time is roughly one-ninth problem time. NESC executed the sample problem in 38 CP seconds on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - FLOOD1, an earlier release, was the first known computer program in the United States to calculate transient reflood rates.

STATUS - Abstract first distributed February 1983.
CDC CYBER176 version submitted August 1981, sample problem executed by NESC November 1982 on a CDC CYBER175.

REFERENCES - R. W. Shumway, Core Reflood Dynamics Code - FLOOD4, EGG-SEMI-5055, October 1979.
INEL-IGS Idaho National Engineering Laboratory Integrated Graphics System Programming Guide, Aerojet Nuclear Company, Computer Science Center, March 1976.
B. Carnahan, H. A. Luther, and J. D. Wilkes, Applied Numerical Methods, John Wiley and Sons, New York, New York, 1969.

11. **HARDWARE REQUIREMENTS** - 114,000 (octal) words of small core memory (SCM) and 121,000 (octal) words of large core memory (LCM) are required on the CDC CYBER176. 215,000 (octal) words of SCM are required on the CDC CYBER175.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS/BE 1.4 (CDC CYBER176), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - NESC supplied dummy routines for the missing INEL Integrated Graphics System (IGS) routines: MODESG, SUBJEG, OBJCTG, SETSMG, RSETMG, PAGEG, EXITG, LINESG, POINTG, GRIDG, LABELG, TITLEG, and SETUPG. Suitable alternatives should be supplied for the computing environment in which the program is implemented to obtain graphical output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. W. Shumway
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
Source (3149 lines)
Sample problem (83 lines)
Sample problem output (28 selected pages)
Reference report, EGG-SEMI-5055, and Excerpts from INEL-IGS Programming Guide

17. **CATEGORY** - H
KEYWORDS - accidents, core flooding systems, fluid flow, loss of coolant, reactor cores, hydrodynamics, PWR reactors, FLOOD1 codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Reactor Safety Research

IDENTIFICATION AND KWIC TITLE - FORCED VIBRATION TEST DATA
FORCED VIBRATION TEST DATA, ANCO KFK HDR tests

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370,303x

DESCRIPTION - A series of intermediate and high-level forced vibration tests were conducted at the Heissdampfreaktor (HDR), a decommissioned, superheated steam nuclear reactor in the Federal Republic of West Germany.

The overall purpose of the HDR test program was to obtain benchmark dynamic properties of the containment and piping systems which would serve to validate analytical and computer methods of structural analysis.

METHOD OF SOLUTION - Forced Vibration tests using eccentric mass vibrator, snapback (hydraulic rams), solid propellant rockets, and buried explosive charges were conducted. The HDR containment structure, primary recirculating piping system, reactor pressure vessel, experimental piping system, and a flood water storage tank were tested under various conditions and the responses monitored. Applied forces, accelerations, displacements, velocities, and strain levels were measured via computer-based data acquisition systems supporting over 230 transducers.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed January 1983.
IBM-compatible tapes submitted June 1981.

REFERENCES - Intermediate and High Level Forced Vibration Tests at the Heissdampfreaktor (HDR), Volume I: Test Report, Revision 1.0, ANCO Final Report 1083-10R, June 1980.
FORCED VIBRATION TEST DATA, NESC No. S1008.370, Description of FORCED VIBRATION TEST DATA Tapes, National Energy Software Center Note 83-35, December 16, 1982.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE -

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
M. G. Srinivasan
Components Technology Division
Argonne National Laboratory

MATERIAL AVAILABLE - Special Distribution (4 tapes)
EBCDIC data (1,222,280 80-character records)

CATEGORY - Z
KEYWORDS - data, nuclear power plants, testing, mechanical vibrations, rockets, explosives, containment systems, pipes, pressure vessels

SPONSOR - NRC Office of Nuclear Regulatory Research

IDENTIFICATION AND KWIC TITLE - SAMPLE TRANSACTION SYSTEM
SAMPLE TRANSACTION SYSTEM, analytical chemists

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC10,20

DESCRIPTION - The SAMPLE TRANSACTION SYSTEM is a set of computer programs developed for use by an analytical chemistry laboratory and its customers. The functions performed include sample management, timekeeping, quality assurance, and data calculation. Sample management tasks log, track, and report customer requests for work. Interactive file maintenance and information retrieval programs and batch programs for some maintenance and reporting functions are included. Interactive work request submission and inquiry programs and batch report and maintenance programs provide customers access to the laboratory's online data files. Timekeeping programs record and bill labor costs incurred as a result of customer work request processing; they also maintain and reference files of valid charge numbers and expected completion times for certain types of work. Quality assurance programs aid in verifying the accuracy of analytical tests performed on customer samples by comparing them to the same analysis performed simultaneously on a control sample. The timekeeping and data calculation programs which pertained specifically to the Oak Ridge environment are not included in the package. The package includes sample management programs: FILEUP, LOOKUP, ACDENQ, LISTER, BAKLOG, CHKFIL, PRECLN, CLENUP, UNCALL, RECALL, ANALUP, ENQUIR, CTFILE, CTDBAK, CMDIN, and quality assurance programs: CNTLIN, CONBAT, MANINQ, SUPV, and TECHN.

METHOD OF SOLUTION - The system's interactive programs are designed to prompt the user for information and to check each response for validity.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed January 1983.
DEC10 version submitted November 1979, replaced January 1983 by revised edition submitted September 1982, compiled by NESC November 1982 on a DEC20.

REFERENCES - J. S. Stanton and P. A. Tilson, Analytical Chemistry Division's Sample Transaction System, ORNL/CSD/TM-81, October 1980.
SAMPLE TRANSACTION SYSTEM, NESC No. 1009, SAMPLE TRANSACTION SYSTEM Tape Description and Implementation Information, National Energy Software Center Note 83-36, December 14, 1982.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - COBOL 68 (99%), Assembler language (1%)

OPERATING SYSTEM - TOPS10 (DEC10), TOPS20 (DEC20).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - CMDIN, A, and S are assembler language routines. LOOKUP uses the CMDIN subprogram. FILEUP, LOOKUP, and ACDENQ can be executed directly or can be called using the S macro program. CTFILE and ENQUIR can be executed directly or can be called using the A macro program.

Control information for batch jobs run at Oak Ridge National Laboratory to produce daily reports and reorganize the ISAM files is included in the package. The timekeeping programs, ANLIZE, BILLING, and CARDS, and the data calculation program, DISTIU, which were not supplied with the package should be replaced with alternatives suitable for the local environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
J. S. Stanton and P. A. Tilson
Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE** –
Source (FILEUP 3786 lines, CTFILE 2309 lines, CNTLIN 935 lines, TECHN 552 lines, LOOKUP 1822 lines, ENQUIR 1041 lines, LISTER 1335 lines, BAKLOG 582 lines, PRECLN 226 lines, CLENUP 419 lines, UNCALL 326 lines, RECALL 367 lines, CHKFIL 365 lines, CONBAT 525 lines, SUPV 499 lines, MANINQ 1861 lines, ACDENQ 1031 lines, CTDBAK 583 lines, ANALUP 609 lines, A 63 lines, S 141 lines, CMDIN 67 lines)
Control information (DAILY1 118 lines, DAILY2 101 lines, DAILY3 101 lines, DAILY4 101 lines, DAILY5 101 lines, DAILY6 96 lines, DAILY7 171 lines, LISTER 46 lines)
Reference report, ORNL/CSD/TM-81, and NESC Note

17. **CATEGORY** – M
KEYWORDS – chemical analysis, quality assurance, information retrieval, interactive computing

18. **SPONSOR** – Oak Ridge National Laboratory,
Analytical Chemistry Division and Chemical Technology Division

IDENTIFICATION AND KWIC TITLE - COGAP
COGAP, nuclear containment H2 control system

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175

DESCRIPTION - COGAP evaluates nuclear power plant containment hydrogen control systems by determining the node (compartment) concentrations of hydrogen, oxygen, nitrogen, and steam, assumed to be ideal gases. The nodes are assumed to be homogeneous and in chemical equilibrium, that is, lumped-parameter nodes. Effects accounted for include: reaction of zirconium and water; radiolysis of core and sump water; corrosion of zinc, aluminum, and copper; recirculation between compartments; hydrogen recombiners; purging; nitrogen addition; and atmospheric steam. Controls are available to determine when options are initiated, e.g., hydrogen recombiners can be started when the hydrogen concentration reaches a user-specified value or after a user-specified time.

METHOD OF SOLUTION - Nodal gas content accounting is determined explicitly, based on addition, removal, or transport of constituents resulting from the effects considered.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
20 hydrogen recombiner connections
20 connections between compartments for recirculation
10 corrosion surfaces
5 compartments

TIMING - The sample problem, which includes two cases, requires about 6 CP seconds on a CDC7600 and 16 CP seconds on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - COGAP is a modification of the COGAP-II program written by D. Shum of the U. S. Nuclear Regulatory Commission.

STATUS - Abstract first distributed February 1983.
CDC7600 version submitted November 1982, sample problem executed by NESC December 1982 on a CDC CYBER175.

REFERENCES - R. G. Gido, COGAP: A Nuclear Power Plant Containment Hydrogen Control System Evaluation Code, NUREG/CR-2847 (LA-9459-MS), January 1983.

U. S. Nuclear Regulatory Commission, Office of Nuclear Reactor Regulation, Standard Review Plan for the Review of Safety Analysis Reports for Nuclear Power Plants, LWR Edition, NUREG-0800 (formerly issued as NUREG-75/087), July 1981.

U. S. Nuclear Regulatory Commission, Office of Standards Development, Regulatory Guide 1.7, Revision 2, Control of Combustible Gas Concentrations in Containment Following a Loss-of-Coolant Accident, November 1978.

D. H. Shum, Development of a Code (COGAP-II) for Evaluation of Combustible Gas Concentrations and Mixing in Various Compartments of a Containment, Memorandum to Z. R. Rosztoczy, Chief, Analysis Branch, Division of Systems Safety, U. S. Nuclear Regulatory Commission, September 16, 1976.

J. A. Kudrick, Computer Program (COGAP) for Predicting Containment Hydrogen and Oxygen Concentrations Following Loss-of-Coolant Accidents, Memorandum to R. L. Tedesco, Assistant Director for Containment Safety, Atomic Energy Commission, Directorate of Licensing, December 2, 1972.

HARDWARE REQUIREMENTS - 55,000 (octal) words of memory are required for CDC7600 execution; the CDC CYBER175 requires 36,000 (octal) words.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -** To duplicate the sample problem output, the FORTRAN compiler option, ROUND, should be invoked.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
R. G. Gido
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE -**
Source (FORTRAN 1339 lines, UPDATE 1353 lines)
Sample problem (55 lines)
Sample problem output (15 pages)
Reference report, NUREG/CR-2847

17. **CATEGORY -** G
KEYWORDS - accidents, radiolysis, hydrogen, gases, recombiners, reactor safety, containment, combustion control, loss of coolant, nuclear power plants

18. **SPONSOR -** NRC Office of Nuclear Reactor Regulation,
Division of Systems Integration

1. **IDENTIFICATION AND KWIC TITLE -** DSM
   DSM, optimal sparse Jacobian matrix estimation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11/780, IBM3033 (designed to be machine-independent)

3. **DESCRIPTION -** DSM is a set of subroutines for estimating a sparse Jacobian matrix with a minimal or nearly minimal number of function evaluations. The set contains two interface routines, DSM and FDJS. DSM partitions the columns of a sparse matrix into groups so that the columns in a given group do not have a nonzero element in the same row position. Given the partition of the columns by DSM, subroutine FDJS determines an approximation to those columns in a given group of the partition. The entire Jacobian matrix is determined by calling FDJS for each group in the partition.

4. **METHOD OF SOLUTION -** The partitioning problem is associated with an equivalent graph coloring problem, and graph coloring heuristics are used to solve the partitioning problem.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -** NESC executed the sample problem in 12 CPU seconds on a DEC VAX11/780 and 3 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE -** DSM is called once to analyze the sparsity structure of the Jacobian matrix producing the partitioning information needed to estimate the Jacobian matrix. This information is stored in an integer array of length equal to the number of variables.

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Abstract first distributed February 1983.
   DEC VAX11/780, IBM3033 version submitted November 1982, sample problem executed by NESC December 1982 on a DEC VAX11/780 and an IBM3033.

10. **REFERENCES -** Thomas F. Coleman and Jorge J. More, Software for Estimating Sparse Jacobian Matrices, ANL-82-37, July 1982.
    Thomas F. Coleman and Jorge J. More, Estimation of Sparse Jacobian Matrices and Graph Coloring Problems, ANL-81-39, June 1981, SIAM Journal on Numerical Analysis, Vol. 20, pp. 189-209, 1983.

11. **HARDWARE REQUIREMENTS -** 156K bytes of virtual memory are required on the DEC VAX11/780; the IBM3033 requires 190K bytes of memory.

12. **PROGRAMMING LANGUAGE -** ANSI FORTRAN 66

13. **OPERATING SYSTEM -** VMS 3.0, UNIX (DEC VAX11/780), OS/MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    T. F. Coleman, B. S. Garbow, and J. J. More
    Mathematics and Computer Science Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE -**
    Source (1470 lines)
    Sample problem (FORTRAN 167 lines)
    Sample problem output (1 page)
    Reference report, ANL-82-37

17. **CATEGORY -** P
    KEYWORDS - mathematics, matrices, nonlinear problems, optimization

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Engineering, Mathematical and Geo-sciences

1. **IDENTIFICATION AND KWIC TITLE** - THREAD
   THREAD, concentration factors for bolt threads

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC6600,CYBER175

3. **DESCRIPTION** - THREAD calculates elastic stress multipliers (concentration factors) and thread load distribution information for the threaded region of the externally threaded member of an engaged connection subject to membrane, bending, and torsional loads. Free-notch stress concentration factors are combined with thread interaction factors caused by mating externally and internally threaded members of the connection. The resultant stress multipliers can be used to calculate peak elastic stresses in the externally threaded member of the connection. The effect of thread load distribution along the engagement length is taken into account.

4. **METHOD OF SOLUTION** - Calculations performed by THREAD are based on an analysis procedure by R. B. Heywood described in reference 2. This procedure, in turn, makes use of expressions for free-notch stress concentration factors and thread interaction factors given in references 3 and 4.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Both internally and externally threaded members are assumed to behave elastically and to have identical elastic properties. Thermal effects are not taken into account. Thread forms must be symmetrical, smoothly transitioned in their root regions (i.e., not undercut), and not tapered along the engagement length. Open-ended load paths through the connection (e.g., turnbuckles) are not treated.

6. **TIMING** - Run times on a CDC6600 are negligible, approximately 0.25 second per problem. NESC executed the sample problems in less than 1 CP second on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed February 1983.
   CDC6600 version submitted September 1982, sample problems executed by NESC January 1983 on a CDC CYBER175.

10. **REFERENCES** - J. M. McKinney, THREAD - A Computer Program for Calculating Elastic Stress Multipliers for Bolt Threads, WAPD-TM-1432(L), May 1980.

R. B. Heywood, Designing by Photoelasticity, Chapman and Hall, London, 1952.

H. Neuber, Theory of Notch Stresses: Principles for Exact Calculation of Strength with Reference to Structural Form and Material, Kerbspannungslehre: Grundlagen fuer genaue Festigkeitsberechnung mit Beruecksichtigung von Konstruktionsform und Werkstoff, Second Edition, Springer-Verlag, Berlin, 1958 (also available as AEC-TR-4547, 1961).

D. G. Sopwith, The Distribution of Load in Screw Threads, Proceedings of the Institute of Mechanical Engineers, pp. 373-383, 391-398, 1948.

11. **HARDWARE REQUIREMENTS** - The program requires 26,000 (octal) words of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.4 (CDC6600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - NESC provided a dummy subroutine for the missing Bettis environmental routine FINISH, used for a standard termination.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. M. McKinney
Bettis Atomic Power Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (436 lines)
    Sample problems (7 lines)
    Reference report, WAPD-TM-1432(L)

17. **CATEGORY** - I
    KEYWORDS - mechanical properties, elasticity, fatigue, stress corrosion, corrosion fatigue, fasteners, stresses, strains, LWBR reactors

18. **SPONSOR** - DOE Division of Naval Reactors

1. **IDENTIFICATION AND KWIC TITLE** - TCU50
   TCU50, timing control unit for LSI-11 systems

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11,LSI11

3. **DESCRIPTION** - TCU50 is a set of three utility routines for use with the Digital Pathways Timing Control Unit (TCU-50), a self-supporting timekeeper board which is designed to operate in a peripheral slot of the LSI-11 system. The three routines are TIMDAT which updates the time and date in the computer to that in the TCU-50 board; TCUSET which sets the TCU-50 board to the time and date in the LSI-11 system; and TCUTST which tests the TCU-50 board.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** - The TCU-50 can operate on its own battery power, with the computer off, for a period of up to three months.

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed February 1983.
   DEC PDP11 version submitted February 1980, routines executed by NESC July 1980 on an LSI-11.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** - 592 words of virtual memory

12. **PROGRAMMING LANGUAGE** - MACRO-11

13. **OPERATING SYSTEM** - RT-11 version 3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - When running TCU50 under RT-11 version 3 or 4, the call to the TCU-50 board must be placed at the end of the startup command file.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. Casterson
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** - Flexible Disk Transmittal
    Source (21 blocks*)
    Object (5 blocks*)
    Compilation listings (57 blocks*)
    Executable images (9 blocks*)
    * The TCU50 transmittal medium is an 8-inch, single sided, single density RX01 diskette written in RT-11 format.

17. **CATEGORY** - P
    KEYWORDS - DEC computers, time measurement, utility routines

18. **SPONSOR** - DOE Division of Military Application

1. **IDENTIFICATION AND KWIC TITLE** – DUST
   DUST, thermal neutron streaming through ducts

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** – IBM370

3. **DESCRIPTION** – DUST simulates thermal neutron streaming through multilegged square concrete ducts in shields.

4. **METHOD OF SOLUTION** – DUST uses the albedo Monte Carlo method. The albedo data used are in the form of empirical formulae based on measured double differential albedo data. Sampling of the reflected polar and azimuthal angles is by a rejection method. Variance reduction techniques such as Russian roulette are used.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** – DUST can handle only thermal neutron streaming through square concrete ducts. Maxima of 5 legs and 50 dose points may be used. The dose points considered are only in the last leg of the multilegged duct.

6. **TIMING** – For a square duct 40 feet in length DUST requires .05 seconds per history. Eight thousand histories give the dose within a plus or minus 15 percent statistical error in the case of a straight duct. The sample problem runs in less than 40 CPU seconds on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** – Optionally, mild biasing of the density function for the reflected polar angle can be introduced, and for the first few reflections the fractional contribution of each order of reflection can be printed.

8. **RELATED AND AUXILIARY SOFTWARE** –

9. **STATUS** – Abstract first distributed March 1983.
   IBM370 version submitted February 1982, sample problem executed by NESC February 1983 on an IBM370/195.

10. **REFERENCES** – R. Indira, K. P. N. Murthy, and R. Shankar Singh, Albedo Monte Carlo Simulation of Thermal Neutron Streaming through Multi Legged Ducts – Code DUST, RRC/FRG/01100/RP-217, January 1982.

DUST, NESC No. 1016, DUST Tape Description, National Energy Software Center Note 83-52, February 11, 1983.

K. P. N. Murthy, R. Indira, and R. Shankar Singh, Simulation of Neutron Streaming through Ducts in Shields Using Albedo Monte Carlo Technique, Internal Note RRC/FRG/RP-122, 1977.

K. P. N. Murthy, R. Indira, and R. Shankar Singh, Albedo Monte Carlo for Neutron Streaming through Ducts, Atomkernenergie, Vol. 34, p. 28, 1979.

11. **HARDWARE REQUIREMENTS** – 100K bytes of memory

12. **PROGRAMMING LANGUAGE** – FORTRAN IV

13. **OPERATING SYSTEM** – OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – Since the albedo data and the subroutines for sampling the reflected polar and azimuthal angles are specifically for concrete ducts, users must provide appropriate data and subroutines for ducts made of other materials.

    DUST uses two local environment timing routines, STIME to initialize the real timer and TTIME to return the elapsed CPU time (in microseconds) since STIME was last called. Dummy subroutines were substituted by NESC. Users who want this feature must provide alternative subroutines suited to their local computing environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
    K. P. N. Murthy, R. Indira, and R. Shankar Singh
    Fast Reactor Group

Reactor Research Centre
India

16. **MATERIAL AVAILABLE** –
Source (1101 lines)
Sample problem (23 lines)
Sample problem output (356 133-character records)
Reference report, RRC/FRG/01100/RP-217, and NESC Note

17. **CATEGORY** – J
KEYWORDS – albedo, radiation streaming, thermal neutrons, reflection, ducts, shields, concretes, Monte Carlo method, computerized simulation

18. **SPONSOR** – India – Department of Atomic Energy,
Reactor Research Centre

1. **IDENTIFICATION AND KWIC TITLE** – PLACID
   PLACID, gamma streaming thru cylindrical ducts

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** – IBM370

3. **DESCRIPTION** – PLACID simulates gamma streaming through straight cylindrical ducts in shields.

4. **METHOD OF SOLUTION** – A straight cylindrical duct located in an infinite shield material is the geometry considered. Monte Carlo simulation is used with variance reduction devices such as Russian roulette and cutoff weight for history termination. For the simulation a Cartesian coordinate system is set up with the origin at the center of the duct mouth and the z-axis along the duct centerline. The source is a plane isotropic disc source, placed at the bottom of the duct. Photon point total cross sections are used. The Klein-Nishina formula is used to compute the differential scattering cross sections. The double rejection technique due to Kahn is employed for sampling the scattered photon energy and the scattering angle. Next event estimators are used for scoring the streaming flux.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** – Only straight cylindrical ducts in shields are simulated.

6. **TIMING** – The simulation of CS-137 photon streaming through a cylindrical duct 100 cm. in length and 5 cm. in radius requires 76 milliseconds per history. About 6400 histories give the total dose at the duct exit within a 10 percent statistical error. The sample problem runs in less than 70 CPU seconds on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** – Contributions of each order of scattering to the total dose are printed. Track length biasing can be incorporated as an option.

8. **RELATED AND AUXILIARY SOFTWARE** –

9. **STATUS** – Abstract first distributed March 1983.
   IBM370 version submitted February 1982, sample problem executed by NESC February 1983 on an IBM370/195.

10. **REFERENCES** – R. Indira and K. P. N. Murthy, Monte Carlo Simulation of Gamma Streaming through Straight Cylindrical Ducts – Code PLACID, RRC/FRG/01100/RP-219, January 1982.
    PLACID, NESC No. 1017, PLACID Tape Description, National Energy Software Center Note 83-51, February 11, 1983.
    K. P. N. Murthy, Tracklength Biasing in Monte Carlo Radiation Transport, M. Sc. Thesis, 1980.
    R. G. Jaeger, Editor, Engineering Compendium on Radiation Shielding, Vol. 1, Springer, Berlin, 1970.

11. **HARDWARE REQUIREMENTS** – 65K bytes of memory

12. **PROGRAMMING LANGUAGE** – FORTRAN IV

13. **OPERATING SYSTEM** – OS/370.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – Users must provide the total cross section routine, SIGT, specific to the shield material considered. The program currently uses iron shields.
    PLACID uses two local environment timing routines, STIME to initialize the real timer and TTIME to return the elapsed CPU time (in microseconds) since STIME was last called. Dummy subroutines were substituted by NESC. Users who want this feature must provide alternative subroutines suited to their local computing environment..

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
    K. P. N. Murthy and R. Indira
    Fast Reactor Group

Reactor Research Centre
India

16. **MATERIAL AVAILABLE** –
Source (768 lines)
Sample problem (14 lines)
Sample problem output (884 133-character records)
Reference report, RRC/FRG/01100/RP-219, and NESC Note

17. **CATEGORY** – J
KEYWORDS – Monte Carlo method, gamma radiation, radiation streaming, ducts, shields, cylinders, computerized simulation

18. **SPONSOR** – India – Department of Atomic Energy Reactor Research Centre

IDENTIFICATION AND KWIC TITLE - SLAB
SLAB, response in fluid sinusoidal temperature

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175

DESCRIPTION - SLAB is a subroutine which solves the one-dimensional temperature problem for a solid slab of finite thickness and infinite width and length which is thermally coupled at both faces by constant film coefficient to a fluid with sinusoidally oscillating temperature. SLAB can calculate the temperatures at any arbitrary set of distances from the center plane of the slab at any desired time after a steady periodic temperature wave is established in the solid, the difference between the surface temperature and average temperature in the slab at that time, and the maximum value of the surface-to-average temperature difference during the cycle, as well as the time of occurrence and temperature distribution at that time.

METHOD OF SOLUTION - An analytical solution from Carslaw and Jaeger is used to achieve fast execution time and allow arbitrary nodal spacing without loss of accuracy.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Temperatures can be calculated for up to 100 distances from the center plane.

TIMING - Execution time is dependent on the number of mesh points at which the temperature is desired. NESC executed the sample problems in less than 1 CP second on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE - The maximum surface-to-average temperature difference in the plane, which occurs during the sinusoidal temperature cycle, is determined without plotting and averaging temperature distributions for several different times during the cycle.

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed March 1983.
CDC7600 version submitted July 1980, sample problems executed by NESC February 1983 on an CDC CYBER175.

REFERENCES - A. M. Poindexter, Subroutine SLAB - A Computer Program for Calculating Thermal Response of a Flat Plate in a Fluid with Oscillating Temperature, Subroutine SLAB Users Guide, December 1979.
H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, Clarendon Press, Oxford, 1959.

HARDWARE REQUIREMENTS - 17,000 (octal) words of memory are required for the sample problem.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The driver routine for SLAB is user-supplied.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
A. M. Poindexter
Advanced Energy Systems Division
Westinghouse Electric Corporation

MATERIAL AVAILABLE -
Source (258 lines)
Sample problem (FORTRAN 48 lines, data 10 lines)
Sample problem output (1 page)
Reference Users Guide

17. **CATEGORY** - H
KEYWORDS - heat transfer, fluid flow, temperature distribution, oscillations, slabs, thermal conduction

18. **SPONSOR** - DOE Clinch River Breeder Reactor Project

1. **IDENTIFICATION AND KWIC TITLE** - BACFIRE
   BACFIRE, common cause failure analysis program

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM360,370

3. **DESCRIPTION** - BACFIRE, designed to aid in common cause failure analysis, searches among the basic events of a minimal cut set of the system logic model for common potential causes of failure. The potential cause of failure is called a qualitative failure characteristic. The algorithm searches qualitative failure characteristics (that are part of the program input) of the basic events contained in a set to find those characteristics common to all basic events. This search is repeated for all cut sets input to the program. Common cause failure analysis is thereby performed without inclusion of secondary failures in the system logic model. By using BACFIRE, a common cause failure analysis can be added to an existing system safety and reliability analysis.

4. **METHOD OF SOLUTION** - BACFIRE searches the qualitative failure characteristics of the basic events contained in the fault tree minimal cut set to find those characteristics common to all basic events by either of two criteria. The first criterion can be met if all the basic events in a minimal cut set are associated by a condition which alone may increase the probability of multiple component malfunction. The second criterion is met if all the basic events in a minimal cut set are susceptible to the same secondary failure cause and are located in the same domain for that cause of secondary failure.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Maxima of -
   1001 secondary failure maps
   101 basic events
   10 cut sets

6. **TIMING** - NESC executed the sample problem in less than 1 CPU second on an IBM370/195.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - BACFIRE is similar to COMCAN (NESC 704), another common cause failure analysis program.

9. **STATUS** - Abstract first distributed March 1983.
   IBM360 version submitted November 1979, sample problem executed by NESC February 1983 on an IBM370/195.

10. **REFERENCES** - C. L. Cate and J. B. Fussell, BACFIRE - A Computer Program for Common Cause Failure Analysis, Reliability and Safety Assessment Project document, Nuclear Engineering Department, University of Tennessee, February 1977.
    Gary R. Burdick, Neldon H. Marshall, and James R. Wilson, COMCAN - A Computer Program for Common Cause Analysis, ANCR-1314, May 1976.
    W. E. Vesely and R. E. Narum, PREP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree, IN-1349, August 1970.
    J. B. Fussell, E. B. Henry, and N. H. Marshall, MOCUS: A Computer Program to Obtain Minimal Sets from Fault Trees, ANCR-1156, August 1974.
    J. B. Fussell, D. M. Rasmuson, J. R. Wilson, G. R. Burdick, and J. C. Zipperer, A Collection of Methods for Reliability and Safety Engineering, ANCR-1273, April 1976.

11. **HARDWARE REQUIREMENTS** - 130K bytes of memory are required for execution.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/MVT.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
J. B. Fussell
JBF Associates, Inc.

16. **MATERIAL AVAILABLE -**
Source (615 lines)
Sample problem (95 lines)
Reference BACFIRE computer program document

17. **CATEGORY** - G
KEYWORDS - reliability, fault tree analysis, failures, system failure analysis, COMCAN codes, MOCUS codes, PREP,KITT codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Project

IDENTIFICATION AND KWIC TITLE - TREDRA
TREDRA, drafting report quality fault trees

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM360,370,303x

DESCRIPTION - TREDRA is a computer program for drafting report-quality fault trees. The input to TREDRA is similar to input for standard computer programs that find minimal cut sets from fault trees. Output includes fault tree plots containing all standard fault tree logic and event symbols, gate and event labels, and an output description for each event in the fault tree. TREDRA contains the following features: a variety of program options that allow flexibility in the program output; capability for automatic pagination of the output fault tree, when necessary; input groups which allow labeling of gates, events, and their output descriptions; a symbol library which includes standard fault tree symbols plus several less frequently used symbols; user control of character size and overall plot size; and extensive input error checking and diagnostic oriented output.

METHOD OF SOLUTION - Fault trees are generated by user-supplied control parameters and a coded description of the fault tree structure consisting of the name of each gate, the gate type, the number of inputs to the gate, and the names of these inputs.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - TREDRA can produce fault trees with a minimum of 3 and a maximum of 56 levels. The width of each level may range from 3 to 37. A total of 50 transfers is allowed during pagination.

TIMING - NESC executed each sample problem in less than 2 CPU seconds on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - TREDRA extends the earlier MOTH and HERCULES programs, which used together produce computer drawn fault trees from processing MOCUS or PREP input data, by combining their features into one program. MOCUS (NESC 653) and PREP,KITT (NESC 528) are computer programs for determining minimal cut sets and minimal path sets from existing fault trees. Six of the seven program options in TREDRA require a MOCUS/PREP description of the fault tree structure.

STATUS - Abstract first distributed March 1983.
IBM360 version submitted November 1979, sample problems executed by NESC February 1983 on an IBM3033.

REFERENCES -
L. S. Baker, D. P. Wagner, C. L. Cate, and J. B. Fussell, TREDRA A Computer Program to Draft Fault Trees, JBF Associates, Inc. document, October 1978.

TREDRA, NESC No. 1021, TREDRA Tape Description and Sample Problem Output, National Energy Software Center Note 83-50, March 18, 1983.

J. B. Fussell, E. B. Henry, and N. H. Marshall, MOCUS: A Computer Program to Obtain Minimal Sets from Fault Trees, ANCR-1156, August 1974.

W. E. Vesely and R. E. Narum, PREP and KITT: Computer Codes for the Automatic Evaluation of a Fault Tree, IN-1349, August 1970.

N. H. Marshall, MOTH -- MOCUS to HERCULES, Aerojet Nuclear Company document, August 1974.

J. B. Fussell, Special Techniques in Fault Tree Analysis, Aerojet Nuclear Company document, March 1974.

J. B. Fussell, Particularities of Fault Tree Analysis, Aerojet Nuclear Company document, September 1974.

HARDWARE REQUIREMENTS - 270K bytes of memory are required for execution.

PROGRAMMING LANGUAGE - FORTRAN IV (99%) and BAL (1%)

OPERATING SYSTEM - OS/MVT (IBM360,370), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Function NCHARS, which determines the length of a string, is written in Basic Assembly Language. Graphical output is accomplished through calls to the proprietary CalComp graphics system.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. B. Fussell
JBF Associates, Inc.

16. **MATERIAL AVAILABLE** -
Source (FORTRAN 3551 lines, BAL 25 lines)
Sample problems (190 lines)
Control information (JCL 106 lines)
Reference TREDRA computer program document and NESC Note

17. **CATEGORY** - N
KEYWORDS - fault tree analysis, reliability, computer graphics, diagrams, MOTH codes, HERCULES codes, MOCUS codes, PREP,KITT codes

18. **SPONSOR** - University of Tennessee
Union Carbide Corporation Nuclear Division

IDENTIFICATION AND KWIC TITLE - PLUTO
PLUTO, molecular & crystal structure plotting

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM303x, DEC VAX11/780

DESCRIPTION - PLUTO may be used for drawing individual molecules in a crystalline arrangement. The drawings may be thought of in three principal aspects, the content, the style, and the viewpoint. The content of the drawing requires the definition of items such as molecules, atoms within molecules, connections between atoms, labels for atoms and unit cell representation. The style of the drawing may be like a stick model or a solid ball and spoke model with variable sizes for atoms and bonds. The atoms may be shaded to enhance the solid appearance. Drawings may be made in parallel projection, perspective, or in stereo-pair perspective. The view direction may be chosen with respect to molecular features such as lines and planes defined by atom names or by reference to the cell and orthogonal axial systems. The view direction may be further modified by rotation about the plotting reference axes.

METHOD OF SOLUTION - There are three distinct axial systems involved in drawing a crystal structure. The input coordinates are usually with reference to the unit cell axes and are in fractional form. These are converted internally to an orthogonal system. The final plotting coordinates are in millimeters and refer to the direction on the plotting paper. All these axes are right-handed, and absolute configuration is preserved in all rotations.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The maximum number of input atoms is 500.

TIMING - The longest running sample problem required less than 12 seconds of CPU time on an IBM3033.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. ORTEP2 (NESC 938) also draws crystal structure illustrations.

STATUS - Abstract first distributed March 1983.
DEC VAX11/780 version submitted February 1981, sample problems executed by NESC May 1982 on an IBM3033.

REFERENCES - Sam Motherwell, PLUTO A Program for Plotting Molecular and Crystal Structures, revised and implemented at the Weizmann Institute of Science by Joel L. Sussman, Zippora Shakked, and David Barnett, Rehovot, Israel, May 1979.

HARDWARE REQUIREMENTS - 350K bytes of memory and a plotting device

PROGRAMMING LANGUAGE - FORTRAN IV (97%) and Assembly language (3%)

OPERATING SYSTEM - MVS (IBM3033).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - PLUTO uses the proprietary CalComp plotting software.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
W. D. S. Motherwell
University Chemical Laboratory
England

MATERIAL AVAILABLE -
Source (FORTRAN 2503 lines, BAL 79 lines)
Sample problems (103 lines)
Reference report

17. **CATEGORY** - U
KEYWORDS - crystal structure, molecular structure, plotters, x-ray diffraction, crystallography, computer graphics, diagrams

18. **SPONSOR** - University Chemical Laboratory, Cambridge, England
The Weizmann Institute of Science, Rehovot, Israel

1. **IDENTIFICATION AND KWIC TITLE** - PROGRAM H
   PROGRAM H, transonic airfoil w/boundary layer

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC6600,7600,CYBER175

3. **DESCRIPTION** - PROGRAM H was designed for the analysis of transonic airfoils with a turbulent boundary layer correction.

4. **METHOD OF SOLUTION** - The analysis program with boundary layer correction is the solution of the finite difference representation of the compressible flow equations. The physical plane is mapped onto the unit circle where the difference scheme is solved using a discrete Poisson Solver for the elliptic part of the problem and a number of relaxation iterations for the entire grid. A turbulent boundary layer correction based on the work of Nash-MacDonald has been incorporated into the program. It is solved iteratively with the flow calculations.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - The running time of the test case is approximately 170 seconds on the CDC6600. NESC executed the sample problem in 55 CPU seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - PROGRAM K (NESC 1024) is a design code for transonic airfoils, turbine or compressor blades.

9. **STATUS** - Abstract first distributed June 1983.
   CDC6600 version submitted December 1976, sample problems executed by NESC March 1983 on a CDC CYBER175.

10. **REFERENCES** - Frances Bauer, Paul Garabedian, David Korn, and Anthony Jameson, Supercritical Wing Sections II, Lecture Notes in Economics and Mathematical Systems, Vol. 108, M. Beckmann and H. P. Kuenzi, Springer-Verlag, 1975.
    PROGRAM H, NESC No. 1023, PROGRAM H Tape Description, National Energy Software Center Note 83-70, March 15, 1983.

11. **HARDWARE REQUIREMENTS** - 112,000 (octal) words are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    F. Bauer
    Courant Institute of Mathematical Sciences
    New York University

16. **MATERIAL AVAILABLE** -
    Source (2566 lines)
    Sample problem (137 lines)
    Control information (10 lines)
    Machine-readable documentation (56 lines)
    Sample problem output (17 pages)
    NESC Note

17. **CATEGORY** - H
    KEYWORDS - transonic flow, airfoils, compressible flow, boundary layers, turbulent flow, Fourier transformation, PROGRAM K codes

18. SPONSOR - AEC
NASA

1. **IDENTIFICATION AND KWIC TITLE** - PROGRAM K
   PROGRAM K, transonic airfoil and blade design

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC6600,7600,CYBER175

3. **DESCRIPTION** - PROGRAM K is a design code for transonic airfoils, turbine or compressor blades.

4. **METHOD OF SOLUTION** - The design program results from the ability to solve the partial differential equations of two-dimensional inviscid gas dynamics by analytic continuation into the domain of two independent complex characteristic coordinates. The domain of integration is mapped conformally onto the unit circle in the plane of one of these coordinates. On the circle it is possible to formulate a boundary value problem for the stream function that is well-posed even in the case of transonic flow. Two boundary value problems are solved by means of the fast Fourier Transform and complex extension. Thus, a procedure is developed for the calculation of an airfoil on which the speed q is prescribed as a function of arc length s. For subsonic flow an exact solution of this non-linear problem is obtained. For the transonic case a shockless flow results which assumes the assigned subsonic values of the speed q exactly but the resulting supersonic values of speed are near the given values.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** - The running time for the test case is approximately 290 seconds on the CDC6600. NESC executed the sample problem in 117 CPU seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - PROGRAM H (NESC 1023) was developed for the analysis of transonic airfoils with a turbulent boundary layer correction.

9. **STATUS** - Abstract first distributed June 1983.
   CDC6600 version submitted December 1976, sample problem executed by NESC March 1983 on a CDC CYBER175.

10. **REFERENCES** - Frances Bauer, Paul Garabedian, and David Korn, Supercritical Wing Sections III, Lecture Notes in Economics and Mathematical Systems, Vol. 150, M. Beckmann and H. P. Kuenzi, Springer-Verlag, 1977.
   PROGRAM K, NESC No. 1024, PROGRAM K Tape Description, National Energy Software Center Note 83-71, April 12, 1983.

11. **HARDWARE REQUIREMENTS** - 132,000 (octal) words are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    F. Bauer
    Courant Institute of Mathematical Sciences
    New York University

16. **MATERIAL AVAILABLE** -
    Source (4692 lines)
    Sample problem (40 lines)
    Control information (11 lines)
    Machine-readable documentation (167 lines)
    Sample problem output (5 pages)
    NESC Note

17. **CATEGORY** - H
KEYWORDS - transonic flow, design, airfoils, turbine blades, compressor blades, boundary-value problems, Fourier transformation, PROGRAM H codes

18. **SPONSOR** - AEC
NASA

1. **IDENTIFICATION AND KWIC TITLE** - HONDO5
   HONDO5, ab initio Hartree-Fock structure

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600,CYBER175

3. **DESCRIPTION** - HONDO5 is a program written for ab initio molecular structure calculations at the Hartree-Fock level. The program calculates RHF or UHF SCF molecular wavefunctions, optimizes molecular geometries using the gradient of the RHF or UHF energy with respect to the 3*N nuclear coordinates, calculates the Cartesian force constant matrix of the molecule and the vibrational frequencies, and calculates the following properties of the RHF or UHF wavefunction: dipole moment, Mulliken population analysis, and atomic spin density.

4. **METHOD OF SOLUTION** - HONDO5 uses Cartesian Gaussian basis functions of S-, P-, and D-type. Hartree-Fock equations are formulated and solved using the conventional Roothaan expansion method. A special feature of the program is the calculation of electron repulsion integrals by a numerical quadrature based on the Rys polynomials. The program also takes advantage of molecular symmetry.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - HONDO5 can handle a maximum of 30 atoms with up to 70 unique shells for a total of 240 primitive Gaussian basis functions and 100 contracted functions.

6. **TIMING** - NESC executed the sample problem in 2 CP seconds on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library.

9. **STATUS** - Abstract first distributed August 1983.
   CDC7600 version submitted February 1981, sample problem executed by NESC March 1983 on a CDC CYBER175.

10. **REFERENCES** - HONDO5, NESC No. 1025.7600, HONDO5 Tape Description, National Energy Software Center Note 83-74, March 30, 1983.
    Harry F. King and Michel Dupuis, Numerical Integration using Rys Polynomials, Journal of Computational Physics, Vol. 21, pp. 144-165, 1976.
    Michel Dupuis, John Rys, Harry F. King, Evaluation of molecular integrals over Gaussian basis functions, Journal of Chemical Physics, Vol. 65, pp. 111-116, July 1976.
    Michel Dupuis and Harry F. King, Molecular Symmetry and Closed-Shell SCF Calculations I., International Journal of Quantum Chemistry, Vol. XI, pp. 613-625, 1977.
    Michel Dupuis and Harry F. King, Molecular symmetry. II. Gradient of electronic energy with respect to nuclear coordinates, Journal of Chemical Physics, Vol. 68, pp. 3998-4004, 1978.

11. **HARDWARE REQUIREMENTS** - 176,000 (octal) words are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (99%) and COMPASS (1%)

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    M. Dupuis
    Lawrence Berkeley Laboratory
    J. Rys and H. F. King
    State University of New York at Buffalo

16. **MATERIAL AVAILABLE** -
Source (21,998 lines)
Sample problem (26 lines)
Sample problem output (276 132-character records)
Auxiliary information (machine-readable documentation 1000 lines)
Control information (140 lines)
NESC Note

17. **CATEGORY** - W
KEYWORDS - Hartree-Fock method, wave functions, self-consistent field, energy, Gauss potential, S states, P states, D states

18. **SPONSOR** - DOE Office of Energy Research,
Office of Basic Energy Sciences,
Chemical Sciences Division
NSF

IDENTIFICATION AND KWIC TITLE - SAMS
SAMS, coupled channel molecular scattering

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER175, CDC7600

DESCRIPTION - SAMS solves the coupled, second-order differential equations of quantum inelastic molecular scattering theory. The solution is provided in terms of the scattering matrix. The physical problem is defined by user-supplied subroutines, POT and LIST.

METHOD OF SOLUTION - The coupled differential equations are reformatted in terms of coupled Volterra integral equations, which are solved using the trapezoid-rule quadrature method of Sams and Kouri.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - SAMS is not designed for production run calculations in which many total angular momentum S-matrices are desired.

TIMING - Execution times may range from 2 seconds to 2 hours depending on the complexity of the system. The computing time increases as the cube of the number of coupled equations. NESC executed the sample problem in less than 1 CP second on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE - The program tends to execute fast for short-range potentials and slowly when long-range interaction potentials, such as in ion-molecule scattering, are involved.

RELATED AND AUXILIARY SOFTWARE - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. An auxiliary program, COEF, is included which defines the list of quantum numbers and evaluates the R-independent F-coefficients.

STATUS - Abstract first distributed August 1983.
CDC CYBER175 version submitted January 1982, sample problem executed by NESC March 1983 on a CDC CYBER175.

REFERENCES - Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980.

Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980.

SAMS, NESC No. 1026, SAMS Tape Description, National Energy Software Center Note 83-73, April 11, 1983.

W. Neal Sams and Donald J. Kouri, Noniterative Solutions of Integral Equations for Scattering. I. Single Channels, Journal of Chemical Physics, Vol. 51, No. 11, pp. 4809-4814, December 1, 1969.

W. Neal Sams and Donald J. Kouri, Noniterative Solutions of Integral Equations for Scattering. II. Coupled Channels, Journal of Chemical Physics, Vol. 51, No. 11, pp. 4815-4819, December 1, 1969.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest, and R. B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

HARDWARE REQUIREMENTS - 64,000 (octal) words are required to execute the sample problem. Dimensions may be reduced if a small problem is being solved.

PROGRAMMING LANGUAGE - FORTRAN IV CDC Extended Version 4.6

OPERATING SYSTEM - NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – Subroutines POT and LIST, which define the physical problem, must be supplied by the user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

K. McLenithan and D. Secrest
School of Chemical Sciences
University of Illinois

16. **MATERIAL AVAILABLE** –

Source (810 lines)
Sample problem (FORTRAN 336 lines, data 14 lines)
Auxiliary information (COEF 464 lines, data 11 lines, machine-readable documentation 263 lines)
Control information (38 lines)
Sample problem output (6 pages)
Excerpts from reference reports, LBL-9501 Vols. I and II, and NESC Note

17. **CATEGORY** – W
KEYWORDS – S matrix, inelastic scattering, collisions, energy transfer, Schroedinger equation, wave functions, Bessel functions

18. **SPONSOR** – NSF

IDENTIFICATION AND KWIC TITLE - LDEF-SS
LDEF-SS, two-phase fluid flow in spray dryers

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,6600,CYBER175, IBM303x,4331

DESCRIPTION - LDEF-SS solves the equations for the two-phase fluid flow in spray dryers. It calculates, by a particle method, the dynamics and vaporization of a single component liquid spray. The spray is fully-coupled to a two-component gas, consisting of an inert species and the vapor of the liquid. The effects of drop collisions and coalescence are included. The geometry is spatially two-dimensional and axisymmetric, and swirling motion is permitted about the dryer axis. A wide variety of dryer parameters, such as dryer size and geometry and atomizer size and speed, and operating conditions, such as gas-flow rates and temperatures, can be specified by user-supplied parameters. Program output includes contour, vector, and spray plots, supplemented by numerical results.

METHOD OF SOLUTION - The equations for a single-component liquid moving and evaporating in a two-component gas composed of air and the vapor of the liquid are solved by finite-difference methods. LDEF-SS incorporates the basic methodology of the stochastic parcel (SP) method, as well as many other features of the numerical solution procedure of Dukowicz, in conjunction with the Implicit Continuous-fluid Eulerian (ICE) method. An algorithm was added to calculate the effects of drop collisions. The ordinary differential equations governing the changes in drop properties are approximated by first-order methods. The finite-difference equations for the gas-phase properties are obtained by a control-volume derivation. An eddy diffusivity approximation is used to calculate the turbulent transport of mass, momentum, and energy in the gas.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - LDEF-SS does not calculate the gas-phase transport of sulfur dioxide and its dissolution and reaction with the liquid.

TIMING - NESC executed the sample problem in 36 CP minutes on a CDC CYBER175 and in less than 6 CPU hours on an IBM4331.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed August 1983.
CDC7600 version submitted September 1982, replaced October 1985 by revised Edition B, sample problem, without plotting, executed by NESC March 1983 on a CDC CYBER175.
IBM3033 version submitted August 1984, sample problem, without plotting, executed by NESC October 1984 on an IBM4331.

REFERENCES - Peter J. O'Rourke and Willard R. Wadt, A Two-Dimensional, Two-Phase Numerical Model for Spray Dryers, LA-9423-MS, July 1982.
Gail Rein, J501 SC-4020 Emulation, User Manual, LANL PIM-2 Program Library Write-Up, May 1981.
LDEF-SS, NESC No. 1027.7600B, LDEF-SS CDC Version Tape Description and Implementation Information, National Energy Software Center Note 86-03, October 25, 1985.
LDEF-SS, NESC No. 1027.3033, LDEF-SS IBM Version Tape Description and Implementation Information, National Energy Software Center Note 86-04, October 25, 1985.
John K. Dukowicz, A Particle-Fluid Numerical Model for Liquid Sprays, Journal of Computational Physics, Vol. 35, No. 2, pp. 229-253, April 1980.

