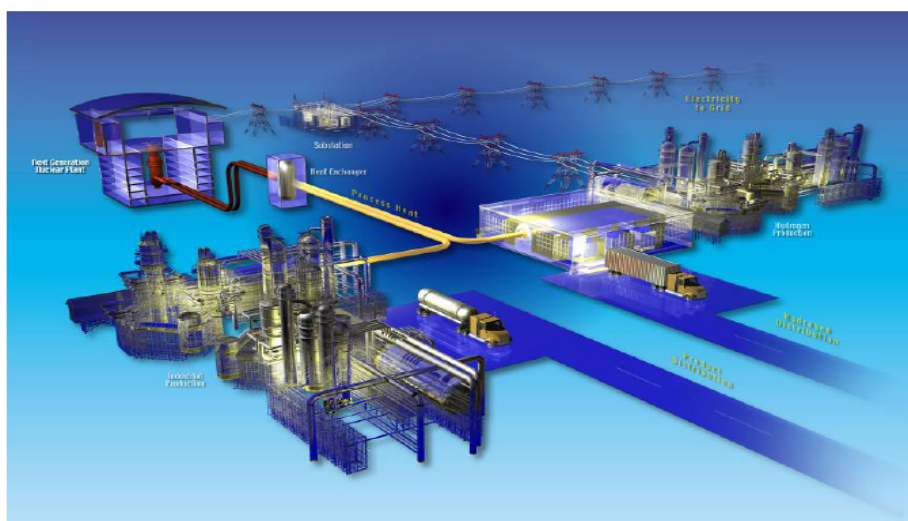# COMBINE7.0 – A Portable ENDF/B-VII.0 Based Neutron Spectrum and Cross-Section Generation Program

W. Y. Yoon
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September 2008

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Idaho National Laboratory

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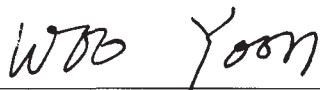Idaho Falls, Idaho 83415

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COMBINE7.0—A Portable ENDF/B-VII.0 Based Neutron Spectrum and Cross-Section Generation Program

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ABSTRACT

COMBINE7.0 is a FORTRAN 90 computer code that generates multigroup neutron constants for use in the deterministic diffusion and transport theory neutronics analysis. The cross-section database used by COMBINE7.0 is derived from the Evaluated Nuclear Data Files (ENDF/B-VII.0). The neutron energy range covered is from 20 MeV to 1.0E-5 eV. The Los Alamos National Laboratory NJOY code is used as the processing code to generate a 167 fine-group cross-section library in MATXS format for Bondarenko self-shielding treatment. Resolved resonance parameters are extracted from ENDF/B-VII.0 File 2 for a separate library to be used in an alternate Nordheim self-shielding treatment in the resolved resonance energy range. The equations solved for energy dependent neutron spectrum in the 167 fine-group structure are the B-3 or B-1 approximations to the transport equation. The fine group cross sections needed for the spectrum calculation are first prepared by Bondarenko self-shielding interpolation in terms of background cross section and temperature. The geometric lump effect, when present, is accounted for by augmenting the background cross section. Nordheim self-shielded fine group cross sections for a material having resolved resonance parameters overwrite correspondingly the existing self-shielded fine group cross sections when this option is used. The fine group cross sections in the thermal energy range are replaced by those self-shielded with the Amouyal/Benoist/Horowitz method in the three region geometry when this option is requested. COMBINE7.0 coalesces fine group cross sections into broad group macroscopic and microscopic constants. The coalescing is performed by utilizing fine-group fluxes and/or currents obtained by spectrum calculation as the weighting functions. The multigroup constant may be output in any of several standard formats including ANISN 14** free format, CCCC ISOTXS format, and AMPX working library format. ANISN-PC, a one-dimensional, discrete-ordinate transport code, is incoporated into COMBINE7.0. As an option, the 167 fine-group constants generated by COMBINE portion in the program can be used to cacluate regionwise spectra in the ANISN portion, all internally to reflect the one-dimensional transport correction. Results for the criticality validation calculations are included as a part of verification and validation.

ACKNOWLEDGMENTS

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ACRONYMS

ABH   Amouyal/Benoist/Horowitz

ENDF   Evaluated Nuclear Data Files

INL   Idaho National Laboratory

MLBW   Multilevel Breit-Wigner

R-M   Reich-Moore

SLBW   single level Breit-Wigner

MND   mixed number density

COMBINE7.0—A Portable ENDF/B-VII.0 Based Neutron Spectrum and Cross-Section Generation Program

1.   INTRODUCTION

COMBINE7.0 is a FORTRAN 90 computer code for generation of spectrum-averaged, multigroup, neutron, cross-section data suitable for use in the deterministic diffusion and transport theory reactor design analysis. The cross-section database used by COMBINE7.0 is derived from Evaluated Nuclear Data Files (ENDF/B-VII.0[1]). The neutron energy ranging from 20 MeV to 1.0E-5 eV is treated by a total of 167 discrete energy groups. The equations solved for the energy-dependent neutron spectrum are the B_3 or B_1 approximations to the transport equation.