HARDWARE REQUIREMENTS - 127,000 (octal) words of memory are required to execute the sample problem on a CDC CYBER175; the IBM version requires 460K bytes of memory on an IBM4331.

PROGRAMMING LANGUAGE - FORTRAN 77 (CDC7600), FORTRAN 77 (88%) and BAL (12%) (IBM3033)

13. **OPERATING SYSTEM** - LTSS (CDC7600), NOS 1.4 (CDC CYBER175), VM/CMS (IBM4331), MVS/TSO (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Due to the iterative nature of the calculations in LDEF-SS, machine round-off error may produce slightly different results on different machines.

For the CDC version, the FORTRAN compiler option, ROUND, should be invoked to duplicate the sample problem output. This version includes NESC-provided dummy routines for the LANL Stromberg-Carlson plotter routines: ADV, DRV. GPLOT, GRPHFTN, GRPHLUN, LIB4020, LINCNT, PLT, and SETFLSH, which should be replaced with suitable alternatives for the environment in which the program is being executed to obtain graphical output.

In the IBM3033 version, subroutines DTIME and DATES are written in assembly language; they return the time of day and date information, respectively. Proprietary CalComp plotting routines PLOT, PLOTS, NEWPEN, WHERE, NUMPEN, and SYMBOL, used to provide the graphic output in the IBM version, are not included and should be replaced with alternatives suited to the local computing environment for graphical output.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

7600 P. J. O'Rourke
Los Alamos National Laboratory

3033 M. D. Marks
Dow Chemical U.S.A.

16. **MATERIAL AVAILABLE** -

Source (7600-2750 lines, 3033-FORTRAN 3163 lines, BAL 426 lines)
Sample problems (7600-15 lines, 3033-11 lines)
Control information (3033-JCL 88 lines)
Sample problem output (7600-20 selected pages, 3033-23 selected pages)
Reference report, LA-9423-MS, NESC Note, appropriate to version, and LANL Write-Up (CDC version)

17. **CATEGORY** - H
KEYWORDS - two-phase flow, spray drying, fluid flow, particles, flue gas, desulfurization, ICE method, finite difference method

18. **SPONSOR** - DOE Morgantown Energy Technology Center
DOE Office of Basic Energy Sciences

IDENTIFICATION AND KWIC TITLE - TRIPM
TRIPM, water & solute transport porous media

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370,303x

DESCRIPTION - TRIPM is a mathematical model designed to predict the transport of radionuclides and their decay products in a saturated-unsaturated vertical plane of a phreatic aquifer under isothermal conditions. The model is composed of two modules: the first calculates the pressure distribution in the domain of interest, enabling one to compute the velocities and soil moisture; the second calculates the migration of the various species by taking into account the major processes associated with the transport phenomena of a dissolved substance in porous media, i.e. advection, mechanical dispersion, molecular diffusion, radioactive decay and sorption. The influence of soil-water pH on the distribution coefficient is also considered. The first module may be used independently of the second.

METHOD OF SOLUTION - The two-dimensional finite-element method used in TRIPM is based on the weighted residual technique. The model can accept two types of elements, quadrilateral and triangular. In the application of the method, the flow equation, which has nonlinear coefficients is solved by a Bubnov-Galerkin type method, using an iterative technique with a backward-difference scheme coupled with a mass lumping of the coefficients of the time-derivative term. The solute equation is solved by a Petrov-Galerkin type method using a Crank-Nicolson scheme.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - TRIPM can accept only isoparametric linear quadrilateral and triangular elements.

TIMING - NESC executed the five sample problems in 6, 4, 1, 1, and 18 CPU minutes, respectively, on an IBM3033 and IBM370/195.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed April 1984.
IBM370 version submitted October 1981, replaced by revised edition November 1982, sample problems executed by NESC March 1983 on an IBM3033 and IBM370/195.

REFERENCES - A. Berge Gureghian, TRIPM: A Two-Dimensional Finite-Element Model for the Simultaneous Transport of Water and Reacting Solutes through Saturated and Unsaturated Porous Media, ONWI-465, July 1983.
A. B. Gureghian, B. R. Stitt, L. P. Sanathanan, Calculation of Unsaturated Hydraulic Conductivity, ANL/EIS-14, June 1982.
TRIPM, NESC No. 1028, TRIPM Tape Description, Implementation Information, and Sample Problem Output, National Energy Software Center Note 84-24, May 24, 1983.

HARDWARE REQUIREMENTS - 900K bytes of memory are required to execute the largest sample problem.

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - OS/MVT (IBM370), MVS (IBM3033).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The user must properly DIMENSION the BAND, BANDP, and BANDG arrays in the MAIN routine for each TRIPM problem. Generally, the user will be able to determine the proper values for a simple mesh configuration; however, for an elaborate mesh the user can obtain the proper values from TRIPM output by an abbreviated run, if necessary.
To produce graphic output, TRIPM uses the Integrated Software Systems Corporation's (ISSCO) proprietary graphics software product, DISSPLA.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

A. B. Gureghian
Office of Nuclear Waste Isolation
Battelle Project Management Division

16. **MATERIAL AVAILABLE –**

Source (6356 lines)
Sample problems (3822 lines, 224 133-character records)
Auxiliary information (machine-readable documentation 1579 133-character records)
Control information (JCL 108 lines)
Sample problem output (18,032 133-character records)
Reference report, ONWI-465, and NESC Note

17. **CATEGORY** – R
KEYWORDS – aquifers, radionuclide migration, ground water, daughter products, finite element method, mill tailings, low-level radioactive wastes, soils

18. **SPONSOR** – DOE Office of Nuclear Waste Isolation
NRC Division of Waste Management

IDENTIFICATION AND KWIC TITLE - A-THREE
A-THREE, optical model for elastic scattering

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600,CYBER175

DESCRIPTION - A-THREE is an optical model code for elastic scattering, specifically designed for the requirements of heavy-ion projectiles. Fast search procedures for fitting model parameters to experimental data are provided. Because of structural similarity, provision for bound state calculation has also been included. The non-relativistic radial Schroedinger equation with complex potential is solved partial wave by partial wave to obtain phase shifts, from which total reaction cross sections, elastic scattering angular distributions, and polarization angular distributions are obtained. Optionally, radial wave functions may be retained. Provisions to search for an eigenvalue or potential which produces a given eigenvalue in the bound state case, and to fit given data or sets of data, with or without angular resolution, in the scattering case are included. The parameter space may also be "scanned", without search.

METHOD OF SOLUTION - The radial differential equation is integrated by the Noumerov method, with mesh refinement, if necessary; the principal search method is a variable metric minimization after Fletcher-Powell and Davidon.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Partial waves are limited to l=800 for no spin and l=400 with spin; the total number of partial waves actually computed is limited to 400, absorption for the lower uncomputed partial waves being set to 1.0. Potential specification must be made in an equally-spaced grid of not over 500 intervals.

TIMING - Typical running time on a CDC7600 for a 100 partial wave problem and 1000 integration steps per partial wave is 1.881 seconds; search times vary with distance from the minimum. NESC executed the sample problem in 60 CP seconds on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE - All arrays requiring more significant figures than 32-bit machines provide are noted; similarly for alphanumeric words of more than four characters.

RELATED AND AUXILIARY SOFTWARE - A-THREE is a descendant of the ABACUS2 and ABACUS-HI program; it has, however, been completely rewritten.

STATUS - Abstract first distributed August 1983.
CDC7600 version submitted September 1982, sample problem executed by NESC March 1983 on a CDC CYBER175.

REFERENCES - E. H. Auerbach, A-THREE A User's Manual, BNL 23001, PD Report No. 127, June 1977.

E. H. Auerbach, A-THREE: A General Optical Model Code Especially Suited to Heavy-Ion Calculations, Computer Physics Communications, Vol. 15, pp. 165-192, 1978.

R. Fletcher and M. J. D. Powell, A rapidly convergent descent method for minimization, Computer Journal, Vol. 6, pp. 163-168, 1969.

HARDWARE REQUIREMENTS - 73,000 (octal) words are required to execute the sample problem.

PROGRAMMING LANGUAGE - FORTRAN IV (Fortran Extended)

OPERATING SYSTEM - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
E. H. Auerbach
Brookhaven National Laboratory

16. **MATERIAL AVAILABLE** –
Source (3701 lines)
Sample problem (36 lines)
Sample problem output (10 pages)
Reference report, BNL 23001

17. **CATEGORY** – W
KEYWORDS – optical models, potential scattering, Schroedinger equation, total cross sections, elastic scattering, angular distribution, wave functions, heavy ions, phase shift

18. **SPONSOR** – DOE Office of High Energy and Nuclear Physics,
Division of Nuclear Physics

1. **IDENTIFICATION AND KWIC TITLE** - RMAT
   RMAT, coupled channel molecular scattering

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,CYBER175

3. **DESCRIPTION** - RMAT solves the coupled, second-order differential equations of atomic and molecular quantum scattering theory. The program is independent of the chemical system or the method (close coupling, coupled states, etc.). The physical problem is defined by user-supplied subroutines, POT and LIST.

4. **METHOD OF SOLUTION** - The R-matrix propagation method for the numerical integration of second-order differential equations without explicit first derivatives is used. Perturbation corrections to the R-matrix may be included. The S-matrix is computed directly from the R-matrix by assuming that the wave function and derivative, which are not found explicitly, may be matched to spherical Bessel functions.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - The number of coupled equations which can be solved depends on the amount of main memory available.

6. **TIMING** - RMAT required 0.7 CP seconds for a 2-channel problem and 71 CP seconds for a 28-channel problem on a CDC7600. NESC executed the sample problem in less than 1 CP second on a CDC CYBER175.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - RMAT selects its own step-size given an error parameter, but step-sizes of arbitrary value are easily introduced into the program.

8. **RELATED AND AUXILIARY SOFTWARE** - This program was transferred in February 1981 from the National Resource for Computation in Chemistry's software library. An auxiliary program, COEF, is included which defines the list of quantum numbers and evaluates the R-independent F-coefficients. Other general integration programs used to solve the coupled equations of molecular scattering theory are DEVOG (NESC 920), PC (NESC 921), MNN (NESC 942), and SAMS (NESC 1026).

9. **STATUS** - Abstract first distributed August 1983.
   CDC7600 version submitted February 1981, sample problem executed by NESC April 1983 on a CDC CYBER175.

10. **REFERENCES** - Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume I, Proceedings of the Workshop held at Argonne National Laboratory, June 25-27, 1979, CONF-790696 (LBL-9501), Vol. I, NRCC Proceedings No. 5, July 1980.

Lowell Thomas, Ed., Algorithms and Computer Codes for Atomic and Molecular Quantum Scattering Theory, Volume II, Proceedings of the Workshop Reconvened at Lawrence Berkeley Laboratory, October 26-27, 1979, CONF-790696 (LBL-9501), Vol. II, NRCC Proceedings No. 5, July 1980.

RMAT, NESC No. 1030, RMAT Tape Description, National Energy Software Center Note 83-94, May 23, 1983.

Ellen B. Stechel, Robert B. Walker, and John C. Light, R-matrix solution of coupled equations for inelastic scattering, Journal of Chemical Physics, Vol. 69, No. 8, pp. 3518-3531, October 15, 1978.

L. D. Thomas, M. H. Alexander, B. R. Johnson, W. A. Lester, Jr., J. C. Light, K. D. McLenithan, G. A. Parker, M. J. Redmon, T. G. Schmalz, D. Secrest, and R. B. Walker, Comparison of Numerical Methods for Solving the Second-Order Differential Equations of Molecular Scattering Theory, Journal of Computational Physics, Vol. 41, No. 2, pp. 407-426, June 1981, also available as LBL-11233, July 1980.

11. **HARDWARE REQUIREMENTS** - 77,000 (octal) words are required to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), NOS 1.4 (CDC CYBER175).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** – Subroutines POT and LIST, which define the physical problem, must be supplied by the user.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

T. G. Schmalz
Department of Marine Sciences
Texas AR University at Galveston

16. **MATERIAL AVAILABLE** –

Source (1495 lines)
Sample problem (FORTRAN 1060 lines, data 11 lines)
Auxiliary information (COEF 324 lines, data 27 lines, machine-readable documentation 230 lines)
Control information (38 lines)
Sample problem output (11 pages)
Excerpts from reference reports, LBL-9501 Vols. I and II, and NESC Note

17. **CATEGORY** – W
KEYWORDS – R matrix, S matrix, inelastic scattering, Schroedinger equation, wave functions, Bessel functions, DEVOG codes, PC codes, MNN codes, SAMS codes

18. **SPONSOR** – DOE Office of Basic Energy Sciences
NSF

1. **IDENTIFICATION AND KWIC TITLE** - TRAC-BD1
   TRAC-BD1, best estimate analysis BWR LOCA

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC CYBER176,CDC6600

3. **DESCRIPTION** - TRAC-BD1 performs best estimate analyses of loss-of-coolant accidents (LOCA) and other transients in boiling water reactors (BWRs). The program provides LOCA analysis capability for BWRs and for many BWR-related thermal-hydraulic experimental facilities. The program features a three-dimensional treatment of the BWR pressure vessel, a detailed model of a BWR fuel bundle including multi-rod, multi-bundle, radiation heat transfer, and leakage path modeling capability; flow-regime-dependent constitutive equation treatment; reflood tracking capability both for falling films and bottom flood quench fronts; and consistent treatment of the entire accident sequence. Dump/restart capabilities are also provided.

4. **METHOD OF SOLUTION** - The system of partial differential equations describing the two-phase flow and heat transfer is solved by use of finite difference techniques. The heat transfer equations are treated as one-dimensional using a semi-implicit differencing technique. The finite difference equations for hydrodynamic phenomena form a system of coupled, nonlinear equations solved by a Newton-Raphson iteration procedure.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - All storage arrays in the program are dynamically allocated; the only limit on the size of a problem is the amount of memory available. The number of reactor components in the problem and the manner in which they are coupled is arbitrary. Reactor component models available in TRAC-BD1 include pipes, pumps, separator-dryers, tees, valves, fuel channels, jet pumps, and vessels with associated internals.

6. **TIMING** - Running time is highly problem-dependent and is a function of the total number of mesh cells and the maximum allowable time-step size. Total run time can be estimated from a unit run time of 2 to 3 ms per mesh cell per time step and an average time-step size of 5 ms. The longest running sample problem requires about 2.5 minutes of CPU time on the CDC6600.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - TRAC-BD1 is a highly versatile program that can describe many thermal-hydraulic experiments in addition to the wide variety of BWR reactor system designs. The program was developed under stringent quality control measures that provide a detailed historical account of the entire development process.

8. **RELATED AND AUXILIARY SOFTWARE** - One of the output files written by TRAC contains graphics information that can be used to produce plots. Auxiliary programs that read the plot file are provided separately in the Idaho National Engineering Laboratory Scientific Data Management System (ISDMS) software (NESC 1034).

9. **STATUS** - Abstract first distributed April 1984.
   CDC CYBER176 version of TRAC-BD1 submitted February 1981, revised March 1983, sample problems executed April 1983 on a CDC6600.

10. **REFERENCES** - J. W. Spore, M. W. Giles, G. L. Singer and R. W. Shumway, TRAC-BD1: An Advanced Best Estimate Computer Program for Boiling Water Reactor Loss-of-Coolant Accident Analysis, NUREG/CR-2178, Volumes 1, 2, 3, and 4, October 1981.

TRAC-BD1, NESC No. 1031.C176, TRAC-BD1 Tape Description and Implementation Information, National Energy Software Center Note 84-29, April 30, 1984.

TRAC-BD1, NESC No. 1031.C176B, TRAC-BD1 Edition B Non-CDC System Tape Description and Implementation Information, National Energy Software Center Note 84-30, April 30, 1984.

M. M. Aburomia, BWR Refill-Reflood Program, TRAC-BWR Component Development, NUREG/CR-2135 (EPRI NP-1583/GEAP-24941), December 1981.

Craig M. Kullberg, Overview of TRAC-BD1 (Version 12) Assessment Studies, NUREG/CR-4196 (EGG-2382), April 1985.

11. **HARDWARE REQUIREMENTS** - CDC CYBER176 computer with 65K words of small core memory (SCM) and 220K words of large core memory (LCM). Minor changes to the standard version are needed to reduce the SCM requirements to this size, since the standard version uses approximately 123K words to obtain maximum efficiency.

12. **PROGRAMMING LANGUAGE** - CDC FORTRAN Extended Version 4 and COMPASS

13. **OPERATING SYSTEM** - CDC CYBER176 NOS/BE 1.4 operating system and OVERLAY loader.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Memory should be set to zero prior to execution. FORTRAN equivalents of the COMPASS matrix inversion routines are included in the package.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

J. W. Spore, M. W. Giles, G. L. Singer,
and R. W. Shumway
EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -

Source (C176 TRAC-BD1 UPDATE source 408 records•, C176 TRAC-BD1 FORTRAN and COMPASS source 887 records•, C176B TRAC-BD1 50,336 records+)
Run (C176 401 records•)
Sample problem input (C176 18 records•, C176B 1965 lines)
Sample problem output (21 selected pages, C176 98 records•, C176B 10,482 135-character records)
Data libraries (C176 99 records•, C176B 2479 records+)
Control information (C176 5 records•, C176B 237 lines)
Auxiliary information (C176 680 records•. C176B 288 lines)
Reference reports, NUREG/CR-2178, Vols. 1, 2, 3, and 4 and NESC Note, appropriate to version

• maximum record size 3840 bytes
+ 90-byte records

17. **CATEGORY** - G
KEYWORDS - accidents, reactor safety, thermodynamics, heat transfer, reactor kinetics, two-phase flow, BWR reactors, loss of coolant, transients

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research

1. **IDENTIFICATION AND KWIC TITLE** - POOLS
   POOLS, estimating swimming pool heating costs

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600,CYBER175, IBM370,303x

3. **DESCRIPTION** - POOLS was developed to compare in detail a wide range of outdoor swimming pool energy conservation measures and solar heating options. The POOLS model can simulate a specific pool at a given location with specified weather, wind, and shading conditions, and a variety of energy saving measures to assess the effects of a combination of insulated and uninsulated pool covers, solar collectors, thermostat settings, night thermostat setback, and changes in the length of heating seasons. POOLS also performs 30-year life-cycle cost calculations. The life-cycle cost represents the present worth of all future costs needed to heat the pool for its assumed 30-year lifetime. The life-cycle cost analysis includes the original equipment and installation costs, equipment design life, and maintenance costs for the 30-year period.

4. **METHOD OF SOLUTION** - Pool heat gains and losses are calculated in two-hour steps. The pool temperature at the end of each step is raised or lowered according to the net pool heat gain or loss during that time. This procedure is repeated for successive time intervals. The pool is simulated over a year's time by making over 4300 successive two-hour heat balance calculations. The hour-by-hour weather and solar data used in the heat balance calculations are based on an "average day" for each month. Twelve average days, one for each month, are used to define the insolation and weather for each city. The data used in the calculations for each average day include values of dry-bulb temperature, wet-bulb temperature, wind speed, cloud cover, and insolation for each two-hour interval. Information used to specify these is taken from National Climatic Center "Local Climatological Data" summaries or the California Solar Data Manual. The calculation of evaporation, convection, and conduction heat losses from an uncovered pool are based on work by Paul Klotz (reference 5).

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Up to eight types of energy conservation measures can be used at the same time in a life-cycle cost analysis. These measures can be active, passive, or both.

6. **TIMING** - NESC executed the sample problem in 97 CP seconds on a CDC CYBER175 and in 126 CPU seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed June 1983.
   CDC7600 version submitted August 1979, sample problem executed by NESC May 1983 on a CDC CYBER175.
   IBM370 version submitted July 1980, sample problem executed by NESC May 1983 on an IBM3033.

10. **REFERENCES** - John Wei, Harry Sigworth, Jr., and Claudette Lederer, User's Manual for "POOLS" Program, LBL-10152, November 1979.

John Wei, Harry Sigworth, Jr., Claudette Lederer, and A. H. Rosenfeld, A Computer Program for Evaluating Swimming Pool Heat Conservation, LBL 9388, July 1979.

Harry Sigworth, Jr., John Wei, and A. H. Rosenfeld, Reducing Swimming Pool Heating Costs: Comparison of Pool Covers, Solar Collectors and Other Options, LBL 9039, received April 1980.

P. Berdahl, D. Grether, M. Martin, and M. Wahlig, California Solar Data Manual, March 1978.

P. S. Klotz, Heating Requirements of Swimming Pools, Thesis, Department of Aeronautics and Astronautics, Stanford University, 1977.

11. **HARDWARE REQUIREMENTS** - 128K bytes of memory are required for execution with the IBM370 version; the CDC7600 version requires 33,000 (octal) words of memory.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE2.1 (CDC7600), NOS 1.4 (CDC CYBER175), OS/MVT (IBM370), MVS (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
C. Lederer and H. Sigworth, Jr.
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
Source (7600-2354 lines, 370-2523 lines)
Sample problems (143 lines)
Control information (370-57 lines)
Sample problems output (7600-50 pages, 370-51 pages)
Reference reports, LBL 9039, LBL 9388, LBL-10152

17. **CATEGORY** - R
KEYWORDS - swimming pools, energy conservation, heaters, life-cycle cost, meteorology, solar collectors, solar water heating, temperature

18. **SPONSOR** - DOE Office of Conservation and Solar Applications,
Division of Building and Community Systems

1. **IDENTIFICATION AND KWIC TITLE -** LSAP, DIGLIB
   LSAP/DIGLIB, linear systems analysis program

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11,PDP11,LSI11

3. **DESCRIPTION -** LSAP (Linear Systems Analysis Program) is an interactive program with graphics capability provided through DIGLIB (Device Independent Graphics Library) that can be used for the analysis and design of linear control systems. Nearly all the classical design tools are available, including manipulation of transfer functions and generation of root locus, time response, and frequency response plots. The program is capable of working with continuous time systems and sampled data systems. For continuous time systems, the Laplace transform is used and for sampled data systems, the Z-transform is used. The capability to convert from a Laplace transform to a Z-transform is provided. The program is intended primarily for the analysis of feedback control systems. The system configuration or parameters can be changed easily, allowing the user to design compensation networks and perform sensitivity analyses in a very convenient manner.

   DIGLIB is a collection of general graphics subroutines. It was designed to be small, reasonably fast, device-independent, and compatible with RT-11, RSX-11M, and VMS and readily usable by casual programmers for two-dimensional plotting. DIGLIB has device drivers for Tektronix 4010, 4012, 4014, 4025, and 4027 terminals; VT100 terminals with the retrographics option; GIGI terminals, CalComp 1012 plotters, and Lexidata 3400 color graphics systems.

4. **METHOD OF SOLUTION -** LSAP performs its modeling by defining and operating upon polynomial fraction representations of transfer functions. It is a command oriented program. A command is entered, together with any necessary data, and then executed. The program is then ready for the next command. The MAIN procedure accepts a command and calls the appropriate command procedure, until the program is halted. Each command procedure uses any utilities required for the execution of the command. The commands interact with global data in two basic ways. All defined transfer functions are global records, which exist in a linked list. All commands except HALT and HELP operate upon these records. Also included in global data are switches, flags, pointers, and scalars which describe the state of the program and control the operations performed by the commands.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -** The program can only be applied to systems which can be described by a collection of rational transfer functions that are either Laplace or Z-transforms. The order of the numerator or denominator polynomials cannot exceed 20.

6. **TIMING -** This varies according to the nature of the systems, the number of generated plots, the speed at which the user can specify input data, and other factors.

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -** LSAP is based on an IBM PL/I program developed by D. J. Duven at Iowa State University.

9. **STATUS -** Abstract first distributed August 1983.
   DEC VAX11 version submitted May 1983, sample problem executed by NESC May 1983 on a DEC VAX11/780 using a Tektronix 4025 terminal.

10. **REFERENCES -** Thomas P. Weis, Linear System Analysis Program Programmer's Manual, UCID-30183, February 15, 1981.

    Charles J. Herget and Thomas P. Weis, Linear Systems Analysis Program User's Manual, UCID-30184, October 15, 1980.

    LSAP,DIGLIB, NESC No. 1033, LSAP,DIGLIB Tape Description and Programmer Information, National Energy Software Center Note 83-83, August 22, 1983.

    H. R. Brand and R. K. Yamauchi, PLTLIB, Graphics Library for Tektronix 4025 and 4027 Terminals, UCID-18981, January 25, 1981.

11. **HARDWARE REQUIREMENTS** - One of the graphics terminals listed in item 3.

12. **PROGRAMMING LANGUAGE** - FORTRAN, PASCAL, and MACRO-11 (LSAP), FORTRAN and MACRO-11 (DIGLIB).

13. **OPERATING SYSTEM** - RSX-11M (PDP11, LSI11), VMS 3.2 (VAX11).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - LSAP was developed using the PASCAL 1.0 compiler. NESC attempted to test the program using PASCAL 2.0 and was unable to obtain a usable LSAP executable module. However, LSAP was executed successfully by NESC using the executable modules supplied by the authors. PASCAL 1.0 is required for this release of the program.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

LSAP	C. J. Herget
DIGLIB	H. R. Brand Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (263 blocks*)
    Object library (132 blocks*)
    Auxiliary information (machine-readable documentation 49 blocks*)
    Control information (28 blocks*)
    Reference reports, UCID-30183, UCID-30184, and NESC Note
    * 2048-character records

17. **CATEGORY** - N
    KEYWORDS - control systems, feedback, computer graphics, systems analysis, response functions, transfer functions, interactive computing

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
    Division of Engineering, Mathematical and Geo-sciences

1. **IDENTIFICATION AND KWIC TITLE** - ISDMS
   ISDMS, INEL scientific data management system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER176

3. **DESCRIPTION** - The Idaho National Engineering Laboratory (INEL) Scientific Data Management System, ISDMS, is a generalized scientific data processing system designed to meet the needs of the various organizations at the INEL. It consists of a set of general and specific processors running under the control of an executive processor which serves as the interface between the system and the user. The data requirements at the INEL are primarily for time series analyses. Data acquired at various site facilities are processed on the central CDC CYBER computers. This processing includes: data conversion, data calibration, computed parameter calculations, time series plots, and sundry other applications. The data structure used in ISDMS is CWAF, a common word addressable format. A table driven command language serves as the ISDMS control language. Execution in both batch and interactive mode is possible. All commands and their input arguments are specified in free form. ISDMS is a modular system both at the top executive or MASTER level and in the independent lower or sub-level modules. ISDMS processors were designed and isolated according to their function. This release of ISDMS, identified as 1.3A by the developers, includes processors for data conversion and reformatting for applications programs (e.g. RELAP4), interactive and batch graphics, data analysis, data storage, and archival and development aids.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Abstract first distributed November 1985.
   CDC CYBER176 version submitted March and May 1982, FORTRAN source compiled by NESC May 1982 on a CDC7600 and CYBER175.

10. **REFERENCES** - H. R. Bruestle, K. D. Russell, D. M. Snider, and H. D. Stewart, Idaho National Engineering Laboratory Scientific Data Management System Release 1.2, EGG-IS-5528, August 1981.
    ISDMS, NESC No. 1034, IDSMS Tape Description and Implementation Information, National Energy Software Center Note 86-11, November 22, 1985.

11. **HARDWARE REQUIREMENTS** - ISDMS will execute on CDC CYBER mainframes running under the NOS/BE operating system only. 250K (octal) words of SCM and 100K (octal) words of LCM storage.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV and COMPASS

13. **OPERATING SYSTEM** - NOS/BE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Proprietary CDC common decks and Record Manager BAMLIB/AAMLIB libraries and the ISSCO DISSPLA 9.0 and Tektronix PLOT-10 graphics software required to implement ISDMS are not included. SYSTEXT, PFMTEXT, TXTCRM, CPUTEXT, and IOTEXT used at INEL are not included. These or similar system texts are necessary to assemble the various ISDMS macros.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    H. R. Bruestle, K. D. Russell,
    D. M. Snider, and H. D. Stewart
    EG&G Idaho, Inc.

16. **MATERIAL AVAILABLE** -
    Source (270,659 lines)
    Control (1,774 lines)
    Reference report and NESC Note

17. **CATEGORY** - M
    KEYWORDS - data processing, digital filters, data analysis, data base management, computer graphics

18. **SPONSOR** - EG&G Idaho, Inc.
    Idaho National Engineering Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - ALICE/LIVERMORE82
   ALICE/LIVERMORE82, precompound compound decay

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600 (designed to be machine-independent)

3. **DESCRIPTION** - ALICE/LIVERMORE82 calculates particle spectra and yields for precompound plus compound decay, including fission competition. Multiple decay of neutron (n), proton (p), alpha, and deuteron (d) particles may be considered. The program can perform a standard Weisskopf-Ewing evaporation calculation with multiple particle emission or an s-wave approximation calculation which gives an upper limit to the enhancement of gamma ray de-excitation due to angular momentum effects. The evaporation calculation can include fission competition according to the Bohr-Wheeler approach, using angular momentum dependent ground state and saddle point energies. (The latter values are derived from Cohen rotating liquid drop model.) Provision to permit precompound emission via the hybrid and geometry-dependent hybrid models is included.

4. **METHOD OF SOLUTION** - In the Weisskopf evaporation calculation, the inverse reaction cross sections may be provided as input data or computed with a classical sharp cutoff algorithm or an optical model routine. In the s-wave approximation the calculation is performed for every partial wave in the entrance channel. The transmission coefficients for the entrance channel partial waves may be provided as input data or by the parabolic model or optical model calculation. The Myers-Swiatecki/Lysekil mass formula is used to calculate the Q value for formation of the compound nucleus and the n, p, alpha, and d binding energies for all nuclides of interest in the evaporation chain.

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - Excitation energies of the compound nucleus up to 200 MeV can be considered in the Weisskopf evaporation calculation. In the s-wave approximation it is assumed that the rotational energy for each partial wave is irrevocably committed to rotational motion and, therefore, unavailable for particle emission.

6. **TIMING** - The sample problem execution time is approximately 10 seconds on a CDC7600 and 40 seconds on an IBM3033.

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** - ALICE/LIVERMORE82 is a revision of the earlier ALICE and OVERLAID ALICE codes.

9. **STATUS** - Abstract first distributed April 1984.
   CDC7600 version submitted November 1983, sample problem executed by NESC December 1983 on an IBM3033.

10. **REFERENCES** - M. Blann and J. Bisplinghoff, CODE ALICE/LIVERMORE82, UCID-19614, November 5, 1982.
    ALICE/LIVERMORE82, NESC No. 1036, ALICE/LIVERMORE82 Tape Description and Implementation Information, National Energy Software Center Note 84-28, April 30, 1984.
    M. Blann, OVERLAID ALICE: A Statistical Model Computer Code including Fission and Preequilibrium Models, COO-3494-29, August 1976.

11. **HARDWARE REQUIREMENTS** - NESC used approximately 244K bytes on an IBM3033 to execute the sample problem.

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE (CDC7600), OS/MVT (IBM3033).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The FORMAT statements contain " delimiters.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**

M. Blann
Lawrence Livermore National Laboratory
J. Bisplinghoff
Institut fuer Strahlen und Kernphysik
Bonn University
Germany

16. **MATERIAL AVAILABLE -**

Source (4286 lines)
Sample problem input (7 lines)
Sample problem output (607 120-character records)
Reference report, UCID-19614, and NESC Note

17. **CATEGORY - W**

KEYWORDS - evaporation model, compound-nucleus reactions, precompound-nucleus emission, Weisskopf model, Bohr-Wheeler theory, nuclear models

18. **SPONSOR -** DOE Office of Basic Energy Sciences

IDENTIFICATION AND KWIC TITLE - BIMOND
BIMOND, monotone bivariate interpolation code

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE - any computer with a FORTRAN 77 compiler

DESCRIPTION - BIMOND is a FORTRAN 77 subroutine for piecewise bicubic interpolation to data on a rectangular mesh, which reproduces the monotonicity of the data. A driver program, BIMOND1, is provided which reads data, computes the interpolating surface parameters, and evaluates the function on a mesh suitable for plotting.

METHOD OF SOLUTION - Monotonic piecewise bicubic Hermite interpolation is used.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - The current version of the program can treat data which are monotone in only one of the independent variables, but cannot handle piecewise monotone data.

TIMING - Running time varies with the computer used. Less than 8 CPU seconds were required on an IBM3033 to compile and execute the sample problem.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE - BIMOND calls subroutine PCHIM from the univariate piecewise cubic interpolation package PCHIP (NESC 9917). This subroutine is included as a separate file in the BIMOND package.

STATUS - Abstract first distributed October 1984.
BIMOND submitted December 1983, sample problem executed by NESC January 1984 on an IBM3033.

REFERENCES - F. N. Fritsch and R. E. Carlson, BIMOND: Monotone Bivariate Interpolation Code, UCID-30197, December 1983.
R. E. Carlson and F. N. Fritsch, Monotone Piecewise Bicubic Interpolation, UCRL-86449, Rev. 1 Preprint, September 1983.
F. N. Fritsch, PCHIP Final Specifications, UCID-30194, August 1982.
BIMOND, NESC No. 1037, BIMOND Tape Description and Implementation Information, National Energy Software Center Note 85-10, October 22, 1984.

HARDWARE REQUIREMENTS - On the IBM3033 1028K bytes of virtual storage and 216K bytes of system storage were required. Logical unit 5 is used for input, 6 for printed output, 7 for plotted output, and 59 for interactive terminal communication.

PROGRAMMING LANGUAGE - FORTRAN 77

OPERATING SYSTEM - NESC executed the sample problem on an IBM3033 with a MVS operating system.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The only new FORTRAN 77 features used are IF-THEN-ELSE control statements, PARAMETER statements, and quote delimiters for character strings. A minimum of four characters per word is assumed.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
F. N. Fritsch and R. E. Carlson
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (3589 lines)
Sample problem (120 lines)
Sample problem output plot file (40 lines)
Sample problem output (240 120-character records)
Reference reports, UCID-30197 and UCRL-86449, Rev. 1 Preprint, and NESC Note

17. CATEGORY - P
KEYWORDS - interpolation, numerical data, algorithms, PCHIP codes

18. SPONSOR - DOE Office of Basic Energy Sciences

IDENTIFICATION AND KWIC TITLE - LAYFLO
LAYFLO, radionuclide transport geologic medium

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER74,175

DESCRIPTION - LAYFLO predicts the one-dimensional convective-dispersive and nondispersive transport of a three-member decay chain in a stratified geologic medium. The dispersive solution is restricted to six layers, while the nondispersive solution can handle any number of layers. The accuracy of LAYFLO was tested on a selected number of problems for which analytical solutions or experimental data were available.

METHOD OF SOLUTION - The set of differential equations describing the migration process is solved by the Laplace transformation technique using a semi-analytical approach subject to either of two types of boundary conditions, a continuous source or a band release from the source mode.

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM - Maxima of -
6 layers (dispersive solution)
3 species
The code has only been used for Peclet number much greater than one.

TIMING - NESC executed all of the sample problems in less than 3 CP minutes on a CDC CYBER175.

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Abstract first distributed June 1984.
CDC CYBER74 version submitted April 1983, sample problems executed by NESC February 1984 on a CDC CYBER175.

REFERENCES - A. B. Gureghian and G. Jansen, LAYFLO: A One-Dimensional Semianalytical Model for the Migration of a Three-Member Decay Chain in a Multilayered Geologic Medium, ONWI-466, May 1983.

LAYFLO, NESC No. 1038, LAYFLO Tape Description and Implementation Information, National Energy Software Center Note 84-31, June 1, 1984.

U. Y. Shamir and D. R. F. Harleman, Numerical and Analytical Solutions of Dispersion Problems in Homogeneous and Layered Aquifers, Massachusetts Institute of Technology Report No. 89, 1966.

HARDWARE REQUIREMENTS - 54,000 (octal) words of memory are required for execution.

PROGRAMMING LANGUAGE - FORTRAN 77

OPERATING SYSTEM - NOS/BE 1.5 (CDC CYBER74), NOS 1.4 (CDC CYBER175).

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS - The VAX version of LAYFLO and auxiliary graphic program mentioned in the ONWI-466 reference report are not available from the authors.

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
A. B. Gureghian and G. Jansen
Office of Nuclear Waste Isolation
Battelle Project Management Division

MATERIAL AVAILABLE - Restricted Distribution
Source (3270 lines)
Sample problems (536 lines)
Sample problems output (3397 133-character records)
Reference report, ONWI-466, and NESC Note

17. **CATEGORY** - R
KEYWORDS - radioactive waste storage, radionuclide migration, convection, ground water, geologic formations, layers, Laplace transformation

18. **SPONSOR** - DOE National Waste Terminal Storage Program Office

1. **IDENTIFICATION AND KWIC TITLE -** TOOLPACK1
   TOOLPACK1, software tools for FORTRAN 77

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11, Apollo, ICL PERQ

3. **DESCRIPTION -** TOOLPACK1 consists of the following categories of software: (1) an integrated collection of tools intended to support the development and maintenance of Fortran 77 programs, in particular moderate-sized collections of mathematical software; (2) three user/Toolpack interfaces, one of which is selected for use at any particular installation; (3) three implementations of the tool/system interface, called TIE (Tool Interface to the Environment). The tools are written in Fortran 77 and are portable among TIE installations. The source contains symbolic constants as macro names and must be expanded with a suitable macro expander before being compiled and loaded. A portable macro expander is supplied in TOOLPACK1.

   The tools may be divided into three functional areas: general, documentation, and FORTRAN processing. One tool, the macro processor, can be used in any of these categories.

   General Tools

   ISTDC This data comparison tool is designed mainly for comparing files of numeric values, though it is also capable of comparing files with embedded text.

   ISTFI This tool will find all the include files mentioned in a specified file, including those that are nested.

   ISTFL This tool will measure the length of a sequential file in lines and characters.

   ISTGP This is a general pattern-matching tool similar to the Unix grep facility.

   ISTHP This tool will provide limited help information about tools. The user enters regular expressions which are matched against keyword lists to trigger text output. The information in the help system is based on that provided in the Tool Quick Reference Guide.

   ISTMP The macro processor may be used to preprocess a file. The processor provides macro replacement, inclusion, conditional replacement, and processing capabilities for complex file processing. (This tool also has uses in FORTRAN processing and documentation preparation.)

   ISTSP This is a TIE-conforming version of the SPLIT utility to split up the concatenated files used on the tape.

   ISTSV This is a save/restore utility to save and restore sub-trees of the Portable File Store (PFS).

   ISTTD This is a text file comparison tool.

   ISTVC This is a simple text file version controller. Version files may be created and recalled either by version number or date/time.

   Documentation Generation Tools

   ISTDX This is a tool used to strip comments identified by source embedded directives from a Fortran source file, permitting use of embedded documentation within a program unit.

   ISTMP The macro processor may be used to expand formatting commands from the TOOLPACK documentation macro definitions into standard ISTRF commands. The documentation macros provide a much higher degree of control over document formatting. The macro processor can read the macros and process them to produce output suitable either for ISTRF or the Unix nroff/troff tool. (This tool also has uses in Fortran processing and general macro expansion.)

   ISTRF This is a text formatter similar to the Unix nroff/troff facility. The formatter reads

unformatted text and embedded formatting commands and produces formatted output text suitable for immediate printing.

Fortran 77-Oriented Tools

ISTAN This is an instrumentor for Fortran 77 that permits the collection of run time execution frequency information, tracing information, and assertion violation counts.

ISTDS This is a declaration standardizer that rebuilds the declarative parts of a Fortran 77 program unit according to a programmable template.

ISTED This is a line-based editor derived from the Software Tools ED editor. ISTED has additional capabilities to assist the Fortran 77 programmer, including a macro facility with all keywords predefined. The editor includes programming capabilities and some intrinsic functions.

ISTFD This is a comparison tool for token streams rather than source text, allowing the comparisons to disregard layout and (optionally) comments.

ISTGI This tool will change all intrinsic function references within Fortran 77 code to their generic forms (where this is legal or possible).

ISTLX This is a low-level tool that scans Fortran 77 source text and produces a token stream and separate comment file. The token stream does not include information about layout but provides identification of keywords and string/numeric values within the original source.

ISTMP The macro processor may be used to process Fortran source text. The 'eval' expression evaluation facility of ISTMP includes the Fortran intrinsic functions in addition to arithmetic facilities. As ISTMP is loaded with the host libraries the intrinsic functions will be the same as those that the processed program will use; this can be useful in the expansion of fixed constants within portable tools. (This tool also has uses in general macro expansion and documentation preparation.)

ISTPL This is a Fortran 77 formatter or "pretty printer." The options for this tool may be set or changed using the separate menu-driven polish options editor ISTPO.

ISTPO This is the polish options editor (see ISTPL).

ISTPT This is an automatic precision converter for Fortran 77. It can convert between REAL and DOUBLE PRECISION, changing intrinsics, constants, formats, and declarations.

ISTVS This tool will format the symbol table for a program unit into a form suitable for display or printing.

ISTVT This tool will format a parse tree for a program for viewing on a terminal (using the WINDOW supplementary library capability) or printing on a printer.

ISTYP This is a parse tree builder.

ISTYF This is a parse tree flattener.

NEWTON The Newton system is a set of tools to instrument a Fortran 77 program to provide a portable, interactive run time debug system. In TOOLPACK1 this is only a development system.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** - In order to run the TOOLPACK tools, an implementation of TIE must be running on the host computer system. The three

implementations of TIE are Fortran 77, C, and a version for VAX/VMS in PASCAL. The Fortran 77 implementation contains macro constants that must be specified for each host machine. Further, several host-dependent routines must be supplied by the installer and various host-sensitive routines must be checked. Installation guides for TIE and the tools are included with the documentation.

One of the user/Toolpack interfaces is a collection of Unix shell scripts. The other two are written in FORTRAN and conform to TIE.

6. **TIMING** - Running time varies with problem size. NESC executed the test command procedures in an interactive session using a small input FORTRAN program of about 50 lines in approximately 30 seconds on a DEC VAX11/780 running under VMS 4.2.

7. **UNUSUAL FEATURES OF THE SOFTWARE** - User documentation and installation guides are in machine-readable form.

8. **RELATED AND AUXILIARY SOFTWARE** - The tools source code needs to be split up using the SPLIT utility program and the results preprocessed using the TIEMAC macro expander utility. Both of these programs are provided.

9. **STATUS** - Abstract first distributed December 1985.
   DEC VAX11/780 version of TOOLPACK1 submitted March 1985, revised August 1985, revised October 1985, sample problems executed by NESC November 1985 on a DEC VAX11/780.

10. **REFERENCES** - W. R. Cowell, S. J. Hague, and R. M. J. Iles, Toolpack/1 - Introductory Guide, NP1007, February 1985.
    TOOLPACK1, NESC No. 1056.VX11, TOOLPACK1 Version 1.3 DEC VAX11/780 Tape Description, Implementation Information for DEC VAX11/780 VMS Systems, and TOOLPACK/1 Introductory Guide Errata, National Energy Software Center Note 86-08, December 9, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77 (96%), PASCAL V2 (1%), and C (3%).

13. **OPERATING SYSTEM** - VMS 4.2 (DEC VAX11).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - Installation of TIE on the host computer is required prior to implementation of TOOLPACK1. Guides for TIECODE, machine-specific versions of TIE, and for installing the tools are provided on the transmittal tape in a form formatted for line printer output. Unformatted copies are also provided for formatting using the TOOLPACK1 tools ISTMP and ISTRF and the Toolpack Documentation Macros. NESC implemented TOOLPACK1 in the VAX11/780 virtual memory environment.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    W. R. Cowell
    Mathematics and Computer Science Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (FORTRAN-147,744 lines, C-4267 lines, PASCAL-1511 lines)
    Machine-readable documentation (40,801 lines)
    Control information (4086 lines)
    Reference report and NESC Note

17. **CATEGORY** - P
    KEYWORDS - utility routines, programming, DEC computers, interactive computing, FORTRAN

18. **SPONSOR** - DOE Office of Basic Energy Sciences
    NSF Computer Sciences Division
    United Kingdom Science and Engineering Research Council

1. **IDENTIFICATION AND KWIC TITLE** - WAPPA
   WAPPA, waste package performance assessment

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - WAPPA, the WAste Package Performance Assessment program, is intended to serve as a tool for evaluating both the relative and the absolute performance of waste package design concepts, for guiding or selecting a preliminary design among conceptual designs, and for support of licensing activities. WAPPA is a barrier degradation code for a nuclear waste package in a geologic repository. The WAPPA model includes five distinct degradation process models (radiation, thermal, mechanical, corrosion, and leaching), which are driven internally by waste decay and externally by repository stress and fluids. The modeling approach is barrier-integrated and process-sequential, allowing modification of the entire waste package by the sequential operation of five process models within each time-step. The process models are coupled at the system level via state and coupling variables. The penetration of water into the waste package and its effects on the barriers it contacts are tracked radially inwards. The WAPPA model describes and predicts the temporal and spatial extent of the loss of containment capability for each barrier and for the entire waste package, on any time scale up to one million years after isolation.

   Input includes the radial geometry and material properties of each component, degradation rates for each process modeled, and time-dependent boundary conditions (fluid flux, mechanical stress, and temperature) at the waste package/repository interface. The output quantifies the residual state of integrity of waste package components as a function of time and calculates the heat and radionuclide fluxes output to the repository. Other output at each calculation time point includes: the temperature and nuclide concentration profiles internal to the waste package, residual mass fractions of radionuclides in the wasteform and residual waste mass fraction, and various barrier status degradation indices and parameters. In addition, summary output includes the total mass for each nuclide output to the repository and the barriers' status history used to pinpoint times of failure.

   The fluid flux required as an input boundary condition to WAPPA can be calculated by STFLO (NESC 9852) as a function of time and stored in the geology-specific boundary conditions file. Similarly, the DOT-BPMD (NESC 9833) program can be used at the front-end to simulate time-dependent temperatures at the waste package/repository boundary.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1986.
   DEC VAX11/780 version submitted December 1985.

10. **REFERENCES** - INTERA Environmental Consultants, Inc., WAPPA: A Waste Package Performance Assessment Code, ONWI-452, April 1983.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
G. Kilshtok
Office of Nuclear Waste Isolation
Battelle Project Management Division

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (12,844 lines)
The reference report and WAPPA source, sample problem input and output, libraries, and auxiliary information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – R
KEYWORDS – waste management, decay, radioactive waste disposal, licensing, waste-rock interactions, high-level radioactive wastes, spent fuels, SCEPTER project, ORIGEN2 codes, STFLO codes, DOT-BPMD codes

18. **SPONSOR** – DOE Salt Repository Project Office

IDENTIFICATION AND KWIC TITLE - PHREEQE
PHREEQE, geochemical speciation mass transfer

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC CYBER176

DESCRIPTION - PHREEQE is designed to model geochemical reactions. Based on an ion pairing aqueous model, PHREEQE can calculate pH, redox potential, and mass transfer as a function of reaction progress. It can be used to describe geochemical processes for both far-field and near-field performance assessment and to evaluate data acquisition needs and test data. It can also calculate the composition of solutions in equilibrium with multiple phases. The data base, including elements, aqueous species, and mineral phases, is independent of the program and is completely user-definable. PHREEQE requires thermodynamic data for each solid, gaseous, or dissolved chemical species being modeled. The two data bases, PREPHR and DEQPAK7, supplied with PHREEQE are for testing purposes only and should not be applied to real problems without first being carefully examined.

The conceptual model embodied in PHREEQE is the ion-association model of Pearson and Noronha. In this model a set of mass action equations are established for each ion pair (and controlling solid phases when making mass transfer calculations) along with a set of mass balance equations for each element considered. These sets of equations are coupled using activity coefficient values for each aqueous species and solved using a continued fraction approach for the mass balances combined with a modified Newton-Raphson technique for all other equations. The activity coefficient expressions in PHREEQE include the extended Debye-Huckel, WATEQ Debye-Huckel, and Davies equations from the original United States Geological Survey version of the program.

The auxiliary preprocessor program PHTL, which is derived from EQTL, converts EQ3/6 (NESC 886) thermodynamic data to PHREEQE format so that the two programs can be compared. PHREEQE can be used to determine solubility limits on the radionuclides present in the waste form. These solubility constraints may be input to the WAPPA (NESC 9673) leach model.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed January 1986.
CDC CYBER176 version submitted December 1985.

REFERENCES - INTERA Environmental Consultants, Inc., PHREEQE: A Geochemical Speciation and Mass Transfer Code Suitable for Nuclear Waste Performance Assessment, ONWI-435, April 1983.

David L. Parkhurst, Donald C. Thorstenson, and L. Niel Plummer, PHREEQE - A Computer Program for Geochemical Calculations, U. S. Geological Survey, Water Resources Investigations, pp. 80-96, November 1980.

T. J. Wolery, Calculation of Chemical Equilibrium Between Aqueous Solution and Minerals: The EQ3/6 Software Package, UCRL-52658, February 1979.

HARDWARE REQUIREMENTS - 56K (octal) words

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM - NOS 1.4.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
G. Kilshtok
Office of Nuclear Waste Isolation
Battelle Project Management Division

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2624 lines)
The ONWI-435 reference report and PHREEQE and PHTL source, PHREEQE sample problems input and output, DEQPAK7 input, and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
KEYWORDS - geochemistry, equilibrium, aqueous solutions, mass transfer, water chemistry, redox potential, SCEPTER project, EQ3/6 codes, PHTL codes, EQTL codes, WAPPA codes

18. **SPONSOR** - DOE Salt Repository Project Office

IDENTIFICATION AND KWIC TITLE - ALIS3.0
ALIS3.0, ab initio MCSCF & CI calculations

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM370

DESCRIPTION - ALIS (Ames Laboratory Iowa State) is a system of 20 stand-alone programs and related routines. ALIS performs ab-initio quantum mechanical calculations of the electronic structure of atoms and molecules with particular, although not exclusive, emphasis on the multi-configuration self-consistent-field approach.

Generally contracted, even-tempered, Cartesian Gaussian functions are used to evaluate all one- and two-electron integrals necessary to evaluate stationary state electronic wavefunctions in the Born-Oppenheimer approximation. Some restricted Hartree-Fock wavefunctions may be evaluated. The Brillouin-Levy-Berthier theorem and natural orbitals are used to generate orbitals that are self-consistent for a list of given configurations.

ALIS currently evaluates only s, p, and d functions with no storage rectrictions on the number of functions or atoms. Only systems with closed shells or just one open shell can be evaluated at the RHF level. At the MCSCF level, no spin eigenfunction may have more than eight unpaired electrons. Run time considerations usually restrict MCSCF calculations to fewer than 30 configurations and CI calculations to fewer than 2000 configurations.

This release is identified as ALIS3.0; it supersedes the original CDC version which was transferred from the National Resource for Computation in Chemistry's software library.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed January 1986.
CDC7600 version of ALIS submitted February 1981, replaced April 1981 by IBM370 version of ALIS3.0.

REFERENCES - K. Ruedenberg, L. M. Cheung, and S. T. Elbert, MCSCF Optimization through Combined Use of Natural Orbitals and the Brillouin-Levy-Berthier Theorem, International Journal of Quantum Chemistry, Vol. 16, pp. 1069-1101, 1979.

HARDWARE REQUIREMENTS - 320K bytes

PROGRAMMING LANGUAGE - FORTRAN IV and Assembler

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
S. T. Elbert
Ames Laboratory
Iowa State University

MATERIAL AVAILABLE -
Source (45,864 lines)
Sample problems output and the ALIS3.0 source, object, sample problems input, control information, and ALIS Reference Manual in machine-readable form on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - W

KEYWORDS - electronic structure, Gauss function, quantum mechanics, self-consistent molecules, Hartree-Fock method, wave functions, configuration interaction

18. **SPONSOR** - DOE Office of Basic Energy Sciences,
Division of Chemical Sciences
Ames Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - BARMOM
   BARMOM, fission barriers & moments of inertia

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
MPLN (designed to be portable)

3. **DESCRIPTION** - BARMOM is a collection of three FORTRAN 77 subroutines: BARFIT, MOMFIT, and LPOLY. BARFIT calculates the fission barrier height (in Mev), the rotating ground-state energy (in Mev), and the maximum angular moment possible in a system of atomic number IZ, atomic mass IA, and angular momentum IL (in units of h-bar). MOMFIT calculates the three principal axis moments of inertia of the saddle-point shape with IZ, IA, and IL. LPOLY calculates Legendre polynomials and is called by BARFIT and MOMFIT. The values of all quantities calculated result from multiparameter fits to calculated properties of fission saddle points and ground states. These subroutines will give an approximation to the calculated fission barrier height, ground-state energy, Lmax, and saddle-point moments of inertia for Z between 20 and 100, A between 1.47+0.009Z**2 and 20+3Z, and L between 0 and Lmax, where Lmax is the value of angular momentum at which the fission barrier vanishes. The subroutines, as distributed, are written for single precision long word-length (60- or 64-bit) computers. Double precision statements for short word-length (32-bit) machines are included as comments.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1985.
   BARMOM submitted November 1985.

10. **REFERENCES** - Arnold J. Sierk, Macroscopic Model of Rotating Nuclei, LA-UR-85-4007, December 1985, submitted to Physical Review C.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
A. J. Sierk
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
   Source (781 lines)
   The BARMOM source on magnetic tape is available from NESC on an "As Is" basis.

17. **CATEGORY** - W
KEYWORDS - fission barrier, angular momentum, ground states, moment of inertia, nuclear structure

18. **SPONSOR** - DOE Office of Military Application

IDENTIFICATION AND KWIC TITLE - CRI
CRI, Cray multitasking compatibility package

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC VAX11/780-4

DESCRIPTION - CRI is a subroutine library and set of utilities which allow the use of a four-processor shared memory DEC VAX11/780-4 computer for parallel processing in a manner compatible with the present use of Cray Research, Inc.'s (CRI's) multitasking primitives on Cray computers. Included in the library are subroutines to perform resource initialization, task functions, lock operations, event signals, file sharing, and work queueing synchronization. A task consists of code and data that can be scheduled for execution on a CPU. Locks are the facility for monitoring critical regions of code. Events allow signaling between tasks; they have two states: cleared and posted. Posting an event allows all other tasks waiting on that event to resume execution. The CRI utilities consist of command procedures for creating the files needed to use the shared memory; for compiling and linking a multitasking program; for starting the logical processors on the physical processors after the time specified by submitting the job(s) to the selected generic batch queue and, optionally, interactively relinquishing control to the multiprocessor debugger; and for removing jobs from the batch queue and, optionally, unmapping specified global sections from shared memory. The CRIDEBUG utility does not work properly in this release.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed December 1985.
DEC VAX11/780 version submitted November 1985.

REFERENCES - Nancy E. Werner and Steven W. Van Matre, Parallel Processing on the Livermore VAX 11/780-4 Parallel Processor System with Compatibility to Cray Research, Inc. (CRI) Multitasking, Version 1, UCRL-92624 Preprint, May 1985.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN (51%), MACRO (47%), PASCAL (2%)

OPERATING SYSTEM - VMS.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
N. E. Werner and S. W. Van Matre
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (3440 lines)
The reference report and CRI source, control information, and machine-readable documentation on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

CATEGORY - P
KEYWORDS - parallel processing, utility routines, DEC computers, Cray computers

18. **SPONSOR** – Lawrence Livermore National Laboratory

IDENTIFICATION AND KWIC TITLE - GEM2D
GEM2D, 2-d electromagnetics Galerkin FEM

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
Cray1

DESCRIPTION - GEM2D, the 2D version of the Galerkin finite element Electro-Magnetics code, solves Maxwell's curl equations in two dimensions. The solution is based on the Galerkin weighted residual technique using the four node isoparametric element. The user can choose from rectangular or cylindrical field symmetry. The time integration can be performed using several different methods, including the LSODE (NESC 592) variable size time-step solver. Preprocessing of data can be done with MAZE (NESC 9907) and postprocessing with ORION (NESC 9906). GEM2D uses 5 units besides the standard input/output units and calls several library routines unique to the LLNL computing environment; these routines are not included.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed December 1985.
Cray1 version submitted January 1985.

REFERENCES -

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
N. Madsen and J. C. Peterson
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (7028 lines)
The GEM2D source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - X
KEYWORDS - electromagnetic fields, Maxwell equations, finite element method, two-dimensional, LSODE codes, MAZE codes, ORION codes

SPONSOR - DOE Office of Military Application

IDENTIFICATION AND KWIC TITLE - POSSOL
POSSOL, nonlinear grid poisson equation solver

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
Cray1

DESCRIPTION - POSSOL is a two-dimensional Poisson equation solver for problems with arbitrary non-uniform gridding in Cartesian coordinates. It is an adaptation of the uniform grid PWSCRT routine developed by Schwarztrauber and Sweet at the National Center for Atmospheric Research (NCAR). POSSOL will solve the Helmholtz equation on an arbitrary, non-uniform grid on a rectangular domain allowing only one type of boundary condition on any one side. It can also be used to handle more than one type of boundary condition on a side by means of a capacitance matrix technique. There are three types of boundary conditions that can be applied: fixed, derivative, or periodic. The two sample problems call some library routines unique to the LLNL computing environment; these are not included. LINPACK routines are used in place of the author's original DEC/SOL combination to solve the capacitance matrix equation.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed December 1985.
Cray1 version submitted November 1985.

REFERENCES - William J. Orvis, POSSOL Poisson Equation Solver, UCID-20539, August 1985.
P. Schwarztrauber and R. Sweet, Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations, NCAR/TN-109+IA, July 1975.
N. K. Madsen, An Application of a Capacitance Matrix Technique to Expand the Usefulness of a PDE Software Package, Technical Memorandum 77-3, Numerical Mathematics Group, Lawrence Livermore National Laboratory, February 1977.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
W. J. Orvis
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (2196 lines)
The UCID-20539 reference report and POSSOL source and sample problems on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - P
KEYWORDS - Poisson equation, Cartesian coordinates, two-dimensional, nonlinear problems, PWSCRT codes

SPONSOR - Lawrence Livermore National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - DEM3_06
   DEM3_06, Deming's general least square fitting

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM PC, GRiD 1139

3. **DESCRIPTION** - DEM3_06 is a generalized least square fitting program based on Deming's method. Functions built into the program for fitting include linear, quadratic, cubic, power, Howard's, exponential, and Gaussian; others can easily be added. The program has the following capabilities: (1) entry, editing, and saving of data; (2) fitting of any of the built-in functions or of a user-supplied function; (3) plotting the data and fitted function on the display screen, with error limits if requested, and with the option of copying the plot to the printer; (4) interpolation of x or y values from the fitted curve with error estimates based on error limits selected by the user; and (5) plotting the residuals between the y data values and the fitted curve, with the option of copying the plot to the printer. If the plot is to be copied to a printer, both the IBM PC and GRiD computers require an addition to the operating system. On an IBM PC or PC-compatible, "GRAPHICS" should be called from the operating system disk before the BASIC interpreter is loaded. On a GRiD Systems Compass II Model 1139, "Screenwatch" must be running in the background before GW-Basic is loaded. To generate the sounds called for by the program, a GRiD user must also have the driver "Sound" as a title in the "Programs" subject. On an IBM PC or PC-compatible the statement "BASIC/D" is used to bring the interpreter into the computer; the calculations require the double-precision interpreter. The GriD version of GW-Basic should also have double-precision capability.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1985.
   IBM PC version submitted October 1985.

10. **REFERENCES** - Phillip M. Rinard and Gerald E. Bosler, User Notes for Curve Fitting with Deming's Procedure Implemented for GW-Basic on IBM-PC Clones and GRiD 1139 Computers, Los Alamos National Laboratory Note 533u, July 2, 1985.
    W. E. Deming, Statistical Adjustment of Data, John Wiley, New York, 1943.
    J. R. Wolberg, Prediction Analysis, D. Van Nostrand, Princeton, New Jersey, 1967.

11. **HARDWARE REQUIREMENTS** - 64K bytes

12. **PROGRAMMING LANGUAGE** - Microsoft GW-BASIC Version 2.0

13. **OPERATING SYSTEM** - DOS 2.11 (IBM PC).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    P. M. Rinard and G. E. Bosler
    Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (1634 lines)
    The reference LANL Note and sample problem output and DEM3_06 source on an IBM PC 5.25 inch, double-sided, double-density flexible disk cartridge are available from NESC on an "As Is" basis. A source listing is available as an alternative to the FDC upon request.

17. **CATEGORY** - P
KEYWORDS - least square fit, experimental data, interpolation, data analysis, computer graphics

18. **SPONSOR** - DOE Office of Safeguards and Security

1. **IDENTIFICATION AND KWIC TITLE** - PC EASI
   PC EASI, adversary sequence interruption model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM PC

3. **DESCRIPTION** - PC EASI is an IBM personal computer or PC-compatible version of an analytical technique for measuring the effectiveness of physical protection systems. PC EASI utilizes a methodology called Estimate of Adversary Sequence Interruption (EASI) which evaluates the probability of interruption (PI) for a given sequence of adversary tasks. Probability of interruption is defined as the probability that the response force will arrive before the adversary force has completed its task. The EASI methodology is a probabilistic approach that analytically evaluates basic functions of the physical security system (detection, assessment, communications, and delay) with respect to response time along a single adversary path. It is important that the most critical scenarios for each target be identified to ensure that vulnerabilities have not been overlooked. If the facility is not overly complex, this can be accomplished by examining all paths. If the facility is complex, a global model such as Safeguards Automated Facility Evaluation (SAFE) may be used to identify the most vulnerable paths.

   PC EASI is menu-driven with screen forms for entering and editing the basic scenarios. In addition to evaluating PI for the basic scenario, the sensitivities of many of the parameters chosen in the scenario can be analyzed. These sensitivities provide information to aid the analyst in determining the tradeoffs for reducing the probability of interruption.

   PC EASI runs under the Micro Data Base Systems' proprietary database management system Knowledgeman. KMAN provides the user environment and file management for the specified basic scenarios, and KGRAPH the graphical output of the sensitivity calculations. This software is not included. Due to errors in release 2 of KMAN, PC EASI will not execute properly; release 1.07 of KMAN is required.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1985.
   IBM PC version submitted October 1985.

10. **REFERENCES** - L. D. Chapman and C. P. Harlan, PC EASI Estimate of Adversary Sequence Interruption on an IBM PC, SAND85-1105, October 1985.

11. **HARDWARE REQUIREMENTS** - 256K RAM and two disk drives or hard disk

12. **PROGRAMMING LANGUAGE** - Knowledgeman V1.07

13. **OPERATING SYSTEM** - DOS 2.0.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. D. Chapman and C. P. Harlan
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (approximately 1875 lines)

The reference report and PC EASI source, object modules, and sample problem on 5.25-inch, double-sided, double-density flexible disk cartridge are available from NESC on an "As Is" basis.

17. **CATEGORY** - M
KEYWORDS - physical protection, safeguards, adversaries, probabilistic estimation, EASI codes, SAFE codes

18. **SPONSOR** - DOE Office of Safeguards and Security

IDENTIFICATION AND KWIC TITLE - ICARUS-LLNL
ICARUS-LLNL, one-dimensional heat conduction

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600

DESCRIPTION - ICARUS-LLNL was developed to solve one-dimensional planar, cylindrical, or spherical conduction heat transfer problems. The model accounts for material phase change (solidification or melting), multiple material regions, temperature-dependent material properties, and time- or temperature-dependent boundary conditions. Finite difference techniques are used to solve the governing differential equations. The finite difference equations are formulated to allow the user to specify a fully implicit, explicit, or a Crank-Nicolson solution type. The resulting system of equations is solved using a tridiagonal reduction algorithm. The NAMELIST convention is used to specify input data.

A typical problem requires 0.15 msec/node-timestep without phase change and 0.45 msec/node-timestep with phase change. The code was first developed in 1974 to allow easy modeling of complex one-dimensional systems. Its original application was to problems in the nuclear explosive testing program. Since then it has undergone extensive revision and been applied to problems dealing with laser fusion target fabrication, heat loads on underground tests, magnetic fusion switching tube anodes, and nuclear waste isolation canisters. This release is designated as Version 17 by the author. ICARUS makes a number of calls to LLNL system and graphics library subroutines; these routines are not included.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed November 1985.
CDC7600 version submitted November 1985.

REFERENCES - S. B. Sutton, ICARUS - A General One-Dimensional Heat Conduction Code, UCID-20125, July 20, 1984.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - LRLTRAN

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
S. B. Sutton
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (3977 lines)
The reference report and ICARUS-LLNL source on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - H
KEYWORDS - heat transfer, phase change materials, thermal conduction, convection, thermal radiation, temperature dependence, finite difference method

SPONSOR - DOE Office of Military Application

IDENTIFICATION AND KWIC TITLE - MULTITASKER
MULTITASKER, multitasking environment kernel

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC VAX11/780

DESCRIPTION - MULTITASKER implements a multitasking kernel for the C and FORTRAN programming languages that runs under UNIX. The kernel provides a multitasking environment which serves two purposes. The first is to provide an efficient portable environment for the development, debugging, and execution of production multiprocessor programs. The second is to provide a means of evaluating the performance of a multitasking program on model multiprocessor hardware. The performance evaluation features require no changes in the application program source and are implemented as a set of compile- and run-time options in the kernel. The multitasking kernel is written almost entirely in C with machine dependencies isolated in just a few routines. Thus, the kernel can be readily moved to new multiprocessors once a C compiler has been developed for the target machine. The kernel is compatible with the UNIX symbolic debugger, dbx. The compatibility of the kernel with a symbolic debugger is a very powerful feature which is lacking in most multitasking implementations.

The FORTRAN interface to the kernel is identical in function to the CRI multitasking package provided for the Cray XMP. This provides a migration path to high speed (but small N) multiprocessors once the application has been coded and debugged. With use of the UNIX m4 macro preprocessor, source compatibility can be achieved between the UNIX code development system and the target Cray multiprocessor. The kernel also provides a means of evaluating a program's performance on model multiprocessors. Execution traces may be obtained which allow the user to determine kernel overhead, memory conflicts between various tasks, and the average concurrency being exploited. The kernel may also be made to switch tasks every cpu instruction with a random execution ordering. This allows the user to look for unprotected critical regions in the program. These features, implemented as a set of compile- and run-time options, cause extra execution overhead which is not present in the standard production version of the kernel.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed November 1985.
DEC VAX11/780 version submitted September 1985.

REFERENCES - Eugene D. Brooks III, A Multitasking Kernel for the C and Fortran Programming Languages, UCID-20167, September 1984.
MULTITASKER, NESC No. 9684, MULTITASKER Tape Directory, National Energy Software Center Note 86-09, November 21, 1985.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - C

OPERATING SYSTEM - UNIX.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
E. D. Brooks, III
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE -**
Source (224 10,240-character records)
The reference report and NESC Note and MULTITASKER source, object, sample problems, machine-readable documentation, and control information on magnetic tape, in VAX/UNIX TAR format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
KEYWORDS - parallel processing, multiprocessors, computerized simulation, FORTRAN, C

18. **SPONSOR** - DOE Office of Military Application

. **IDENTIFICATION AND KWIC TITLE -** FATHOM360,FATHOM360S
FATHOM360,FATHOM360S, LMFBR thermal hydraulics

. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
Cray1S

. **DESCRIPTION -** The FATHOM codes calculate, at any axial position, the detailed coolant velocity and temperature profile around the rod circumference in LMFBR core assemblies, as well as the rod radial and circumferential temperature profiles. Fuel, radial blanket, and control assemblies can be investigated. FATHOM360 applies to inboard rods, while FATHOM360S applies to side rods. Both wire wrapped and bare rods can be analyzed. The codes are used in conjunction with subchannel analysis codes, which calculate the bulk subchannel coolant velocity and temperature specified as input to FATHOM which performs a detailed evaluation of the velocity and temperature fields. Detailed three-dimensional evaluations at the desired axial levels are obtained by coupling the two-dimensional (r,theta) FATHOM program with the three-dimensional subchannel code. The FATHOM finite difference program solves the conservation equations over a very detailed mesh. Separate energy equations are formulated for fuel, cladding, and coolant regions and coupled by the appropriate boundary conditions. An enhanced eddy diffusivity model accounts for the forced diversion flow effect caused by the wire. Typical design applications of the FATHOM programs are: calculation of the wire wrap hot spot factor, calculation of local cladding and fuel temperatures, calculation of the effect of pellet eccentricity on cladding and fuel temperatures, and consideration of the effect of power skew across the rod pellet.

FATHOM360 can consider heat generation in the cladding, in addition to heat generation in the pellet; heat generation in the wire wrap is not considered, but can be added easily if deemed significant. FATHOM360 does not analyze the case of a displaced rod in the channel (e.g., due to stack-up of tolerances) or rod axis distortions due to bowing.

FATHOM360S permits the unequal heating of duct walls to simulate the actual heat transfer across side walls in fuel assemblies.

Earlier editions of FATHOM were limited to a bare rod model and analysis of 30 and 60 degree rod sectors rather than the entire rod.

. **METHOD OF SOLUTION -**

. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

. **TIMING -**

. **UNUSUAL FEATURES OF THE SOFTWARE -**

. **RELATED AND AUXILIARY SOFTWARE -**

. **STATUS -** Summary first distributed November 1985.
Cray1 version submitted June 1985, replaced July 1985.

. **REFERENCES -** M. D. Carelli, Verification of the FATHOM Codes for Prediction of Local Thermohydraulics in Wire Wrapped Rods of LMFBR Cores, WAESD-TR-85-0041, May 1985.

M. C. Chuang and M. D. Carelli, FATHOM-360: A Code for Prediction of the Detailed Thermal-Hydraulic Field in a Wire Wrapped Inboard Rod of an LMFBR Core, WAESD-TR-85-0040, May 1985.

M. C. Chuang and M. D. Carelli, FATHOM-360S: A Code for Prediction of the Detailed Thermal-Hydraulic Field in a Wire Wrapped Side Rod of an LMFBR Core, WAESD-TR-85-0039, May 1985.

. **HARDWARE REQUIREMENTS -**

. **PROGRAMMING LANGUAGE -** FORTRAN IV

. **OPERATING SYSTEM -**

. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
R. A. Markley
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (FATHOM360 6189 lines, FATHOM360S 5027 lines)
The reference reports and FATHOM360 and FATHOM360S source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – H
KEYWORDS – fuel rods, fuel pellets, reactor cores, finite difference method, temperature distribution, liquid metal cooled reactors, Clinch River Breeder Reactor, FATHOM codes

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

IDENTIFICATION AND KWIC TITLE - LSODP
LSODP, ODE system solver projection method

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600, IBM3033 (designed to be portable)

DESCRIPTION - LSODP is a set of FORTRAN subroutines for solving the initial value problem for stiff and nonstiff systems of ordinary differential equations. LSODP is an experimental variant of LSODE (NESC 592). In solving stiff systems, LSODP uses a combination of Newton iteration and a projection method for the corrector iteration. The projection method is the Incomplete Orthogonalization Method (IOM) based on Arnoldi's method, with scaling. The implementation is matrix-free, meaning that there is no explicit storage of the Jacobian (or related) matrix required. The projection method, and hence LSODP, is experimental because the scope of problems for which it is effective is not well known, and users should be forewarned that LSODP may or may not be competitive with traditional methods for their problems. The LSODP source is commented extensively to facilitate modification. Both a single-precision version for long word-length machines (e.g. CDC) and a double-precision version for short word-length machines (e.g. IBM) are available.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed November 1985.
CDC7600 (S.P.) version submitted October 1985.
IBM3033 (D.P.) version submitted October 1985.

REFERENCES - Peter N. Brown and Alan C. Hindmarsh, Matrix-Free Methods for Stiff Systems of ODE's, UCRL-90770, Rev. 1, Preprint, May 1985.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN IV

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
A. C. Hindmarsh
Mathematics and Statistics Division
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (single-precision version 3478 lines, double-precision version 3492 lines)
The reference report and LSODP source and demonstration program on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - P
KEYWORDS - ordinary differential equations, algorithms, initial-value problems, numerical solution, LSODE codes

SPONSOR - DOE Office of Energy Research,
Applied Mathematical Sciences Research Program

IDENTIFICATION AND KWIC TITLE - KIVA
KIVA, 2- & 3-d reactive flows with fuel sprays

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
Cray1

DESCRIPTION - KIVA solves the equations of transient multicomponent chemically reactive fluid dynamics, together with those for the dynamics of an evaporating liquid spray. The program has been developed with applications to internal combustion engines specifically in mind, and contains a number of features to facilitate such applications. However, most of the program structure is quite general, and the program can be adapted to a variety of other applications with only minor modifications. The formulation is fully three-dimensional, but planar and axisymmetric two-dimensional options are also provided. KIVA is a time-marching finite-difference program that uses an acoustic subcycling method for efficiency at low Mach number. Spatial differences are formed with respect to a generalized three-dimensional mesh of arbitrary hexahedrons whose corner locations are specified functions of time. This feature allows a Lagrangian, Eulerian, or mixed description, and is particularly useful for representing curved or moving boundaries. A subgrid scale turbulence model including turbulent energy transport is included, and a turbulent law-of-the-wall boundary layer option is provided. Arbitrary numbers of species and chemical reactions are allowed. The latter are subdivided into kinetic and equilibrium reactions, which are treated by different algorithms. A discrete-particle technique is used to represent an evaporating liquid spray, including the effects of droplet collisions and coalescence.

KIVA is essentially a three-dimensional version of the earlier CONCHAS-SPRAY program (NESC 9993). It makes extensive use of Cray vectorization features, but there are no inherent features that prevent adaptation to other machines. For a typical engine calculation with 4000 cells, 12 species, and 2000 spray particles, the memory requirement is about 400K, including libraries. More generally, the requirement ranges from about 150K upward, depending on the number of cells, chemical species, and spray particles. Execution times vary from several minutes to an hour or more depending on the complexity of the problem.

KIVA calls a number of LANL system subroutines. These routines are not included, but are described in the reference report. Several routines called from LINPACK (NESC 800) and SLATEC2.0 (NESC 820) are included. KIVAPP, a postprocessor which is included, initializes the graphics file using the LANL routines GPLOT and LIBDISP; these routines are not included. KIVAPP uses the proprietary ISSCO graphics software system, DISSPLA, to produce graphical output.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed November 1985.
Cray1 version submitted October 1985, revised January 1986.

REFERENCES - A. A. Amsden, J. D. Ramshaw, P. J. O'Rourke, and J. K. Dukowicz, KIVA: A Computer Program for Two- and Three-Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays, LA-10245-MS, February 1985.

A. A. Amsden, J. D. Ramshaw, L. D. Cloutman, and P. J. O'Rourke, Improvements and Extensions to the KIVA Computer Program, LA-10534-MS, October 1985.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN (Cray CFT)

13. **OPERATING SYSTEM** - CTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
A. A. Amsden, J. D. Ramshaw, P. J. O'Rourke,
J. K. Dukowicz, and L. D. Cloutman
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE** -
Source (KIVA 8620 lines, KIVAPP 1602 lines)
The reference reports and KIVA source, sample problem, and auxiliary program on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - U
KEYWORDS - three-dimensional, two-dimensional, chemical reactions, particles, sprays, ICE method, finite difference method, fluid flow, CONCHAS-SPRAY codes, APACHE codes, SALE2D codes, SALE3D codes, LINPACK codes, SLATEC codes

18. **SPONSOR** - DOE Division of Energy Conversion and Utilization Technologies

IDENTIFICATION AND KWIC TITLE - GKS
GKS, minimal graphical kernel system C Binding

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC VAX11/780

DESCRIPTION - GKS (the Graphical Kernel System) is both an American National Standard (ANS) and an ISO international standard graphics package. It conforms to ANS X3.124-1985 and to the May 1985 draft proposal for the GKS C Language Binding standard under development by the X3H3 Technical Committee. This implementation includes level ma (the lowest level of the ANS) and some routines from level mb. The following graphics capabilities are supported: two-dimensional lines, markers, text, and filled areas; control over color, line type, and character height and alignment; multiple simultaneous workstations and multiple transformations; and locator and choice input. Tektronix 4014 and 4115 terminals are supported, and support for other devices may be added.

Since this implementation was developed under UNIX, it uses makefiles, C shell scripts, the ar library maintainer, editor scripts, and other UNIX utilities. Therefore, implementing it under another operating system may require considerable effort.

Also included with GKS is the small plot package (SPP), a direct descendent of the WEASEL plot package developed at Ssndia. SPP is built on the GKS; therefore, all of the capabilities of GKS are available. It is not necessary to use GKS functions, since entire plots can be produced using only SPP functions, but the addition of GKS will give the programmer added power and flexibility. SPP provides single-call plot commands, linear and logarithmic axis commands, control for optional plotting of tick marks and tick mark labels, and permits plotting of data with or without markers and connecting lines.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed October 1985.
DEC VAX11 Version submitted October 1985.

REFERENCES - Sandia C GKS Documentation, Sandia National Laboratories Memorandum, received October 1985.

GKS Author's Notes, received October 17, 1985.

GKS, NESC NO. 9689, GKS Tape Directory, National Energy Software Center Note 86-07, October 28, 1986.

Randall W. Simons, Minimal GKS, Computer Graphics, Vol. 17, No. 3, pp. 183-189, July 1983.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - C

OPERATING SYSTEM - UNIX BSD 4.2.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
R. W. Simons
Sandia National Laboratories, Albuquerque

MATERIAL AVAILABLE -
Source (139 10,240-character records)

The SNLA memorandum, GKS Author's Notes, and NESC Note and GKS source, maintenance procedures, test routines, auxiliary programs, and machine-readable documentation on magnetic tape, in VAX/UNIX TAR format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
KEYWORDS - computer graphics, interactive computing, interactive display devices, standards, SPP codes, WEASEL codes

18. **SPONSOR** - DOD Air Force Technical Applications Center

1. **IDENTIFICATION AND KWIC TITLE -** GRAFAID
   GRAFAID, interactive x-y data analysis & plots

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11/750

3. **DESCRIPTION -** GRAFAID is an interactive x-y data tool, which is built upon the Sandia Graphics Compatibility System (GCS) library subroutines and the Sandia Virtual Device Interface (SVDI) library subroutines (NESC 9985). Initially developed for the analysis and comparison of shock and vibration data for the generation of weapons component specifications, GRAFAID has evolved into a general-purpose data summary and analysis tool. It provides an interactive capability for simultaneously plotting and comparing multiple sets of x-y data, and it contains a number of utility routines for creating curve definitions and analyzing and manipulating x-y data. Utilities are provided to add to existing x-y data sets, to create curve definitions by performing calculations on existing x-y data, for editing data, for enveloping data, for calculating Fast Fourier Transform approximations of data, for integrating and differentiating data, for applying a prescribed window to the data, and for statistical calculations on existing data. A direct-access database for storing sets of x-y data and their plot definitions is created and maintained by GRAFAID, and a file system using free format ASCII records is provided for communicating x-y data into, and out of, a GRAFAID database.

   Neither the SVDI library subroutines nor the GCS library subroutines are included.

   The most significant limitations are: (1) the maximum number of data pairs that can be included in a curve definition is 4096; (2) the curve definition is limited to real x and y data; (3) most of the curve utilities that sample and/or interpolate curve data require that the curve data be monotonically increasing in x; (4) the curve utilities that apply digital signal analysis techniques require both monotonically increasing x data and a uniform x data sample spacing (equal intervals); and (5) the DESINE curve utility for creating a curve definition that is the shock spectra of a user-defined decayed sine time history pulse is limited to a maximum of 25 decayed sine pulses including the compensation pulse.

   The graphics terminals supported by GRAFAID include all alphanumeric terminals; the AED 512; Envision Models 215, 220, and 230; Tektronix 4100 series, 4014, and 4010 Emulator for graphics with an auxiliary VT100 compatible terminal equipped with a printer port and RS-232 switch or the DEC VT100 with Retro-Graphics enhancement.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed October 1985.
   DEC VAX11 version submitted September 1985.

10. **REFERENCES -** C. R. Adams, GRAFAID Code User Manual Version 2.0, SAND84-1725, September 1985.

    GRAFAID, NESC No. 9690, GRAFAID Tape Contents File Name Directory, National Energy Software Center Note 86-06, October 25, 1985.

    GCS, the Graphics Compatibility System Reference Manual, Sandia National Laboratories.

    Karen M. Erickson and Randall W. Simons, Functional Specification of the Sandia Virtual Device Interface (SVDI), SAND81-1900, December 1981.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN

13. **OPERATING SYSTEM** - VMS 4.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
C. R. Adams
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
Source (1008 8192-character records)
The SAND84-1725 reference report and NESC Note and GRAFAID source, message files, HELP files, font table, sample problem, executable images, command procedures, and machine-readable documentation on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - N
KEYWORDS - computer graphics, numerical data, data analysis, engineering, time-series analysis, SVDI codes

18. **SPONSOR** - DOE Office of Military Application

IDENTIFICATION AND KWIC TITLE - SWAC13E
SWAC13E, sodium-water reaction two-phase flow
SWAC13, sodium-water reaction two-phase flow

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM3033

DESCRIPTION - SWAC13E and SWAC13 are designed to analyze the quasi-steady flow of the liquid sodium and hydrogen gas mixture which results from large-scale water leaks in the steam generator of an LMFBR. The treatment is generally a two-phase flow treatment where pure sodium or all gas are special cases. The geometric configuration of a problem or model is defined by input data; hence, the code is a general-purpose code.

In SWAC13E, the set of governing differential equations used consists of the five two-phase flow equations with a drift-flux model for the relative velocity between the phases. Specifically, the set of equations includes two continuity equations, one for each phase, a mixture momentum equation, and two energy equations, again one for each phase. In SWAC13, the set of governing differential equations used are three two-phase flow equations with a slip flow model between the phases. Specifically, these include two continuity equations, one for each phase, and a mixture momentum equation. The method used to solve the equations is that of the node and link developed earlier by Porsching et al. The SWAC13E energy equations are not solved implicitly with the continuity and momentum equations. Instead, first the continuity and momentum equations are advanced for each time-step, then the results are used in advancing the energy equations.

Both programs allow maxima of 40 nodes and 55 links, and a total of 3 steam generators are permitted in the system.

On an IBM3033, approximately 8 CPU minutes are required to execute 6 seconds of real-time transient run for the SWAC13E sample problem with 28 nodes and 34 links, and approximately 6 CPU minutes are required to execute 6 seconds of real-time transient run for the SWAC13 sample problem with 22 nodes and 31 links.

SWAC13E is an extension of SWAC13 with the temperature field added to calculate the thermal transient in addition to hydrodynamic transients. Both the SWAC13 and SWAC13E codes, developed by Japan's Power Reactor and Nuclear Fuel Development Corporation, were validated against the large-leak SWAT-3 test data obtained for the Monju reactor steam generator design with large covergas space. They were converted to run on the IBM computer system at ANL.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed October 1985.
IBM3033 version of SWAC13E submitted September 1985.
IBM3033 version of SWAC13 submitted October 1985.

REFERENCES - Y. W. Shin, U. S. Choi, and S. O. Nelson, User's Input Manual for Quasi-Steady Sodium/Water Reaction Analysis Computer Program SWAC-13E, ANL-85-43, August 1985.

Osam Miyake and Minoru Sato, Interim Report on SWAC-13E Development for Analysis of Long-Term Transients of Large-Scale Sodium-Water Reaction, PNC SN941 83-133, August 1983.

Y. W. Shin, U. S. Choi, and S. O. Nelson, User's Input Manual for SWAC-13, A Quasi-Steady Two-Phase Flow Analysis Computer Code for Large-Leak Sodium/Water Reactions in an LMFBR Steam Generator System, ANL-85-52, September 1985.

Osam Miyake, Yoshihisa Shindo, and Minoru Sato, Computer Code for Large Leak Sodium-Water Reaction Analysis -SWACS/REG3- (Program Description), PNC SN952 79-19Tr, September 1979.

Osam Miyake, Yoshihisa Shindo, and Minoru Sato, Computer Code for Large Leak Sodium-Water Reaction Analysis -SWACS/REG3- (Input Manual), PNC SN952 79-20Tr, September 1979.

11. **HARDWARE REQUIREMENTS** - 1250K bytes (SWAC13E), 750K bytes (SWAC13)

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - MVS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

Y. W. Shin
Components Technology Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (SWAC13E 15,244 lines, SWAC13 5991 lines)
For SWAC13E, the ANL-85-43 and PNC SN941 83-133 reference reports and SWAC13E source, sample problem input and output, load module, and control information on magnetic tape are available from NESC on an "As Is" basis. For SWAC13, the ANL-85-52 and PNC SN952 79-19Tr reference reports and SWAC13 source, sample problem input and output, load module, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - G
KEYWORDS - molten metal-water reactions, two-phase flow, LMFBR reactors, steam generators, heat transfer, leaks, SWAAM2 codes, SWAAM-LT codes, RELAP4 codes

18. **SPONSOR** - DOE Office of Advanced Reactor Programs

IDENTIFICATION AND KWIC TITLE - PLOTLIB
PLOTLIB, FR80, TMDS & RJET graphics library

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
CDC7600, Cray1,X-MP

DESCRIPTION - PLOTLIB is a basic graphics library which allows the user to plot lines and text to the FR80, RJET, and TMDS systems. With PLOTLIB a user can receive microfiche from the FR80, print Versatec output with RJET, and display TMDS output. In PLOTLIB, line plots may be a series of disjoint line segments or a connected line, and text plots may be text or markers. Line and text appearance are determined by selection from a large number of available global attributes; and after all the lines and text are plotted, the picture can be displayed or printed. PLOTLIB consists of three types of subroutines: low-level, high-level, and three-dimensional. The low-level subroutines are small, single-function routines which, for example, initialize a view surface, set a buffer size, or plot a line. The high-level routines are larger, multi-function routines which, for example, plot vectors, a reference grid, a filled polygon, or a contour map. The three-dimensional routines are a prototype extension of the library to plot lines and text in three dimensions or a surface with hidden lines removed. PLOTLIB can plot up to 16 view surfaces at one time and can record a maximum of 16 view surface identifiers.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed October 1985.
CDC7600,Cray version submitted September 1985.

REFERENCES - Joyce Moulden, Lynd Stringer, Mark Blair, and Jim Kohn, PLOTLIB User's Manual, LCSD-439, February 1985.
John C. Fletcher, TMDS Manual, UCID-30118, February 9, 1976.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - LRLTRAN (99%) and CAL (1%)

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
L. M. Stringer, M. Blair, J. Kohn, E. Mueller,
G. Cronshagen, and K. O'Hair
Lawrence Livermore National Laboratory

MATERIAL AVAILABLE -
Source (31,399 lines)
The LCSD-439 reference report and PLOTLIB source and font library on magnetic tape are available from NESC on an "As Is" basis.

CATEGORY - N
KEYWORDS - computer graphics, plotters, computer output devices, display devices, three-dimensional

SPONSOR - DOE Office of Military Application

IDENTIFICATION AND KWIC TITLE - CONTROLITE1.0, CONTROLITE SOURCE
CONTROLITE1.0, lighting control energy savings
CONTROLITE SOURCE, lighting energy analysis

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM PC

DESCRIPTION - CONTROLITE1.0 is a lighting energy analysis program designed to calculate the energy savings and cost benefits obtainable using lighting controls in buildings. The program can compute the lighting energy reductions that result from using daylighting, scheduling, and other control strategies.

To compute energy savings, CONTROLITE1.0 calculates how much electric light (and thus, how much power) is necessary to satisfy the user-specified design light level in the modeled building space. When modeling daylight control systems, the program uses QUICKLITE to compute the daylight illuminances at specified points 5 times a day, 12 days a year (the 21st of each month), and for two sky conditions (clear and overcast skies). Fourier series techniques are used to fit a continuous curve through the computed illuminance points. The energy use for each of the 12 days is then computed given user-specified power-in/light-out characteristics of the modeled control system. The monthly and annual energy usage for overcast and clear conditions are found separately by fitting two long-term Fourier series curves to the energy use computed for each of the 12 days. Finally, the monthly energy use is calculated by taking a weighted average for the monthly energy use computed for the overcast and clear sky conditions. The program only treats the energy use directly attributable to lighting. The impact of lighting control strategies on building thermal loads is not computed. The program allows input of different control schedules (i.e., on/off times for the lighting system) for each day of the week, but every week of the year is treated the same; thus, holidays cannot be modeled explicitly. When used for daylighting purposes, CONTROLITE1.0 understands only clear and overcast conditions. User-supplied values for the proportion of clear and overcast hours for each month of the year are required to accommodate different climatic conditions. CONTROLITE1.0 permits modeling of continuous or stepped control systems, modeling of linear and nonlinear light-output versus power-input relationships, automatic calculation and reporting of daylight illuminance values or the entry of empirically measured daylight data or values computed by other programs. Input data are entered with a menu-driven, screen-oriented worksheet. The program output is a listing of the computed lighting energy for the modeled lighting control system and the savings relative to an uncontrolled base case lighting system. The computed life-cycle costs for the controlled and base case systems are listed as well as the Savings Investment Ratio (SIR) for the controls investment. QUICKLITE is incorporated within CONTROLITE1.0 as a subroutine and may be executed independently to perform interior daylight calculations.

For a relatively complex control system simulation (i.e., daylighting control system with QUICKLITE computing daylight illuminances at 10 workplane points), running time is 15 to 20 minutes with the 8087 co-processor. Without the co-processor, running time is much longer.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed September 1985.
IBM PC version of CONTROLITE1.0 submitted June 1985, replaced July 1985.
IBM PC version of CONTROLITE SOURCE submitted September 1985.

REFERENCES - CONTROLITE1.0 Lighting Control Systems and Daylighting Analysis Program: User's Manual, LBL-17444 Rev., January 1985, revised July 1985.

H. J. Bryan, R. D. Clear, J. Rosen, and S. Selkowitz, QUICKLITE 1: New Procedure for Daylighting Design, Solar Age, Vol. 6, No. 8, pp. 37-47, August 1981.

H. J. Bryan and R. D. Clear, Calculating Interior Daylight Illumination with a Programmable Hand Calculator, Journal of the Illuminating Engineering Society, Vol. 10, No. 4, pp. 219-227, July 1981.

11. **HARDWARE REQUIREMENTS** -
256K with two floppy disk drives or hard disk.

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - DOS 2.0.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** - The CONTROLITE1.0 program is distributed in executable form only because the Lighting Technologies user interface incorporated in this edition of the program is proprietary.

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
F. Rubinstein
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
The LBL-17444 reference report and CONTROLITE1.0 executable image, sample problem input and output, auxiliary information, and control information on two 5.25-inch, double-sided, double-density flexible disks are available from NESC on an "As Is" basis.
The FORTRAN source code for an earlier edition, without the user-friendly interface features, is available upon special request.

17. **CATEGORY** - T
KEYWORDS - lighting systems, illuminance, daylighting, energy analysis, cost benefit analysis, sky, schedules, QUICKLITE codes

18. **SPONSOR** - DOE Office of Building Energy Research and Development, Building Equipment Division

. **IDENTIFICATION AND KWIC TITLE -** SPECTR3T
SPECTR3T, 3-d time dependent resistive MHD

. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
Cray1

. **DESCRIPTION -** SPECTR3T solves the three-dimensional, time-dependent, compressible, resistive magnetohydrodynamic equations in periodic cylindrical (r,theta,z) geometry. The program solves the spatial approximation using finite differences for the radial direction r, and the pseudospectral method for approximation in the two periodic coordinates, theta and z. Leapfrog time advancement is used for advective terms and a first-order explicit method for resistive terms. Fast Fourier transforms are used to communicate between configuration and Fourier space. Diffusion terms are treated implicitly to avoid several time-step restrictions. The theta and z meshes must be powers of 2. The Cray running time is approximately 0.09 milliseconds per meshpoint per time-step. SPECTR3T produces history binary data files to be analyzed by user-supplied postprocessors. The program uses fast Fourier transform routines from the Cray Research OMNILIB library and other LANL environment routines; these routines are not included.

. **METHOD OF SOLUTION -**

. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

. **TIMING -**

. **UNUSUAL FEATURES OF THE SOFTWARE -**

. **RELATED AND AUXILIARY SOFTWARE -**

. **STATUS -** Summary first distributed September 1985.
Cray1 version submitted August 1985.

. **REFERENCES -** D. D. Schnack, D. C. Baxter, and E. J. Caramana, A Pseudospectral Algorithm for Three-Dimensional Magnetohydrodynamic Simulation, Journal of Computational Physics, Vol. 55, No. 3, pp. 485-514, September 1984.
A. Y. Aydemir, D. C. Barnes, E. J. Caramana, A. A. Mirin, R. A. Nebel, D. D. Schnack, and A. G. Sgro, Compressibility as a Feature of Field Reversal Maintenance in the Reversed-Field Pinch, Physics of Fluids, Vol. 28, No. 3, pp. 898-902, March 1985.

. **HARDWARE REQUIREMENTS -**

. **PROGRAMMING LANGUAGE -** LRLTRAN

. **OPERATING SYSTEM -** CTSS.

. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
D. D. Schnack
Science Applications International Corporation

. **MATERIAL AVAILABLE -**
Source (2787 lines)
The SPECTR3T source on magnetic tape is available from NESC on an "As Is" basis.

. **CATEGORY -** X
KEYWORDS - three-dimensional, magnetohydrodynamics, plasma simulation, cylindrical configuration, reverse-field pinch, Cray computers

. **SPONSOR -** DOE Office of Fusion Energy

IDENTIFICATION AND KWIC TITLE - SALT-ANL
SALT-ANL, systems analysis process simulation

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
IBM3033

DESCRIPTION - SALT (Systems Analysis Language Translator), a systems-analysis and process-simulation program for steady-state and dynamic systems, can also be used for optimization and sensitivity studies. SALT employs state-of-the-art numerical techniques including a hybrid steepest-descent/quasi-Newtonian multidimensional nonlinear equation solver, sequential quadratic programming methods for optimization, and multistep integration methods for both stiff and nonstiff systems of differential equations. Based on a preprocessor concept where a 'new' system driver can be written for each application, SALT-ANL contains precompiled component models, several flow types, and a number of thermodynamic and transport property routines, including a gas chemical-equilibrium code. It has been applied to the study of open-cycle and liquid-metal magnetohydrodynamic systems, fuel cells, ocean thermal energy conversion, municipal solid-waste processing, fusion, breeder reactors, and geothermal and solar-energy systems. Models available include: combustor, compressor, deaerator, gas-diffuser, fuel-dryer, feedwater-heater, flash-tank, gas-turbine, heater, heat-exchanger, flow-initiator, fuel-flow-initiator, molten-carbonate fuel-cell, liquid-metal diffuser, magnetohydrodynamic-generator, liquid-metal magnetohydrodynamic-generator, liquid-metal nozzle, liquid-metal pipe, flow-mixer, gas-nozzle, phosphoric acid fuel-cell, pump, pipe-calculator, steam-condenser, steam-drum, liquid-gas separator, stack, solid-oxide fuel-cell, flow-splitter, steam-turbine, two-phase diffuser, two-phase mixer, and two-phase nozzle.

Input data to the SALT program describe the system configuration for the specific problem to be analyzed and provide instructions defining system constraints, objective functions, parameter sweeps, etc. to generate a PL/I program representing the system problem and performing the various analytic tasks.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed September 1985.
IBM3033 version submitted August 1985.

REFERENCES - Howard K. Geyer and Gregory F. Berry, The Systems Analysis Language Translator (SALT): User's Guide, ANL/FE-85-3, January 1985.
Howard K. Geyer and Gregory F. Berry, The Systems Analysis Language Translator (SALT): Programmer's Guide, ANL/FE-85-4, March 1985.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - PL/I

OPERATING SYSTEM - MVS.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
G. F. Berry and H. K. Geyer
Energy and Environmental Systems Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** –
Source (18,576 lines)
The reference reports and SALT source, models, sample problems, load modules, library data, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – T
KEYWORDS – systems analysis, optimization, sensitivity analysis, mathematical models, simulation, thermodynamic properties

18. **SPONSOR** – DOE Office of Fossil Energy

IDENTIFICATION AND KWIC TITLE - CLASTR, NEWRATETR
CLASTR,NEWRATETR, 3-atom classical trajectory

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
DEC VAX11/780,PDP11/45

DESCRIPTION - CLASTR is a Monte Carlo quasiclassical trajectory program for calculating reactive scattering cross sections for three-atom systems with potential energy surfaces represented by generalized London-Eying-Polanyi-Sato functions.

NEWRATETR, a modification of the CLASTR program, calculates bimolecular reaction rate constants instead of reactive scattering cross sections. NEWRATETR also differs from CLASTR in that it employs Monte Carlo selection of the reactant rotational state from the Boltzmann distribution at the specified temperature and importance sampling of the collision energy and impact parameter. The same temperature is used in both the rotational state and collision energy selection; a slight modification of the code is required to accommodate different internal (rotational) and translational temperatures. Due to the use of importance sampling, the trajectories from NEWRATETR do not have equal statistical weights. The statistical weight of each trajectory is calculated by the program and written to the output and data analysis files. These statistical weights must be used in the analysis of the computed results.

Other potential functions may be used with minor modifications of the programs. These programs represent later releases of an original CDC version of CLASTR transferred from the National Resource for Computation in Chemistry's software library in February 1981.

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed August 1985.
DEC VAX11/780,PDP11/45 version submitted August 1985.

REFERENCES - R. B. Bernstein, Ed., Atom-Molecule Collision Theory: A Guide for the Experimentalist, Plenum Press, New York, 1979.

M. B. Faist, J. T. Muckerman, and F. E. Schubert, Importance sampling and histogramic representation of reactivity functions and product distributions in Monte Carlo quasiclassical trajectory calculations, Journal of Chemical Physics, Vol. 69, No. 1, pp. 4087-4096, November 1, 1978.

J. T. Muckerman and M. B. Faist, Rate Constants from Monte Carlo Quasi-Classical Trajectory Calculations. A Procedure for Importance Sampling, Journal of Physical Chemistry, Vol. 83, No. 1, pp. 79-88, 1979.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN

OPERATING SYSTEM -

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -
J. T. Muckerman
Chemistry Department
Brookhaven National Laboratory

16. **MATERIAL AVAILABLE** –
Source (CLASTR 2126 lines, NEWRATETR 2337 lines)
The CLASTR,NEWRATETR source, sample problems input and output, and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – W
KEYWORDS – atom collisions, nuclear reactions, three-nucleon transfer reactions, Monte Carlo method, scattering, cross sections

18. **SPONSOR** – DOE Office of Basic Energy Sciences

1. **IDENTIFICATION AND KWIC TITLE -** CRAB2
   CRAB2, rod bundle hydraulics & scram dynamics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Cray1

3. **DESCRIPTION -** CRAB2 (Control Rod Assembly Behavior) calculates the hydraulics, scram dynamics, and flotation behavior of primary control assemblies (PCAs) of the rod bundle type used in LMFBR core designs. The program predicts control assembly steady-state and scram performance including: flow split between bypass channel and rod bundle, rod bundle pressure drop, assembly mass flow rate, and rod bundle position, velocity, and acceleration. CRAB2 also accounts for assembly weight and buoyancy, scram spring, sliding friction, fluid shear, and time-dependent forces. In addition, CRAB2 features a gas expansion model for the CRDM bellows, a dashpot model, calculation of assembly mass flow rate during scram (variable to satisfy condition of constant pressure drop across core), and calculation of the transient increase in rod bundle pressure drop due to rod bundle acceleration. CRAB2 can calculate scram characteristics under seismic conditions.

   CRAB2 is based on first principles and on the three control volume model of the PCA. The program retains the original one control volume model of the rod bundle only from the original CRAB program as an option, for use in scoping analyses because of its very short running time. The approach taken is to apply the equations of continuity, conservation of momentum, and conservation of energy to each control volume. The resulting system of equations are then coupled by the two continuity equations at the control volume interfaces, and the overall boundary condition is that the pressure drop across the entire PCA is constant and equal to the core pressure drop. These equations are then reduced to a system of first order differential equations which are integrated using a standard Runge-Kutta method and solved simultaneously.

   In addition to its use as a primary design tool, CRAB2 can be useful in parametric studies (e.g. sensitivity of scram to rod bundle wear pad dimension variations within design tolerance or scram analysis assuming a missing scram spring), feasibility studies, and in optimizing designs.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed August 1985.
   Cray1 version submitted June 1985.

10. **REFERENCES -** M. D. Carelli, J. P. Sechrist, and J. M. Willis, CRAB-II: A Hydraulics and Scram Dynamics Code for Rod Bundle Type Control Assemblies User's Manual, WAESD-TR-85-0042, May 1985.

    J. P. Sechrist and M. D. Carelli, Verification of the CRAB-II Code for Prediction of the Hydraulics and Scram Dynamics of Rod Bundle Type Control Assemblies, WAESD-TR-85-0043, May 1985.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN IV

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

M. D. Carelli, J. P. Sechrist, and J. M. Willis
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** – Restricted Distribution

Source (4349 lines)

The reference reports and CRAB2 source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – H

KEYWORDS – rod bundles, reactor cores, hydraulics, scram, reactor control systems, pressure drop, seismic effects, LMFBR reactors, Clinch River Breeder Reactor, CRAB codes

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - FULMX
   FULMX, reactor rod bundle thermal-hydraulics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - Honeywell6000

3. **DESCRIPTION** - FULMX is a generic bundle thermal-hydraulic analysis code developed specifically for LMFBR core applications. It exists as two programs - FULMIX for fuel/blanket assemblies and FULSCA for control assemblies. FULMIX can be used for hexagonally arranged fuel or blanket bundles with 7 to 271 fuel rods. It performs the steady-state calculation of average temperatures for each fuel rod and coolant flow cell in the bundle at an arbitrary number of axial planes. Flow splits between cells are calculated from input dimensions assuming no radial pressure gradients. The magnitude of turbulent mixing between adjacent cells can be varied from zero (i.e., only molecular conduction) to values representative of grid-speed and wire-wrapped bundles. Edge swirl induced by wire wraps can be simulated. Any desired power distribution can be assumed.

   FULSCA is a revision of FULMIX to handle the Clinch River Breeder Reactor Plant (CRBRP) circular secondary control assembly bundle with 31 rods and 6 filler pins. The adiabatic duct, wall temperature conditions were replaced by adjacent fuel/blanket duct wall temperatures to account for heat transfer to adjacent fuel and/or blanket assemblies. FULSCA calculates detailed subchannel coolant and absorber rod temperatures while accounting for heat transfer through the bundle tube, bypass flow, guide tube, Secondary Control Assembly (SCA) duct wall, and the interassembly gap to the adjacent assembly duct wall. Temperatures of this wall must be specified as input and can be obtained from CORTM (NESC 9759).

   FULMIX requires about 0.03 minutes of running time per axial plane for a 127-rod bundle problem.

   FULMIX should give results comparable to COBRA2 for nominal bundles in which flow redistribution does not occur or is very small. FULMIX does not calculate diversion crossflow from one channel to another correctly. First, FULMIX is unable to identify the adjacent channel from which the crossflow occurs. It incorrectly assumes that the added flow (resulting from crossflow) has the same enthalpy as that originally in the channel. This results in excessively high temperatures behind severe blockages. Second, FULMIX cannot "see" a blockage before the axial flow reaches the blockage. Flow redistribution is instantaneous at a blockage rather than gradual. Another limitation is that FULMIX cannot handle two-phase flow.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed August 1985.
   Honeywell6000 version submitted January 1985.

10. **REFERENCES** - Verification for Computer Code FULMX, GE ARSD Spec. 23A3051, May 29, 1985.
    D. J. Bender and P. M. Magee, Turbulent Heat Transfer in a Rod Bundle with Liquid Metal Coolant, GEAP-10052, July 1969.
    D. S. Rowe, COBRA-II: A Digital Computer Program for Thermal-Hydraulic Subchannel Analysis of Rod Bundle Nuclear Fuel Elements, BNWL-1229, February 1970.

11. **HARDWARE REQUIREMENTS** - 26K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** –

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

P. M. Magee
Advanced Reactor Systems Department
General Electric Company

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (FULSCA 1198 lines, FULMIX 1913 lines)
The 23A3051 reference document and FULSCA source and sample problem and FULMIX source, sample problem, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – H
KEYWORDS – rod bundles, fuel assemblies, reactor cores, thermal conduction, breeding blankets, temperature, LMFBR reactors, Clinch River Breeder Reactor, CORTM codes, COBRA2 codes

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - FORE2M
   FORE2M, LMFBR reactor code transient analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - FORE2M, a modification of the FORE2 program (NESC 174), is a coupled thermal-hydraulics point-kinetics program designed to calculate significant reactor core parameters under steady-state conditions, or as functions of time during transients. Variable inlet coolant flow rate and temperature are considered. The code calculates the reactor power, the individual reactivity feedbacks, and the temperature of coolant, cladding, fuel, structure, and additional material for up to seven axial positions. Various plant protection system trip functions can be simulated, and the control rod shutdown worth can be prescribed as a function of time from the trip signal. By specifying appropriate hot channel or spot factors, the transient behavior of an average, peak, and hot fuel rod can be analyzed. The heat of fusion accompanying fuel melting and the spatial time variation of the fuel-cladding gap coefficient (due to changes in gap size) are considered. The feedback reactivity includes contributions due to the Doppler effect, coolant density changes, and dimensional changes (including bowing and radial expansion).

   The modified edition contains changes to several of the FORE2 models and the addition of new models. The calculation of the fuel centerline temperature has been changed to yield more accurate results. Built-in tables of sodium properties have been updated to reflect more recent data. New additions to the FORE2M program include: a sintering model, which simulates the sintering behavior of regions of fast reactor oxide fuel pellets which operate at high temperature (1600-1800C) and tend to become more dense; two new routines for determining pressure drop and channel flow rates during a transient; a variable (axial) conductance correction factor which allows the user to vary the gap conductance in all three channels (i.e. average, peak, and hot channel); an alternate method by which the heat transfer from certain structural materials (e.g., fuel assembly ducts) or other materials (e.g., control rods) can be evaluated in a gross (lumped) manner; two additional reactivity feedback mechanisms; and flexibility in the method of specifying a flow coastdown.

   FORE2M is valid as long as the core retains its initial geometry (i.e. up to the point of gross fuel pin melting). Only one size pin is modeled at a time. Seven fuel geometry and four types of scram options are available. FORE2M allows maxima of 10 radial fuel nodes, 7 axial coolant nodes, and 7 axial cladding nodes. The thermal conductivity of the cladding can be specified as a constant value or as a variable, temperature-dependent, conductivity.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed August 1985.
   CDC7600 version submitted June 1985.

10. **REFERENCES** - J. V. Miller and R. D. Coffield, FORE-2M: Modified Version of the FORE-II Computer Program for the Analysis of LMFBR Transients, CRBRP-ARD-0142, November 1976.

    R. D. Coffield, R. K. Sievers, and R. F. Wright, FORE-2M Verification Summary, WAESD-TR-85-0038, May 1985.

    J. N. Fox, B. E. Lawler, and H. R. Butz, FORE II, A Computational Program for the Analysis of Steady-State and Transient Reactor Performance, GEAP-5273, September 1966.

    FORE2M, NESC No. R9699, FORE2M Implementation Information and Sample Problem Output, National Energy Software Center Note 85-82, July 29, 1985.

11. **HARDWARE REQUIREMENTS** - 135K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. N. Fox, B. E. Lawler, H. R. Butz, J. V. Miller, and R. D. Coffield
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (9200 lines)
The reference reports and NESC Note and sample problem output on microfiche and FORE2M source and sample problem input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - reactor cores, reactor kinetics, power distribution, temperature, flow rate, fuels, coolants, Clinch River Breeder Reactor, FORE2 codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - AVPROG
   AVPROG, MC simulation of system availability

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - IBM3033

3. **DESCRIPTION** - AVPROG is a large-scale simulation program used to estimate steady-state availability of a system, typically a large production unit. The system is modeled as a success logic flow block diagram of equipment affecting the production output. AVPROG simulates system operation over a specified time period using Monte Carlo techniques. System components are failed and restarted using numerous types of distributions that are available. Among the distributions available are the exponential and the lognormal. AVPROG computes availability based on averages from a number of simulation cases (batches) for the specified production time interval. It also ranks unavailability contributors to permit investigation of design modifications that have the greatest impact on availability. AVPROG uses Monte Carlo simulations to estimate availability based on time histories of production developed from failure and restore data for each logic block (on the logic diagram representing the system operation) and from specified additional restore time data for the failed system.

   Input to AVPROG consists of system geometry (as defined on logic diagrams), mean time between failures, mean time to restore (MTTR), and mean plant delta (MPD) for each logic block. MTTR is defined to include access time, equipment preparation time, actual replace time, cleanup time, and time to restore the equipment and associated subsystem to normal operation. MPD is defined as additional time to restore full production after the equipment in the logic block has been restored. AVPROG is unique in its ability to handle MPD in a parallel logic configuration. AVPROG can handle K-out-of-N parallel configurations where the components are not identical. It can also handle weighted and normalized parallel configurations. In considering parallel configurations in the logic diagram, all components are assumed to be operating normally and not on standby. The output shows not only the system availability, but also the contribution of each block to system unavailability, ranked in order of size of the contribution.

   Execution time is dependent on the number of blocks in the system, the number of batches, and the simulation time (years) for each batch. A problem, consisting of 49 blocks run at 10 batches for 5000 years each, produced an average of 13,446 failures per batch with a standard deviation of 0.0000015 and took 2.75 minutes of CPU time. A much more complicated problem with 1048 blocks run for 10 batches for 500 years produced an average of 70,749 failures per batch with a standard deviation of 0.000014 and required almost 129 minutes of CPU time.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed July 1985.
   IBM3033 version submitted July 1985.

10. **REFERENCES** - P. W. McGrady, AVPROG User's Manual, Y/PO-87-02 Revision 1, March 23, 1984, revised July 25, 1985.
    R. Balsam, Gas Centrifuge Enrichment Plant Availability Analysis Procedures Manual, Y/PO-87-1, August 1, 1983.

11. **HARDWARE REQUIREMENTS** - 372K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - MVS/JES2.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
P. W. McGrady and L. D. Reynolds
Martin Marietta Energy Systems, Inc.

16. **MATERIAL AVAILABLE -**
Source (2669 lines)
The reference reports and AVPROG source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY -** P
KEYWORDS - availability, Monte Carlo method, simulation, production, systems analysis, AVANAL codes

18. **SPONSOR -** DOE Systems Management Branch

1. **IDENTIFICATION AND KWIC TITLE** - CATFISH
   CATFISH, LMFBR primary flow network analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - CATFISH (Core Assemblies Tailored Flow Identification Self-adjusting pump Head) was developed to perform parametric and design studies of reactor flow distribution and pressure drop in an LMFBR primary system and to detail the core hydraulic characteristics and performance. Emphasis is placed on detailing the flow distribution throughout the core. A branched network models the various flow paths: fuel, blanket, primary and secondary control assemblies, radial shield, vessel and core barrel, and leakage. For each individual assembly, the hydraulic resistance of every component is accounted for including lower internals, assembly nozzles, orifices, shield, rod bundle, etc. The entire primary system is thus modeled with the pump characteristics equation representing the boundary condition, or, more accurately, the closure of the network. CATFISH also sizes the orifices (number of plates, size, and number of holes) to better satisfy the specified flow orificing requirements. The data handling capability of the program allows a number of specific flow and orificing problems to be solved; for example, it is possible to analyze flow distributions in manifolds which supply different combinations of different types of core assemblies. The only limitation of the program is that the parallel flow network solution is accurate as long as large density differences are absent.

   CATFISH calculates the unique hydraulic parameters (flows and orificing) that satisfy user-specified constraints. Input error testing helps prevent the user from defining an over- or under-constrained problem. The types of problems that can be solved fall into two general categories: 1) When the hydraulic characteristics of every network component (including the pump and orifices) is specified, the program calculates the flow in every flow path. This feature is used in analyzing existing designs. 2) When some orifice hydraulic resistances are not specified, the code calculates the unspecified orifices to satisfy flow constraint specified by the user (i.e., total reactor flow rate and/or core flow distribution). This feature is used in determining the core design.

   The main input consists of the pressure drop characteristics of all flow channels and the head versus flow relationship of the supply pump. The program calculates the flow in each channel and, if they are not given, can specify the characteristics of orifice plates required to control the flow to specific paths. It matches the overall head loss of the system with the pump characteristics. Parameters defining the flow network are specified by the user. Subject to program dimension limitations, a large number of parallel assemblies (1212) and of orificing zones (31) is allowed; each core assembly can be divided into a maximum of 10 hydraulic components with each component having its own unique hydraulic law; any number of lower inlet modules is allowed; and any number of assemblies can be placed in a given lower inlet module. The current release of the program is restricted to one pump and one loop. Uncertainty analysis is performed by either applying a factor to each flow resistance or by calculating root mean square flow deviations for all flow rates.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed August 1985.
   CDC7600 version submitted July 1985.

10. **REFERENCES** - M. D. Carelli and J. M. Willis, CATFISH: A Primary System and Core Hydraulic Flow Network Code for LMFBRs User's Manual, WAESD-TR-85-0025, April 1985.

M. D. Carelli and F. C. Engel, Verification of the LMFBR Primary Flow Network Code CATFISH, WAESD-TR-85-0026, April 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
M. D. Carelli and J. M. Willis
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2327 lines)
The reference reports and CATFISH source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - reactor cores, pumps, fluid flow, reactor components, reactor cooling systems, orifices, Clinch River Breeder Reactor, LMFBR reactors, COBRA-WC codes, FLOWDIV codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - OCTOPUS
   OCTOPUS, optimizing LMFBR core flow orificing

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - OCTOPUS (Optimization Core Temperatures, Orificing, Pressures, Upper Structure) determines the relative flow allocated to the fuel and blanket assemblies in the core region of a Liquid Metal Fast Breeder Reactor (LMFBR). Core orificing is needed since the power generation across the core is radially non-uniform, and therefore, an equal flow distribution among the assemblies is unsuitable for proper cooling. Consequently, a criterion must be established as to how an "optimum" allocation of flow to the various assemblies is to be achieved.

   OCTOPUS optimizes the flow among the various assemblies on the basis of the following general criteria: a. the cumulative cladding strain and damage function of the limiting rod in every assembly is less than or equal to an allowable limit; b. the maximum subchannel coolant temperature must be less than or equal to a specified allowable limit during transient events; c. the maximum assembly exit temperatures must be compatible with upper internals structure (UIS) limitations; and d. the core assemblies mixed mean coolant exit temperatures are equalized and minimized in order to reduce both temperature levels and thermal gradients across the core outlet. The first three criteria are achieved by redefining the constraints in a form analytically more amenable for calculation as follows: 1) The maximum cladding/coolant temperature of the limiting rod/subchannel in each core assembly is equal to or less than a specified limiting temperature. 2) The flow allocated to each assembly is equal to or greater than that required to keep the mixed mean coolant exit temperature below that dictated by UIS design constraints.

   The limiting temperature for each assembly is developed external to the OCTOPUS code and represents the maximum temperature the cladding (or coolant) can be allowed to reach without exceeding limits on such items as cladding strain, cumulative damage, or transient margin. These limits are generated based on analysis of individual rod characteristics, such as linear power rating, cladding temperature history, and internal pressure.

   OCTOPUS is written in two primary modules (called phases). The first either solves for the minimum flow rate in each assembly that does not cause the specified maximum temperature to exceed the assembly limiting temperature (which is input) or takes the input flow requirement and calculates the associated cladding and coolant temperatures. In either case, an array of assembly flow rates results, and OCTOPUS then groups the assemblies in orificing zones to minimize the total flow. The second phase then rearranges the excess flow, if any (total allocated flow to fuel and blanket minus total flow calculated in the first phase), to satisfy the second criterion without exceeding the first. This reallocation of flow is accomplished primarily by finding the flow distribution which produces the minimum variance between the coolant mixed mean outlet temperatures of the orificing zones. In the case there is inadequate flow to achieve the limiting temperature or flow constraints, then either the specified constraints should be relaxed or an increase in the total allocated flow to fuel and blanket is required.

   The orificing capability of OCTOPUS allows a range of specifications from a single orificing zone for all assemblies to one zone for each assembly. The only restriction on this capability is that the running time is a function of the orificing scheme and could become prohibitive when a very large number of assemblies and orificing zones is involved. Both fuel and blanket assemblies can be orificed simultaneously. Uncertainty factors are included in calculating the cladding and coolant temperatures.

   Input for OCTOPUS can be directly provided by the user or an option can be selected to accept input from a tape prepared by an assembly subchannel code, such as COTEC. A typical OCTOPUS problem requires 10 to 20 CP seconds on an CDC7600. OCTOPUS makes use of some local WAESD system routines; these routines are not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed July 1985.
CDC7600 version submitted June 1985.

10. **REFERENCES -** W. C. Chiang, M. D. Carelli, and P. W. Rosenthal, OCTOPUS: A Flow Orificing Optimization Code for LMFBR Cores User's Manual, WAESD-TR-85-0044, May 1985.
W. C. Chiang, P. W. Rosenthal, and M. D. Carelli, Verification of the LMFBR Core Orificing Optimization Code OCTOPUS, WAESD-TR-85-0045, May 1985.

11. **HARDWARE REQUIREMENTS -** 126K (octal) words SCM and 147K (octal) words LCM

12. **PROGRAMMING LANGUAGE -** FORTRAN IV

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
W. C. Chiang, M. D. Carelli, and P. W. Rosenthal
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE -** Restricted Distribution
Source (2979 lines)
The reference reports and OCTOPUS source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY -** H
KEYWORDS - reactor cores, orifices, temperature distribution, flow models, optimization, Clinch River Breeder Reactor, LMFBR reactors, COTEC codes, FATHOM360 codes

18. **SPONSOR -** DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - LCR-BASED DESIGN TOOL
   LCR-BASED DESIGN TOOL, LCR/SSF & energy plots

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   HP1000

3. **DESCRIPTION** - LCR-BASED DESIGN TOOL is a set of programs for maintaining a database of Load Collector Ratio (LCR) data and producing graphics output plots using an HP2647A graphics terminal with attached HP9872S plotter. New locations can be added to the database along with pertinent data including city name, state abbreviation, latitude, and LCR/SSF ratios for ten different building types and five values for average annual heating degree days. The software can plot LCR/SSF (Solar Savings Fraction) ratios for up to 10 different building types on a single sheet or on continuous-roll paper. One or more cities may be selected at a time. Data points are retrieved from the database and used to generate a 'least squares' polynomial to produce a smooth curve. Plots of auxiliary energy requirements can be produced also. Cities may be selected by reference number or those for a particular state or all database entries may be plotted. The LCR database and the Hewlett-Packard IMAGE/1000 database software, which is used extensively by the programs, are not included. Developer support is not available for the LCR-BASED DESIGN TOOL software.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed July 1985.
   HP1000 version submitted March 1982.

10. **REFERENCES** - LCR-BASED DESIGN TOOL Software Package, Southern Solar Energy Center, Inc., Technical Services Division document, August 17, 1981.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 4X

13. **OPERATING SYSTEM** - RTE IVB.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   G. B. Graves
   Southern Solar Energy Center

16. **MATERIAL AVAILABLE** -
   Source (2374 lines)
   The reference document and LCR-BASED DESIGN TOOL source, plotter commands, database schema, and terminal screen input form on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - M
   KEYWORDS - load collector ratio, passive solar heating systems, data base management, HP computers, computer graphics, plotters

18. **SPONSOR** - DOE Office of Conservation and Renewable Energy

1. **IDENTIFICATION AND KWIC TITLE -** BCPL
   BCPL, block-structured recursive language

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   MODCOMP IV/35

3. **DESCRIPTION -** BCPL is a block-structured recursive language which has the ability to access core locations directly. This makes it useful for systems programming. While BCPL is a highly structured language, it shares with assembly languages the lack of an explicit notion of type. The programmer has complete freedom to model objects of any kind and is provided with a large number of basic operations to perform transformations on these objects. BCPL has been used to implement operating systems, editors, algebra manipulation programs, compilers, and many systems programs. The language is mainly composed of declarations, expressions, and commands.
   The BCPL compiler, itself written in BCPL, consists of a syntax analyzer which reads a BCPL source program and converts it into a tree structure called the Applicative Expression tree (AE tree). The translation phase of the compiler then operates on the AE tree and translates it into a sequence of statements in an intermediate object code (OCODE). The compiler's code generator then translates the OCODE statements into machine code.
   BCPL was developed originally by Dr. M. Richards of the University of Cambridge. It has been used extensively at CERN and at LBL; compilers existed on CDC6000 and DEC PDP11 machines as well as the MODCOMP.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed July 1985.
   MODCOMP IV version submitted July 1981.

10. **REFERENCES -** Van Jacobson, John Lynch, Steve Mellor, Bob Upshaw, and Nick Jacobs, BCPL Version 1.1, Lawrence Berkeley Laboratory, Real Time Systems Group draft document, May 28, 1981.
    Listing of BCPL Files, Lawrence Berkeley Laboratory document, July 9, 1981.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** BCPL

13. **OPERATING SYSTEM -** MAX IV.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    V. Jacobson, J. Lynch, S. Mellor, and B. Upshaw
    Real Time Systems Group
    Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE -**
    Source (approximately 37,625 lines)
    The LBL documents and BCPL source, interface routines, SOFTWARE TOOLS primitives, and control information on magnetic tape, in source editor COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY -** P
    KEYWORDS - programming languages, real time systems, operating systems, text editors

18. **SPONSOR** - Lawrence Berkeley Laboratory

1. **IDENTIFICATION AND KWIC TITLE -** WATRE
   WATRE, heated concrete water and gas release

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   UNIVAC1100

3. **DESCRIPTION -** WATRE is a one-dimensional, finite difference program designed to calculate the rate and quantity of water and carbon dioxide gas released from heated concrete. The WATRE model is based on a series of partial differential equations that describe the flow of mass and energy within heated concrete. An equation of state and a number of auxiliary equations describing water/cement equilibrium and various fluid and concrete physical properties are also used. Changes in the temperature field within a concrete structure are determined by the exposure it receives from external sources and by the generation and flow of energy within the structure.

   According to the WATRE model, energy can be transported by thermal conduction and by fluid flowing from one region to another. Phase changes, chemical reactions, and other phenomena such as nuclear decay heating provide energy sources and sinks. The internal energy content of concrete due to its temperature can change also. Mass transfer is described by a series of continuity equations. WATRE solves four continuity equations to account for transport of liquid water, water vapor, air, and carbon dioxide. Fluids can be transported by pressure gradients or by molecular diffusion. Phase changes act as sources or sinks for the fluid species. The quantity of fluid stored at a particular location can change also. Any one of four types of concrete may be selected to provide concrete properties for WATRE calculations. If one of the three standard concrete types is chosen (limestone, basalt, or magnetite), appropriate properties are calculated by the program. If alternate properties are desired, they may be specified by selecting the fourth option for user-defined concrete.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed July 1985.
   UNIVAC1100 version submitted June 1985.

10. **REFERENCES -** S. W. Claybrook and L. D. Muhlestein, WATRE: An Improved Computer Program to Analyze Water and Gas Released from Heated Concrete, HEDL-TME 84-27, September 1984.

11. **HARDWARE REQUIREMENTS -** 24K words

12. **PROGRAMMING LANGUAGE -** FORTRAN 77

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    S. W. Claybrook and L. D. Muhlestein
    Hanford Engineering Development Laboratory

16. **MATERIAL AVAILABLE -** Restricted Distribution
    Source (3248 lines)
    The reference report and WATRE source and sample problems input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - G
KEYWORDS - concretes, containment buildings, temperature effects, water vapor, carbon dioxide, reactor accidents, fires

18. **SPONSOR** - DOE Office of Breeder Technology Projects

1. **IDENTIFICATION AND KWIC TITLE** - SMACS
   SMACS, probabilistic seismic analysis system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - The SMACS (Seismic Methodology Analysis Chain with Statistics) system of computer programs is one of the major computational tools of the U. S. NRC Seismic Safety Margins Research Program (SSMRP). It links seismic input with the calculation of soil-structure interaction (SSI), major structure response, and subsystem response. Seismic input is defined by ensembles of acceleration time histories in three orthogonal directions. SSI and detailed structure response are determined simultaneously using the substructure approach to SSI as implemented in the CLASSI family of computer programs. Subsystem response is determined from spectral accelerations at specified frequencies or by multi-support time history analysis of piping systems. Uncertainty in soil, structures, and subsystems is incorporated through selected parameter variations. In the SSI link, the selected parameters are the shear modulus and material damping in the soil; in the major structure and subsystem links, frequencies and modal damping properties are chosen.

   SMACS performs repeated deterministic analyses, each analysis simulating an earthquake occurrence. Uncertainty is accounted for by performing many such analyses using different definitions of the seismic input and varying different system parameters according to a Latin hypercube experimental design. SMACS is comprised of the core program SMAX, which performs the SSI response analyses, five preprocessing programs, and two postprocessors. The preprocessing programs include: GLAY and CLAN, which generate the nominal impedance matrices and wave scattering vectors for surface-founded structures; INSSIN, which projects the dynamic properties of structures to the foundation in the form of modal participation factors and mass matrices; SAPPAC, which projects the dynamic and pseudostatic properties of multiply-supported piping systems to the support locations, and LNGEN, which can be used to generate the multiplication factors to be applied to the nominal soil, structural, and subsystem properties for each of the response calculations in accounting for random variations of these properties. The postprocessors are: PRESTO, which performs statistical operations on the raw data from the response vectors that SMAX produces to calculate best fit lognormal distributions for each response location, and CHANGO, which manipulates the data produced by PRESTO to produce other results of interest to the user.

   Also included is the computer program SAP4 (a modified version of the University of California, Berkeley SAPIV program), a general linear structural analysis program used for eigenvalue extractions and pseudostatic mode calculations of the models of major structures and subsystems. SAP4 is used to prepare input to the INSSIN and SAPPAC preprocessing programs. The GLAY and CLAN programs were originally developed by J. E. Luco (UCSD) and H. L. Wong (USC).

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed July 1985.
   CDC7600 version submitted June 1985.

10. **REFERENCES** - Oleg R. Maslenikov, James J. Johnson, Lu Woon Tiong, Michael J. Mraz, Stan Bumpus, and Michael A. Gerhard, SMACS - A System of Computer Programs for Probabilistic Seismic Analysis of Structures and Subsystems, Volume I, User's Manual, UCID-20413, Vol. 1, March 1985.

    Oleg R. Maslenikov, James J. Johnson, Lu Woon Tiong, Michael J. Mraz, Stan Bumpus, and Michael A. Gerhard, SMACS - A System of Computer Programs for Probabilistic Seismic Analysis of Structures and Subsystems, Volume II, Example Problem, UCID-20413, Vol. 2, March 1985.

J. J. Johnson, G. L. Goudreau, S. E. Bumpus, and O. R. Maslenikov, Seismic Safety Margins Research Program Phase I Final Report – SMACS – Seismic Methodology Analysis Chain with Statistics (Project VIII), NUREG/CR-2015, Vol. 9 (UCRL-53021, Vol. 9), July 1981.

SMACS Descriptions of "Missing" IMSL and LLNL Environmental Subroutines, Lawrence Livermore National Laboratory Note, July 1985.

Steven J. Sackett, Users Manual for SAP4, A Modified and Extended Version of the U.C. Berkeley SAPIV Code, UCID-18226, May 1979.

11. **HARDWARE REQUIREMENTS –**

12. **PROGRAMMING LANGUAGE –** FORTRAN IV

13. **OPERATING SYSTEM –**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS –**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**

J. J. Johnson, O. R. Maslenikov, L. W. Tiong,
and M. J. Mraz
Structural Mechanics Associates
S. Bumpus and M. A. Gerhard
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE –**

Source (40,674 lines)

The reference reports and the LLNL Note and SMACS source, SAP4 source, sample problems input and output, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY –** I

KEYWORDS – seismic effects, soil-structure interactions, earthquakes, mechanical structures, reactor safety, nuclear power plants, response functions, probabilistic estimation, SAP4 codes, GEMINI codes, CLASSI codes, SEISIM codes, HAZARD codes, SIMQ codes

18. **SPONSOR –** NRC Office of Nuclear Regulatory Research

1. **IDENTIFICATION AND KWIC TITLE** - SISAL,IF1
   SISAL,IF1, parallel machine data-flow language

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - SISAL (Streams and Iteration in a Single-Assignment Language) is a functional data-flow language intended for use on a variety of sequential, vector, multi-, and data-flow processors. It is designed to express algorithms for execution on computers capable of highly concurrent operation. The application area supported is numerical computation which strains the limits of high performance machines. IF1 is a set of programs which take IF1 (Intermediate Format) files produced by the SISAL compiler and prepare them for execution on the LLNL debugger/interpreter, which can be used to debug and execute IF1 programs. The set of IF1 programs includes the debugger/interpreter, a prettyprinter for IF1 files, a common subexpression eliminator, an IF1 file structural checker, a loop invariant remover, a loop and test inverter, and programs to topologically sort IF1 files, expand functions inline, and count nodes in IF1 files.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC VAX11/780 version submitted January 1985, replaced May 1985.

10. **REFERENCES** - James McGraw, Stephen Skedzielewski, Stephen Allan, Rod Oldehoeft, John Glauert, Chris Kirkham, Bill Noyce, and Robert Thomas, SISAL: Streams and Iteration in a Single Assignment Language, Language Reference Manual Version 1.2, Lawrence Livermore National Laboratory - University of California, Davis Memorandum M-146, Rev. 1, March 1, 1985.

    Stephen Skedzielewski, Michael Welcome, and R. Kim Yates, SISAL/IF1 User's Guide, Lawrence Livermore National Laboratory Memorandum M-163, April 26, 1985.

    SISAL,IF1, NESC No. 9707, SISAL,IF1 Tape Directory, National Energy Software Center Note 85-79, June 28, 1985.

    KNOWN PROBLEMS WITH THE sc COMPILER as Distributed with the SISAL/IF1 Package, LLNL Note, November 6, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - PASCAL

13. **OPERATING SYSTEM** - UNIX BSD 4.2.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    S. K. Skedzielewski
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (378 10,240-character records)
    The LLNL Memoranda, LLNL Note, and NESC Note and SISAL,IF1 source and object files, sample problems, and machine-readable documentation on magnetic tape, in VAX/UNIX TAR format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
KEYWORDS - data-flow processing, parallel processing, vector processing, algorithms, DEC computers, programming languages, performance testing

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - ELTEMP
   ELTEMP, ASME code stress evaluation of piping

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - ELTEMP was developed for the structural evaluation of elevated temperature Class 1 piping systems and components. Stresses and deformations are evaluated against the combined requirements for piping of the 1974 ASME Boiler and Pressure Vessel Code Section III, Division 1 (1975) and ASME B&PV Code Case 1592-7 (1975), as amended and augmented by RDT Standard F9-4T. The program begins from a specification of local loadings in the piping system and carries the analysis forward to obtain local stress intensities based upon elastic behavior and to obtain an assessment of compliance with the limits of Code Case 1592 and RDT F9-4T. Both the mandatory load-controlled limits and the permissive deformation-controlled limits are evaluated. Loading due to weight, seismic and mechanical forces, anchors, and thermal expansion is treated. The numerical values for such loadings are presumed to be available at the data points throughout the piping system. These values are generally the result of a flexibility analysis of the piping system. Pressure and thermal transient loadings are also considered. Pressure values are usually the result of hydraulic analysis. These pressure and thermal transient loadings are identified separately from the types of loadings which result from flexibility analyses.

   Each loading condition is referred to as a 'load case'. A load cycle consists of a pair of load cases. It is assumed that the two extremes of an operating cycle can be identified and represented with the two load cases which comprise a load cycle. The geometry of the piping system is specified in terms of basic cross-section data. Then, the types of components are identified with the type of cross section. The types of components include straight, curved, tee, branch, and reducer sections. Additionally, the connecting welds, discontinuities, and ovality are specified and considered. The analysis performed by ELTEMP corresponds to the local component analyses presented in NB-3650, which is based upon the use of stress indices with one exception. The elbow analysis is the type covered by NB-3200.

   ELTEMP was originally developed by H. Y. Chow at the Bechtel Power Corporation for the AEC Fast Flux Test Facility program.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed July 1985.
   CDC7600 version submitted July 1975, replaced June 1985.

10. **REFERENCES** - R. H. Mallett, S. Kumar, M. E. Karabin, and K. Thomas, ELTEMP: A Computer Program For Structural Evaluation of Elevated Temperature Piping - Users' Manual, WAESD-TR-85-0033, June 1985.

   K. Thomas, Verification of the ELTEMP Computer Program for Structural Evaluation of Elevated Temperature Piping, WAESD-TR-85-0034, June 1985.

   ASME Boiler and Pressure Vessel Code Case 1592-7, Class 1 Components in Elevated Temperature Service, Section III, Division 1, American Society of Mechanical Engineers, New York, New York, 1975.

   ASME Boiler and Pressure Vessel Code, Section III, Division 1, Rules for Construction of Nuclear Power Plant Components, American Society of Mechanical Engineers, New York, New York, 1975.

11. **HARDWARE REQUIREMENTS** - 156K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. H. Mallett, S. Kumar, and K. Thomas
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (9031 lines)
The WAESD-TR-85-0033 and WAESD-TR-85-0034 reference reports and ELTEMP source and sample problems input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - stress intensity factors, deformation, pipes, sodium cooled reactors, mechanical properties, creep, performance testing, FFTF reactor, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - UCMD92
   UCMD92, mass properties analysis AGS/880 file

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11/34

3. **DESCRIPTION** - UCMD92 is an interactive FORTRAN program which analyzes and stores the mass properties of geometrical shapes, point masses, and assemblies represented in an Applicon AGS/880 drawing file. Access to the drawing file is accomplished via the Applicon 881-I FORTRAN User Command Interface Option package. UCMD92 will compute weight, area or volume, center of gravity, and moments and products of inertia of items in the file. The geometry of these items is restricted to solids of revolution and right prisms bounded by multi-vertex polyarcs. The number of vertices or arcs in which an item may be constructed is limited only by the drawing file size and the file size allocation. Items of any type geometry with known mass properties may be treated as point masses. The mass properties parameters are stored in the Applicon drawing file as a data record which is attached to the item under investigation. Other capabilities of UCMD92 enable the designer to total or combine the mass properties and compute the principal moments and axes and the ballast for static balancing of selected items stored in the Applicon drawing file. UCMD92 is executed as a user command from either a graphics station or a nongraphics terminal. It operates under version 8.5 of the AGS/880 operating system.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC PDP11/34 version submitted May 1985.

10. **REFERENCES** - James E. Malloch, UCMD92 Mass Properties Analysis User Guide, SAND79-2284, December 1979.
    James E. Malloch, UCMD92 Mass Properties Analysis Programmer Guide, SAND79-2285, January 1980.

11. **HARDWARE REQUIREMENTS** - 98K words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV V01C-03 (98%) and MACRO-11 (2%)

13. **OPERATING SYSTEM** - RSX-11M 3.2 and AGS/880-I Applicon Graphics System.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    N. J. Nelson
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (approximately 1300 lines)
    The reference reports and UCMD92 source, object library, and control information on magnetic tape, in PDP11 DOS FLX format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
    KEYWORDS - computer graphics, PDP computers, display devices, computer-aided design, computer-aided manufacturing, mass, weight, moment of inertia, geometry

18. **SPONSOR** - Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - TOXRISK
   TOXRISK, toxic gas accident analysis release

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER170/855

3. **DESCRIPTION** - TOXRISK is an interactive program developed to aid in the evaluation of nuclear power plant control room habitability in the event of a nearby toxic material release. The program uses a model which is consistent with the approach described in the NRC Regulatory Guide 1.78. Release of the gas is treated as an initial puff followed by a continuous plume. The relative proportions of these as well as the plume release rate are supplied by the user. Transport of the gas is modeled as a Gaussian distribution and occurs through the action of a constant velocity, constant direction wind. Dispersion or diffusion of the gas during transport is described by modified Pasquill-Gifford dispersion coefficients. Great flexibility is afforded the user in specifying the release description, meteorological conditions, relative geometry of the accident and plant, and the plant ventilation system characteristics.

   Two types of simulation can be performed: multiple case (parametric) studies and probabilistic analyses. Upon execution, TOXRISK presents a menu, and the user chooses between the Data Base Manager, the Multiple Case program, and the Probabilistic Study program.

   The Data Base Manager provides a convenient means of storing, retrieving, and modifying blocks of data required by the analysis programs. The Multiple Case program calculates resultant gas concentrations inside the control room and presents a summary of information that describes the event for each set of conditions given. Optimally, a time history profile of inside and outside concentrations can also be produced. The Probabilistic Study program provides a means for estimating the annual probability of operator incapacitation due to toxic gas accidents on surrounding transportation routes and storage sites.

   A skeleton database, which contains weather data for 29 cities, is included along with two auxiliary programs which convert the database from card-image to random-access format for use by TOXRISK and vice versa.

   Substantial effort would be required for conversion of the program to a non-CDC computer due to the strong dependence of the Data Base Manager on the CDC mass storage file system.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   CDC CYBER170 version submitted May 1985.

10. **REFERENCES** - D. I. Chanin, A. W. Shiver, and D. E. Bennett, Toxic Gas Accident Analysis Code User's Manual, NUREG/CR-3685 (SAND84-0367), August 1984.

    U. S. Nuclear Regulatory Commission, Office of Standards Development, Regulatory Guide 1.78, Assumptions for Evaluating the Habitability of a Nuclear Power Plant Control Room During a Postulated Hazardous Chemical Release, June 1974.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 5

13. **OPERATING SYSTEM** - NOS 2.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
D. E. Bennett, D. I. Chanin, and A. W. Shiver
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE -**
Source (7518 lines)
The NUREG/CR-3685 reference report and TOXRISK source, skeleton database, auxiliary programs, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
KEYWORDS - nuclear power plants, accidents, control rooms, reactor operators, toxic materials, ventilation, interactive computing

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Risk Analysis and Operations

1. **IDENTIFICATION AND KWIC TITLE** - COAL DIESEL
   COAL DIESEL, diesel engine performance study

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   XEROX Sigma 9

3. **DESCRIPTION** - COAL DIESEL calculates the performance of a diesel engine using coal/water slurry as fuel and diesel oil as pilot fuel. The diesel cycle is divided into nine regimes, and macroscopic equilibrium is assumed at regime interfaces. The regimes considered are: turbo-compression, intercooling, diesel compression, constant volume combustion, constant pressure combustion, constant temperature combustion, diesel expansion, exhaust and scavenging, and turbo-expansion. Conservation of mass, the first law of thermodynamics, and the properties of air and combustion gases are utilized in the macroscopic model. It is assumed that the ideal gas law is applicable and homogeneous thermodynamic equilibrium always achievable.
   Two COAL DIESEL programs are included. In Program A, heat transfer during the combustion portion of the cycle is accounted for by adjusting the cycle efficiency by a constant value. Heat transfer during other portions of the cycle is ignored, and all state points are based on an ideal cycle (i.e., without heat transfer and expansion inefficiencies). In Program B, heat transfer during the combustion and diesel expansion phase relative to a base case is calculated based on the Woschni correlation.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   XEROX Sigma 9 version submitted February 1985.

10. **REFERENCES** - Thermo Electron Corporation, The Development of a Coal/Water Slurry-Fueled Diesel Engine for Industrial Cogeneration, Task 1.0 - Topical Report Thermodynamic Analysis, TE4319-54-84, May 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - Extended FORTRAN IV

13. **OPERATING SYSTEM** - CPV.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. P. Davis and C. C. Wang
Energy Systems Division
Thermo Electron Corporation

16. **MATERIAL AVAILABLE** -
   Source (Program A 388 lines, Program B 427 lines)
   The reference report and COAL DIESEL source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - diesel engines, cogeneration, diesel fuels, coal, fuel slurries

18. **SPONSOR** - DOE Office of Industrial Programs

1. **IDENTIFICATION AND KWIC TITLE** - IGES/RIM PARSER & CONVERTER
   IGES/RIM PARSER & CONVERTER, IGES to RIM DBMS

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - IGES/RIM PARSER & CONVERTER converts a file in IGES (Initial Graphics Exchange Specification) format to a form suitable for loading into the RIM relational database management system. A schema for IGES is provided.
   Each section of the IGES file is processed separately. The IGES Start, Global, and Directory sections are each treated as one relation. The Parameter Data section has one or more relations for most IGES entity types. All pointers to other entities, whether in the Directory or Parameter Data section, are put into one relation. The output is a sequential character file containing directives to the RIM (Relational Information Manager) database interleaved with data from the IGES file. This output file is then used as input to RIM. After loading, the IGES data are accessible either directly via RIM commands or through the RIM FORTRAN interface. A summary of the contents of the IGES file, including a listing of the Start Section and Global Section contents, and a tabulation of the entities in the Directory and Parameter Data sections are produced. Most of the entities required for the transfer of mechanical CAD/CAM data are supported, including all of the annotation entities. An IGES file with 889 entities takes less than 3 minutes to process on a DEC VAX11/780. Loading the data into the RIM database requires an additional twenty minutes.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC VAX11/780 version submitted May 1985.

10. **REFERENCES** - R. E. Isler, IGES/RIM Parser/Converter Users Guide, SAND85-8219, May 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. E. Isler
    Sandia National Laboratories, Livermore

16. **MATERIAL AVAILABLE** -
    Source (21,917 lines)
    The reference report and IGES/RIM PARSER & CONVERTER source and IGES schema on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
    KEYWORDS - computer-aided design, computer-aided manufacturing, data base management, computer graphics, RIM codes

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - CHERN R1045
   CHERN R1045, 1-d inelastic structural analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - CHERN R1045 is a one-dimensional, plane strain, thick cylinder, static, small displacement, small strain, elastic-plastic-creep structural analysis program. The loadings considered are internal and external pressure, axial stress or strain, and temperature as a function of radius. Temperature-dependent material properties are permitted. The program will evaluate the structural response to a user-specified number of loading cycles and then perform a creep-fatigue evaluation. The creep equation, stress-rupture limits, and fatigue limits are provided by the user either as subroutines or functions. The MATLIB library can be used to provide the thermal creep rates, stress-rupture limits, and fatigue limits for CHERN R1045.

   The program calculates the structural response of a typical cross-section of a right circular cylinder of uniform thickness. There are three plane strain options available; the total axial strain is uniform across the wall in each option: a) generalized plane strain, where the total axial strain is initially unknown and the axial stress, uniform across the section, is specified as a function of time; b) plane strain, where the total axial strain is always zero at all radial locations; and c) generalized plane strain, where the total axial strain, which is uniform across the section, is specified by the user as a function of time.

   CHERN R1045 was originally written by Dr. J. Chern at the Foster Wheeler Energy Corporation under DOE contract.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed July 1985.
   CDC7600 version submitted April 1979, replaced December 1984, replaced April 1985.

10. **REFERENCES** - A. L. Snow and H. J. Konish, A User's Manual for Chern R-1045 A One Dimensional Elastic-Plastic-Creep Analysis Program, WAESD-SD-94000-26, November 1984.

    CHERN R1045, NESC No. R9713, CHERN R1045 Sample Problem Output Differences, National Energy Software Center Note 85-80, July 30, 1985.

    J. M. Chern, Elastic-Plastic-Creep Analysis of a Thick-Walled Cylinder Subjected to Time Dependent Pressure, Temperature and Axial Loads or Displacements, FWR-35 Rev. 1, April 28, 1973.

    J. M. Chern and D. H. Pai, New Tools to Simplify Inelastic Analysis, Research and Development, pp. 30-32, May 1976.

    J. M. Chern and D. H. Pai, A Simplified Tool for the Elevated Temperature Cyclic Analysis of Pressure Components, ASME Second International Conference on Pressure Vessel Technology, Part I, Design and Analysis, San Antonio, pp. 263-275, 1973.

    H. J. Konish and A. L. Snow, MATLIB: A Computer Library of Material Properties User's Manual, WARD-SD-3045-15, December 1978, Rev. 2 1980, Rev. 3 October 21, 1982, Rev. 4 August 8, 1983.

    H. J. Konish and A. L. Snow, MATLIB: A Computer Library of Material Properties Verification Manual, WARD-SD-94000-2, July 1979.

11. **HARDWARE REQUIREMENTS** - 150K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** –

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –

J. Chern, A. L. Snow, and H. J. Konish
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (9492 lines)
The WAESD-SD-94000-26 reference report, NESC Note, and selected sample problems output and CHERN R1045 source and sample problems input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – I
KEYWORDS – strains, mechanical properties, static loads, creep, elasticity, plasticity, one-dimensional, cylinders, fatigue, pressure, temperature, MATLIB codes

18. **SPONSOR** – DOE Office of Breeder Technology Projects

1. **IDENTIFICATION AND KWIC TITLE** - FASTBUS STANDARD ROUTINES
   FASTBUS STANDARD ROUTINES, basic operations

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11

3. **DESCRIPTION** - The FASTBUS STANDARD ROUTINES make up a software library for performing basic FASTBUS system operations such as block transfers, control operations, etc. The software is designed for the Unibus Processor Interface (UPI) and Input Output Register FASTBUS Interface (IORFI) operating under RSX-11M (V4.1).

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC PDP11 version submitted May 1985.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** - approximately 20K words

12. **PROGRAMMING LANGUAGE** - MACRO-11 (99%) and FORTRAN (1%)

13. **OPERATING SYSTEM** - RSX-11M 4.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. Lesny, R. Pordes, Y. Kim, and A. J. Cohen
    Fermi National Accelerator Laboratory

16. **MATERIAL AVAILABLE** -
    Source (11,740 lines)
    The FASTBUS STANDARD ROUTINES source, executable images, and control information on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - O
    KEYWORDS - data acquisition systems, Fastbus system, PDP computers

18. **SPONSOR** - DOE Chicago Operations Office

1. **IDENTIFICATION AND KWIC TITLE** - FASTBUS SYSTEM MANAGER
   FASTBUS SYSTEM MANAGER, system design tools

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - The FASTBUS SYSTEM MANAGER (FSM) software allows the FASTBUS system user to perform various system design tasks. Because of the flexible topology of FASTBUS, the logistics are more complicated than in CAMAC systems. The hardware configuration must be rigorously specified and verified. Module and segment addresses must be calculated. The paths between devices must be determined and this information loaded into the modules, the segment's ancillary logic, and the segment interconnects. In a sense, a software topology must be specified, also. For example, to determine which modules access which other modules, which modules need their control programs down loaded, and the addresses which must be linked into these programs. FSM assists in performing these tasks. Digital Equipment Corporation's proprietary DATATRIEVE database management system is used to specify record definitions for devices, segments, and segment interconnects; to specify logical relationships between fields in these records; to produce interactive procedures to create and update the database; and to design reports to be generated as needed.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC VAX11/780 version submitted May 1985.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77 (86%), PASCAL (12%), and MACRO-11 (2%)

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    A. J. Cohen
    Fermi National Accelerator Laboratory

16. **MATERIAL AVAILABLE** -
    Source (271 8192-character records)
    The FASTBUS SYSTEM MANAGER source, executable images, example FASTBUS system, machine-readable documentation, and control information on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - M
    KEYWORDS - Fastbus system, DEC computers, data base management, data acquisition systems design, utility routines

18. **SPONSOR** - DOE Chicago Operations Office

1. **IDENTIFICATION AND KWIC TITLE** - RSX-MULTI
   RSX-MULTI, experiment control & data analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11

3. **DESCRIPTION** - RSX-MULTI is a Fortran-based data analysis program having well-defined interfaces through which it obtains data, makes graphics displays, accomplishes data input and output, and performs user data analysis. It is based on the MULTI program written by J. F. Bartlett at the California Institute of Technology. To generate RSX-MULTI, a complete and general system for acquiring and analyzing data, Fermilab National Accelerator Laboratory (FNAL) integrated MULTI with the FNAL RSX-DA software package, graphics and I/O routines appropriate to the RSX-11M operating system, and with default user analysis subroutines. There are two levels of RSX-MULTI systems. Level 0 or "basic" RSX-MULTI refers to the analysis program and the interface definitions but not the interface routines themselves. Level 1 of RSX-MULTI will acquire data on an event-by-event basis from CAMAC-based experiment hardware, optionally log it onto magnetic tape, and make it available to the analysis system. When enabled for data processing, RSX-MULTI will obtain an event through its interface routine (either from the experiment or, in playback mode, from magnetic tape). It will perform arithmetic computations on the data. These computations may be specified and altered from the keyboard, even while data is being processed. RSX-MULTI will periodically monitor various user-defined quantities by checking that they are within predefined limits and typing out messages when they are out of range. Specialized code tailored to the needs of a particular application may be inserted in the RSX-MULTI system.

   The Level 1 system has considerable dependence on FNAL hardware standards. In cases where FNAL-like hardware is not available, facilities are provided for creating a Level 0.5 of RSX-MULTI. This level is a tape-only analysis system analyzing data tapes generated by RSX-DA. The minimum CPU required to run Level 1 RSX-MULTI is a PDP11 Model 34, 45, or higher processor with full instruction set (including FPU and EIS) and 48K words of memory. RSX-MULTI must be built on a machine with an RK or larger disk and a second block-structured device for the system. Due to the space requirements of RSX-MULTI, it is not recommended that the system be built on fewer than two RK05's. The system is designed for data-logging to, or playback from, industry-standard 9-track magnetic tape. The system can use either TU10 (800 frames/inch), TJU16 (800 or 1600 frames/inch), or STC (1600 or 6250 bpi) transports.

   RSX-MULTI performs its text and graphics display functions on Tektronix 4006 or 4010 display terminals, or equivalent terminals such as the ENVISION terminal or the ADM3 or ADM36 with the retro-graphics board. Versatek model 200A, 80, or 800A matrix printer/plotter unit is supported as a line printer for text output and as a graphics device for histogram display. RSX-MULTI imposes no intrinsic limitations on data acquisition hardware. RSX-MULTI runs with Version 4.X of the RSX-11M operating system. The F77 compiler is required by RSX-MULTI due to the use of INCLUDE statements not supported in F4P. The FNAL CDPACK library is required for use with Level 1 of RSX-MULTI; the CDPACK software is not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   DEC PDP11 version submitted May 1985.

10. **REFERENCES** - L. M. Taff, D. J. Ritchie, E. K. Quigg, and T. D. Lagerlund, Fermilab MULTI User's Guide, Fermilab memorandum PN-97.5, October 1, 1979.

D. J. Ritchie, A Guide to MULTI COMMON Blocks, Fermilab memorandum PN-150, August 23, 1982.

Y. Kang, T. Lagerlund, D. Ritchie, and L. Taff, Programs for Maintaining Text Library Files, Fermilab memorandum PN-125, July 10, 1979.

Peter Heinicke and Penelope Constanta-Fanourakis, Fermilab RSX Software Menu, Fermilab memorandum PN-243.00, December 4, 1984.

E. K. Quigg, T. D. Lagerlund, D. J. Ritchie, and L. M. Taff, MULTI Programming Reference Notes, Fermilab memorandum PN-106, March 26, 1980, with Addendum, June 19, 1981.

Penelope Constanta-Fanourakis, RSXMULTI I/O System, Fermilab memorandum PN-240.01, September 10, 1984.

Peter Heinicke, RSXMULTI System Generation, Fermilab memorandum PN-239.1, received May 2, 1985.

11. **HARDWARE REQUIREMENTS** - 48K words

12. **PROGRAMMING LANGUAGE** - FORTRAN 77 (93%) and MACRO-11 (7%)

13. **OPERATING SYSTEM** - RSX-11M 4.X with Jy411 CAMAC branch driver.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

J. F. Bartlett and P. Constanta-Fanourakis
Fermi National Accelerator Laboratory

16. **MATERIAL AVAILABLE** -

Source (263 2048-character records)

The reference memoranda and RSX-MULTI source, test driver, machine-readable documentation, and control information on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - O
KEYWORDS - data acquisition systems, PDP computers, experimental data, computerized control systems, data analysis, RSX-DA codes, CDPACK codes

18. **SPONSOR** - DOE Chicago Operations Office

1. **IDENTIFICATION AND KWIC TITLE** - SCIENTIFIC WORKSTATION EVALUATION BENCHMARK
   SCIENTIFIC WORKSTATION EVALUATION BENCHMARK

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   MPLN (designed to be portable)

3. **DESCRIPTION** - The SCIENTIFIC WORKSTATION EVALUATION BENCHMARK software includes 16 programs which are executed in a well-defined scenario to measure the following performance capabilities of a scientific workstation: implementation of FORTRAN77, processor speed, memory management, disk I/O, monitor (or display) output, scheduling of processing (multiprocessing), and scheduling of print tasks (spooling).
   The benchmark programs are: DK1, DK2, and DK3, which do Fourier series fitting based on spline techniques; JC1, which checks the FORTRAN function routines which produce numerical results; JD1 and JD2, which solve dense systems of linear equations in double- and single-precision, respectively; JD3 and JD4, which perform matrix multiplication in single- and double-precision, respectively; RB1, RB2, and RB3, which perform substantial amounts of I/O processing on files other than the input and output files; RR1, which does intense single-precision floating-point multiplication in a tight loop; RR2, which initializes a 512x512 integer matrix in a manner which skips around in the address space rather than initializing each consecutive memory cell in turn; RR3, which writes alternating text buffers to the output file; RR4, which evaluates the timer routines and demonstrates that they conform to the specification; and RR5, which determines whether the workstation is capable of executing a 4-megabyte program.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed May 1985.
   SCIENTIFIC WORKSTATION EVALUATION BENCHMARK submitted May 1985.

10. **REFERENCES** - Richard C. Raffenetti, Scientific Workstation Comparisons Using a Benchmark, ANL/TM-415, April 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. C. Raffenetti
    Computing Services-Support Services Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (7688 lines)
    The reference report and SCIENTIFIC WORKSTATION EVALUATION BENCHMARK source and data files on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - Z
    KEYWORDS - benchmarks, performance testing, computers, FORTRAN

18. **SPONSOR** - Argonne National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - SWAAM-LT
   SWAAM-LT, long-term sodium-water reaction

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM3033

3. **DESCRIPTION** - SWAAM-LT (Sodium-Water Advanced Analysis Method - Long Term) analyzes long-term unsteady flow behavior in piping network systems due to sodium-water reactions in a liquid metal fast breeder reactor steam generator. SWAAM-LT is based on incompressible viscous flow equations in which the effects of fluid compressibility that are usually important during the early stages are neglected. SWAAM-LT is written specifically for application to a large-scale sodium-water reaction in the secondary heat transport system of a LMFBR, although it is not limited to such applications. Output includes junction pressures, pipe flow velocities, gas/liquid interface locations, details of gas regions, relief-line flow characteristics, and cover-gas junction details at each time-step of calculation.

   The program is based on the general assumption of one-dimensional single-phase and incompressible pipe flow. However, it has a two-phase flow capability in the relief system connected to the cover-gas region of steam generators. SWAAM-LT can produce analysis results on the long-term response resulting from a large sodium-water reaction (SWR) in a steam generator as long as the system does not encounter a gross two-phase flow situation. As a SWR transient progresses, the relief system becomes activated, the system becomes depressurized, the sodium inventory in the system decreases, and a two-phase flow situation would eventually occur somewhere in the system. The program is designed to detect this situation and stop its calculation.

   SWAAM-LT can analyze a system with up to 50 pipes and 50 junctions; however, these array dimensions can be easily increased to analyze a larger system. SWAAM-LT uses the proprietary ISSCO graphics software system, DISSPLA, to produce graphical output. The solution typically converges in less than one minute of CPU time on an IBM3033.

   SWAAM1 (NESC 885) and SWAAM2, other members of the SWR family of codes for analysis of sodium-water reactions, are designed to analyze short-term behavior.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed May 1985.
   IBM3033 version submitted May 1985.

10. **REFERENCES** - H. Chung, Y. W. Shin, and A. H. Wiedermann, User's Manual for the Long-Term Sodium/Water Reaction Analysis Code SWAAM-LT, ANL-83-41, June 1983.

    H. Chung, Y. W. Shin, and A. H. Wiedermann, Verification of SWAAM-LT Code Capabilities by Use of Sample Problems, ANL-83-38, May 1983.

    H. Tanabe, Y. W. Shin, and H. Chung, SWAAM-LT Validation by SWAT-3 Data, ANL-83-60, November 1983.

    H. Chung and Y. W. Shin, Validation of SWAAM-LT Code with LLTR Series II Test A-3 Data, ANL-84-2, January 1984.

    H. Chung and Y. W. Shin, Validation of SWAAM-LT Code with SWAT-3 Test Data, ANL-84-69, August 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - MVS 3.0.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** –

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
H. Chung, Y. W. Shin, and A. H. Wiedermann
Components Technology Division
Argonne National Laboratory

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (2618 lines)
The ANL-83-41 reference report and SWAAM-LT source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – G
KEYWORDS – steam generators, reactor components, viscous flow, sodium, water, LMFBR reactors, leaks, molten metal-water reactions, SWAAM1 codes

18. **SPONSOR** – DOE Division of Reactor Research and Technology,
Engineered Component Branch

1. **IDENTIFICATION AND KWIC TITLE -** EPACA
   EPACA, 3d thick shell elastic-plastic-creep

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   IBM360

3. **DESCRIPTION -** EPACA is designed for elastic-plastic-creep analysis of thick, three-dimensional shells made up of flat or curved shell elements. Multiple fixed format operating modes are incorporated such that static-elastic, elastic-plastic-creep, free vibration, dynamic time history, and buckling analysis can be performed. EPACA is based on an incremental displacement finite-element approach. Constitutive equations for time-independent plasticity and time-dependent creep behavior are handled through tangential stiffness and initial strain algorithms, respectively. Kinematic descriptions are general; flat and curved, thin- and thick-shell/plate type finite elements are included.
   For steady-state vibration analysis, eigenvalues of the lumped mass system are computed by inverse power iteration with shifts. A Newmark step-by-step solution is carried out for transient response calculations. Bifurcation buckling capabilities are included. Truly three-dimensional structural problems cannot be modeled. The analysis methods of RDT Standard F9-5 are incorporated. Execution times vary from 1 CPU minute to several hours depending on the problem size. EPACA uses proprietary CalComp software to obtain graphical output.
   Developer support is not available for the EPACA software.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed May 1985.
   IBM360 version submitted March 1977.

10. **REFERENCES -** Z. Zudans, M. M. Reddi, H. M. Fishman, and T. Y. Chow, Theory and Users Manual for EPACA General Purpose Elastic-Plastic-Creep Finite Element Program for Three-Dimensional Thick Shell Structures, F-C3038, June 30, 1972.
    J. A. Clinard and S. K. Iskander, ORNL Notes for EPACA (5.2), Oak Ridge National Laboratory Memorandum, February 1977.
    EPACA, NESC No. R9719, EPACA Implementation Information, National Energy Software Center Note 85-78, May 17, 1985.

11. **HARDWARE REQUIREMENTS -** 300K to 1000K bytes

12. **PROGRAMMING LANGUAGE -** FORTRAN IV (99%) and BAL (1%)

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    J. A. Clinard
    Oak Ridge National Laboratory

16. **MATERIAL AVAILABLE -** Restricted Distribution
    Source (18,451 lines)
    The reference report, ORNL Memorandum, and NESC Note and EPACA source, machine-readable documentation, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - deformation, elasticity, plasticity, finite element method, plates, shells, stresses, mechanical structures, three-dimensional, dynamic loads, static loads

18. **SPONSOR** - ERDA Division of Reactor Development and Demonstration

1. **IDENTIFICATION AND KWIC TITLE -** IH
   IH, optical code solar central receiver system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Honeywell Series 60 Level 66

3. **DESCRIPTION -** IH is a set of four optical model programs: NS, RC, IH, and CA offering a generalized approach to performance simulation, optimization, and optical design of central receiver systems based on the exact location and diurnal behavior of each heliostat in the collector field. A solar central receiver system is a means of collecting high quality solar energy by optical transmission from a field containing a large number of mass-produced identical heliostats.

   The NS program is a cellwise performance model which represents the collector field by a set of computational cells that are square and have a north-south orientation. Each cell contains a representative heliostat at the cell center which represents all of the heliostats in that cell. NS requires collector field, receiver, heliostat, and tower geometry as input and determines interception fractions (for RC) and flux distributions (for CA). Daily, monthly, or annual performance data may be produced.

   The RC program is a cellwise optimization program that uses detailed cost and performance models to determine the optimum heliostat spacing in each cell and the optimum trim (boundary) of the collector field. The optimized portion of the system includes land, heliostats, heliostat wiring, receiver, tower, and riser/downcomer. The collector field boundary can be varied about the optimum to obtain cost and performance information covering a range of values. RC produces a set of curve-fit coefficients for the optimized heliostat spacings. The coefficient data are required by IH and may also be input to NS to examine the performance of an optimized collector field.

   The IH program is an individual heliostat representation performance model which provides heliostat coordinates to the power plant constructor. In addition, IH can perform a total system analysis similar to NS.

   The CA program is a cavity radiation program which provides geometry data for NS. It generates zonal decomposition for view factor analysis and convergent flux densities and temperatures.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed July 1985.
   Honeywell Series 60 version submitted March 1985.

10. **REFERENCES -** C. L. Laurence and F. W. Lipps, User's Manual for the University of Houston Individual Heliostat Layout and Performance Code, SAND84-8187, December 1984.

    F. W. Lipps and L. L. Vant-Hull, A Programmer's Manual for the University of Houston Computer Code RCELL: Cellwise Optimization for the Solar Central Receiver Project, DOE/SF/10763-T5 (SAN/0763-1), September 1980.

    Fred W. Lipps and Lorin L. Vant-Hull, Notes on Collector Field Optimization - Extensions of the Basic Theory, DOE/SF/10763-T6 (SAN/0763-5), November 1980.

    C. L. Laurence and F. W. Lipps, A User's Manual for the University of Houston Computer Code - RC Cellwise Optimization for the Central Receiver Project, DOE/SF/10763-T7 (SAN/0763-3), December 1980.

    F. W. Lipps and L. L. Vant-Hull, A User Manual for the University of Houston Solar Central Receiver, Cellwise Performance Model: NS, DOE/SF/10763-T9 (SAN/0763-4), Vols. I and II, December 1980.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE** - FORTRAN V

13. **OPERATING SYSTEM** - GCOS3 Version 4JS3 update 8.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
A. J. Webb
Sandia National Laboratories, Livermore

16. **MATERIAL AVAILABLE** -
Source (25,382 lines)
The SAND84-8187 reference report and IH source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - solar thermal power plants, central receivers, heliostats, optimization, light transmission, solar collectors, performance, concentrating collectors

18. **SPONSOR** - DOE Solar Thermal Division

1. **IDENTIFICATION AND KWIC TITLE -** LRSYS
   LRSYS, PASCAL LR(1) parser generator system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Cray1, DEC VAX11, IBM PC

3. **DESCRIPTION -** LRSYS is a complete LR(1) parser generator system written entirely in a portable subset of Pascal. The system, LRSYS, includes a grammar analyzer program (LR) which reads a context-free (BNF) grammar as input and produces LR(1) parsing tables as output, a lexical analyzer generator (LEX) which reads regular expressions created by the REG process as input and produces lexical tables as output, and various parser skeletons that get merged with the tables to produce complete parsers (SMAKE). Current parser skeletons include Pascal, FORTRAN 77, and C. In addition, the Cray1,DEC VAX11 version contains LRLTRAN and CFT-FORTRAN 77 skeletons. Other language skeletons can easily be added to the system. LRSYS is based on the LR program (NESC 822).

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed May 1985.
   Cray1,DEC VAX11 version submitted February 1985, replaced April 1985.
   IBM PC version submitted April 1985.

10. **REFERENCES -** Kelly O'Hair, The LR System User Manual, LCSD-313 Revision 1 Draft, April 1985.
    C. Wetherell and A. Shannon, LR Automatic Parser Generator and LR(1) Parser, UCRL-82926 Preprint, July 14, 1979.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** Pascal

13. **OPERATING SYSTEM -** CTSS (Cray1), UNIX (DEC VAX11), DOS (IBM PC).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    K. O'Hair
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE -**
    Source (CRA1,VX11-14,557 lines, IBM PC-6472 lines)
    The reference LCSD-313 Revision 1 Draft report and LRSYS source, sample problems, skeletons, and machine-readable documentation on magnetic tape (Cray1,DEC VAX11) or two 5.25-inch, double-sided, double-density flexible disks are available from NESC on an "As Is" basis.

17. **CATEGORY -** P
    KEYWORDS - computers, programming languages, Pascal, LR codes

18. **SPONSOR -** Lawrence Livermore National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - FE3DGW
   FE3DGW, finite element ground water flow model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - FE3DGW (Finite Element 3-Dimensional Ground Water) analyzes flow through large, multilayered, ground-water systems. The code has the capability to model noncontinuous as well as continuous layers, time-dependent and constant sources/sinks, and transient as well as steady-state flow.
   The code offers a wide choice of boundary conditions including prescribed heads, nodal injection or withdrawal, constant or spatially varying infiltration rates, and elemental source/sink. Initial conditions can be prescribed as vertically hydrostatic or variable hydraulic head. The heterogeneity in aquifer permeability can be described by geologic unit or explicitly for given elements. Three-dimensional elements are generated from user-defined well logs at each surface node. To facilitate interaction between disciplines, auxiliary programs are provided to plot the finite-element grid, well logs, contour maps of input and output parameters, and vertical cross sections and to determine ground-water pathlines and travel time from a specified point. FE3DGW does not account for density variation and calculates only the hydraulic heads. The program can be used to support site characterization, evaluate ground-water flow rates, and estimate travel path and time in regional and local ground-water systems. FE3DGW uses the proprietary CalComp and DISSPLA graphics software to generate graphical output.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed May 1985.
   DEC VAX11/780 version submitted April 1985.

10. **REFERENCES** - Sumant K. Gupta, Charlie R. Cole, Frederick W. Bond, and Amy M. Monti, Finite-Element Three-Dimensional Ground-Water (FE3DGW) Flow Model: Formulation, Computer Source Listings, and User's Manual, BMI/ONWI-548, October 1984.

11. **HARDWARE REQUIREMENTS** - 500K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - VMS 3.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    S. K. Gupta and C. R. Cole
    Office of Nuclear Waste Isolation
    Battelle Project Management Division

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (17,394 lines)
    The reference report and FE3DGW source, sample problems input and output, auxiliary programs, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R

KEYWORDS - finite element method, ground water, three-dimensional, radioactive waste management, fluid flow, hydrology, hydraulic conductivity, layers, porosity

18. **SPONSOR** - DOE National Waste Terminal Storage Program

1. **IDENTIFICATION AND KWIC TITLE** - EXPANTR
   EXPANTR, thermal analysis of Na expansion tank

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - EXPANTR calculates thermal transients for the sodium expansion tank of the Intermediate Heat Transport System (IHTS) in the Clinch River Breeder Reactor Plant (CRBRP). As duty cycle events occur in the plant, temperature changes in the IHTS main loop result in expansion and contraction of loop sodium and consequent flow of sodium between the IHTS main loop and the expansion and pump tanks. The resulting temperatures, flow rates, pressures, and levels at the expansion tank define the applicable transients for the tank. EXPANTR generates these transients for a single IHTS loop by calculating (1) the net rate of expansion or contraction of sodium in the main loop, (2) the pressures in the main loop on the basis of defined input flows and pump inlet pressures, and (3) the flows out of and into the main loop on the basis of the results of (2). The net flows of (1) and (3) are compared, and the pump inlet pressure is adjusted in successive iterations until these flows are acceptably close. The specific EXPANTR transient input data for this process (besides fixed quantities such as initial conditions) are time histories of main loop flow rate and sodium temperatures at the inlet of each segment of piping and each major component in the main loop. These quantities are obtained from output generated by the DEMO code (NESC 676). EXPANTR output includes temperatures, pressures, and flows throughout the system, as well as sodium levels in the tanks.
   EXPANTR includes the following subsystems: main IHTS piping of a loop, major in-line components of the loop, sodium pump characteristics, vent piping from the steam generator modules, discharge line from the expansion tank, cold trap line, leakage paths in the pump, and expansion and pump tanks.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed June 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES** - Robert Yaspo, Verification for Computer Code EXPANTR, GE-ARSD Spec. 23A3009, June 24, 1983.
    G. E. Orr, EXPANTR Code Verification, GE-ARSD Memorandum YL-612-00030, April 21, 1980.
    R. A. Luoma, et al., Computer Code for IHTS Sodium Expansion Tank Thermal Transients, GE-ARSD Memorandum, August 30, 1977.
    Clinch River Breeder Reactor Plant Nuclear Island, LMFBR Demonstration Plant Simulation Model (DEMO), WARD-D-0005, Revision 4, January 23, 1976.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. A. Luoma
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (1174 lines)
The YL-612-00030 and 23A3009 reference documents and EXPANTR source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - sodium, fluid flow, flow rate, temperature, pressure, reactor components, tanks, Clinch River Breeder Reactor, DEMO codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - SML
   SML, FORTRAN and CAL source library management

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600 or Cray1

3. **DESCRIPTION** - SML copies FORTRAN and CAL packed ASCII source files into a LIB library of packed ASCII subroutine source files or merges a LIB library of subroutines into a single source file for listing or other purposes. The program can perform a partial copy of the source file and will prompt the user for the subroutine names to be copied. By default, the subroutine names are sorted for the copy; however, an option is available to leave the order unchanged. In the CDC7600 version, the ASCII source files should contain FORTRAN source statements; CAL assembly subprograms as well as FORTRAN can be handled with the Cray1 version. A maximum of 400 subroutines is allowed in a file or library. SML uses LLNL computing environment system subroutines to perform the required input and output operations; these routines are not included. SML allows a programmer to work on a large development program, a subroutine at a time.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   CDC7600,Cray1 version submitted April 1985.

10. **REFERENCES** - Lila L. Chase, SML, UCID-18887, Rev. 1, February 11, 1982.

11. **HARDWARE REQUIREMENTS** - 13K (octal) words (CDC7600), 15K (octal) words (Cray1)

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. L. Chase
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (1938 lines)
    The reference report and SML source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - utility routines, programming, FORTRAN, information systems, information retrieval, SFM codes, LIB codes

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - NIKE3D
   NIKE3D, static & dynamic response of 3d solids

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1, CDC7600

3. **DESCRIPTION** - NIKE3D is a vectorized, fully implicit, three-dimensional, finite-element program for analyzing the finite-strain, static and dynamic response of inelastic solids, shells, and beams. Capabilities currently available include sliding interfaces, body force loads due to base acceleration, body force loads due to spinning (geometry dependent), concentrated nodal loads, pressure boundary conditions (geometry dependent), displacement boundary conditions, thermal stresses, plotfile generation, and problem restart.
   Spatial discretization is accomplished using eight-node solid elements that are integrated using a two-point Gauss quadrature rule, four-node shell elements that use a 2x2 Gauss integration in the surface and from 1 to 5 integration points through the thickness, and two-node thick beam elements using from 1 to 5 integration points in each local direction of the cross section at the center of the beam. Elastic, orthotropic elastic, elastic-plastic, thermo-elastic-plastic, soil and crushable foam, linear viscoelastic, thermo-orthotropic elastic, and thermo-elastic-creep material models are implemented. An incremental-iterative numerical algorithm, based on the Green-Naghdi and Jaumann stress rate formulations, is implemented in NIKE3D. Five iterative schemes are available including the BFGS quasi-Newton method, Broyden's quasi-Newton method, modified Newton-Raphson, full Newton, and full Newton with line search.
   Similar methods in two dimensions are available in NIKE2D (NESC 9923). INGRID, SLIC (NESC 968), and TACO3D (NESC 9838) can be used to prepare NIKE3D input, and the TAURUS (NESC 9908) postprocessor generates graphic output from NIKE3D results.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed May 1985.
   Cray1 version submitted March 1985.

10. **REFERENCES** - J. O. Hallquist, NIKE3D: An implicit finite-deformation, finite element code for analyzing the static and dynamic response of three-dimensional solids, UCID-18822, Rev. 1, July 1984.
    DYNA2D, DYNA3D, NIKE2D, NIKE3D, TAURUS Descriptions of "Missing" LLNL Environmental Subroutines, Lawrence Livermore National Laboratory Note, June 1983.
    NIKE3D, NESC No. 9725, NIKE3D Implementation Information, National Energy Software Center Note 85-77, May 28, 1985.

11. **HARDWARE REQUIREMENTS** - 100K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (98%) and CAL (2%)

13. **OPERATING SYSTEM** - CTSS (Cray1), LTSS (CDC7600).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. O. Hallquist
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** –
Source (19,887 lines)
The reference report and LLNL and NESC Notes and NIKE3D source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – I
KEYWORDS – three-dimensional, finite element method, structural models, dynamic loads, deformation, stress analysis, static loads, creep, plasticity, elasticity, NIKE2D codes, SLIC codes, TAURUS codes, INGRID codes, TACO3D codes

18. **SPONSOR** – DOE Division of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - METACAD
   METACAD, AGS880 data structure usage routines

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - METACAD (the METa file approach to Access of Computer Aided Design data) is a FORTRAN subroutine library used to create a randomly accessible data structure from an Applicon Apple-3D graphics file and to provide a logical method for accessing the data structure from an application program. The METACAD system was designed to ease the development of application programs that use the Applicon 880 system graphics definitions as a database. These applications include database translation (GRAPTRAN,PATRAN), photo-plotting code generation (PREP33,HOST33), design rule checking (NETLIS3/CLRCHK3), hard-copy plotting (CHECKPLOT3D,COM output), and any other postprocessor which must extract data stored in the proprietary Applicon graphics data structure (AGS file).

   The METACAD system was developed to provide an improved interface over what was available (Apple-3D, AP3GCS). Both Apple-3D and AP3GCS allow only sequential access of the data and limited data access capabilities. The Apple-3D data structure is created from the AGS file by IO-121, an Applicon-supplied interface; it is intended primarily for transporting data between Applicon equipment. Its sequential ASCII format makes it unusable as a random access database structure. AP3GCS uses the Apple-3D file as its input while retaining its sequential nature and problems. METACAD eliminates the Apple-3D/AP3GCS problems by creating a linked-list data structure which allows random access.

   The METACAD system consists of two sections: the data structure generation routine and the access routines. The METACAD data structure is generated from an Apple-3D formatted file and placed in resident (virtual) memory by a call to APLIN. The system is designed so that all data manipulation is done through the use of the data access routines for the application program. The METACAD data structure is organized into three major sections: global parameters, component definitions, and component placements. The global parameters consist of variables, such as drawing title, file name, and scaling information, not associated with particular graphics components. The components definitions contain attributes assigned to primitive graphics entities, such as component type, component name, and other information, specific to an individual primitive entity. The component placements section contains entries for the graphics components that have been inserted into the drawing.

   Three utility routines METAWRITE, METAREAD, and METADUMP are included as program development aids. METAWRITE writes the METACAD data structure and state variables to an unformatted file with the logical name METASTRUC. METAREAD reads the METASTRUC file into the data structure restoring the data. METADUMP creates an ASCII printable version of the METACAD data structures. METACAD output is provided as a status file, METASTAT.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed May 1985.
   DEC VAX11/780 version submitted January 1985, replaced March 1985.

10. **REFERENCES** - Victor R. Yarberry, METACAD Programmer's Guide, SAND83-1110, May 1983 and Errata May 16, 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77 V3.0-2

13. **OPERATING SYSTEM** - VMS 3.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
D. L. Janni
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE -**
Source (48 8192-character records)
The reference report and Errata and METACAD source on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - computer-aided design, computer graphics, computer-aided manufacturing, data processing, data base management, DEC computers

18. **SPONSOR** - DOE Albuquerque Operations Office

1. **IDENTIFICATION AND KWIC TITLE** - MF.CH
   MF.CH, Metafont change files typeface design

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - MF.CH is a set of five Metafont change files used to create VAX/VMS Pascal programs for typeface design in conjunction with the Metafont source files and the TANGLE and WEAVE processors of the Web System of Documentation written by Donald E. Knuth at Stanford University. The change files MF.CH, INIMF.CH, GFTYPE.CH, GFTOPXL.CH, and GFTODVI.CH are designed to be used with the source files MF.WEB, GFTYPE.WEB, GFTOPXL.WEB, and GFTODVI.WEB written by Knuth. TANGLE and WEAVE are used to create Pascal programs and TeX documentation files, respectively.
   MF is a program which takes Metafont input files and produces output files which can be used by the other programs to create fonts for computer typesetting. INIMF is the initialization version of MF. GFTYPE checks the output files for internal consistency and produces a symbolic description of their contents. GFTOPXL uses an output file from MF to produce a pixel file of character bitmaps, which can be used by TeX system programs when producing typesetter output. GFTODVI generates a file which can be used by TeX system programs to produce character proofs on a typesetting device. The purpose of the MF.CH set of VAX/VMS change files is to tailor the respective source programs so that they can be compiled and run on a VAX/VMS system.

4 **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   DEC VAX11/780 version submitted December 1984.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - PASCAL and WEB

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. Colman
    Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
    Source (15 8192-character records)
    The MF.CH change files source and machine-readable documentation on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - text editors, DEC computers, METAFONT codes, TEX codes

18. **SPONSOR** - Lawrence Berkeley Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - PART2
   PART2, COMTAL particle counting & analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/750

3. **DESCRIPTION** - PART2 calculates the fractal dimension of binary colloidal particle images recorded by an imaging microscope. The fractal dimension is computed as the slope of the regression line fitted to a log-log plot of each particle's second-order moment against its area. The program also counts the number of closed polygons contained within a closed rectangular region of specified dimensions, generates a cell area histogram, and in addition, computes central moments up to and including order 3. Each particle's central moments are calculated by applying Green's Theorem while traversing the contour. The image to be processed must be a binary-image with black representing the particles and white representing the background. All images and image files are assumed to be 512 x 512 pixels. No provision is available to transfer more or less data to or from the COMTAL. Line at a time disk transfers are possible with existing subroutines. All area and higher-order moment calculations assume that each particle is solid. The PLOTIT program is used to plot the graph of regression data on the Versatec plotter.
   The SNLA image reading and writing routines, TRANFIL and TRANCOM, and the COMTAL-specific routines, CMGET, CMREL, CMWAIT and WTTARG, are not included. PART2 is a modification of an earlier PARTICLE program written by D. Ghiglia. Three minutes of execution time are required for a 512 x 512 image.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   DEC VAX11/750 version submitted March 1985.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS 3.6 and COMTAL Vision One/20 Image Processor.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   G. A. Mastin
   Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
   Source (1471 lines)
   The PART2 source on magnetic tape, in VAX/VMS COPY format, is available from NESC on an "As Is" basis.

17. **CATEGORY** - P
   KEYWORDS - image processing, particles, particle size, colloids, regression analysis, display devices

18. **SPONSOR** - Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - HECTR
   HECTR, containment response to hydrogen event

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600, Cray1, DEC VAX11/780

3. **DESCRIPTION** - HECTR (Hydrogen Event-Containment Transient Response) is a lumped-volume containment analysis program developed for calculating the containment atmosphere pressure-temperature response to hydrogen burns. HECTR was developed primarily for analysis of ice-condenser PWR and Mark III BWR containments, but its use is not restricted to these systems. HECTR is also useful for modeling hydrogen transport and combustion experiments or for analyzing experiments involving only the release of steam and liquid water. Four gases - steam, nitrogen, oxygen, and hydrogen - are modeled along with sumps containing liquid water. To calculate the pressure, temperature, and composition of gases in a containment, the system is divided into compartments with flow between compartments occurring at junctions. Flows between compartments are pressure and buoyancy driven with inertial and resistance terms included. Steam is treated as a real gas, and the other gases are treated as ideal. Gases in each compartment are instantaneously mixed, and source terms are user-specified. Mass, momentum, and energy conservation equations are then solved using a linearized implicit formulation (backward Euler method) to determine compartment and junction conditions during the transient. The thermal response of surfaces and equipment in the containment can also be calculated, using either one-dimensional finite difference slabs or lumped masses. The effects of many important physical phenomena in reactor containments during accidents, as well as many engineered safety features (ESF's) are modeled. The physical phenomena considered are hydrogen combustion, radiative and convective heat transfer, and steam condensation or evaporation. The ESF's modeled are containment sprays, fans, ice condensers, sumps, suppression pools, and heat exchangers.
   Steam explosions, core-concrete interactions, and aerosol transport are not modeled by HECTR.
   A postprocessor program, ACHILES, is included. It processes the time-dependent variable output (compartment pressures, flow junction velocities, surface temperatures, etc.) produced by HECTR. ACHILES can create tables and graphs of these data. The ISSCO proprietary DISSPLA graphics software is required to produce plots.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   CDC7600,Cray1,DEC VAX11/780 version submitted February 1985.

10. **REFERENCES** - Allen L. Camp, Michael J. Wester, and Susan E. Dingman, HECTR Version 1.0 User's Manual, NUREG/CR-3913 (SAND84-1522), February 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - SCOPE 2.1 (CDC7600), COS 1.11 (Cray1), VMS 3.6 (DEC VAX11/780).

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. C. Wong
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (11,261 lines)
The reference report and HECTR source, sample problems, auxiliary program, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - G
KEYWORDS - reactor safety, pressure effects, temperature dependence, combustion, hydrogen, containment systems, ice condensers, PWR type reactors, BWR type reactors, ACHILES codes

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Accident Evaluation,
Containment Systems Research Branch

1. **IDENTIFICATION AND KWIC TITLE** - MRSPAK
   MRSPAK, combinatorial geometry PADL2 add-on

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - MRSPAK is a suite of subroutines designed for installation in the PADL2 solid modeling system developed by the University of Rochester. MRSPAK generates a text file containing Combinatorial Geometry (CG) data corresponding to PADL2 geometry. This allows the users of MORSE, ACCEPT, and other radiation transport analysis packages based on Combinatorial Geometry to create geometry using the PADL2 system and then automatically generate the CG data from the PADL2 representation. This is desirable since creating geometry data in the CG format is tedious and error-prone.
   An inverse translator, which takes CG input and produces a text file containing PADL2 commands that define the corresponding solid in PADL2, is also included. This is a standalone program, and separate from both MORSE and PADL2.
   PADL2 is proprietary software; it is not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   DEC VAX11/780 version submitted January 1985.

10. **REFERENCES** - MRSPAK: A Translation Package, Sandia National Laboratories Memorandum, received January 1985.
    MRSPAK, NESC No. 9730, Author's Notes on MRSPAK Add-on Module for PADL2, National Energy Software Center Note 85-56, March 25, 1985.
    E. E. Hartquist and H. A. Marisa, PADL2 Users Manual, Production Automation Project document UM-10/1.2, University of Rochester, May 1983.
    P. H. Dietz, Solid Modeling at the U. S. Army Ballistics Research Laboratory, Proceedings of the Third Annual Conference and Exposition of the Naval Computer Graphics Association, Vol. II, June 1982.
    L. C. Jones and D. C. McKeon, Generation of Radiation Transport Geometry from Computer Generated Design Data, Transactions of the Nuclear Space and Radiation Effects Conference held July 1984, Vol. NS-31, December 1984.

11. **HARDWARE REQUIREMENTS** - MRSPAK with PADL2 requires 6 Mbytes of virtual memory.

12. **PROGRAMMING LANGUAGE** - FLEX

13. **OPERATING SYSTEM** - VMS 3.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. C. Jones
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (153 8192-character records)
    The SNLA memorandum and NESC Note and MRSPAK source, sample problem input and output, auxiliary programs, and object libraries on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - solids, geometry, radiation transport, PADL2 codes, MORSE codes, ACCEPT codes

18. **SPONSOR** - Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - FURFAN
   FURFAN, fuel and blanket pin failure analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - FURFAN is a program for the general analysis of fuel or blanket pins clad with 20% cold worked 316 stainless steel operating in a LMFBR environment. Each analysis assumes a specific, independent axial position along the pin's length. The pin's overall performance through steady-state and/or transient operation is gauged by the computation of the following three performance indices: the cumulative Creep Damage Function (CDF), the Transient Damage Index (TDI), and the Transient Stress Ratio (TSR). In addition, the cumulative probabilities for failure by creep and by a single transient stress are computed using data-based Weibull distribution functions indexed to the CDF and TSR, respectively. The pin's operating history through steady-state and transient events is simulated by a sequence of linear time segments. A linear time segment is any portion of the overall history in which the power, cladding temperature, cladding stress or gas pressure, and pellet-clad contact pressure can be adequately described by linear functions in time. Thus, each segment is defined by a set of start and end-of-segment values for these operating parameters supplied as input data. Each linear segment in FURFAN is divided into computational increments of equal size defined by the user. Normally, the following performance related phenomena are computed for every computational increment: cladding wastage, the change in the cladding's interstitial content via diffusion to (or from) the sodium and its effect on mechanical properties, annealing of the cladding's mechanical properties, and the degradation of the cladding's transient capability by liquid metal embrittlement.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   CDC7600 version submitted March 1985.

10. **REFERENCES** - Lisa M. Shenton, FURFAN Code User's Manual, WAESD-TN-85-0022, February 27, 1985.
    Lisa M. Shenton, FURFAN Cladding Failure Analysis Computer Code Model Description Report, WAESD-TN-85-0021, February 27, 1985.
    L. M. Shenton, FURFAN Verification Summary Report, WAESD Memorandum SP-85-021, February 28, 1985.
    Lisa M. Shenton, Verification of FURFAN LMFBR Cladding Damage Analysis Computer Code - Part 1, WAESD-TN-84-0152, December 19, 1984.
    Lisa M. Shenton, Verification of FURFAN LMFBR Cladding Damage Analysis Computer Code - Part 2, WAESD-TN-85-0004, January 8, 1985.
    Lisa M. Shenton, Verification of FURFAN LMFBR Cladding Damage Analysis Computer Code - Part 3, WAESD-TN-85-0006, January 18, 1985.
    Lisa M. Shenton, Verification of FURFAN LMFBR Cladding Damage Analysis Computer Code - Part 4 and Appendices, WAESD-TN-85-0020, February 19, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**
R. A. Smith
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE –** Restricted Distribution
Source (4093 lines)
The reference reports and FURFAN source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY –** I
KEYWORDS – fuel pins, performance testing, steady-state conditions, transients, creep, stresses, Clinch River Breeder Reactor

18. **SPONSOR –** DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - NEWPLOT
   NEWPLOT, general-purpose scientific plotting

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - NEWPLOT provides the means of preparing both "quick" (for inspection) and publication-quality x-y data plots with a minimum of effort on a variety of plotting devices. The ISSCO proprietary DISSPLA graphics software system is required. NEWPLOT acts as a convenient user front-end to the DISSPLA subroutine package. Default values that are suitable for most plots are supplied for almost all parameters; if the default value is satisfactory, the user need not specify the parameter explicitly. NEWPLOT can produce linear, semi-log, and log-log plots, with multiple data sets, character strings, lines, and vectors plotted in black-and-white or in color. Data points are read in from disk files; plot parameter input can be read in from either a terminal or a parameter disk file, and can be saved as a disk file for subsequent modification and reuse. The data points can be plotted as symbols only, connected curves only, or both. In addition, individual plot symbols and line segments (or arrows) can be specified and labelled with text to exhibit plot legends, etc. NEWPLOT has provision for convenient recovery from error conditions except for those cases when DISSPLA returns the user to the monitor. This release of NEWPLOT is identified as NEWPLOT3 by the author; it can handle a maximum of 20 data sets each containing up to 2000 points, 100 lines, 50 symbols, and 50 strings to be plotted.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   DEC VAX11/780 version submitted March 1985.

10. **REFERENCES** - J. E. M. Goldsmith, NEWPLOT3 A General-Purpose Scientific Plotting Package, SAND85-8210, February 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. E. M. Goldsmith
    Sandia National Laboratories, Livermore

16. **MATERIAL AVAILABLE** -
    Source (2875 lines)
    The reference report and NEWPLOT source on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - N
    KEYWORDS - computer graphics, data processing, plotters, computer output devices, DISSPLA codes

18. **SPONSOR** - DOE Office of Basic Energy Sciences

1. **IDENTIFICATION AND KWIC TITLE** - UPSON
   UPSON, natural scene ray-tracing graphics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1

3. **DESCRIPTION** - UPSON is a special-purpose, ray-tracing program intended for drawing and animating natural terrain, such as clouds and islands and their reflections in the ocean with light diffusion through clouds and haze. The algorithm assumes that the sun is directly overhead, but gives convincing pictures for other sun directions. The surfaces of the moving waves, the clouds, and the islands are represented mathematically using polynomials, trigonometric functions, and square roots. A line buffer on vertical scan lines is used for the hidden surface computations, together with height field algorithms, which use the fact that the surfaces are single-valued (or double-valued for the clouds) functions of two variables. A bundle of light rays can also be reflected from the water ripples to illuminate an object. The computations are organized so that they can be vectorized on the Cray.
   Output is recorded on magnetic tape and plotted on a Dicomed D-48 color film recorder, at 24 bits per pixel (8 per color), or else at 8 bits per pixel with a color lookup table. UPSON uses the LLNL environment GRAFCORE graphics library and system subroutines; these routines are not included. UPSON is based on the earlier ISLES program which is included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Cray1 version submitted February 1984.

10. **REFERENCES** - Nelson L. Max, Light Diffusion Through Clouds and Haze, UCRL-88411 Preprint, September 29, 1983.
    Nelson L. Max, Vectorized Procedural Models for Natural Terrain: Waves and Islands in the Sunset, ACM/SIGGRAPH Computer Graphics, Vol. 15, No. 3, pp. 317-324, August 1981.
    James F. Blinn, Light Reflection Functions for Simulation of Clouds and Dusty Surfaces, ACM/SIGGRAPH Computer Graphics, Vol. 16, No. 3, pp. 21-29, July 1982.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    N. L. Max
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (ISLES 1402 lines, UPSON 1954 lines)
    The UCRL-88411 reference report and UPSON and ISLES sources on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - computer graphics, photographic films, ISLES codes

18. **SPONSOR** – DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE -** UB1
   UB1, HP subroutine name & location management

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   HP1000

3. **DESCRIPTION -** UB1 is used to keep track of FORTRAN and MACRO subroutines in a software collection. It uses two parallel lists of six-character names for this purpose. The first list contains the subroutine name and the second the name of the source file in which it is found. Either list can be searched for any name and the corresponding entries in the other list will be printed. The entire list can be printed as well, sorted by subroutine name or source file location. Entries in the lists can be changed or deleted. New entries can be added individually or from a list prepared by FIND2. FIND2 will search an entire cartridge for all subroutines and functions. It searches only Type 4 files, but will find assembly language subroutines. It produces a list of these subroutine names and the name of the source file in which it found them in a format UB1 accepts. FINDA searches all Type 4 files for all occurrences of a given string. It produces a list of the file names the string was found in as well as the line numbers at which the string occurred. The auxiliary programs FIND2 and FINDA are included. UB1 is based on an earlier program, SUBS, written by M. Brown.

   This program contains a slightly-modified subroutine from the IMSL Library, proprietary software from International Mathematical and Statistical Libraries, Inc., Houston, Texas. This routine may not be redistributed or removed for use in other applications. It is identified as SRTIT and is derived from IMSL routine VSRTM.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed March 1985.
   HP1000 version submitted September 1984.

10. **REFERENCES -**

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN 77 (84%) and MACRO (16%)

13. **OPERATING SYSTEM -** RTE VI.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    D. E. Perkins and H. H. Bell, Jr.
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE -**
    Source (UB1 65K, FIND2 16K, FINDA 26K)
    The UB1 source, object decks, machine-readable documentation, auxiliary programs, and control information on magnetic tape, in HP1000 RTE VI SAVER format, are available from NESC on an "As Is" basis.

17. **CATEGORY -** M
    KEYWORDS - HP computers, data base management, information systems, information retrieval, SUBS codes, FIND2 codes, FINDA codes

18. **SPONSOR** - DOE Office of Magnetic Fusion Energy

1. **IDENTIFICATION AND KWIC TITLE** - CO2CYCL
   CO2CYCL, huff-n-puff heavy crude oil recovery

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER205,170

3. **DESCRIPTION** - CO2CYCL is a numerical model which simulates multicomponent, multiphase, compressible flow through a horizontal, two-dimensional porous medium bounded on one side by a one-dimensional fracture. The absolute permeability of the fracture is assumed to be much greater (five orders of magnitude or more) than that of the reservoir matrix, so that flow in the matrix is predominantly perpendicular to the fracture face, and flow in the matrix parallel to the fracture can be ignored. The fluid system consists of three components in three phases. Component 1 is the injected fluid, e.g. CO2, and can exist in any of the three phases - gas, oil, and water. Component 2 is the hydrocarbon component and is assumed to be heavy enough so that it exists only in the oil phase. Component 3 is the aqueous component and is restricted to the water phase. All fluid properties, except viscosity and relative permeability, are assumed to be linear functions of pressure and composition. The temperature of the system is taken as constant, and effects due to capillary pressure and gravity are not included.

   The mathematical formulation is based on a set of molar continuity equations (one per component), the phase equilibrium condition, and a volume conservation equation. Reduction of this system of equations to a single equation in pressure leads to a sequential (implicit pressure-explicit moles) method of solution. In-step iterations are performed to increase the implicitness of the method. The algorithm includes time-step control and a volume balance check.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   CDC CYBER205 version submitted December 1984.

10. **REFERENCES** - Roland Begin and David A. Krueger, Computer Simulation of Recovery of Heavy Crude Oil Using Carbon Dioxide Drive or Huff-N-Puff, DOE/BC/10640-21, November 1983.

    F. M. Orr, Jr., Simulation of the One-Dimensional Convection of Four-Phase, Four-Component Mixtures, DOE/ET/12082-8, October 1980.

    J. S. Miller and R. A. Jones, A Laboratory Study to Determine Physical Characteristics of Heavy Oil After CO2 Saturation, SPE/DOE 9789, 1981.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - USOS 2.0 (CDC CYBER205), NOS 2.2 (CDC CYBER170)

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. A. Krueger
    Department of Physics
    Colorado State University

16. **MATERIAL AVAILABLE** -
    Source (1955 lines)

The DOE/BC/10640-21 reference report and CO2CYCL source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - petroleum deposits, miscible-phase displacement, carbon dioxide injection, compressible flow, reservoir engineering, viscosity, computerized simulation

18. **SPONSOR** - DOE Office of Fossil Energy

1. **IDENTIFICATION AND KWIC TITLE -** SPLPKG, WFCMPR, WFAPPX
   SPLPKG,WFCMPR,WFAPPX, Wilson-Fowler spline use

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11/750

3. **DESCRIPTION -** The three programs SPLPKG, WFCMPR, and WFAPPX provide the capability for interactively generating, comparing, and approximating Wilson-Fowler splines. The Wilson-Fowler spline is widely used in Computer Aided Design and Manufacturing (CAD/CAM) systems. It is favored for many applications because it produces a smooth, low curvature fit to planar data points.

   Program SPLPKG generates a Wilson-Fowler spline passing through given nodes (with given end conditions) and also generates a piecewise linear approximation to that spline within a user-defined tolerance. The program may be used to generate a 'desired' spline against which to compare other splines generated by CAD/CAM systems. It may also be used to generate an acceptable approximation to a desired spline in the event that an acceptable spline cannot be generated by the receiving CAD/CAM system. SPLPKG writes an IGES file of points evaluated on the spline and/or a file containing the spline description. Maxima of 100 spline nodes and 1600 evaluation points are considered for the linear approximation. These limits can easily be changed.

   Program WFCMPR computes the maximum difference between two Wilson-Fowler splines and may be used to verify the spline recomputed by a receiving system. It compares two Wilson-Fowler splines with common nodes and reports the maximum distance between curves (measured perpendicular to segments) and the maximum difference of their tangents (or normals), both computed along the entire length of the splines. WFCMPR is limited to a maximum of 100 spline nodes.

   Program WFAPPX computes the maximum difference between a Wilson-Fowler spline and a piecewise linear curve. It may be used to accept or reject a proposed approximation to a desired Wilson-Fowler spline, even if the origin of the approximation is unknown. The maximum deviation between these two curves, and the parameter value on the spline where it occurs are reported. WFAPPX is limited to maxima of 100 spline nodes, 1000 linear curve breakpoints, and 1000 evaluation points along the spline.

   Algorithms used in SPLPKG, WFCMPR, and WFAPPX were provided by J. D. Emery, BKCD, and W. R. Melvin, LANL.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed March 1985.
   DEC VAX11/750 version submitted February 1985.

10. **REFERENCES -** Sharon K. Fletcher, User's Guide for Wilson-Fowler Spline Software SPLPKG,WFCMPR,WFAPPX CADCAM-010, SAND84-1161, February 1985.

    Sharon K. Fletcher, CADCAM-007 Recommended Practices for Spline Usage in CAD/CAM Systems, SAND84-0142, April 1984.

    W. R. Melvin, Error Analysis and Uniqueness Properties of the Wilson-Fowler Spline, LA-9178, August 1982.

    R. M. Dolin and W. R. Oakes, A Comparison Between the Wilson-Fowler Spline and the Circle Spline Routines, LA-10522-MS, November 1985.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN 77

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
S. K. Fletcher
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
Source (SPLPKG 675 lines, WFCMPR 159 lines, WFAPPX 188 lines)
The SAND84-1161 and SAND84-0142 reference reports and SPLPKG,WFCMPR,WFAPPX source and sample problems on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
KEYWORDS - spline functions, computer-aided design, computer-aided manufacturing, numerical data, interpolation, algorithms

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE -** ASEAM
   ASEAM, simplified building energy analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   APPLE II+

3. **DESCRIPTION -** ASEAM is an interactive program developed as an energy analysis tool for commercial buildings. The program is based upon simplified analysis methods using modified annual 'bin' temperature frequency data. It can be used to evaluate the individual or combined effects of various energy design strategies. Algorithms include heating and cooling load calculations based on a methodology documented by the ASHRAE Technical Committee on Energy Calculations (TC4.7) and HVAC system and plant calculation routines with options to size cooling equipment and air flows. The HVAC system and heating and cooling plant routines were developed by W. S. Fleming & Associates. HVAC systems are configured by selecting among eight basic system types, control options, five heating plants, and five cooling plants. The program is structured so that input and output files can be manipulated to perform comparison studies. Temperature frequency bin data from Air Force Manual 88-29, "Engineering Weather Data," are used, although users can supply input data from other sources if desired. In addition to load calculation and HVAC system energy consumption reports, annual estimates for the following seven energy end-use categories are reported: heating, cooling, HVAC pumps, HVAC fans, cooling tower, lighting, and equipment.

   The eight basic system types included are: a double duct or multizone unit, a terminal reheat unit, a variable air volume (VAV) system, a ceiling bypass VAV system, a variable temperature single zone system, a 2- or 4-pipe fan coil system, a water/air heat pump system, and a packaged terminal air conditioner unit. The five heating plant types are: electric resistance, air-to-air heat pump, hot water or steam boiler, district steam or hot water from a central plant system, and forced hot-air furnace. Available cooling plant types are: direct expansion, centrifugal chiller, absorption chiller, district chilled water, and double bundle chiller.

   In deriving a building's annual energy consumption the 'bin' method employed by ASEAM computes the energy consumption rate at selected outdoor temperature intervals. Annual energy consumption for the building is determined by performing the secondary system simulation and passing this consumption rate to the primary system (chillers, boilers, etc.) multiplied by the number of hours duration at the specified temperature intervals. These temperature intervals, or bins, are groups of temperatures, usually in 5-degree Fahrenheit increments. The building's annual energy requirements are estimated by summing the energy requirements from each bin. For additional accuracy the bin calculation is performed separately for occupied and unoccupied hours as well as for heating and cooling seasonal space temperature setpoints.

   ASEAM is intended to be used in estimating the design energy performance of smaller commercial buildings and those which are not extremely complex from an energy standpoint. ASEAM results have been compared and tested against the DOE2.1B hour-by-hour energy analysis program (NESC 782) with good results. The program can be used to examine the energy aspects of alternative building designs or features using conventional construction and mechanical systems. With judgment, the program could also be used to assess energy conservation improvements to existing buildings.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed March 1985.
   APPLE II+ version submitted May 1984.

10. **REFERENCES** - W. S. Fleming and Associates, Inc., ASEAM A Simplified Energy Analysis Method Microcomputer Program Users Manual, DOE/CS/20286-1, July 1983.

11. **HARDWARE REQUIREMENTS** - 48K

12. **PROGRAMMING LANGUAGE** - BASIC

13. **OPERATING SYSTEM** - DOS 3.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
H. P. Misuriello
W. S. Fleming and Associates, Inc.

16. **MATERIAL AVAILABLE** -
Source (414 sectors)
The reference report and ASEAM source and sample problem input and output on 5.25-inch flexible diskette are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - air conditioning, energy consumption, space heating, boilers, weather, economics, buildings, construction, energy analysis, DOE2 codes

18. **SPONSOR** - DOE Office of Building Energy Research and Development,
Building Systems Division,
Building Energy Sciences Branch

1. **IDENTIFICATION AND KWIC TITLE** - KNASA
   KNASA, multi-gas mixture component pressures

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM3033

3. **DESCRIPTION** - KNASA calculates the partial pressures of the species present in a multi-gas mixture as a function of system temperature and total pressure and composition at atmospheric conditions. Compositions are specified in weight percent units. The sample problem requires 2 CPU seconds of execution time. KNASA is a modification of a general-purpose program developed under NASA-sponsorship.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   IBM3033 version submitted January 1985.

10. **REFERENCES** - Jiaren Chen, Sherman Greenberg, and Roger B. Poeppel, The Viscosity of Coal Slags as a Function of Composition, Temperature, and Oxygen Partial Pressure, ANL/FE-83-30, March 1984.

11. **HARDWARE REQUIREMENTS** - 190K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - MVS or VM/CMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. Chen, S. Greenberg, and R. B. Poeppel
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (2224 lines)
    The reference report and KNASA source and sample problem input and output and thermodynamic data on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - U
    KEYWORDS - gases, temperature effects, pressure effects, slags, viscosity, coal gasification

18. **SPONSOR** - DOE Office of Fossil Energy,
    Surface Gasification Materials Program

1. **IDENTIFICATION AND KWIC TITLE** - 2DFLOW
   2DFLOW, 2-d drainage flow air pollution model

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - 2DFLOW is a vertically integrated dynamical drainage flow model developed from conservation equations for momentum and mass in a terrain following coordinate system. Wind fields from the dynamical model drive a Monte Carlo transport and diffusion model. The model needs only topographic data, an Eulerian or Lagrangian time scale, and a surface drag coefficient for input data; it can be started with a motionless atmosphere. The system of dynamical equations is solved numerically with a second-order finite difference scheme. Advection of mass and momentum is calculated by the second upwind differencing or "donor cell" method. 2DFLOW has the following features which make it attractive as a practical tool for estimating the concentrations of pollutants released into nocturnal drainage winds: 1) No wind or temperature data are needed. A surface drag coefficient and Eulerian or Lagrangian time scale are required, but the model is not sensitive to their exact value. High resolution topographic data are required. 2) The model has been successfully tested at sites with rugged mountainous terrain and at a site with gently rolling terrain. 3) The model is two-dimensional (vertically integrated) so its computational requirements are moderate. 4) Maximum pollutant concentrations are predicted to within factors of 2 to 10 at specific points, based on observed and simulated concentration time series.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   DEC VAX11/780 version submitted January 1985.

10. **REFERENCES** - Alfred J. Garrett and Frank G. Smith III, Two-Dimensional Simulations of Drainage Winds and Diffusion Compared to Observations, Journal of Climate and Applied Meteorology, Vol. 23, No. 4, pp. 597-610, April 1984.

11. **HARDWARE REQUIREMENTS** - 500K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS 4.0.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    A. J. Garrett
    Savannah River Laboratory

16. **MATERIAL AVAILABLE** -
    Source (774 lines)
    The reference reprint and sample problem output and 2DFLOW source, sample problem input, and topographical data on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
    KEYWORDS - flow models, air pollution, diffusion, Monte Carlo method, surface air, turbulence, topography, wind, weather, computerized simulation

18. **SPONSOR** - DOE Office of Health and Environmental Research

1. **IDENTIFICATION AND KWIC TITLE** - DAHRS
   DAHRS, CRB auxiliary heat removal system study

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - DAHRS (Demo Auxiliary Heat Removal System) is used to determine the long-term transient heat load on auxiliary heat removal equipment for the Clinch River Breeder Reactor Plant. Auxiliary heat removal for the CRBRP is the task of the Steam Generator Auxiliary Heat Removal System (SGAHRS). DAHRS was developed to assist in the sizing of SGAHRS components, such as the auxiliary feed pumps and the protected water storage tank. The heat load on SGAHRS will come from two sources: decay heat from reactor fuel and stored heat from piping and components throughout the plant. In the context of auxiliary heat removal, 'long term' refers to a period of up to several hours (e.g. 2 to 10 hours) following an incident and the resulting plant shutdown. During the first hours after a shutdown, stored heat will provide the greatest part of the heat load. Thus, DAHRS is designed to account for both heat sources while representing the transport time for delivery of heat to SGAHRS.
   Many different incidents may cause activation of SGAHRS, including events in which one or two heat transport circuits become inoperative. For this reason, DAHRS has multiloop capability to examine faulted-loop incidents of interest.
   DAHRS will compute thermal transients, but it is not intended for use as a thermal transient code. The prime objective of the thermal transients calculated with DAHRS is to provide a conservative estimate of the heat load on SGAHRS to assist in sizing and not detailed input for calculation of component thermal stresses.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES** - A. L. Gunby, Computer Code DAHRS, GE ARSD Spec. 23A2451 Rev. 1, June 3, 1983.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   L. Tiemann
   Advanced Reactor Systems Department
   General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
   Source (2184 lines)
   The reference document and sample problem output and DAHRS source and sample problem input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H

KEYWORDS - steam generators, reactor components, reactor cooling systems, after-heat removal, heat transfer, transients, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - ASEP
   ASEP, CRBR axial support structural evaluation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - Honeywell6000

3. **DESCRIPTION** - The Axial Support Evaluation Program, ASEP Revision 4, was written for the Clinch River Breeder Reactor Plant Intermediate Heat Transport System (IHTS). It performs a structural evaluation of each CRBRP IHTS axial restraint fitting attached to a piping line, based on the dynamic loading conditions at the support. Structural screening rules for the piping components are incorporated in ASEP. The program provides a pressure boundary evaluation based upon screening criteria and a detailed three-dimensional finite element analysis of the axial restraint fitting resulting in enveloping stress equations for each line evaluated. The CRBRP lines evaluated are the IHTS main piping lines A, B, C, D/E, and F. The program is based on CRBRP Drawing 909E127, Revision D-1. The transients used are specific to CRBRP events as defined in the piping specification, and the loading terminology and screening criteria used are specific to the 1974 edition of the ASME Boiler and Pressure Vessel Code through the Winter 1975 addenda. Any other usage will require modification of the ASEP program.
   Two releases of ASEP are included: one runs in the timeshare mode, the other in batch mode.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES** - M. R. Schrag, Verification for Computer Code ASEP, GE-ANTO Spec. 23A2927, June 18, 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (Timeshare 2864 lines, Batch 2875 lines)
    The reference report and the ASEP source, sample problem, control information, and executable binary files on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
    KEYWORDS - pipes, restraints, supports, dynamic loads, thermal stresses, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - DIGMAN
   DIGMAN, sampling waste sites for contamination

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   APPLE II with 64K RAM and 1 disk

3. **DESCRIPTION** - DIGMAN was developed to illustrate the complexities in sampling a commercial low-level radioactive waste site for spills or migration. Monitoring for both purposes is required by 10 CFR Part 61. DIGMAN tests a site manager's ability to locate a contaminated area and to determine its areal extent. In the DIGMAN scenario, it is assumed that contamination is present. By sampling the site, the extent of the contamination must be determined and a decision made as to whether the contaminant has migrated off-site. The site manager (player) is given the prior knowledge that a spill has occurred and subsequently migrated through or over the soil surface. In addition, the location is given for one point where some contamination is known to exist. Such information may or may not be available at actual sites. The player is allowed to take a maximum of 45 samples. The DIGMAN waste site provides the player with 1600 possible sampling sites, which is far fewer than would actually be available. Thus, the situations depicted by DIGMAN are the simplest of the myriad of possible scenarios which might be faced by a site manager. Several different scenarios relating to sampling and costs can be used in playing DIGMAN.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   APPLE II version submitted December 1984.

10. **REFERENCES** - M. A. Simmons, J. R. Skalski, R. Swannack, and J. M. Thomas, DIGMAN: A Computer Program to Illustrate the Complexities in Sampling Commercial Low-Level Waste Sites for Radionuclide Spills or Migration, NUREG/CR-3797 (PNL-5028), April 1984.

11. **HARDWARE REQUIREMENTS** - 64K RAM

12. **PROGRAMMING LANGUAGE** - BASIC

13. **OPERATING SYSTEM** - DOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    M. A. Simmons
    Pacific Northwest Laboratory

16. **MATERIAL AVAILABLE** -
    Source (348 sectors)
    The reference report and DIGMAN source on 5.25 inch, double-sided, double-density flexible disk are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
    KEYWORDS - radionuclide migration, radioactive waste management, sampling, low-level radioactive wastes, radioactive waste facilities, monitoring, statistics, APPLE computers

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
    Division of Health, Siting and Waste Management

1. **IDENTIFICATION AND KWIC TITLE -** IHTSD
   IHTSD, CRBRP heat transport system evaluation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Honeywell6000

3. **DESCRIPTION -** IHTSD calculates and reports information about volumes, pressures, flow rates, and sodium levels at various places in the Clinch River Breeder Reactor Plant Intermediate Heat Transport System (IHTS). The program prints velocities in piping elements; sodium volumes for piping elements, major components, piping subtotals, and system totals; permanent pressure drops for piping elements, subtotals, and totals; sodium levels for the case of equal levels in the expansion tank and pump tank; and sodium levels for the case of unequal levels in the two tanks due to permanent pressure losses between them. For the lines between these two tanks, IHTSD prints a breakdown of the permanent pressure drops and static pressures. IHTSD can be used to size orifices for the superheater vent line, the evaporator vent lines, and the F-line (expansion tank return line) in the IHTS. A trial-and-error method is used in which various orifice sizes are tried until the desired flows and levels are obtained. Once the proper orifice sizes are found, the flows and levels at other loop conditions can be calculated.
   IHTSD logic is as follows: 1) The program calculates the permanent pressure drops and volumes starting at the upper pump tank, going to the pump suction, and continuing progressively upstream. 2) Once the permanent pressure drops in the main line between the sweep-o-let and evaporator vent and superheater vent are known, iterative calculations are used to find the flows in the F-line, superheater vent line, and evaporator vent line. 3) Then, the permanent pressure drops between the expansion tank and upper pump tank are calculated, and the tank sodium levels determined. Steps 1) through 3) are repeated until the change in pressure drop between the superheater vent and the sweep-o-let becomes less than the convergence criterion. Once the convergence criterion is satisfied, IHTSD returns to step 1) once more to repeat the process printing the values as calculated.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed March 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES -** Ted C. Huang, Verification for Computer Code IHTSD, GE ARSD Spec. 23A3056, September 16, 1983.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN IV

13. **OPERATING SYSTEM -** GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE -** Restricted Distribution
    Source (542 lines)

The reference document and IHTSD source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - reactor components, reactor cooling systems, pressure drop, superheaters, pumps, pipes, orifices, sodium, heat transfer, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - SPRAY3B
   SPRAY3B, sodium spray fires within containment

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - SPRAY3B is a modification of the SPRAY3 program (NESC 716) developed at Hanford Engineering Development Laboratory to model the effects of postulated sodium spray release from LMFBR piping within containment chambers. The calculation method utilizes gas convection, heat transfer, and droplet combustion theory to compute the pressure and temperature effects within the enclosure. Droplet motion and large sodium surface area combine to produce rapid heat release and pressure rise within the enclosed volume. For a postulated release of Na or NaK spray in a chamber with or without venting capabilities, the SPRAY3B code can be used to evaluate the spray droplet motion, combustion processes, transfer of heat and mass between the droplet and surrounding gas, the convective flow of gas, and the release of gas and combustion products to the environment. The code was designed for CRBRP use in assessing transient thermal conditions in both inerted and air-filled cells under various design basis sodium fire scenarios. Five different types of vent control are modeled. Two reaction rate efficiency factors are employed, one for the sodium-oxygen reaction and one for the sodium-water reaction. These affect the energy generated by the chemical reaction only; there is no effect upon the heat transfer mechanisms considered. A new iterative procedure has been adopted in SPRAY3B to determine the vapor pressure at the reaction zone interface.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed April 1985.
   CDC7600 version submitted January 1985.

10. **REFERENCES** - Ted C. Huang, The SPRAY-3B Code, GE ARSD Spec. 23A2842, August 15, 1983.
    SPRAY3B, NESC No. R9744, Modifications Required for SPRAY3B Sample Problem 2, National Energy Software Center Note 85-57, April 17, 1985.
    P. R. Shire, SPRAY Code User's Report, HEDL-TME 76-94, March 1977.

11. **HARDWARE REQUIREMENTS** - 41K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (1686 lines)
    The 23A2842 and HEDL-TME 76-94 reference documents, NESC Note, and sample problems output and SPRAY3B source and sample problems input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - G
KEYWORDS - sodium, containment, droplets, sprays, thermodynamics, mass balance, reactor safety, convection, LMFBR reactors, Clinch River Breeder Reactor, SPRAY3 codes, SPRAY-3A codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - CLMPGEN
   CLMPGEN, ANSYS finite-element mesh generator

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - CLMPGEN is a preprocessor finite element mesh generator used with the proprietary ANSYS software for analysis of pipe-to-clamp interactions in the Clinch River Breeder Reactor Intermediate Heat Transport System (IHTS). Because the IHTS is a relatively thin-walled, high temperature piping system subject to rapid thermal transients, special insulated clamps were designed to support the system without introducing unacceptable thermal or mechanical stresses. The clamps/piping interaction requires nonlinear three-dimensional analysis using the Swanson Analysis Systems ANSYS code. To facilitate this analysis CLMPGEN was developed to create node and element input files for use with subsequent ANSYS runs. CLMPGEN can generate meshes for uninsulated clamps as well, and with minor modifications, can be used to develop models for clamps with bolted connections, without gussets, or with several gussets, or gussets of a different shape. The insulation/gap modeling is the most sophisticated aspect of CLMPGEN since the compressive forces these elements transmit are the primary means by which the pipe is locally loaded.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Honeywell6000 version submitted January 1985.

10. **REFERENCES** - R. C. Taylor, Verification of Computer Code CLMPGEN, GE ARSD Spec. 23A3105, January 4, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (2788 lines)
    The reference document and CLMPGEN source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - L
    KEYWORDS - mesh generation, pipes, mechanical structures, thermal stresses, finite element method, Clinch River Breeder Reactor, ANSYS codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - UCMD109
   UCMD109, AGS880 x-y coordinate table generator

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11/34

3. **DESCRIPTION** - UCMD109 is a User Command developed for the Applicon Graphics AGS/880-I System using the DEC PDP11/34 minicomputer. The software generates a table of x and y coordinates of either selected hole centers, cell locations, or multi-vertex polyarc vertices. The coordinates are referenced to a user-defined origin. UCMD109 can be executed from any AGS activity having a graphics display and attached keyboard. UCMD109 must be loaded on the UCMD table, and a drawing file must be loaded on the AGS activity. The program can be executed from either Edit or Edit Component mode. The area of application is primarily in mechanical applications requiring a table of hole-center coordinates for numerical control purposes. The UCMD can be used in hybrid microcircuits for producing a table of hole/cell locations. The UCMD can also produce a table of multi-vertex polyarc vertex locations. UCMD109 consists of the main program, HOLTBL, and ten subroutines.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   DEC PDP11/34 version submitted January 1985.

10. **REFERENCES** - Leo J. LaFrance, User/Programmer Guide for UCMD 109 Hole/Cell/Multi-Vertex Polyarc Coordinate Table Generator, SAND84-1750, August 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV/IAS-RSX 2.5 (94%) and MACRO-11 (6%)

13. **OPERATING SYSTEM** - RSX-11M 3.2 and AGS/880-I Applicon Graphics System.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. J. LaFrance
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (879 lines)
    The reference report and UCMD109 source and control information on magnetic tape, in PDP11 FLX DDS format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
    KEYWORDS - computer graphics, PDP computers, display devices, computer-aided manufacturing, HOLTBL codes

18. **SPONSOR** - Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - UCMD108
   UCMD108, AGS polyarc/path integrity verifier

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC PDP11/34

3. **DESCRIPTION** - UCMD108 is a User Command developed for the Applicon Graphics AGS/880-I System using the DEC PDP11/34 minicomputer. The software performs three tests on path and polyarc components in the AGS view cube. These tests find zero length polyarc/path components, verify the closure of polygons, and verify that the segments of the polyarc/path components, i.e., the portion of a multi-vertex polyarc/path between two vertices, are parallel to their respective coordinate axes. The closure and parallelism tests are independent of the orientation of the polygon. This edition of UCMD108, designated by the developers as Version 2.0, does not correct offending polyarc/path components, but partially selects them. UCMD108 can be executed from any AGS activity having a graphics display with an attached keyboard. UCMD108 must be loaded on the UCMD table, and a drawing file must be loaded on the AGS activity. UCMD108 can be executed from either Edit or Edit Component mode. Applications for UCMD108 are hybrid microcircuits, ground planes of printed wiring boards, odd shaped painted-in areas, and geometry closure of mechanical parts requiring numerical control contouring. The processes in the applications, photoplotting and numerical control contouring, require closing of polygonal areas. Certain applications in photoplotting require the edges of rectangles to be perfectly parallel to the coordinate axes. Zero length polyarc/path instances are also a source of errors in photoplotting. The UCMD will eliminate processing errors due to zero length instances, non-closure, and non-parallelism and generally increase the integrity of the data.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   DEC PDP11 version submitted December 1984.

10. **REFERENCES** - Leo J. LaFrance, User/Programmer Guide for UCMD 108 Multi-Vertex Polyarc/Path Integrity Verifier, SAND84-1749, August 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV/IAS-RSX 2.5 (99%) and MACRO-11 (1%)

13. **OPERATING SYSTEM** - RSX-11M 3.2 and AGS/880-I Applicon Graphics System.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. J. LaFrance
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (318 lines)
    The reference report and UCMD108 source and control information on magnetic tape, in PDP11 FLX DDS format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T

KEYWORDS - computer graphics, PDP computers, electronic circuits, display devices, computer-aided design, computer-aided manufacturing, RECT codes

18. **SPONSOR -** Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE** - CALC
   CALC, programmable calculator with parser

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DG Eclipse MV/10000

3. **DESCRIPTION** - CALC is an interactive program which acts as a programmable calculator. It accepts a statement in the form of an algebraic expression, performs the calculations as specified, and assigns the result to the designated output variable. Statements may be saved for re-use, and the user can define 'programs' that consist of statements or other programs that have been saved previously. CALC accepts any algebraic expression given in the syntax of FORTRAN77 assignment statements. CALC maintains a work space for up to 100 variable names and their numerical values (double-precision). In evaluating a statement, CALC takes the data of input variables from the work space and puts the result in the output variable which is also contained in the work space. The algebraic expression is converted from a string of ASCII characters into a list of lexical elements. The algorithm used for parsing these elements is basically that of left-to-right, bottom-up, rule-based parsing. The following constraints apply: a maximum of 10 statements or "programs" can be saved for re-use; a program may consist of up to 65 statements or statements awaiting execution; and an assignment statement may have maxima of 131 characters, 100 elements (variables, operators, etc.), 16 variables or constants, and 24 operators or calls to intrinsic functions.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   DG Eclipse MV/10000 version submitted November 1984.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - PL/I

13. **OPERATING SYSTEM** - AOS/VS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. J. Yio
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (1327 lines)
    The CALC source and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - algebra, computer calculations, programming, calculators, data analysis

18. **SPONSOR** - Sandia National Laboratories, Albuquerque,
    Test Data Programming Division

1. **IDENTIFICATION AND KWIC TITLE** - STATLIB
   STATLIB, conversational statistical library

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - STATLIB is a conversational statistical program library developed in conjunction with a Sandia National Laboratories applied statistics course intended for practicing engineers and scientists. STATLIB is a group of 15 interactive, argument-free, statistical routines. Included are: analysis of sensitivity tests; sample statistics for the normal, exponential, hypergeometric, Weibull, and extreme value distributions; three models of multiple regression analysis; x-y data plots; exact probabilities for RxC tables; n sets of m permuted integers in the range 1 to m; simple linear regression and correlation; k different random integers in the range m to n; and Fisher's exact test of independence for a 2 by 2 contingency table. Forty-five other subroutines in the library support the basic 15.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   DEC VAX11/780 version submitted October 1984.

10. **REFERENCES** - Herbert E. Anderson, STATLIB, SAND82-1976, September 1982.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN77

13. **OPERATING SYSTEM** - VMS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    H. E. Anderson
    Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
    Source (4683 lines)
    The reference report and STATLIB source on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - data analysis, experimental data, interactive computing, statistics, regression analysis, probability, numerical data

18. **SPONSOR** - Sandia National Laboratories, Albuquerque

1. **IDENTIFICATION AND KWIC TITLE -** REPRO
   REPRO, printing contract bid evaluation system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC PDP10

3. **DESCRIPTION -** REPRO is a prompt-oriented system that automates the multiple bid award process for selecting a printing contractor. The system calculates the costs of printing a document using contracted rates with various printers and then ranks the printers in ascending cost order (i.e. lowest bid first). A maximum of 20 contractors is allowed. A REPRO session consists of a series of questions or prompts that query the user for information the system requires to calculate printing costs for a specific document (for example, number of copies needed, number of pages in the document, type of paper, and type of binding desired, etc.). Many of the prompts are in a menu-type format that allows the user to pick a response from a list of options. The remainder of the prompts are short questions that require numerical input or a yes or no response. The rates used in the program are those negotiated with printing contractors within individual DOE regions by the Government Printing Office. Two releases of REPRO are included. One, REPRO.QOR, is for first-time users; it contains a HELP facility. At any prompt, the user may type HELP to access descriptive information on that specific prompt. The other release, REPRO.FOR, is intended for experienced users and does not contain the HELP facility.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed March 1985.
   DEC PDP10 version submitted January 1985.

10. **REFERENCES -** REPRO SYSTEM USER'S GUIDE, U. S. Department of Energy, Office of Scientific and Technical Information document, March 1984.
    REPRO SYSTEM PROGRAMMER'S GUIDE, U. S. Department of Energy, Office of Scientific and Technical Information document.
    Excerpts from DECsystem-10 BACKUP Program Description, May 1975.

11. **HARDWARE REQUIREMENTS -** 32K words

12. **PROGRAMMING LANGUAGE -** FORTRAN IV

13. **OPERATING SYSTEM -** TOPS-10.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    A. M. Craig
    Office of Scientific and Technical Information
    U. S. Department of Energy

16. **MATERIAL AVAILABLE -**
    Source (68 2720-character records)
    The reference documents and REPRO source, object module, and executable image on magnetic tape, in DECSYSTEM-10 BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY -** M

KEYWORDS - printing and publishing industry, bids, contracts, interactive computing, procurement, cost

18. **SPONSOR** - DOE Office of Scientific and Technical Information

1. **IDENTIFICATION AND KWIC TITLE** - HISTAM2S
   HISTAM2S, superheater sodium-water reaction

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - HISTAM2S predicts sodium flow rates, gas flow rates, and pressures in the CRBRP Intermediate Heat Transport System (IHTS) and the Sodium Water Reaction Products Relief System (SWRPRS) as a function of time during a large sodium-water reaction in a steam generator. In particular, HISTAM2S is written for a Sodium-Water Reaction in a superheater. The code is intended to model the event from the time acoustic pressure pulses and sodium compressibility effects are no longer important until the end of the event. The first portion of the event, up to the time when any of the rupture disks is broken, is modeled with the TRANSWRAP program (NESC 962). HISTAM2S is a hydraulics code which models sodium as incompressible, while TRANSWRAP models sodium as compressible. The code predictions are used as the design basis for the relief line system of the CRBRP steam generators. The code has been used in CRBRP safety assessments to analyze the thermal stress problems of the relief pipings of the CRBRP steam generators.
   Because of the different characteristics of a steam/water leak occurring in a CRBRP superheater or evaporator, two releases of the HISTAM code were developed. HISTAM2S applies to leaks in a CRBRP superheater while HISTAM2E handles any leak inside a CRBRP evaporator. Both model sodium flows in the main IHTS piping, pressures in the IHTS at flow junction points, sodium flow through the steam generators and into or from the expansion and pump tanks, pump performance including coastdown, sodium and hydrogen flow rates into the SWRPRS, pressure in the SWRPRS, gas flow rates out of the SWRPRS, and the sodium-water reaction gas bubble and its location. The SWRPRS is modeled as one large Reaction Products Tank with one constant area vent line to the flare stack.
   A typical problem takes less than 6 minutes of processor time.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted September 1984.

10. **REFERENCES** - K. Chen, Verification for Computer Code HISTAM, GE ARSD Spec. 23A3102, Rev. 0, September 10, 1984.
    TRANSWRAP II Computer Code, GE Specification 23A3033, Rev. 0, September 9, 1983.

11. **HARDWARE REQUIREMENTS** - 27K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (2884 lines)
The 23A3102 reference document and HISTAM2S source, sample problems, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – G
KEYWORDS – hydraulics, superheaters, steam generators, molten metal–water reactions, relief valves, Clinch River Breeder Reactor, TRANSWRAP codes, HISTAM2E codes

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - DYNALSS
   DYNALSS, CRBR control assembly scram dynamics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - DYNALSS was developed to analyze the scram dynamics of a control assembly with hydraulic scram-assist force. It was written specifically for the CRBRP Secondary Control Rod System and is restricted to a configuration where the inlet flow is split in the vicinity of the control rod with part of the flow exiting at the top and the remaining flow going to a low pressure plenum at the bottom. The program traces the control rod position, calculates the flow resistances and flow distribution, and determines the detailed hydrodynamic response of the control rod as it moves into the reactor core. Options exist to accept either time-dependent pressure at the inlet, lower and upper outlet, or time-dependent flows as input boundary conditions for the scram dynamics calculations.

   A major part of the DYNALSS program is concerned with determination of the flow split in the Secondary Control Assembly (SCA) and the hydraulic-scram assist force on the control rod before a scram transient. Due to the complex nature of the flow path, an iterative technique is used to determine three different flows before the flow distribution is determined: the inlet flow, the flow around the outside of the rod, and the flow through the pin bundle. An estimate of the inlet flow is made to start the calculations. The inlet flow is used to determine the pressure drop from the inlet to a point just inside the guide tube holes. Then, an estimate is made of the fraction of the inlet flow which goes around the outside of the pin bundle. This flow is used to determine the pressure drop from the inlet of the control rod to the outlet. The iteration of the flow through the pin bundle continues until the pressure drop through the pin bundle matches the pressure drop along the outside of the bundle from inlet to outlet. Once the pin bundle flow is known, the pressure drop from the inlet to the top of the assembly can be determined. If the computed pressure drop does not match the boundary condition, a new estimate for the flow around the bundle is made, and the procedure is repeated until the pressure drops match. Once the flow exiting at the top of the assembly is known, the remaining flow is used to compute the pressure drop from the guide tube holes to the low pressure plenum. If the computed pressure drop from the inlet to the low pressure plenum does not match the boundary conditions, a new guess for the inlet flow is made, and the whole process is repeated until all pressure boundary conditions match. If flow boundary conditions are provided, the iterative procedure is needed only to determine the flow split between the pin bundle flow and the flow outside of the bundle.

   As the control rod moves, the flow paths around the rod and their resistances change. This, in turn, varies the flow distribution and the hydraulic scram-assist force. The iterative procedure used in the pre-scram flow distribution calculation is repeated at every time-step for transient flow distribution calculations during the scram. A model, which assumes that the control rod is a simple cylinder with time-dependent control rods above, below, and around the rod, is used to determine the effect of the moving control rod on the fluid. Mass and momentum balances are written for the control volumes. A force balance is written for the control rod. In the regions where there is no rod motion, the hydraulic parameters are constant with time; the pressure drop varies only with changes in the flow rate. In the fluid regions with control rod motion, the mass, momentum, and force balance are combined and solved to calculate the rod acceleration and velocity.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted September 1984.

10. **REFERENCES** - J. Wei, Verification for Computer Code DYNALSS, GE ARSD Spec. 23A3089, January 5, 1984.
H. K. Yang, User's Manual for the DYNASCA Program, GE ARSD memorandum YL-606-10008, January 1981.
J. P. Wei, Thermal and Hydraulic Analyses of CRBRP Secondary Control Rod System, CRBRP-GEFR-00542, October 1983.
A. J. Lipps, DYNALSS: A Computer Code to Analyze the Response of a Control Rod with Hydraulic Scram-Assist, CRBRP-GEFR-14040, February 1975.

11. **HARDWARE REQUIREMENTS** - 74K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
L. Tiemann
Advanced Reactor Systems Department
General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2680 lines)
The 23A3089 and YL-606-10008 reference documents and DYNALSS source, sample problems input and output, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - reactor components, reactor control systems, control rod drives, hydrodynamics, scram, dynamics, Clinch River Breeder Reactor, DYALS codes, DYNASCA codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - STALS
   STALS, control rod steady-state hydraulics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - STALS is a steady-state hydraulic performance code developed specificaliy to calculate the steady-state flow and pressure distributions within the CRBRP Secondary Control Assembly (SCA) as well as hydraulic forces acting on the control rod when it is at either the fully-withdrawn or -inserted position. Pressures at the SCA inlet, upper outlet, and lower outlet provide the boundary conditions for the SCA hydraulic performance calculation. STALS calculates flow splits and detailed pressure drop distributions as well as hydraulic forces acting on the control rod at both positions. An option is included to provide statistical results when required ranges of uncertainties and frequencies of random sampling processes are specified. The SCA consists of a movable control rod, a guide tube, a nosepiece assembly, and an outer duct. The hydraulic modeling is based on the following major assumptions: incompressible fluid, one-dimensional flow, axial symmetric flow pattern about the vertical center line of the assembly, and insignificant temperature variation. Because the flow paths are complicated, an iterative technique is used to determine the pressure drop from the inlet to the inlet ports in the guide tube. An iterative procedure is also used to determine the flow split between the pin bundle and the bypass annulus.
   Two releases of STALS are included. The first is designed for use in a time-sharing environment and the second for a batch environment.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Honeywell6000 version submitted September 1984.

10. **REFERENCES** - Verification for Computer Code STALS, GE ARSD Spec. 23A3093, January 5, 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (786 lines)
    The reference document and STALS source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
    KEYWORDS - control elements, hydraulics, steady-state conditions, fluid flow, pressure drop, reactor control systems, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE -** SCRAM
   SCRAM, control rod - guide duct interference

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Honeywell6000

3. **DESCRIPTION -** SCRAM is a two-dimensional geometry comparison code which calculates clearances between a control rod and its guide duct during the control rod scram travel. Interference analysis with SCRAM consists of: combining the nominal geometries with fabrication tolerances and operational deformations to define distorted control rod and guide duct geometries; translating the distorted control rod along the distorted guide duct to simulate scram travel; and calculating the clearances at selected intervals along the scram path to evaluate margins to interference. Distorted geometries of the control rod and guide duct are defined separately in different coordinate systems by superimposing the user-supplied information on the nominal geometries and deformations. Scram is simulated by translating the control rod coordinate system relative to the guide duct coordinate system. The interference analysis at any instant during scram consists of moving the control rod to one side of the guide duct envelope through a series of rigid body translations and rotations and calculating the minimum guide duct/control rod clearance (maximum interference) on the opposite side. For complex geometries and bowed shapes of the guide duct, there may be several such configurations at a given elevation. SCRAM searches through these alternative configurations to identify the "best" configuration providing maximum value for the clearance at the point of closest approach between the control rod and guide duct. Interference is predicted only if a negative clearance is calculated for the "best" configuration. SCRAM was developed to evaluate potential for interference between the control rod and guide duct in the Clinch River Breeder Reactor Secondary Control Rod System during scram travel; however, it is sufficiently general to permit evaluation of interference potential in other systems involving relative movement between two co-axial elements.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed February 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES -** M. Patel, SCRAM - Control Rod/Guide Duct Interference Evaluation Code, CRBRP-GEFR-00675, October 1983.
    D. A. Braun, Verification for Computer Code SCRAM, GE ARSD Spec. 23A3043, August 9, 1983.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** FORTRAN IV

13. **OPERATING SYSTEM -** GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (1393 lines)
The reference documents and SCRAM source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - reactor components, control rod drives, reactor control systems, scram, deformation, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - PRECOMP
   PRECOMP, LRLTRAN macroprocessor & translator

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1

3. **DESCRIPTION** - PRECOMP is a precompilation macroprocessor and translator for LRLTRAN source code. It can produce output for compilation by the CHAT, CIVIC (NESC 9757), FENIX, and CFT compilers. PRECOMP processes PARAMETER and MACRO definition statements. An output file is created with PARAMETER and MACRO statements, conditional compilation blocks (DIF statements), and CLICHE definitions deleted. Parameters are replaced by their defined values. MACRO statements are replaced by the expanded text. The output file is compilable. PRECOMP has the ability to translate some LRLTRAN statements into CFT-acceptable statements. Other statements, not translated and unacceptable to CFT, are flagged. PRECOMP can also be used as an assembler for the CPU76 assembly language producing relocatable binary files. PRECOMP may be executed in an interactive debug mode. This feature allows one to stop on the expansion of a particular macro, the definition or usage of a particular parameter, etc. The value of a parameter, arguments of a macro, etc. may then be displayed.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Cray1 version submitted January 1985.

10. **REFERENCES** - Dennis E. Johnson, PRECOMP, Lawrence Livermore National Laboratory Utility Routine report UR-920, September 28, 1979.

11. **HARDWARE REQUIREMENTS** - 24K (octal) words

12. **PROGRAMMING LANGUAGE** - LRLTRAN (50%) and CAL (50%)

13. **OPERATING SYSTEM** - LTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. E. Johnson
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (13,307 lines)
    The reference report and PRECOMP source and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - programming languages, LRLTRAN, translators, Cray computers, CIVIC codes

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE -** DDT
   DDT, LRLTRAN dynamic symbolic debugging tool

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   Cray1

3. **DESCRIPTION -** DDT is a dynamic symbolic debugging tool for the LRLTRAN language. It allows users to look at current values of any of their program's variables without recompiling and using PRINT statements. DDT, using a function called BREAKPOINTS, permits the user to trace each of the logic paths in a program by executing a few statements or even a few instructions at a time. DDT has three types of breakpoints: permanent breakpoints, which stay at the location specified until the user requests that they be released; temporary breakpoints, which are automatically released when reached; and tracing breakpoints, which will not cause a stop at a location until the location has been reached a specified number of times. DDT allows the user to identify variables for viewing by name and to display them in the appropriate form (i.e, floating-point, character, octal, etc.) It is also possible to display the contents of registers and vectors, and to change the value of a variable at a breakpoint. DDT may also be used to trace subroutine calls made in a program. A history file is created which contains all input commands to DDT and the output from those commands. This information is left on disk to provide users with a record of their debug session.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed February 1985.
   Cray1 version submitted January 1985.

10. **REFERENCES -** Dave Seberger, DDT, LCSD-1620 Rev. 0, November 24, 1981.

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** LRLTRAN

13. **OPERATING SYSTEM -** LTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    D. Seberger
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE -**
    Source (23,998 lines)
    The reference report and DDT source and CLICHE definitions on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY -** P
    KEYWORDS - programming, utility routines, LRLTRAN, validation, testing

18. **SPONSOR -** DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - CIVIC
   CIVIC, Cray1 compiler for the LRLTRAN language

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1

3. **DESCRIPTION** - CIVIC is a compiler for the Lawrence Livermore National Laboratory's LRLTRAN language. LRLTRAN, a programming language derived from FORTRAN, is the scientific programming language supported by the LLNL Computation Department. It contains the most widely used features in FORTRAN and other unique extensions, including macro processing; bit, byte, and character manipulation; vector extensions; and dynamic storage allocation. CIVIC is a multipass (8-pass) compiler which translates LRLTRAN source statements to relocatable binary object code. Symbolic debugging records, which facilitate symbolic debugging with DDT (NESC 9756) in a dynamic or static mode, are produced for all identifiers in each subprogram compiled. Options exist to produce a cross-reference code analysis listing, a CAL object-code listing, or Cray1 assembly mnemonics. In general, up to four steps may be required for a program to complete macro processing, compilation, loading, and execution of the controllee. CIVIC can function as a job controller to initiate this sequence as a single step. CIVIC allows separate compilations to proceed simultaneously from different user suffixes. Each program unit is compiled independently. Macro expansion, parameter replacement, and conditional compilation for CIVIC are performed by the PRECOMP (NESC 9755) preprocessor program. The controllee program can be executed under CTSS. CIVIC may be executed directly from a terminal, or it may be started by a batch controller, such as COSMOS.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed March 1985.
   Cray1 version submitted January 1985.

10. **REFERENCES** - William S. Derby, John T. Engle, and Jeanne T. Martin, LRLTRAN Language Used with the CHAT and CIVIC Compilers, LCSD-302 Rev. 1, June 1, 1982.
    CIVIC, NESC No. 9757, CIVIC Author's Implementation Information, National Energy Software Center Note 85-54, February 11, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** - LTSS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    J. T. Engle
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (76,405 lines)
    The reference report and NESC Note and CIVIC source, HELP file, and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - programming languages, Cray computers, LRLTRAN

18. **SPONSOR** – DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - DUMP-GE
   DUMP-GE, sodium dump rate prediction CRBRP

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - DUMP-GE is used to predict the hydraulic performance in the CRBRP Intermediate Heat Transport System (IHTS) as a result of an instantaneous dump valve actuation in the sodium dump line. DUMP models the events after the pump coastdown is complete, and both the IHTS loop flow rate and the pump heat pressure are assumed to be zero. The program predicts sodium flows in the main IHTS piping, steam generator vent lines, and dump lines; sodium dump rate and total volume of sodium dumped as a function of time; pressures in the pipes and tanks of the IHTS; cover gas pressure and volume; sodium levels in the expansion tank, pump tank, and dump tank; and sodium slug lengths in pipes during a pipe clearing period.
   The general method of predicting the system performance during the events is to start with a steady-state zero flow condition and use the values of pressures, volumes, flow rates, elevations, etc. at that point in time, t, to calculate the time derivatives of these variables, and then to integrate them over a finite time-step, delta t, to determine a new set of values at time t plus delta t. A hydraulic solution is calculated at each time-step to determine the pressure profile in the loop, satisfying continuity at all junction points in the system. With this pressure profile, accelerations of sodium flow in pipes can be found by using the momentum conservation equations. These calculations continue until the vent lines of the steam generator are cleared of sodium. After that, all the pipes and dump lines in the IHTS are combined into four individual subsystems, and the sodium flow in each subsystem is calculated, assuming a quasi-steady condition.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted January 1985.

10. **REFERENCES** - K. Chen, Verification for Computer Code DUMP-GE, GE ANTO Spec. 23A3098, Rev. 0, October 18, 1984.
    Asher H. Shapiro, The Dynamics and Thermodynamics of Compressible Fluid Flow, Volume I, Ronald Press Co., New York, 1953.

11. **HARDWARE REQUIREMENTS** - 19K words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Nuclear Systems Technology Operation
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (1008 lines)

The reference document and DUMP source, sample problem, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - reactor components, reactor cooling systems, sodium cooled reactors, hydraulics, relief valves, performance testing, Clinch River Breeder Reactor, HISTAM2 codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - CORTM
   CORTM, steady-state core thermal-hydraulics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - CORTM is a steady-state core-wide thermal-hydraulic code developed specifically for LMFBR applications with explicit consideration of intra-assembly and inter-assembly heat transfer. CORTM includes the following features: analysis of one-twelfth (30-degree) sector of up to 21 radial rings (121 assemblies) as a full adiabatic representative portion of the core; treatment of up to six different types of assemblies: fuel, radial blanket, primary control, secondary control, special shield, and inner blanket; modeling of fuel and blanket wire-wrapped assemblies in the tri-grid form; modeling of control and radial shield assemblies in the tri-grid form; heat generation due to gamma heating in the duct wall and the bypass sodium in the interstitial gaps; an option for treating the bypass sodium with zero or finite velocity; a maximum of five primary and three secondary control assemblies in the core sector; an option for partial insertion of the primary control assemblies; and the capability of separating the assembly bundle power and gamma heating input for the control assemblies. Circumferential swirl flow is not treated; turbulent mixing is used as an approximation. CORTM has been used to determine CRBRP core-wide temperature distributions to set duct wall temperatures and heat transfer as boundary conditions for secondary control assembly temperatures using the FULSCA version of the FULMX program. CORTM has also been incorporated in the core-wide orifice optimization code, ORIFOPT.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted January 1985.

10. **REFERENCES** - J. Wei, Verification for Computer Code CORTM, GE ARSD Spec. 23A3063, January 5, 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (5766 lines)
    The reference document and CORTM source, sample problem, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H

KEYWORDS - reactor cores, heat transfer, temperature distributions, steady-state conditions, reactor core restraints, Clinch River Breeder Reactor, ORIFOPT codes, FULMX codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

IDENTIFICATION AND KWIC TITLE - RECON
RECON, simulating waste repository operations

COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -
UNIVAC1100/44

DESCRIPTION - RECON is designed to estimate costs of mined geologic repositories based on parametric input data. Input parameters describe facilities, construction times, shafts, mine design, emplacement limitations, waste flows available for disposal, waste processing parameters (labor, materials, utility, and equipment requirements), facility construction costs and unit labor, materials, utility, and equipment costs. Using this information, RECON determines the facility requirements for receiving, packaging, transporting, and emplacing the wastes. Based on the facility requirements, RECON calculates labor, material, and equipment requirements. Labor requirements are calculated in shifts based on available working days. From the shifts and days worked, utility requirements are calculated. Equipment replacement requirements are calculated based on equipment life (stated in years or units processed) and processing rates. All of the above requirements are calculated year-by-year for each of up to 10 waste types, thereby simulating actual repository operations.

Output tables provide summaries of total construction, waste operations, rock operations, and decommissioning costs by waste type. Further breakdowns of costs within these categories are shown in backup tables as a function of time. Levelized unit costs are calculated per unit mass, unit volume, and per package using an input-specified discount rate. Supporting tables show summaries of emplacement descriptions, rock logistics, waste operation logistics, and backfilling logistics.

Because of the large amount of input data required for RECON, an auxiliary program, PREPROCESSOR, is included to aid the user in developing input data. PREPROCESSOR is a menu-driven, interactive program that creates an input data file for execution by the RECON model. The data file may be created using data from an existing case, a reference data library, or completely new data entered via the terminal. Following data entry, the user has the option of verifying, and changing if necessary, data in the newly developed file or exiting and writing the file to disk prior to RECON execution .

METHOD OF SOLUTION -

RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -

TIMING -

UNUSUAL FEATURES OF THE SOFTWARE -

RELATED AND AUXILIARY SOFTWARE -

STATUS - Summary first distributed February 1985.
UNIVAC1100 version submitted January 1985.

REFERENCES - L. L. Clark, B. M. Cole, G. W. McNair, and M. E. Schutz, RECON: A Computer Program for Analyzing Repository Economics, Documentation and User's Manual, PNL-4465, May 1983.

RECON, NESC No. S9760, RECON Reference Report PNL-4465, National Energy Software Center Note 85-52, February 5, 1985.

L. L. Clark and B. M. Cole, An Analysis of the Cost of Mined Geologic Repositories in Alternative Media, PNL-3949, February 1982.

HARDWARE REQUIREMENTS -

PROGRAMMING LANGUAGE - FORTRAN ASCII

OPERATING SYSTEM - EXEC8.

OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** –
L. L. Clark
Pacific Northwest Laboratory

16. **MATERIAL AVAILABLE** – Special Distribution
Source (7620 lines)
The PNL-4465 reference report and NESC Note and RECON source, sample problem input and output, and auxiliary program on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – R
KEYWORDS – radioactive waste storage, mines, waste management, economic analysis, operating cost, waste processing

18. **SPONSOR** – DOE Office of Civilian Radioactive Waste Management

1. **IDENTIFICATION AND KWIC TITLE** - ADEPT
   ADEPT, aerosol deposition in cylindrical pipes

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   NAS5000, IBM370

3. **DESCRIPTION** - ADEPT calculates the deposition of aerosols in straight cylindrical pipes during turbulent air flow. Aerosol deposition is calculated in a time-dependent manner based on empirical correlations for turbulent flow in pipes. The calculated deposition during a single time interval is cumulative with that of previous time intervals and results in a decreasing inner diameter of the pipe. The calculated deposition is assumed uniform over the length of the pipe. The entering aerosol distribution is specified by the user in the form of a log-normal distribution of accumulated mass versus particle size and may be time dependent. Entering flow conditions are also specified by the user and may also be time dependent. For simplicity and generality, the geometry implicit in the program is that of a cylindrical pipe with no bends or fittings. The flow is turbulent and monodirectional; only one set of inlet conditions may be applied at a given time. The flow parameters are not calculated along the length of pipe; therefore, the dynamic behavior of the aerosol within the pipe as well as the effects of reentrainment cannot be determined explicitly. A typical problem requires 2 minutes of CPU time.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   NAS5000 version submitted January 1985.

10. **REFERENCES** - "ADEPT" Computer Code User's Manual, Burns and Roe, Inc., received January 1985.

    N. A. Fuchs, The Mechanics of Aerosols, Pergamon Press, Oxford, New York, 1964.

    G. A. Sehmel, Particle Deposition from Turbulent Air Flow, Journal of Geophysical Research, Vol. 75, No. 9, pp. 1766-1781, March 20, 1970.

11. **HARDWARE REQUIREMENTS** - 512K words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - MVS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    P. Fazekas
    Burns and Roe, Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (287 lines)
    The reference User's Manual and ADEPT source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
    KEYWORDS - aerosols, deposition, turbulent flow, pipes, plugging, particle resuspension

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - PCON
   PCON, fuel-pin failure analysis pellet contact

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - PCON, a Clinch River Breeder Reactor Plant (CRBRP) program, calculates the effects of transient factors that ultimately affect LMFBR fuel-pin performance. PCON employs a fuel-clad displacement balance to compute the contact pressures developed during a rapid reactivity insertion. This displacement balance incorporates the dimensional changes associated with thermal expansion, fuel swelling, and plastic-elastic deformation. In addition to computing the developed contact pressure due to fuel-cladding mechanical interaction during the reactivity insertion, PCON also computes the Cumulative Mechanical Damage Function (CDF) worth of the transient and the contact pressure that would cause failure. These quantities determine the fuel pin's ability to survive the event at a specific time in life. Both the developed and allowable contact pressures are intimately related to the fuel pin's prior history, specifically, the pellet micro-structure, prior environmental effects to the clad, and the clad's accrued CDF.
   The two latter items may be obtained directly from the CRBRP FURFAN program (NESC 9731). FURFAN deals exclusively with the clad and its reaction to applied loads. The sample problem requires less than 1 CP second on a CDC7600.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   CDC7600 version submitted January 1985.

10. **REFERENCES** - David C. Jacobs, The Development and Application of a CDF Related Procedure for LMFBR Fuel-Pin Failure Analysis During Rapid Reactivity Insertions, Westinghouse ARD memorandum RA-76-148, August 13, 1976.
    D. C. Jacobs, Strain Rate and Fluence Dependent Models for the Tensile Properties of 20% Cold-Worked, 316 Stainless Steel Tubing, Westinghouse ARD memorandum LRA-77-292, March 1977.
    A. L. Stiehl, Verification of the PCON Computer Program, Westinghouse ARD memorandum LRA-80-63, May 20, 1980.
    A. L. Stiehl, Fuel/Blanket Pin Mechanical Design PCON Verification, Westinghouse ARD memorandum LRA-FR-80-12, Rev. 0, May 21, 1980.
    A. L. Stiehl, Westinghouse ARD memorandum LRA-FR-80-9, Rev. 1, October 22, 1980.
    A. L. Stiehl, Fuel/Blanket Pin Mechanical Design PCON Verification, Westinghouse ARD memorandum LRA-FR-80-1, Rev. 0, April 28, 1980.
    A. L. Stiehl, Fuel/Blanket Pin Mechanical Design 2-sigma Plastic Design CDF-PCON, Westinghouse ARD memorandum LRA-FR-79-24, Rev. 0, August 2, 1979.
    A. L. Stiehl, Fuel/Blanket Pin Mechanical Design PCON Material Properties Verification, Westinghouse ARD memorandum LRA-FR-79-22, Rev. 0, May 31, 1979.
    A. L. Stiehl, Fuel/Blanket Pin Mechanical Design B/A 201 AFMS/M Analysis, Westinghouse ARD memorandum LRA-FR-79-20, Rev. 0, June 4, 1979.
    D. C. Jacobs, The Development and Application of a Cumulative Mechanical Damage Function for Fuel-Pin Failure Analysis in LMFBR Systems, CRBRP-ARD-0115, August 1976.

11. **HARDWARE REQUIREMENTS** - 35K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.5 Level 512.102.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

D. C. Jacobs
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2333 lines)
The reference memoranda and sample problem output and PCON source and sample problem input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - fuel-cladding interactions, fuel pellets, reactivity insertions, elasticity, plasticity, Clinch River Breeder Reactor, LMFBR reactors, FURFAN codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - LEAK
   LEAK, sodium flow heat transport system leaks

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - Honeywell6000

3. **DESCRIPTION** - LEAK is used to determine the time history of sodium flow rate to, and spilled volume through, leaks at various locations in the main piping of the Intermediate Heat Transport System (IHTS) of the Clinch River Breeder Reactor Plant (CRBRP). This information is used for purposes such as analysis of sodium fires, sizing of sodium catch pans, and determining effects of sodium leaks on building supports and concrete.

   The calculations start at the time when the expansion tank and pump tanks have just emptied and the main flow in the IHTS has stopped. At this point, steady-state conditions are assumed since dynamic effects are negligible. Also, since the flow resistances in the main loop pipes and components are negligible compared with that of the leak, they are ignored and the model becomes the equivalent of a large tank of rather complicated geometry with a leak at some arbitrarily chosen point. LEAK calculates the leak flow from the time of the start of emptying of the system to arrival of the sodium surface at the leak, or to hydraulic equilibrium.

   Basic assumptions used in the program are as follows: the expansion tank and pump have just emptied and IHTS main flow has stopped; friction losses in the main piping and components are negligible in view of the low flow rate; flows are based upon steady-state conditions at each calculation point; average flow between calculation points is found by linear interpolation; calculations are made when the geometry at the sodium surface elevation changes (transition from vertical to nearby horizontal pipe, emptying of a flow path, etc.); the free surfaces of the sodium in contact with the cover gas assume a common level as they fall; if hydraulic equilibrium is achieved before the break elevation is uncovered, bubbling is assumed to occur; the cell pressure is constant at 14.7 psia; and gas entering the IHTS from the cell during bubbling does not react with the sodium.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES** - R. A. Luoma, Computer Code LEAK, GE ARSD Spec. 23A2833, October 29, 1981.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (150 lines)

The reference document and LEAK source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - reactor components, reactor cooling systems, sodium cooled reactors, leaks, flow rate, performance testing, Clinch River Breeder Reactor, LMFBR reactors, SPILL codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - DUMPHTF
   DUMPHTF, temperature transients in dump lines

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Honeywell6000

3. **DESCRIPTION** - DUMPHTF calculates the effect of heat transfer from the sodium moving in a dump line to the dump line wall. In this sense, the code is a transient analysis code. Primary output is a table of the temperature of sodium entering the dump tanks versus time. The code also calculates the temperature-time response of the dump line wall. Although a sodium dump is performed following a sodium water reaction, DUMPHTF is limited to consideration of a single phase fluid. DUMPHTF models a sodium dump line by dividing the length of piping into axial segments. Each axial segment has a specifiable number of radial nodes, up to a maximum of 10, starting at the inner surface of the pipe and ending at the outer surface. The initial fluid conditions (temperature and flow velocity) are input functions. In addition, the initial piping preheat temperature and pipe thermal conductivity are given where the pipe thermal conductivity is a function of the temperature. DUMPHTF uses finite differences to calculate heat transfer from the fluid to the pipe wall and within the pipe wall.

   The information generated by DUMPHTF is used in the stress analysis of the dump line wall and the stress analysis of the dump tank and dump tank nozzle.

   DUMPHTF was developed for the Clinch River Breeder Reactor Plant (CRBRP) assessment of the sodium dump piping system. As a general purpose program, DUMPHTF can be applied to any system which can be modeled as an insulated pipeline which is given an initial temperature distribution along its length and given a time-dependent hot fluid, with a time-dependent velocity fluid entering one end of it.

   Three properties of liquid sodium at standard pressure as a function of temperature are incorporated in the program. If another liquid is used the user must replace the values of the Prandtl number which is correct for the temperature range from 300 to 1100 degrees F, kinematic viscosity, which is valid for the same temperature range, and the conductive heat transfer coefficient given in the program.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed February 1985.
   Honeywell6000 version submitted August 1984.

10. **REFERENCES** - R. Yaspo, Computer Code DUMPHTF, GE ARSD Spec. 23A3006, March 17, 1983.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - GCOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    L. Tiemann
    Advanced Reactor Systems Department
    General Electric Company

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (235 lines)
The reference document and DUMPHTF source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – H
KEYWORDS – temperature distribution, time dependence, sodium cooled reactors, reactor components, pipes, Clinch River Breeder Reactor, LMFBR reactors

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - CONROD2
   CONROD2, breeder reactor absorber pin analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600,6600

3. **DESCRIPTION** - CONROD2 is a neutron absorber lifetime behavior prediction code. It is a modification of the CNRD2 program written at Hanford Engineering Development Laboratory to analyze FFTF absorber pins. CONROD2 is able to analyze absorber pin lifetime performance within user-specified environmental conditions. Thermal-hydraulic behavior, boron carbide gas release and swelling, clad swelling, clad stress and strain, and pellet-to-clad and bundle-to-duct clearances are calculated as a function of time. FFTF-specific model elements have been removed and modifications made to allow geometric variations of the bundle, more straightforward nucleonics input, a stepped pellet option, and more extensive behavior parameter output. The program is applicable to any fast reactor primary or secondary absorber assembly.

   The code breaks the pin column into one inch segments which are treated as uniform elements. After the flow and heating rate parameters are determined, a time marching scheme is employed to solve for the thermal-hydraulic and mechanical behavior of each of the elements. CONROD2 makes the following assumptions: each axial section is treated independently, the only axial coupling being the fluid temperature and the initial gas pressure; 'time hardening' creep accumulation is used; B4C material is assumed isotropic in its absorption characteristics; there is no coupling between the mechanical and thermal equations, i.e., flow channels retain their original size and shape; pin failure is assumed to occur when pellet-clad contact occurs; the control rod is assumed stationary and in steady-state operation; neutron heating takes place in the B10 and clad materials only, gamma heating occurs in all constituent materials; all the gas is at the average temperature of the plenums weighted by their respective volumes; and a bundle is comprised of one-third "peak" (highest power) pins and two-thirds "average" pins.

   The equations used in the thermal-hydraulic modules are solved simultaneously at each node with iteration on both the gap radiation and conduction. The solution scheme governing the mechanical behavior is a time marching incrementation which assumes constant behavior (stresses, strains, loads) between time-steps. The helium release, and the pellet and clad inelastic strains are computed incrementally and summed at each time-step. B10 depletion causes the rate of helium release and pellet swelling to decrease with time while the clad strains, which are fluence driven, proceed unabated. The stability of this procedure is dependent on time-step size.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted August 1984.

10. **REFERENCES** - D. Heisser, CONROD-II, A User's Guide to the Modified CNRD-II Code for Absorber Pin Evaluation, GE-ANTO Memorandum YL-604-840119, June 14, 1984.
    D. Heisser, Verification for Computer Code CONROD-II, GE Spec. 23A3087, January 5, 1984.
    A. L. Pittner, User's Manual for CNRD2--A Design Analysis Code for LMFBR Control Rods, HEDL-TME-81-50, January 1982.

11. **HARDWARE REQUIREMENTS** - 54K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

L. Tiemann
Advanced Reactor Systems Department
General Electric Company

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (2039 lines)
The YL-604-840119 and 23A3087 reference documents and CONROD2 source and sample problems input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - heat transfer, reactor cores, control rod worths, swelling, creep, neutron absorbers, control elements, burnable poisons, FFTF reactor, Clinch River Breeder Reactor, CNRD2 codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - T-HEMP3D
   T-HEMP3D, elastic-plastic flow in 3-d & time

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Prime750

3. **DESCRIPTION** - T-HEMP3D (Transportable HEMP3D) is a derivative of the STEALTH three-dimensional thermodynamics code developed by Science Applications, Inc. Changes were made primarily in three areas: material specification, coordinate generation, and the addition of sliding surface boundary conditions. STEALTH itself is based entirely on the HEMP3D code written at LLNL. HEMP3D solves problems in solid mechanics involving dynamic plasticity and time-dependent material behavior and problems in gas dynamics. The equations of motion, conservation equations, and constitutive relations for stresses, strains, hydrostatic pressure, the von Mises yield condition, and artificial viscosity are solved by finite difference methods following the format of the HEMP code (NESC 775). The physical object is divided into zones defined by 8 grid points. The grid (i,j,k) moves with the material, and the mass within a zone remains constant. HEMP3D is formulated in Lagrange coordinates in three dimensions and time. T-HEMP3D divides boundary conditions into two categories, momentum and thermal. Available momentum boundary conditions include pressure and velocity histories, wall interaction (stonewalls) and grid interaction (slide planes). Thermal boundary conditions include temperature and heat flux histories.
   Two auxiliary programs, VMESH and GREMP, are included. VMESH creates meshes, or grids, suitable for use with any three-dimensional Lagrangian finite difference program, such as T-HEMP3D. GREMP is a postprocessor which plots the problem grid in three dimensions.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   Prime750 version submitted September 1983.

10. **REFERENCES** - David Turner, T-HEMP3D User Manual, UCID-19873, August 1983.
    M. L. Wilkins, R. E. Blum, E. Cronshagen, and P. Grantham, A Method for Computer Simulation of Problems in Solid Mechanics and Gas Dynamics in Three Dimensions and Time, UCRL-51574 Rev. 1, May 30, 1975.
    David Turner, T-HEMP3D Programmer's Guide, Machine Dependencies in T-HEMP3D, Lawrence Livermore National Laboratory Memorandum, August 17, 1983.
    Jo Anne L. Levatin, GREMP User's Manual, Lawrence Livermore National Laboratory Memorandum, received September 22, 1983.
    Solveig Shearer, VMESH--Semiautomatic Coordinate Generator of Three-Dimensional Meshes, Lawrence Livermore National Laboratory Memorandum, July 1983.
    T-HEMP3D, NESC No. 9766, T-HEMP3D Author's Notes, National Energy Software Center Note 85-46, September 8, 1983.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    D. P. Turner
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (70,627 lines)
The reference reports, memoranda, and NESC Note and T-HEMP3D source, material properties library, and auxiliary programs on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - thermodynamics, three-dimensional, fluid mechanics, Navier-Stokes equations, finite difference method, Lagrange equations, elasticity, plasticity, STEALTH codes, HEMP3D codes, HEMP codes, GREMP codes, VMESH codes, GRADIS codes

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - RCTRMO
   RCTRMO, zinc ferrite coal-gas desulfurization

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780, IBM3083

3. **DESCRIPTION** - RCTRMO simulates the dynamics of the desulfurization and regeneration phases of the hot coal-gas desulfurization process, which uses a fixed-bed of extruded zinc ferrite pellets. The primary desulfurization and regeneration chemical reactions occur between H_2S and a mixture of ZnO and Fe_3O_4, and between O_2 and a mixture of ZnS and FeS, respectively.

   The gas and solid continuity equations used assume that: (1) plug flow prevails in the reactor, (2) a pseudo steady-state condition exists relative to the gas in both the pellets and bed (i.e., neglect gas sorbate accumulation terms), and (3) the chemical reactions are irreversible and occur isothermally at the particle level. The energy continuity equation used assumes that: (1) the reactor is adiabatic, (2) there is no radial transfer of heat, (3) no temperature gradients reside in the particles, (4) rapid heat transfer occurs between gases and solids, (5) gases are in plug flow, (6) energy accumulation in the gas is negligible compared to that in the solid, and (7) gas density is independent of composition.

   The partial differential equations derived are solved using standard numerical methods. A modified Euler's method is applied to start the solution followed by application of the Milne's 4th order predictor method with Hamming's corrector procedure. The energy balance equation is solved using a finite element method.

   Two BASIC programs, STEPC and STEPN, which can assist the user in selecting the time and length step RCTRMO input parameters, are listed in the reference report.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   DEC VAX11/780 version submitted November 1984.
   IBM3083 version submitted November 1984.

10. **REFERENCES** - J. T. Schrodt, Dynamic Simulation of a Fixed-Bed Zinc/Iron Oxide High Temperature Desulfurization Process, DOE/MC/21582-1500, February 21, 1983.
    RCTRMO, NESC No. 9767, RCTRMO Programming Information, National Energy Software Center Note 85-47, January 29, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. R. Gansley
    Morgantown Energy Technology Center

16. **MATERIAL AVAILABLE** -
    Source (VX11-1513 lines, 3083-1509 lines)

The reference report and NESC Note and RCTRMO source and sample problem input on magnetic tape are available from NESC on an "As Is" basis. In addition, sample problem output is included on the DEC VAX11 version magnetic tape.

17. **CATEGORY** - U
KEYWORDS - desulfurization, regeneration, coal gas, zinc, iron oxides, chemical reactions, high temperature

18. **SPONSOR** - DOE Office of Fossil Energy

1. **IDENTIFICATION AND KWIC TITLE** - DILATE
   DILATE, fuel assembly duct dilation analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - DILATE calculates duct corner and midflat radial dilation (in inches) as a function of time during normal reactor operation. Developed for use in CRBRP fuel assembly design, the program takes into account elasticity, thermal expansion, and irradiation induced creep and swelling. Multiple cycle capability can be invoked by specifying a negative thickness as input. Creep and swelling are calculated using a summation of incremental values and fluence rates over each cycle. Irradiation induced creep and swelling properties are provided by user-supplied subroutines CRP and SWL, respectively. The standard CRP and SWL subroutines for 20% CW 316 stainless steel are included. DILATE thermally expands the reactor pitch, which is established by the lower core support structure, from room temperature to reactor inlet temperature. The burnup or time in a given cycle when the radial duct dilation will equal the thermally expanded radial pitch is calculated by linear interpolation between printout points (every 5th iteration). Temperatures should not be so high that thermal creep becomes an important deformation mechanism.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted October 1984.

10. **REFERENCES** - R. M. Duritsa, DILATE Computer Code Verification, Westinghouse ARD Memorandum LRA-84-052, October 15, 1984.
    B. A. Bishop, DILATE Verification/ANSYS Comparison, Westinghouse ARD Memorandum LRA-FR-78-26, September 12, 1978.
    B. A. Bishop, Duct Dilation/Evaluate Impact of First Core Steel Creep and Swelling for Initial Cycles of Reference Core, Westinghouse ARD Memorandum LRA-FR-77-1, August 16, 1976.
    B. A. Bishop, Duct Dilation/Verification, Westinghouse ARD Memorandum LRA-FR-77-11, June 7, 1977.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. C. Haberstroh
    Advanced Energy Systems Division
    Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (155 lines)
    The reference memoranda and DILATE source and sample problems on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - physical radiation effects, creep, ducts, swelling, neutron fluence, reactor components, Clinch River Breeder Reactor

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - DENS
   DENS, CRBRP fuel rod densification analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - DENS determines the core average gap and the maximum gap in the peak power fuel rod for average maximum and minimum densification and provides input data for subsequent plotting of this information with peak fuel pellet burnup. DENS is applicable to LMFBR fuel manufactured to RDT E-13-6 specifications. Maxima of 20 each radial and axial regions are allowed. The program is limited to CRBRP fuel density of 90.4% and to cycles 1 and 2 of RFMS core operation. The sample problems require less than 1 CP second on a CDC7600.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted September 1984.

10. **REFERENCES** - Bruce A. Bishop, Impact of Fuel Densification on CRBRP Fuel Performance, CRBRP-ARD-0168, June 1977.
    J. J. Huba, Code Verification/Verify the DENS Computer Program, Westinghouse ARD Memorandum LRA-FR-79-12, May 31, 1979.
    Attachment I, Input Data Description, 8/1/78 Version of DENS, Westinghouse ARD Memorandum, received September 1984.
    B. A. Bishop, Fuel Densification Behavior of FFTF/CRBRP Fuel, Westinghouse ARD Memorandum LRA-FR-77-8, April 15, 1977.
    B. A. Bishop, Fuel Densification/Effect on AFMS Initial Core Fuel Performance, Westinghouse ARD Memorandum LRA-FR-77-33, October 11, 1977.
    B. A. Bishop, Fuel Densification Effects on AFMS Initial Core Fuel Performance, Westinghouse ARD Memorandum LRA-77-811, October 11, 1977.
    DENS, NESC No. R9769, DENS Implementation Information, National Energy Software Center Note 85-45, January 29, 1985.

11. **HARDWARE REQUIREMENTS** - 15K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    B. A. Bishop
    Advanced Energy Systems Division
    Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (337 lines)
    The reference report, memoranda, NESC Note, and sample problems output and DENS source and sample problems input on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I

KEYWORDS - fuel densification, nuclear fuels, performance testing, LMFBR reactors, fuel rods, Clinch River Breeder Reactor

18. SPONSOR - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - SLIB77
   SLIB77, source library file maintenance system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780, DEC20, Prime, CDC, Cray, IBM, Data General, HP1000, Harris, UNIVAC, Apollo

3. **DESCRIPTION** - SLIB77 is a source librarian program designed to maintain FORTRAN source code in a compressed form on magnetic disk. The program was prepared to meet program maintenance requirements for ongoing program development and continual improvement of very large programs involving many programmers from a number of different organizations. SLIB77 automatically maintains in one file the source of the current program as well as all previous modifications. Although written originally for FORTRAN programs, SLIB77 is suitable for use with data files, text files, operating systems, and other programming languages, such as Ada, C, and COBOL. It can handle libraries with records of up to 160 characters. Records are grouped into DECKS and assigned deck names by the user. SLIB77 assigns a number to each record in each DECK. Records can be deleted or restored singly or as a group within each deck. Modification records are grouped and assigned modification identification names by the user. The program assigns numbers to each new record within the deck. The program has two modes of execution, BATCH and EDIT. The BATCH mode is controlled by an input file and is used to make changes permanent and create new library files. The EDIT mode is controlled by interactive terminal input, and a built-in line editor is used for modification of single decks. Transferring of a library from one computer system to another is accomplished using a Portable Library File created by SLIB77 in a BATCH run. Other features of SLIB77 include: user-controlled switches which can be used to control records being placed onto the compile file, the capability of reverting to an earlier library condition, options for controlling listings of deck records, provisions such that if a COMMON deck is modified all decks which call it will automatically be updated, and groups of records within a COMMON deck may be given a group name and selectively incorporated into any deck.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   SLIB77 submitted November 1984, replaced by Edition B August 1985.

10. **REFERENCES** - SLIB77 A Source Librarian Written in Fortran 77 - User's Guide, Western Area Power Administration memorandum, August 31, 1983, revised June 15, 1985.
    SLIB77 A Source Librarian Written in Fortran 77 - Installation Manual, Western Area Power Administration memorandum, June 1, 1984, revised June 15, 1985.
    SLIB77 A Source Librarian Written in Fortran 77 - Demonstration Guide, Western Area Power Administration memorandum, June 1, 1984, revised June 15, 1985.
    SLIB77 A Source Librarian Written in Fortran 77 - Modifications Manual, Western Area Power Administration memorandum, June 1, 1984, revised June 15, 1985.

11. **HARDWARE REQUIREMENTS** - 1 Mbyte

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR –**
A. Lunsford
Western Area Power Administration
U. S. Department of Energy

16. **MATERIAL AVAILABLE –**
Source (approximately 19,000 lines)
The WAPA memoranda and SLIB77 source, portable library input, and latest modification sets on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – M
KEYWORDS – libraries, maintenance, data processing, retrieval systems, FORTRAN, programming languages, utility routines

18. **SPONSOR** – DOE Western Area Power Administration,
Division of System Engineering

1. **IDENTIFICATION AND KWIC TITLE** - GEOTEMP2
   GEOTEMP2, advanced wellbore thermal simulator

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC CYBER170, CDC7600,6600

3. **DESCRIPTION** - GEOTEMP2, which is based on the earlier GEOTEMP program, is a wellbore thermal simulator designed for geothermal well drilling and production applications. The code treats natural and forced convection and conduction within the wellbore and heat conduction within the surrounding rock matrix. A variety of well operations can be modeled including injection, production, forward and reverse circulation with gas or liquid, gas or liquid drilling, and two-phase steam injection and production. Well completion with several different casing sizes and cement intervals can be modeled. The code allows variables, such as flow rate, to change with time enabling a realistic treatment of well operations. Provision is made in the flow equations to allow the flow areas of the tubing to vary with depth in the wellbore. Multiple liquids can exist in GEOTEMP2 simulations. Liquid interfaces are tracked through the tubing and annulus as one liquid displaces another. GEOTEMP2, however, does not attempt to simulate displacement of liquids with a gas or two-phase steam or vice versa. This means that it is not possible to simulate an operation where the type of drilling fluid changes, e.g. mud going to air.
   GEOTEMP2 was designed primarily for use in predicting the behavior of geothermal wells, but it is flexible enough to handle many typical drilling, production, and injection problems in the oil industry as well. However, GEOTEMP2 does not allow the modeling of gas-filled annuli in production or injection problems. In gas or mist drilling, no radiation losses are included in the energy balance. No attempt is made to model flow in the formation. Average execution time is 50 CP seconds on a CDC CYBER170. This edition of GEOTEMP2 is designated as Version 2.0 by the contributors.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted September 1982, replaced by CDC CYBER170 version January 1985.

10. **REFERENCES** - Lisa A. Mondy and Leonard E. Duda, Advanced Wellbore Thermal Simulator GEOTEMP2 User Manual, SAND84-0857, November 1984.
   Robert F. Mitchell, Advanced Wellbore Thermal Simulator GEOTEMP2 Research Report, SAND82-7003/1, February 1982.
   G. R. Wooley, Wellbore and Soil Thermal Simulation for Geothermal Wells - Development of Computer Model and Acquisition of Field Temperature Data, Part I Report, SAND79-7119, March 1980.
   G. R. Wooley, Wellbore and Soil Thermal Simulation for Geothermal Wells - Comparison of GEOTEMP Predictions to Field Data and Evaluation of Flow Variables, Part II Report, SAND79-7116, March 1980.
   G. R. Wooley, User's Manual for GEOTEMP, A Computer Code for Predicting Downhole Wellbore and Soil Temperatures in Geothermal Wells, Appendix to Part I Report, SAND79-7118, March 1980.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 5

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
L. E. Duda
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
Source (3555 lines)
The SAND84-0857 and SAND82-7003/1 reference reports and GEOTEMP2 source and sample problems input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - geothermal wells, computerized simulation, heat transfer, well drilling, well stimulation, forced convection, rock drilling, GEOTEMP codes

18. **SPONSOR** - DOE Division of Geothermal and Hydropower Technologies

1. **IDENTIFICATION AND KWIC TITLE** - ARCHIVE
   ARCHIVE, NOS2.2 permanent file backup system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER170,175

3. **DESCRIPTION** - The ARCHIVE system is a NOS2.2 subsystem designed to backup permanent files on CDC Cyber machine systems. A Mass Storage Subsystem (MSS) runs at a control point, monitoring archive activity. Archive activity consists of: (1) creating backup files by dumping disk files to magnetic tape storage, (2) processing user-initiated requests for backed-up files, (3) controlling disk space by releasing disk files that have been backed up to tape, and (4) recycling old backup tapes so they may be reused. Additionally, ARCHIVE provides a fail-safe environment for the site, in case hardware or software errors destroy the permanent file base, and for users, in case they erroneously purge or irremediably alter a file. The archive itself is a set of magnetic tapes with each tape having a twin, for maximum data security. Once a file is copied, ARCHIVE may change its residence from one disk device to another, in order to improve track utilization, or it may evict the file from disk, to release space needed for growth of other files. If a file has been evicted, it may still be attached. ARCHIVE locates the tape copy of the file and restores it to disk. Users may access the database identifying the locations in the archive of all known versions of any of their files and then direct ARCHIVE to retrieve any version. To prevent the archive from growing forever, a recycling process is implemented. Recycling takes old archive tapes and by a direct tape to tape copy moves the still active files to new archive tapes and makes the recycled tape available for reuse.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC CYBER170 version submitted December 1984.

10. **REFERENCES** - FERMILAB ARCHIVE System, NOS2.2, FERMILAB Memorandum, July 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN V and COMPASS

13. **OPERATING SYSTEM** - NOS 2.2 Level 596/587.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    S. Ahlgrim
    Fermi National Accelerator Laboratory

16. **MATERIAL AVAILABLE** -
    Source (approximately 7000 lines)
    The reference memorandum and ARCHIVE source, control information, and documentation; REQUEST source, library, and control information; NUMBERS source and control information; and FSS source, library, and documentation on magnetic tape, in CDC NOS INTERNAL format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - CDC computers, operating systems, information systems, management

18. **SPONSOR** - Fermi National Accelerator Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - RMATRX
RMATRX, R-matrix atomic continuum processes

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
CDC7600

3. **DESCRIPTION** - RMATRX is a set of three programs, STG1, STG2, and STG3, to calculate atomic continuum processes using the R-matrix method. The atomic processes include electron-atom, electron-ion and photoionization cross sections, and atomic polarizabilities.

STG1 calculates all one-electron, two-electron, and multipole radial integrals involving bound and continuum orbitals in the inner region. The radial integrals enable electron-atom or electron-ion scattering, photoionization or frequency dependent polarizabilities to be calculated for a general atomic system. The bound orbitals are specified analytically; STG1 calculates the continuum orbitals. The integrals are saved for input to STG2.

STG2 reads the radial integrals calculated by STG1 and then calculates the Hamiltonian matrix elements, the asymptotic potential coefficients, and the dipole length and velocity matrix elements from a given initial state to the final state specified by L, S, and the channel quantum numbers. These quantities are stored for use in STG3.

STG3 reads the Hamiltonian matrix elements calculated by STG2 and then diagonalizes the Hamiltonian matrix and calculates the R-matrix and its Buttle correction. Then either the electron-atom or electron-ion cross section, the photoionization cross section and beta asymmetry parameter or the frequency dependent polarizability is calculated, for a range of incident energies or frequencies. In a photoionization or polarizability calculation, the initial state is treated in exactly the same way as the final states.

Up to 5 bound orbitals and 20 continuum orbitals can be included for each angular momentum up to l=14. The maximum size of the Hamiltonian matrix that can be treated is 200, and the maximum number of channels is 12. The maximum number of incident energies which can be dealt with in one STG3 run is 50. RMATRX assumes that L and S are good quantum numbers and neglects effects due to the spin-orbit interaction.

STG1 running time depends approximately on the square of the number of bound orbitals, on the square of the number of continuum orbitals for each angular momentum, and on the number of continuum angular momenta. STG2 running time depends on the square of the number of shells and the number of configurations included.

This software, identified as RMATOM, was transferred in February 1981, from the National Resource for Computation in Chemistry's software library.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
CDC7600 version submitted February 1981.

10. **REFERENCES** - K. A. Berrington, P. G. Burke, M. Le Dourneuf, W. D. Robb, K. T. Taylor, and Vo Ky Lan, A New Version of the General Program to Calculate Atomic Continuum Processes Using the R-Matrix Method, Computer Physics Communications, Vol. 14, pp. 367-412, 1978.

P. G. Burke, J. J. Chang, A. T. Chivers, W. D. Robb, and K. T. Taylor, A General Program to Calculate Atomic Continuum Processes Using the R-Matrix Method, Computer Physics Communications, Vol. 8, pp. 149-198, 1974.

P. G. Burke and W. D. Robb, R-Matrix Method, Advances in Atomic and Molecular Physics, Vol. 11, p. 143, 1975.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -

L. D. Thomas
NRCC
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -

Source (STG1 5377 lines, STG2 10,897 lines, STG3 7660 lines)

The RMATRX source, sample problems input and output, control information, and machine-readable documentation on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - W

KEYWORDS - R matrix, electron-atom collisions, electron-ion collisions, photoionization, cross sections, polarizabilities, scattering, RMATOM codes

18. **SPONSOR** - Queen's University, Belfast, U.K.
United Kingdom Science Research Council

1. **IDENTIFICATION AND KWIC TITLE** - CHEMTRN
   CHEMTRN, 1d chemical transport in porous media

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - CHEMTRN simulates the transport of chemical species in groundwater systems. The program is based on thermodynamic principles. Equilibrium is assumed in all chemical reactions, and thermodynamic activities of all reacting species are related by mass-action expressions. The mass action and transport equations are expressed as a set of differential/algebraic equations which are solved simultaneously. CHEMTRN can simulate either one-dimensional or purely radial flow in porous media using a grid with either a uniform or a variable spacing. The program includes the effects of dispersion/diffusion, advection, sorption via ion exchange or surface complexation model, complexation in the aqueous phase, precipitation or dissolution of solids, and the dissociation of water. In the surface complexation model, the effect of the electric double layer has been included. The user must supply the equilibrium constants and the stoichiometric coefficients for the reactions of interest.
   The four sample cases include, in addition to the transport of the species in the porous media, the chemical effects of (1) sorption via ion exchange, (2) aqueous complexation with sorption via ion exchange and precipitation of solids, (3) sorption via a surface complexation model and aqueous complexation, and (4) precipitation and dissolution of solids.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted August 1983, replaced by revised edition April 1985, replaced by revised edition May 1985.

10. **REFERENCES** - C. W. Miller, CHEMTRN User's Manual, LBL-16152, March 1983.
    Supplement to CHEMTRN User's Manual, April 26, 1985.
    CHEMTRN, NESC No. 9774, Errata to CHEMTRN Reference Report, LBL-16152, National Energy Software Center Note 85-67, May 3, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. W. Miller
    Earth Sciences Division
    Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
    Source (2462 lines)
    The reference report, Supplement, and NESC Note and CHEMTRN source and sample problems on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
KEYWORDS - ground water, chemical effluents, diffusion, advection, sorption, porous materials, radionuclide migration, ion exchange, chemical reactions

18. **SPONSOR** - NRC Office of Nuclear Regulatory Research,
Division of Health, Safety and Waste Management,
Waste Management Branch

1. **IDENTIFICATION AND KWIC TITLE** - EQUILIN
   EQUILIN, temperature distribution for concrete

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - EQUILIN calculates an equivalent linear temperature distribution from a given nonlinear distribution through a concrete wall or a slab, according to the techniques described in the American Concrete Institute's "Code Requirements for Nuclear Safety Related Concrete Structures". A maximum of 10 points (temperatures) may be specified at various locations through the thickness of the wall, including the temperature of each face. Any value may be selected for the thickness of the wall. If the wall thickness is less than the depth at which the last temperature is specified, the temperature at the outer surfaces is linearly interpolated from the input values. The nonlinear temperature distribution specified as input to EQUILIN must be monotonically increasing or decreasing through the thickness.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted September 1984.

10. **REFERENCES** - EQUILIN User's Manual, Burns and Roe, Inc. document, received September 1984.
American Concrete Institute, Code Requirements for Nuclear Safety Related Concrete Structures, ACI 349-80, 1980.
American Concrete Institute, Code Requirements for Nuclear Safety Related Concrete Structures, ACI 349-80, Appendix A, and commentary, 1980.

11. **HARDWARE REQUIREMENTS** - 40K words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. E. Palm
    Burns and Roe, Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (151 lines)
    The reference User's Manual and EQUILIN source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
    KEYWORDS - concretes, buildings, walls, slabs, temperature distribution

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - ILUIR
   ILUIR, incomplete LU with iterative refinement

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1

3. **DESCRIPTION** - ILUIR solves a linear system Ax=b using incomplete LU decomposition with iterative refinement (also known as SIP, Strongly Implicit Procedure). The matrix is specified by supplying arrays containing the nonzero elements of the matrix, their row numbers, and their column numbers.
   ILUIR uses the dynamic memory management provided by the LRLTRAN POINTER statement in conjunction with the Lawrence Livermore National Laboratory environment subroutines GETSPACE and RELSPACE; these routines are not included. This feature can be replaced by specifying dimensions for the required arrays.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   Cray1 version submitted December 1984.

10. **REFERENCES** -

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    A. Greenbaum
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (956 lines)
    The ILUIR source on magnetic tape is available from NESC on an "As Is" basis.

17. **CATEGORY** - P
    KEYWORDS - matrices, algebra, equations, algorithms, mathematics

18. **SPONSOR** - DOE Office of Energy Research

1. **IDENTIFICATION AND KWIC TITLE** - REVERT
   REVERT, processing spent fuel test-climax data

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - REVERT is used by the Spent Fuel Test-Climax Project to reconvert data values collected on a Hewlett-Packard 1000 database at the Nevada Test Site. The system also converts raw data (electrical units of measure) to engineering units. Both the raw and engineering data values, along with time (Julian days to five decimal digits) and two device identifying fields (a 'license plate' and 'channel number'), are periodically written onto magnetic tape along with data conversion coefficients and control parameters from several tables on the HP system. These tapes are delivered to Livermore to produce a printed record of their contents and for REVERT processing. REVERT has two independent paths of control. One is to read the tapes created by the HP system and make a file that, two, can be randomly read for coefficients during the "re-conversion" process. Basically, there are five uses for REVERT: to make a CDC7600 compatible database from an HP tape file, to merge an HP tape file with a database, to modify a database, to list a database, and to use a database to process a data file compensating for thermal effects, individual calibrations, instrument geometries, etc.

   Two auxiliary preprocessor programs, BREAD and MFAB, are included. BREAD processes a family of data files copied from a HP-generated data tape, translating the data to CDC7600 BCD code and sorting it by license and time into a single file. MFAB converts BREAD output BCD file(s) to a binary data file with space allocated for the reconverted data values (fifth word per data point). It can also merge files of either type into a binary data file, with a time-range constraint.

   REVERT, BREAD, and MFAB make use of LLNL-environment routines contained in the ORDERLIB library; these routines are not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted December 1984.

10. **REFERENCES** - Glenn Hage, A User's Guide to REVERT A CDC 7600 Program for Converting Spent Fuel Test - Climax Data to Engineering Units, with Corrections, UCID-30206, October 1984.

    Glenn L. Hage, BREAD A CDC 7600 Program that Processes Spent Fuel Test-Climax Data, UCID-19814, April 1983.

    Glenn Hage, File Merging and Conversion Program, MFAB, Lawrence Livermore National Laboratory Memorandum, June 3, 1982.

    Edna Carpenter, Stanley V. Solbeck, and Karl Dusenburg, Livermore Timesharing System Part 4: Library Files Chapter 304: ORDERLIB Subroutine Library, LCSD-408, October 22, 1980.

11. **HARDWARE REQUIREMENTS** - 220K (octal) words

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -

G. L. Hage
Lawrence Livermore National Laboratory

16. MATERIAL AVAILABLE -

Source (3974 lines)

The UCID-30206 and UCID-19814 reference reports, LCSD-408 excerpt, and LLNL memorandum and REVERT, BREAD, and MFAB source on magnetic tape are available from NESC on an "As Is" basis.

17. CATEGORY - O

KEYWORDS - data acquisition, data processing, HP computers, CDC computers, BREAD codes, MFAB codes

18. SPONSOR - DOE Office of Civilian Radioactive Waste Management

1. **IDENTIFICATION AND KWIC TITLE** - TWOHEX
   TWOHEX, 2-d x,y triangular mesh Sn transport

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
Cray1 or Cray-XMP

3. **DESCRIPTION** - TWOHEX solves the two-dimensional, multigroup transport equation on an equilateral triangular mesh in the x,y plane. Both regular and adjoint, inhomogeneous (fixed source) and homogeneous problems are solved. Three problem domains are treated by TWOHEX. The 'whole core' domain is a 60-degree parallelogram with vacuum boundary conditions on each face. The 'third core' domain is a 120-degree parallelogram with two vacuum and two rotational boundary conditions. The 'sixth core' domain is a 60-degree parallelogram with two vacuum and two rotational boundary conditions. General anisotropic scattering is allowed, and an anisotropic inhomogeneous source may be input as cell averages. TWOHEX numerically solves the two-dimensional, multigroup form of the neutral-particle, steady-state Boltzmann transport equation. The discrete-ordinates form of approximation is used for treating the angular variation of the particle distribution, and a linear characteristic/nodal scheme is used for spatial discretization. There is no negative flux fixup since few if any negative fluxes are generated by this numerical scheme. A standard inner (within-group) iteration, outer (energy-group-dependent source) iteration technique is used. Both inner and outer iterations are accelerated using the Chebyshev acceleration method. The code is designed for a three-level hierarchy of data storage: a small, fast central memory (SCM), a fast-access peripheral large memory (LCM), and random-access peripheral storage. TWOHEX accepts, uses, and creates standard interface files as defined by the Committee on Computer Code Coordination.

   ONEDANT (NESC 9970) style free-field, card-image input capability is provided for the user. The program is basically the same with the one-dimensional SOLVER module of ONEDANT replaced with a two-dimensional SOLVER module.

   Running time is directly related to problem size and to central processor and data transfer speeds. On a Cray1, a four-group calculation of the eigenvalue of a midplane 'whole core' model of the Fast Test Reactor took 45 seconds. The calculation used transport corrected P0 cross sections, and S4 angular quadrature with 12 angles per hemisphere, and a 60x30 spatial mesh (six triangles per subassembly).

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   Cray1 version submitted December 1984.

10. **REFERENCES** - Wallace F. Walters, Forrest W. Brinkley, and Duane R. Marr, User's Guide for TWOHEX: A Code Package for Two-Dimensional Neutral-Particle Transport in Equilateral Triangular Meshes, LA-10258-M, October 1984.
    R. Douglas O'Dell, Forrest W. Brinkley, Jr., and Duane R. Marr, User's Manual for ONEDANT: A Code for One-Dimensional Diffusion-Accelerated Neutral-Particle Transport, LA-9184-M, February 1982.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - COS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
W. F. Walters, F. W. Brinkley, and D. R. Marr
Los Alamos National Laboratory

16. **MATERIAL AVAILABLE -** Restricted Distribution
Source (42,405 lines)
The LA-10258-M reference report and TWOHEX source, sample problem input and output, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY -** C
KEYWORDS - two-dimensional, Boltzmann equation, multigroup theory, discrete ordinate method, x-y, anisotropic scattering, space dependence, triangular configuration, ONEDANT codes

18. **SPONSOR -** DOE Office of Breeder Reactor Technology

1. **IDENTIFICATION AND KWIC TITLE** - RESPECTPLOT
   RESPECTPLOT, response spectra calculation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC6600

3. **DESCRIPTION** - RESPECTPLOT computes and plots acceleration response spectra at specified frequencies or periods from digitized input seismic time-history motions. It will also compute response spectra values at additional frequencies (or periods), if required. The response spectra can be calculated for different values of spectral damping ratios as well. A response spectrum is a plot of the maximum response of a family of single-degree-of-frequency damper oscillators with different frequency characteristics when the base of the oscillator is subjected to an appropriate time history record. To construct the response spectra, it is necessary to find the maximum values of the acceleration during a given excitation. This is done by calculating the response at discrete time intervals and monitoring the response parameter to retain the maximum values. As an option, RESPECTPLOT broadens computed response spectra from a time history motion by plus or minus 10% of the frequencies corresponding to the peaks. RESPECTPLOT makes use of proprietary CalComp graphics software to produce graphical output. A typical problem requires 50 CP seconds on a CDC6600.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC6600 program listing submitted September 1984.

10. **REFERENCES** - RESPECTPLOT User's Manual, Burns and Roe document, received September 1984.
    N. C. Nigam and P. C. Jenning, Digital Calculation of Response Spectra from Strong-Motion Earthquake Records, Earthquake Engineering Research Laboratory, California Institute of Technology, Pasadena, June 1968.

11. **HARDWARE REQUIREMENTS** - 100K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS or SCOPE 3.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. E. Palm
    Burns and Roe, Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution
    Source (644 lines)
    The RESPECTPLOT reference document containing the RESPECTPLOT source, sample problem input and output, and control information listings is available from NESC on an "As Is" basis.

17. **CATEGORY** - I
    KEYWORDS - response functions, acceleration, spectral response, seismic events, frequency response testing

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - CODES
   CODES, design of concrete walls and shells

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - CODES designs reinforced concrete wall and shell structures according to ACI 318-77, the American Concrete Institute's "Building Code Requirements for Reinforced Concrete". Either the principal stress option or the axial load with shear option can be used. CODES calculates load combinations and designs the amount of reinforcement for each load combination. The maximum reinforcement for each element to be designed is tabulated. In addition, the maximum reinforcement areas for each group of elements is tabulated after all elements of the group have been designed. The program has the option of adjusting the thermal moment based on the cracked section of concrete. For wall design, the inplane shear forces are resisted by shear reinforcement for shell design. All inplane forces are combined into principal forces. The component of principal forces in the directions of the reinforcement are combined with moment for flexural design. CODES accepts up to a maximum of 36 load conditions and can handle up to 14 available load combinations and up to 10 element groups to be designed with a maximum of 20 elements per group. A typical design problem requires 70 CP seconds on a CDC7600. The output from STARDYNE, a general purpose finite element analysis program, is acceptable as CODES input.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC7600 program listing sumitted September 1984.

10. **REFERENCES** - "CODES" User's Manual, CODES - A Computer Program for the Design of Reinforced Concrete Wall and Shell Structures, Burns and Roe document, received September 1984.

11. **HARDWARE REQUIREMENTS** - 200K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - NOS.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   R. E. Palm
   Burns and Roe, Inc.

16. **MATERIAL AVAILABLE** - Restricted Distribution
   Source (838 statements)
   The CODES reference document containing the CODES source, sample problem input and output, and control information listings is available from NESC on an "As Is" basis.

17. **CATEGORY** - I
   KEYWORDS - reinforced concrete, shells, walls, bending, shear, STARDYNE codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - GEODYN
   GEODYN, rock formation drill string dynamics

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11/780

3. **DESCRIPTION** - GEODYN Phase I is the initial stage of an ongoing effort to analyze the dynamic behavior of a drill string within a borehole. Phase I solves the bit/formation interaction problem. GEODYN is a three-dimensional finite element program which models a polycrystalline diamond compact (PDC) bit drilling in a user defined formation, which can be non-homogeneous. The program accommodates nonlinear, time-dependent, loading and boundary conditions. GEODYN models the drill string using eight-node isoparametric brick elements, three-dimensional linear beam elements, and ghost cutter sub-elements. The eight-node brick elements are used to model the bit; the linear beams to model the drill collar and drill pipe, and the ghost cutters to model the teeth on the bit. GEODYN cannot completely model 20-node bricks, infinite bricks, or nonlinear beams.

   GEODYN accomplishes two major tasks. The first of these (subprogram GENDYN) is the generation of a finite element drill string model and the solution of the model's eigenvalues and eigenvectors. The second task (subprogram RUNDYN), which cannot be performed until the first is completed, is the solution of the response of the model to dynamic loading.

   The formation model utilized consists of a collection of discrete points located systematically in space. These points, if connected, would map the wellbore's surface. The model is comprised of three separate portions (or submodels), i.e. a 'bottom' surface, a 'side wall' surface, and an 'incline' surface, for which the direction of ghost cutter penetration varies. A uniform grid pattern is employed for each of the three portions. Each formation point has a penetration coordinate associated with it. This penetration coordinate is used to compute a penetration resistance force if a ghost cutter has penetrated the formation at this point. Constitutive formation properties, which are defined for each formation point, include a linear stiffness resisting ghost cutter penetration, the maximum attainable coefficient of friction in the rock, and the velocity at which this maximum attainable coefficient of friction is attained. Different constitutive formation properties may be defined for different formation points constituting the model. A mesh generator is incorporated to facilitate the description of the formation model.

   The solution process utilized embodies the totality of the three submodels described above to provide the capability of representing the transient dynamic response of the PDC bit system arising from nonlinear, time-dependent loading and formation interaction behavior. The solution algorithm incorporates an iterative solution technique employing a Newton-Raphson approximation within the incremental time-step process to obtain a converged equilibrium solution. Newmark's method is utilized to integrate the modal transformed equations of motion of the PDC bit system. Intermittent formation interaction forces, externally applied upstring boundary forces (i.e., weight-on-bit, torque, etc.), gravity forces, and centrifugal body forces are all accounted for in the solution process.

   An auxiliary utility program, GEOIN, is included which creates interactively a GEODYN input file for reuse or use in a batch environment.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   DEC VAX11/780 version submitted October 1984.

10. **REFERENCES** - Jerold A. Baird, Michael C. Apostal, Richard L. Rotelli, Jr., Mark A. Tinianow, and David N. Wormley, Phase 1 Theoretical Description A Geological Formation - Drill String Dynamic Interaction Finite Element Program (GEODYN), SAND84-7101, June 1984.
Mark A. Tinianow, Richard L. Rotelli, Jr., and Jerold A. Baird, Phase 1 User Instruction Manual A Geological Formation - Drill String Dynamic Interaction Finite Element Program (GEODYN), SAND84-7102, June 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS 3.4.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
B. C. Caskey
Sandia National Laboratories, Albuquerque

16. **MATERIAL AVAILABLE** -
Source (67,011 records)
The reference reports and GEODYN source, sample problem input and output, and auxiliary programs on magnetic tape, in VAX/VMS COPY format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - R
KEYWORDS - rock drilling, boreholes, drilling equipment, drill bits, finite element method, dynamic loads

18. **SPONSOR** - DOE Geothermal and Hydropower Technologies Division

1. **IDENTIFICATION AND KWIC TITLE** - PWBSTAT
   PWBSTAT, printed wiring board yield prediction

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER174 with graphics terminal

3. **DESCRIPTION** - PWBSTAT is a menu-driven program used to predict yields for printed wiring boards before production begins by comparing design characteristics against statistical models of fabrication processes. A PWBSTAT database contains characteristic curves for conductor width change (CWC), plated hole reduction (PHR), hole-to-land mislocation (HLM), contour deviation (CD), and hole registration (HR). Each of these curves conforms to the criteria for a normal distribution curve, and all are modeled as such. Because of this conformity, several curves can be combined by using statistical methods to produce a single normal distribution curve to represent the combined effect and to assess a DWB feature that results from the combination of several variables, such as a minimum angular ring prediction. The on-screen display of digital design definitions has been shown to contribute to greater, more predictable and reliable yields for complex multilayer and double-sided designs. Engineers are able to identify and correct manufacturing problem areas and predict risk before production. PWBSTAT can also be used to develop automated panel layouts, work directions, illustrations, and tooling.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC CYBER174 version submitted November 1984.

10. **REFERENCES** - K. D. Foreman, Computer-Aided Process Preparation for Printed Wiring Boards, BDX-613-2707, November 1981.
    J. L. Wilson and C. W. Jennings, Sandia/Bendix Standard Capability Study of Printed Wiring Boards, BDX-613-1349, August 1976.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 3.3.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    K. D. Foreman
    Kansas City Division
    The Bendix Corporation

16. **MATERIAL AVAILABLE** -
    Source (1081 lines)
    The BDX-613-2707 reference report and PWBSTAT source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
    KEYWORDS - manufacturing, yields, display devices, statistical models, computer-aided design, printed circuits

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE** - HOTDAMAGE
   HOTDAMAGE, thermal transient structural damage

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC CYBER170 Series 800

3. **DESCRIPTION** - HOTDAMAGE performs rapid calculation of creep and fatigue damage resulting from thermal transients and long-term exposure to high temperatures such as those common to Liquid Metal Fast Breeder Reactors. HOTDAMAGE is capable of analyzing several transients comprising a duty cycle, of performing transient thermal analyses, and of calculating creep and fatigue damage for a strain range and residual stress obtained by other means. The normal application is that of finding the response of a flat plate subjected to a thermal transient event and calculating the damage which will ensue from that event. Several thicknesses may be studied in the parametric mode, possibly to investigate the value of a design change in mitigating the effects of a transient. The duty cycle option may also be used to determine the cumulative damage resulting from a series of events. In evaluating a duty cycle, HOTDAMAGE proceeds on the assumption that the individual transients occur in the most severe sequence possible.

   The program is based on a simplified inelastic analysis technique which uses a plasticity correction factor to adjust the strain obtained from an elastic analysis. HOTDAMAGE determines the strains and stresses for a specified thermal transient by first solving the elastic thermal stress problem, then applying a correction factor to the elastic strains to include plasticity. The peak and initial residual stresses are obtained from a stress-strain curve which has been adjusted for environmental effects and cyclic hardening. Creep damage is calculated over the specified steady-state hold time with relaxation effects included. Fatigue damage is calculated as a function of strain range and peak temperature for the specified material. Material property data for types 304 and 306 stainless steels are incorporated in the program. Creep and fatigue damage values are determined for these materials.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC CYBER170 version submitted December 1984.

10. **REFERENCES** - J. L. Houtman, H. A. Mitchell, and M. A. Todd, HOTDAMAGE--A Computer Program for Simplified Evaluation of Cumulative Structural Damage Due to Thermal Transients User's Manual, AS-84-98, November 1984.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    M. A. Todd
    Advanced Energy Systems Division
    Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (1226 lines)
The reference report and HOTDAMAGE source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – I
KEYWORDS – thermal stresses, mechanical properties, LMFBR reactors, creep, damage, thermal fatigue, strains, transients

18. **SPONSOR** – DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - FRST
   FRST, fuel rod strains due to transients

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - The FRST, Fuel Rod Strain-Transient, program is a modification of the earlier FRS program which calculates fuel rod cladding strains caused by primary and secondary thermal creep, thermal stresses, irradiation induced creep and irradiation swelling. The program is used to determine fuel rod lifetimes by comparing the calculated strains to a design limit. All materials properties equations and steady-state stress and strain calculation subroutines used in FRST are identical to those used in FRS. Likewise, most of the input data for the FRS and FRST codes are the same. In FRST, a single type of upset and emergency transient is considered for a given problem. FRST calculates the cladding strains due to primary and secondary thermal creep during the transient, and adds these strains to the accumulated steady-state and transient cladding strain at the beginning of the transient. Whenever the cladding equivalent stress exceeds the yield stress, the cladding plastic deformation is calculated and included in the cladding total strain.

   The cladding thermal creep and plastic strains due to the emergency transient are calculated in the same way as the upset transient strains. FRST applies an emergency transient to the cladding each time an upset transient occurs. The emergency transient cladding strains are added to the accumulated cladding strain, and this total strain is compared to the emergency strain limit of 0.7%. If this limit is not exceeded, the cladding strains resulting from the emergency transient are deleted from the total cladding strain, and the program continues. If the limit is exceeded, a cladding end-of-life message is printed along with the cladding stresses, strains, and temperatures during the emergency transient, and the program moves on to the next problem. Thus, the cladding lifetime for FRST is defined as the time at which the occurrence of an emergency transient causes the cladding emergency strain limit to be exceeded. If the program calculates that the emergency strain limit is not exceeded at the specified end-of-life, the emergency transient is applied at end-of-life. The total end-of-life cladding strains due to steady state operation, the specified number of upset transients, and the single end-of-life emergency transient are then calculated and printed.

   Limitations of the FRST program are: more than one time-step must be specified, and at least two temperatures must be specified for a transient.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   CDC7600 version submitted October 1984.

10. **REFERENCES** - J. J. Huba and E. C. Schwegler, Description of FRST Computer Program, Westinghouse ARD Memorandum LRM-74-1552, December 2, 1974.

    J. J. Huba, User's Instruction Package for the "FRST" Program, Westinghouse ARD Memorandum RA-79-66, February 2, 1979.

    J. J. Huba, Verify the "FRS" and "FRST" Programs, Westinghouse ARD Memorandum LRA-FR-78-22, July 17, 1978.

    M. L. Travis, FRS Computer Program Description, Westinghouse ARD Memorandum LRM-74-1408, October 25, 1974.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
R. A. Smith
Advanced Energy Systems Division
Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** - Restricted Distribution
Source (1443 lines)
The reference memoranda and sample problem input and output and FRST source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - I
KEYWORDS - fuel rods, strains, creep, thermal stresses, thermal expansion, fuel-cladding interactions, Clinch River Breeder Reactor, FRS codes

18. **SPONSOR** - DOE Clinch River Breeder Reactor Plant Project Office

1. **IDENTIFICATION AND KWIC TITLE** - TALKPLOT
   TALKPLOT, plotting U.S. drill hole locations

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - TALKPLOT is an interactive computer program which plots locations of drill holes from the Continental Scientific Drilling Program (CSDP) database on a United States map. The entire United States, individual states, counties, or latitude-longitude areas can be plotted. Multiple input files can be plotted with different markers on the same map. A warning is given when points in the input file lie outside the area designated for plotting.
   The CSDP database was originally established at LLNL in 1979. It currently contains information on 1927 drill holes, and is maintained as a FRAMIS (NESC 9915) database. TALKPLOT utilizes the LLNL computing environment graphics library, GRAFLIB, to produce graphic output. The geographic data used is obtained from a very large resident database, over 2.5M (octal) words. The data are U.S. Bureau of Census data obtained from Lawrence Berkeley Laboratory and adapted to the LLNL computing environment. The CSDP database, geographic data, and GRAFLIB library are not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC7600 version submitted November 1984.

10. **REFERENCES** - W. W. Richardson, TALKPLOT: An Interactive Code for Plotting Locations of Drill Holes from Continental Scientific Drilling Program Data Base, UCRL-53408, April 7, 1983.
    G. Pawloski, N. Howard, G. Hage, M. L. Higuera, W. Richardson, The Continental Scientific Drilling Program Data Base, UCRL-53284, April 1982.
    S. Jones, D. Ries, L. Lyles, A. Dittli, K. Johnson, FRAMIS Reference Manual, LCSD-555, April 1981.
    P. Keller, K. O'Hair, J. Rowe, GRAFLIB Reference Manual, LCSD-432, October 1982.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    W. W. Richardson
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (930 lines)
    The UCRL-53408 reference report and TALKPLOT source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - R

KEYWORDS - interactive computing, drilling, data base management, computer graphics, FRAMIS codes, GRAFLIB codes

18. **SPONSOR** - DOE Office of Basic Energy Sciences

1. **IDENTIFICATION AND KWIC TITLE** - COULOMB, RSUM, GSUM
   COULOMB,RSUM,GSUM, evaluation of Coulomb sums

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Cray1

3. **DESCRIPTION** - COULOMB,RSUM,GSUM is a set of three subroutines written to evaluate the first and second derivatives of Coulomb interaction using the standard Ewald method. The subroutine COULOMB sums over the shells in the direct and reciprocal spaces and determines when the sums have converged. RSUM performs the sum over the direct space. GSUM performs the sum over the reciprocal space. The subroutines are part of a FORTRAN program representing a generalization of Weber's Adiabatic Bond Charge (ABC) model applied to generate the equilibrium configurations and phonon spectra for continous random network models of amorphous Group IV semiconductors with periodic boundary conditions. In the ABC model, massless, point bond charges are introduced at the midpoint of each bond. This gives an effective three-body interaction between bonds and provides the shear strength of the diamond structure. Ions and bond charges are free to move in response to forces derived from the ABC model potentials. The four basic interactions in the ABC model are the Coulomb, the Keating, the ion-ion, and the ion-bond charge interactions. The equilibrium configuration is that set of ion and bond charge coordinates which makes the forces on all the ions and on all the bond charges vanish simultaneously. Once the ions and bond charges are relaxed to their equilibrium position with the specified ABC model interactions, the dynamical matrix may be calculated for the phonon spectra.
   The LLNL computing environment routines BOX, PICXY, ENDPIC, LINK, and TIMEUSED are called; these routines are not included. The three subroutines have been vectorized to reduce calculation time on the Cray1. Only the IF-THEN-ELSE construct of the FORTRAN 77 language is used in the driver program.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   Cray1 version submitted September 1984.

10. **REFERENCES** - K. Winer and F. Wooten, Generalization of Weber's Adiabatic Bond Charge Model to Amorphous Group IV Semiconductors, UCRL-90726, received September 1984.
    Werner Weber, Adiabatic Bond Charge Model for the Phonons in Diamond, Si, Ge, and Alpha-Sn, Physical Review B, Vol. 15, No. 10, pp. 4789-4803, May 15, 1977.
    A. Goldberg, M. El-Batanouny, and F. Wooten, Effect of Geometric Deformation of Tetrahedral Bonding on the Vibrational Properties of Group-IV Semiconductors: Si in the BC-8 Structure, Physical Review B, Vol. 26, No. 12, pp. 6661-6668, December 15, 1982.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    K. Winer
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (1144 lines)
The UCRL-90726 reference report and COULOMB,RSUM,GSUM source on magnetic tape a
available from NESC on an "As Is" basis.

17. **CATEGORY** - W
KEYWORDS - electromagnetic interactions, Coulomb field, semiconductor materials, silicon
germanium, interactive computing

18. **SPONSOR** - Lawrence Livermore National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - SIG
   SIG, signal processing, analysis, & display

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   DEC VAX11

3. **DESCRIPTION** - SIG is a general-purpose signal processing, analysis, and display program. Its main purpose is to perform manipulations on time- and frequency-domain signals. However, it has been designed to ultimately accommodate other representations for data such as multiplexed signals and complex matrices. Two user interfaces are provided in SIG - a menu mode for the unfamiliar user, and a command mode for more experienced users. In both modes errors are detected as early as possible and are indicated by friendly, meaningful messages. An on-line HELP package is also included. Many different operations can be performed on time- and frequency-domain signals including operations on the samples of a signal, operations on the entire signal, and operations on two or more signals. Signal processing operations that can be performed are digital filtering (median, Bessel, Butterworth, and Chebychev), ensemble average, resample, auto and cross spectral density, transfer function and impulse response, trend removal, convolution, Fourier transform and inverse window functions (Hamming, Kaiser-Bessel), simulation (ramp, sine, pulsetrain, random), and read/write signals. User definable signal processing algorithms are also featured. SIG has many options including multiple commands per line, command files with arguments, commenting lines, defining commands, and automatic execution for each item in a "repeat" sequence.

   Graphics is accomplished with the LLNL-developed DIGLIB graphics software; this software is included. Graphical operations on signals and spectra include: x-y plots of time signals; real, imaginary, magnitude, and phase plots of spectra; scaling of spectra for continuous or discrete domain; cursor zoom; families of curves; and multiple viewports. Graphics devices compatible with SIG include DEC VT100 terminal with Retrographics, DEC VT125 and 240; Tektronix 4105, 4010, 4012, 4014, 4025, and 4027 (color) terminals; the RAMTEK 9600; the Versatec and LXY11 printer/plotters; QMS Lasergrafix printer; the HP2623 and HP2648; the Vectrix VX128 and VX384; and the IBM PC with PC-Plot Tektronix terminal emulator.

   SIG was written in the Structured Fortran (SF) preprocessor language which produces either standard FORTRAN66 or FORTRAN77. Both the SF and FORTRAN77 sources are provided. The SF preprocessor is a proprietary product; it is not included.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed January 1985.
   DEC VAX11 version submitted August 1984, replaced Edition B October 1985.

10. **REFERENCES** - Darrel Lager and Stephen Azevedo, SIG, A General-Purpose Signal Processing Program, UCID-19912, Rev. 1, May 9, 1985.

    SIG Installation Procedure-VMS, Lawrence Livermore National Laboratory memorandum, received October 1985.

    SIG A General-Purpose Signal Processing, Analysis, and Display Program, Lawrence Livermore National Laboratory brochure, received October 1985.

    SIG, NESC No. 9787, SIG Tape Contents File Name Directory, National Energy Software Center Note 86-01, October 15, 1985.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN 77

13. **OPERATING SYSTEM** - VMS 4.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
D. Lager and S. Azevedo
Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (1177 8192-character records)
The reference report, LLNL memorandum and brochure, and NESC Note and SIG sourc executable images, HELP files, sample problems, and machine-readable documentation magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - digital filters, Fourier transformation, time dependence, data transmissio spectral density, digital frequency analysis, signals, plotters, DIGLIB codes

18. **SPONSOR** - DOE Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE -** TRUST84
   TRUST84, sat-unsat flow in deformable media

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -** CDC7600

3. **DESCRIPTION -** TRUST84 solves for transient and steady-state flow in variably saturated deformable media in one, two, or three dimensions. It can handle porous media, fractured media, or fractured-porous media. Boundary conditions may be an arbitrary function of time. Sources or sinks may be a function of time or of potential. The theoretical model considers a general three-dimensional field of flow in conjunction with a one-dimensional vertical deformation field. The governing equation expresses the conservation of fluid mass in an elemental volume that has a constant volume of solids. Deformation of the porous medium may be nonelastic. Permeability and the compressibility coefficients may be nonlinearly related to effective stress. Relationships between permeability and saturation with pore water pressure in the unsaturated zone may be characterized by hysteresis. The relation between pore pressure change and effective stress change may be a function of saturation.

   The basic calculational model of the conductive heat transfer code TRUMP (NESC 771) is applied in TRUST84 to the flow of fluids in porous media. The model combines an integrated finite difference algorithm for numerically solving the governing equation with a mixed explicit-implicit iterative scheme in which the explicit changes in potential are first computed for all elements in the system, after which implicit corrections are made only for those elements for which the stable time-step is less than the time-step being used. Time-step sizes are automatically controlled to optimize the number of iterations, to control maximum change to potential during a time-step, and to obtain desired output information. Time derivatives, estimated on the basis of system behavior during the two previous time-steps, are used to start the iteration process and to evaluate nonlinear coefficients. Both heterogeneity and anistropy can be handled. The sample problem required less than 90 CP seconds on a CDC7600.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed November 1984.
   CDC7600 version submitted November 1984.

10. **REFERENCES -** T. N. Narasimhan, P. A. Witherspoon, and A. L. Edwards, Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media. 2. The Algorithm, Water Resources Research, Vol. 14, No. 2, pp. 255-260, April 1978.

T. N. Narasimhan and P. A. Witherspoon, Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media. 3. Applications, Water Resources Research, Vol. 14, No. 6, pp. 1017-1034, December 1978.

TRUST Glossary, Lawrence Berkeley Laboratory memorandum, August 17, 1978.

T. N. Narasimhan, TRUST: A Computer Program for Transient and Steady State Fluid Flow in Multidimensional Variably Saturated Deformable Media under Isothermal Conditions, Lawrence Berkeley Laboratory memorandum, March 2, 1984.

T. N. Narasimhan and P. A. Witherspoon, Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media. 1. Theory, Water Resources Research, Vol. 13, No. 3, pp. 657-664, June 1977.

John F. Pickens, Robert W. Gillham, and Douglas R. Cameron, Finite-Element Analysis of the Transport of Water and Solutes in Tile-Drained Soils, Journal of Hydrology, Vol. 40, pp. 243-264, 1979.

11. **HARDWARE REQUIREMENTS -** 144K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
T. N. Narasimhan
Lawrence Berkeley Laboratory

16. **MATERIAL AVAILABLE** -
Source (4261 lines)
The reference Water Resources Research paper parts 2 and 3, LBL memoranda, and selected sample problem output and TRUST84 source, sample problem input, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - H
KEYWORDS - ground water, fluid flow, porous materials, soil mechanics, drainage, permeability, geothermal energy, deformation, TRUMP codes

18. **SPONSOR** - DOE Division of Geothermal Energy

1. **IDENTIFICATION AND KWIC TITLE -** CDMS
   CDMS, cost data management spread sheet

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   DEC VAX11/780 with VT-100

3. **DESCRIPTION -** The CDMS, Cost Data Management System, program is a user-friendly interactive tool for collecting and describing the costs associated with the construction of a plant or project in varying levels of detail. The detail can change for both the cost elements and the plant structure. Notes can be provided for the plant items, and reports can be issued using the varied level of detail. The program is a sophisticated spreadsheet with instantaneous summations of the subtotals and total costs. CDMS was written to manage cost data for the Solar Thermal Central Receiver program, but is not specific to that power generation technology. Features of CDMS include on-line help facilities, the ability to record detailed notes, automatic incorporation of plant detail titles, a rapid data input capability, and accommodation of varied levels of report detail. The customizing of account structures for any plant or project is easy, and cost totals are automatically updated.
   This release of CDMS, designated as version 1.1E by the contributor, is limited to maxima of 9 plant structure levels and 36 cost element columns. The notes are each limited to 4000 characters; however, any number of notes about any plant structure detail can be used. CDMS will not operate properly with terminals which cannot emulate a DEC VT-100 terminal. CDMS utilizes the DEC VAX EDT text editing program to create or revise notes and to modify the elements-of-work list.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed January 1985.
   DEC VAX11/780 version submitted October 1984.

10. **REFERENCES -** J. M. Weingart, Solar Thermal Central Receiver Cost Data Management System (CDMS) Software Users' Guide CDMS Version 1.1, SAND83-8175, October 1984.
    J. M. Weingart and P. B. Bos, Solar Thermal Central Receiver Cost Data Management System (CDMS) - Final Report, SAND83-8176, October 1984.
    CDMS, NESC No. 9789, CDMS Tape Description, National Energy Software Center Note 85-43, January 2, 1985.

11. **HARDWARE REQUIREMENTS -** 52K bytes

12. **PROGRAMMING LANGUAGE -** FORTRAN 77

13. **OPERATING SYSTEM -** VMS 3.5.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
    H. F. Norris, Jr.
    Sandia National Laboratories, Livermore

16. **MATERIAL AVAILABLE -**
    Source (17 8192-character blocks)
    The reference reports and NESC Note and CDMS and REWRITE executable images, library data, and control information on magnetic tape, in VAX/VMS BACKUP format, are available from NESC on an "As Is" basis.

17. **CATEGORY** - M
KEYWORDS - program management, cost, solar receivers, central receivers, data bas management, planning, construction

18. **SPONSOR** - Sandia National Laboratories, Livermore

1. **IDENTIFICATION AND KWIC TITLE** - PIFITE
   PIFITE, CRBR HCDA cover gas pipeline analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** - CDC7600

3. **DESCRIPTION** - During an energetic hypothetical core disruptive accident (HCDA), primary sodium could be forced down auxiliary system gas lines attached to the reactor vessel. PIFITE calculates the penetration into, and continued sodium flow through, these lines. The output of the PIFITE program is the slug interface location and velocity, and static pressure and temperature histories for selected locations along the line. In addition, axial forces on elbows are calculated.

   PIFITE employs one-dimensional equations both for fluid flow and heat transfer. The fluid flow is represented by an equation which describes the conservation of slug momentum. This equation and the equation describing the slug motion along the piping are solved by the fourth order Runge-Kutta-Gill method. The gas pipe may have a heater rod and an insulation layer. The axial temperatures of the sodium slug and the pipe, together with the radial temperatures of the pipe and insulation layers, can be calculated. Conduction, convection, and radiation heat transfer mechanisms are included.

   The original version of PIFITE is a modified version of the CACECO program (NESC 762); both programs were developed at the Hanford Engineering Development Laboratory. Major limitations of PIFITE are: the gas pipe has a constant diameter along its entire length; the gas pipe cannot branch; end condition modeling does not allow for back-pressurization; the program does not consider shock wave propagation or check valve response to the penetrating slug, or energy lost in pipe response; and elbow loss coefficients are limited to built-in correction for equivalent frictional length.

   Approximately 7 CP seconds are required on a CDC7600 for a typical 2 second real-time problem with 256 time-steps at approximately 41 steps per second. PIFITE requires that the memory be preset to zero before execution.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed December 1984.
   CDC7600 version submitted October 1984.

10. **REFERENCES** - I. M. Tang, PIFITE Code Application in Clinch River Breeder Reactor, WARD-D-0144, June 1976.
    R. D. Peak, User's Guide to CACECO Containment Analysis Code, HEDL-TC-859, June 1977.

11. **HARDWARE REQUIREMENTS** - 155K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - SCOPE 2.1.5 Level 512.1.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    R. E. Lacko
    Advanced Energy Systems Division
    Westinghouse Electric Corporation

16. **MATERIAL AVAILABLE** – Restricted Distribution
Source (3852 lines)
The WARD-D-0144 reference report and PIFITE source and sample problem input and output on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** – G
KEYWORDS – Clinch River Breeder Reactor, sodium cooled reactors, reactor core disruption, cover gas, pipes, fluid flow, temperature, pressure, CACECO codes

18. **SPONSOR** – ERDA Division of Reactor Research and Development

1. **IDENTIFICATION AND KWIC TITLE -** ROSET
   ROSET, solar thermal electric power simulation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC7600

3. **DESCRIPTION -** ROSET (Representation Of Solar Electric-Thermal) consists of five programs (WTPREAD, FIELD, POWERT, POWERE, and HISTO) to calculate the energy output of a solar thermal electric power system. The ROSET programs provide two distinct functions. The first four (WTPREAD, FIELD, POWERT, and POWERE) use hourly weather data for a year to calculate hourly electric energy output for a solar thermal system. The last program (HISTO) uses one or more electric energy output files created by the first four programs to provide an energy distribution for each hour of a typical day (one typical day per month).

   WTPREAD accepts hourly weather data in WTP format, extracts solar radiation and temperature data, calculates wet bulb temperature and packs the results in a form compatible with the remaining programs. FIELD calculates the position of the sun at each hour and the resultant amount of solar energy collected. The types of collector systems that can be simulated include the point-focus central receiver; line-focus central receiver; point-focus distributed receiver; fixed-mirror distributed focus; line-focus distributed receiver, tracking collector; line-focus distributed receiver, tracking receiver; low-concentration nontracking collector and Fresnel lens; and shallow solar ponds.

   The collected energy is transferred to a working fluid, and once the working fluid reaches a minimum temperature, the energy is transferred from the fluid to a heat engine. The effects of losses and thermal mass on the temperature of the working fluid are calculated by POWERT. The output of POWERT is the energy available for conversion to electricity. Given the available thermal energy, program POWERE computes the electrical energy output, taking into account the heat engine and the electric generator. POWERE employs several strategies for storing thermal or electric energy to smooth the output energy profile.

   HISTO uses hourly results for one or more years to produce energy distributions for each hour of a typical day each month. Up to ten input files, each containing data for one year, can be accommodated. The output of ROSET is a set of energy distributions that can be used by program ULMOD as part of the overall utility value determination process.

   While ROSET is set up to simulate one system at a time, its constituent programs are also capable of performing parametric trade studies in a stand-alone mode. The trade studies can yield valuable information on sizing a solar thermal electric power system. Only when a single system is simulated, however, are the outputs of the various programs compatible and able to produce input for ULMOD.

   Auxiliary program FINAM performs an economic analysis to determine the value of solar thermal energy systems to electric utilities.

   ROSET is one of a series of programs that evaluate the value of energy systems to electric utilities. The others are the wind simulation model ROSEW, which is part of the WECS package (NESC 932); the photovoltaics model ROSEPV (NESC 9792); and the OTEC model ROSEB (NESC 9793). A typical problem requires 30 CP seconds of execution time on a CDC7600.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed November 1984.
   CDC7600 version submitted June 1982.

10. **REFERENCES** - James R. Harper and C. David Percival, Solar Electric Technologies: Methods of Electric Utility Value Analysis, SERI/TR-214-1362, May 1982.
Robert O'Doherty, ROSET: A Solar Thermal Electric Power Simulation User's Guide, SERI/TR-214-1449, August 1982.
David Percival and James Harper, Electric Utility Value Determination for Wind Energy, Volume I: A Methodology, SERI/TR-732-604, Vol. 1, February 1981.
David Percival and James Harper, Electric Utility Value Determination for Wind Energy, Volume II: A User's Guide, SERI/TR-732-604, Vol. 2, February 1981.

11. **HARDWARE REQUIREMENTS** - 47K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV (FTN)

13. **OPERATING SYSTEM** - SCOPE.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
J. R. Harper
Solar Energy Research Institute

16. **MATERIAL AVAILABLE** -
Source (3234 lines)
The reference reports and ROSET, WTP, ULMOD, and FINAM source and ROSET and WTP sample problems, weather data library, and ROSET control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - T
KEYWORDS - solar thermal power plants, electric utilities, power generation, solar receivers, planning, computerized simulation, solar energy, WTPREAD codes, FIELD codes, POWERT codes, POWERE codes, HISTO codes, WTP codes, ULMOD codes, FINAM codes, ROSEW codes, ROSEPV codes, ROSEB codes, WECS codes

18. **SPONSOR** - DOE Office of Solar Power Applications

1. **IDENTIFICATION AND KWIC TITLE** - ROSEPV
   ROSEPV, photovoltaic electric power simulation

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - ROSEPV (Representation Of Solar Electric-PhotoVoltaic) estimates the electrical generation from photovoltaic systems modeled by the solar resource data provided by either WTP or WETHR. The solar resource data used by ROSEPV include not only hour-by-hour data but probability information on insolation. This probabilistic insolation normally is provided for each hour of a typical day each month. This ability better represents the solar resource than that provided by the more typical use of a single year of hourly data. Auxiliary program WETHR may be used to develop this probability data from one or more years of weather data. For the hour-by-hour data, ROSEPV can alternatively use the results of the WTP program. ROSEPV was developed by modifying the Sandia National Laboratories, Albuquerque, program SOLCEL2 (NESC 937) to fit within the SERI value analysis methodology.

   The original SOLCEL2 program and ROSEPV can model a wide variety of photovoltaic systems. A total of nine different PV-collector cooling options exist - three variations of active and passive cooling, each for flat-plate, linear-focus, and point-focus collector systems. In addition, there are 12 different PV-collector orientation possibilities that vary from nontracking flat-plate to fully tracking line-focus or point-focus systems. The inverter system also has options, and certain design specifications can be optimized parametrically. (The optimization feature, however, should not be used when ROSEPV is used for utility value analysis).

   ROSEPV can also consider the probability of a loss of PV generation caused by a failure in the collector and/or inverter subsystems. The PV modeling is for a single system. To obtain results for many identical systems, ROSEPV uses multiplication by a user input number of systems to increase the PV generation on the special data file created for ULMOD. All other reported results are for a single PV system.

   Auxiliary program ULMOD uses ROSEPV output to modify the hourly utility load forecast, which is in turn processed by utility planning models. The planning models are not included. Given the utility model results, the auxiliary program FINAM calculates the present worth economics to determine the break-even amount the utility could afford to pay for the solar-electric capacity of each scenario.

   ROSEPV is one of a series of programs that evaluate the value of energy systems to electric utilities. The others are the wind simulation model ROSEW, which is part of the WECS package (NESC 932); the solar thermal model ROSET (NESC 9791); and the OTEC model ROSEB (NESC 9793). A typical ROSEPV problem requires approximately 15 CP seconds on a CDC7600.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed November 1984.
   CDC7600 version submitted June 1982.

10. **REFERENCES** - James R. Harper and C. David Percival, Solar Electric Technologies: Methods of Electric Utility Value Analysis, SERI/TR-214-1362, May 1982.

   David Percival and James Harper, Electric Utility Value Determination for Wind Energy, Volume I: A Methodology, SERI/TR-732-604, Vol. 1, February 1981.

   David Percival and James Harper, Electric Utility Value Determination for Wind Energy, Volume II: A User's Guide, SERI/TR-732-604, Vol. 2, February 1981.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
J. R. Harper
Solar Energy Research Institute

16. **MATERIAL AVAILABLE -**
Source (117 lines)
The reference reports and ROSEB, ULMOD, and FINAM source and ROSEB sample problem and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY -** T
KEYWORDS - ocean thermal power plants, biomass, rankine cycle power systems, electric utilities, solar power plants, planning, power generation, computerized simulation, ULMOD codes, FINAM codes, WECS codes, ROSEPV codes, ROSET codes

18. **SPONSOR -** DOE Office of Solar Power Applications

1. **IDENTIFICATION AND KWIC TITLE** - HELIOSTAT CONTROLLER
   HELIOSTAT CONTROLLER, Solar 1 collector system

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   Motorola M6801

3. **DESCRIPTION** - HELIOSTAT CONTROLLER is Motorola M6801 microprocessor software developed for the collector (heliostat) subsystem at the 10-MWe Solar Thermal Central Receiver Pilot Plant (Solar One). Listings of two versions of the collector subsystem software are provided. One listing, identified as Version A02, is a listing of the assembler software developed for programming of the sixty-four field control microprocessors used in the collector subsystem, each of which controls up to thirty-two individual heliostats. The second listing, identified as Version A11-Barstow, is the assembler source program for the 1,818 individual heliostat microprocessors.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed November 1984.
   Motorola M6801 listing submitted July 1984.

10. **REFERENCES** - Martin Marietta, Heliostat Field Controller Software Source Listing Version A02, DOE/SF/10539-4 (STMPO-564), February 13, 1980.
    Martin Marietta, Heliostat Controller Software Source Listing Version A11-Barstow, DOE/SF/10539-15 (STMPO-565), October 22, 1980.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - Assembler

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    S. D. Elliott, Jr.
    DOE San Francisco Operations Office
    U. S. Department of Energy

16. **MATERIAL AVAILABLE** -
    Source (A02 2266 statements, A11-Barstow 1553 statements)
    The reference source listings are available from NESC.

17. **CATEGORY** - T
    KEYWORDS - Barstow solar pilot plant, solar thermal power plants, solar collectors, microprocessors, heliostats

18. **SPONSOR** - DOE Solar One Project Office

1. **IDENTIFICATION AND KWIC TITLE** - NOX
   NOX, nitrogen oxides in MHD radiant boiler

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   IBM370

3. **DESCRIPTION** - NOX, a modification of the earlier NASA chemical kinetics program, is used to calculate the gas-phase decomposition of nitrogen oxides in an open-cycle MHD radiant boiler. NOX uses chemical kinetics, fluid flow, and heat transfer models to compute the cross-sectional area or diameter of a cylindrical boiler for a given plant size (thermal size) when an inlet gas velocity is specified. These models were combined with the NASA program, which numerically solves the stiff kinetic differential equations using a modified Runge-Kutta method and the other differential equations involving the temperature and overall density. Time histories of the NOx concentration are obtained for various boiler diameters and initial gas compositions. The compositions were obtained from the NASA equilibrium code described in NASA SP-237 by S. Gordon and B. J. McBride.
   The chemical kinetics model is limited to 30 gas-phase chemical reactions. The kinetics constants are restricted to the 1000K to 3000K temperature range. When initial chemical species, except NO, are near equilibrium conditions, the running time is about 2 CPU minutes on an IBM370. Otherwise, the running time may be as long as 10 CPU minutes. The program can produce simple X-Y plots using the proprietary ISSCO DISSPLA graphics package. Calls to DISSPLA are localized in subroutine MICPLT and currently commented out.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed November 1984.
   IBM370 version submitted April 1982.

10. **REFERENCES** - A. J. Sistino, Analytical Studies of NOX Decomposition in the Radiant Boiler of an Open-Cycle MHD Power Plant, ANL/MHD-79-7, April 1979.
    David A. Bittker and Vincent J. Scullin, General Chemical Kinetics Computer Program for Static and Flow Reactions, with Application to Combustion and Shock-Tube Kinetics, NASA TN D-6586, January 1972.
    NOX, NESC No. 9795, Errata to NOX Reference Report, ANL/MHD-79-7, and NOX Nomenclature Sheet, National Energy Software Center Note 85-34, November 28, 1984.

11. **HARDWARE REQUIREMENTS** - 250K bytes

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** - OS/MVT.

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    A. J. Sistino
    Engineering Division
    Argonne National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (4337 lines)
    The reference reports, NESC Note, and sample problem output and NOX source, sample problem input and plot output, thermodynamic database, and control information on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - U
KEYWORDS - chemical reactions, chemical reaction kinetics, thermodynamic properties, magnetohydrodynamics, boilers, pollution

18. **SPONSOR** - DOE Office of Fossil Energy,
Division of Magnetohydrodynamics

1. **IDENTIFICATION AND KWIC TITLE** - ECRCSD
   ECRCSD, ion source charge-state distribution

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - ECRCSD calculates the equilibrium charge-state distribution of ions that can be extracted from a two-stage electron cyclotron resonance (ECR) ion source. It is used for the design of ion sources for cyclotrons and/or atomic physics studies. The study of design parameters is emphasized, hence the atomic physics used is often subject to approximations. Production of ions is caused by the impact ionization of the charge gas from ECR heated electrons of a few keV. Loss of an ion of a given charge state is from charge exchange and radiative recombination resulting from thermal electrons. In the second (main) stage of the ion source, electrons trapped in a minimum-B geometry, composed of a superposition of solenoidal and hexapolar fields, are heated to several keV by ECR interaction. Here they step-wise strip ions of their electrons, and the ions are extracted out the end of the device. The energetic ions, trapped in the minimum-B geometry, are assumed to be approximately in thermal equilibrium at a temperature of a few keV. They are assumed also to be at approximately their energy of formation described by a temperature of a few keV.
   Input data consist of gas neutral density, hot-electron temperature and density, ion temperature, cold electron temperature, mirror ratio, physical dimensions, and atomic physics data. ECRCSD calculates charge-state distribution and power requirements as output information. Execution times range from 10 CP seconds for argon to 60 CP seconds for mercury on a CDC7600.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed November 1984.
   CDC7600 version submitted October 1984.

10. **REFERENCES** - H. I. West, Jr., Calculation of Ion Charge - State Distribution in ECR Ion Sources, UCRL-53391, December 8, 1982.

11. **HARDWARE REQUIREMENTS** - 123K (octal) words

12. **PROGRAMMING LANGUAGE** - FORTRAN IV

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
   H. I. West, Jr.
   Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
   Source (567 lines)
   The reference report and ECRCSD source and sample problem on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - W
   KEYWORDS - ion sources, electron cyclotron-resonance, charge exchange, ECR heating

18. **SPONSOR** - Lawrence Livermore National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - PATTER
   PATTER, pattern recognition data analysis

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600

3. **DESCRIPTION** - PATTER is an interactive program with extensive facilities for modeling analytical processes and solving complex data analysis problems using statistical methods, spectral analysis, and pattern recognition techniques. PATTER addresses the type of problem generally stated as follows: given a set of objects and a list of measurements made on these objects, is it possible to find or predict a property of the objects which is not directly measurable but is known to define some unknown relationship? When employed intelligently, PATTER will act upon a data set in such a way that it becomes apparent if useful information, beyond that already discerned, is contained in the data.

   In order to solve the general problem, PATTER contains preprocessing techniques to produce new variables that are related to the values of the measurements which may reduce the number of variables and/or reveal useful information about the "obscure" property; display techniques to represent the variable space in some way that can be easily projected onto a two- or three-dimensional plot for human observation to see if any significant clustering of points occurs; and learning techniques based on both unsupervised and supervised methods, to extract as much information from the data as possible so that the optimum solution can be found.

   The use of PATTER's "process instructions" allows the user a great deal of flexibility in the data analysis procedure. The verbs of these instructions are grouped into the following functional areas: pattern analysis, data preprocessing, spectral analysis, display routines, supervised learning, unsupervised learning, and utility routines.

   PATTER is a smaller, faster, more efficient code than the earlier RECOG program with additional capabilities. RECOG-ORNL (NESC 9867) is a modification of RECOG.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed October 1984.
   CDC7600 version submitted October 1984.

10. **REFERENCES** - L. A. Cox, Jr. and C. F. Bender, PATTER: A Polyalgorithm for the Analysis of Generalized Data Sets. Principles and Practice, UCID-16915, October 1975.
    L. A. Cox, Jr., R. H. Pritchard, and C. F. Bender, RECOG: A Polyalgorithm for the Analysis of Generalized Data Sets, An Operator's Manual, UCID-16443, Rev. 1, April 9, 1975.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - FORTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    C. F. Bender
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
Source (5530 lines)
The UCID-16915 reference report and PATTER source on magnetic tape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P
KEYWORDS - algorithms, data processing, statistics, pattern recognition, data analysis, learning, correlations, RECOG codes, RECOG-ORNL codes

18. **SPONSOR** - ERDA Office of Military Application

1. **IDENTIFICATION AND KWIC TITLE -** ZOOM
   ZOOM, Omnimax view of diamond crystal lattice

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE -**
   CDC7600

3. **DESCRIPTION -** ZOOM computes perspective vector views of the diamond crystal lattice, distorted for projection through an Omninax projector, onto a planetarium dome.

4. **METHOD OF SOLUTION -**

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM -**

6. **TIMING -**

7. **UNUSUAL FEATURES OF THE SOFTWARE -**

8. **RELATED AND AUXILIARY SOFTWARE -**

9. **STATUS -** Summary first distributed October 1984.
   CDC7600 version submitted August 1983.

10. **REFERENCES -**

11. **HARDWARE REQUIREMENTS -**

12. **PROGRAMMING LANGUAGE -** LRLTRAN

13. **OPERATING SYSTEM -**

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS -**

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR -**
   N. L. Max
   Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE -**
   Source (999 lines)
   The ZOOM source on magnetic tape is available from NESC on an "As Is" basis.

17. **CATEGORY -** P
   KEYWORDS - crystal lattices, computer graphics, photographic films

18. **SPONSOR -** Lawrence Livermore National Laboratory

1. **IDENTIFICATION AND KWIC TITLE** - ATOMLLL
   ATOMLLL, 3d opaque molecular modeling

2. **COMPUTER FOR WHICH SOFTWARE IS WRITTEN AND OTHER MACHINE VERSIONS AVAILABLE** -
   CDC7600 and Varian minicomputer

3. **DESCRIPTION** - ATOMLLL draws color, shaded, hidden surface pictures and movies of 'ball-and stick' and 'space-filling' molecular models. ATOMLLL can simulate hard-sphere bouncing of atoms or nuclei and contains the following features: rotation of coordinates, interpolation between key frames, distortion of planetarium dome projection, shadows cast by one atom onto another, transparent atoms, and sorting of large data sets into windows. From a file containing coordinates of atomic centers, radii, colors, and descriptions of bounds, if any, ATOMLLL computes the visible portions of each atom and writes these descriptions to a file which can be copied to tape. The tape is then read by the Varian DNI postprocessor shading program which controls the plotting on a Dicomed D-48 color miccrofilm recorder. The DNI algorithm makes use of the Dicomed's color compensation tables. The QUAD assembly language routine is not included. A suitable replacement will have to be supplied for the user's computing environment.
   The original ATOMS program was written at Bell Laboratories by Kenneth Knowlton and Linda Cherry to compute the visible regions of a scene consisting of potentially intersecting spheres or cylinders. The LLNL edition contains enhancements to add shading and highlights and to render the spheres on film as ellipses, so that they would appear round when projected in various wide-screen formats.

4. **METHOD OF SOLUTION** -

5. **RESTRICTIONS ON THE COMPLEXITY OF THE PROBLEM** -

6. **TIMING** -

7. **UNUSUAL FEATURES OF THE SOFTWARE** -

8. **RELATED AND AUXILIARY SOFTWARE** -

9. **STATUS** - Summary first distributed October 1984.
   CDC7600 version of ATOMA submitted August 1983, replaced by ATOMLLL January 1986.

10. **REFERENCES** - N. L. Max, ATOMLLL - A Three-D Opaque Molecule System (Lawrence Livermore Laboratory Version), UCRL-52645, January 11, 1979.
    N. L. Max, ATOMLLL: ATOMS with Shading and Highlights, UCRL-82137 Rev. 1 Preprint, May 11, 1979.

11. **HARDWARE REQUIREMENTS** -

12. **PROGRAMMING LANGUAGE** - LRLTRAN

13. **OPERATING SYSTEM** -

14. **OTHER PROGRAMMING OR OPERATING INFORMATION OR RESTRICTIONS** -

15. **NAME AND ESTABLISHMENT OF AUTHOR OR CONTRIBUTOR** -
    N. L. Max
    Lawrence Livermore National Laboratory

16. **MATERIAL AVAILABLE** -
    Source (ATOMLLL 3826 lines, DNI 459 lines)
    The reference reports and ATOMLLL and DNI source and sample problem input and output on magnetictape are available from NESC on an "As Is" basis.

17. **CATEGORY** - P

KEYWORDS – molecular models, computer graphics, photographic films, three-dimensional calculations, ATOMS codes, ATOMA codes, DNI codes

18. **SPONSOR** – DOE Office of Military Application

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