COMBINE7.0 has evolved from its predecessor Versions 5 and 6. The earlier version, COMBINE/PC—a Portable ENDF/B Version 5 Neutron Spectrum and Cross-Section Generation Program[2] (COMBINE5)—combined the preexisting neutron spectrum codes, PHROG[3] (fast) and INCITE[4] (thermal spectrum), previously developed at Idaho National Laboratory (INL), by suitably integrating them into a single package, thus, the name COMBINE. The cross-section database used by COMBINE5 is derived from the ENDF/B-V[5]. In the fast spectrum calculation, the B_3 spherical harmonics equations are solved by Gauss elimination and the B_1 spherical harmonics equations are solved simultaneously, beginning with the highest energy group. In INCITE, the B_1 thermal equations have been cast in the form of a normalized Gauss-Seidel iterative scheme where extrapolation and iteration in both directions have been included as options. The fast and thermal energy ranges are coupled by using slowing down theory and energy-dependent scattering and spectra data to generate average transfer cross sections from the PHROG broad groups into INCITE broad groups. The results are then normalized to the total scatter below the fast range cutoff as produced by PHROG.

The 1990 release of ENDF/B-VI nuclear data[6] of ENDF-6 format created problems for the INL's Version 5 processing codes used to generate cross-section libraries for COMBINE5, requiring major revisions of these codes. An alternative to the modifications of the INL's processing codes was to utilize the NJOY code system[7] developed at the Los Alamos National Laboratory. NJOY optionally processes all resonance self-shielding through the Bondarenko approximation. In the Bondarenko model,[8] the narrow resonance (NR) approximation and the B_N approximation for large systems are invoked.[9] Two cross section libraries were generated by NJOY for the fast (72 group) and thermal (101 energy points) spectrum calculations, maintaining the same energy structures as in COMBINE5. The fast cross section library was based on sets of background cross sections and temperatures for Bondarenko self-shielding interpolation. The geometric effects of fuel lump and lattice are accounted for by the combination of Rational Approximation and Dancoff-Ginsburg correction, including a double heterogeneity due to fuel grains present within the macroscopic fuel lump by augmenting the background cross section. The weakness of the Bondarenko model occurs for thermal reactor analysis in the "epithermal" energy region from about 4 eV to around 200 to 300 eV.[10] In this region, the resonances are no longer "narrow" and the flux shape given by Bondarenko method is no longer sufficiently accurate. An alternate approach is the Nordheim resonance integral treatment method.[11] A separate resolved resonance library was also created, including formats in single level Breit-Wigner (SLBW), Multilevel Breit-Wigner (MLBW), Reich-Moore (R-M), and no resonance, extracted directly from ENDF/B-VI nuclear data files to be used in the Nordheim self-shielding treatment in the resolved resonance energy range. The Version 5 code was modified to handle the new cross section and resolved resonance libraries. The new code was designated as COMBINE6.[12] The ENDF/B-VI derived thermal cross-section library is based on the infinite dilution and temperature dependence is only present if thermal scattering data is available for an isotope. This format of the thermal cross-section library is same as that of COMBINE5's. The INCITE portion of COMBINE5 is therefore fully retained, including the Amouyal/Benoist/Horowitz (ABH) option for self-shielding in the thermal energy range. The energy range treated is from 0.001 eV to 16.905 MeV spanned

by a total of 166 discrete energy points/groups. A routine was also retained to calculate a Dancoff-Ginsburg correction factor in conjunction with the resonance calculation for either a rectangular or hexagonal arrangement of cylindrical absorber pins. Several routines to process MLBW and R-M resonance formats were adopted from the NJOY code. Nordheim self-shielded cross sections, when requested for a material having resolved resonance parameters, overwrite the corresponding multigroup Bondarenko self-shielded cross sections. An iterative scheme was also introduced for better fission-rate weighted χ values. In both COMBINE5 and COMBINE6, the energy boundary between the fast spectrum module and thermal spectrum module can be chosen by the user at one of the eight overlapping mutual energy group boundaries, the highest being 2.3824 eV and the lowest 0.414 eV. No resonance treatment is considered below the chosen energy boundary. No thermal upscattering is allowed into the energy above the highest boundary. Thermal upscattering does not take place between the highest (2.3824 eV) and chosen boundary of less energy, even though it is possible from below to above the boundary when the boundary is below the highest. The adequate self-shielding treatment of resonances in the thermal energy range is critical where thermal upscattering is also significant because of high operating temperature. Overlap and interference effect of resonances among admixed absorbing isotopes was not accounted.

COMBINE7.0 has been modified to resolve the above issues. The B_1 and B_3 transport algorithms for the full range multigroup treatment, including thermal upscattering, were identified and implemented to unify fast and thermal spectrum calculations. The neutron energy ranging from 20 MeV to 1.0E-5 eV is treated by a total of 167 discrete energy groups, adding one more group (20–16.905 MeV) to the previous versions' group structure. The thermal upscattering takes place between 1.0E-5 eV and 5.0435 eV (high enough for most reactor applications) with no energy boundary restriction. Up to g-wave resonances are now treated to obtain the elastic scattering cross section, although the isotropic scattering is still used for energy transfer. In the Nordheim resonance treatment, up to three admixed resonance absorbers can be present to account for the resonance overlap and interference effect. Thermal upscattering was also added in the resonance treatment solution. The interpolation algorithm in the Bondarenko scheme to self-shield cross sections has been modified for improvement and revamped to afford additional temperature-only-dependent thermal scatterings, free and/or $S(\alpha,\beta)$. The interpolation is now performed first for the background cross sections at each temperature and the generated cross sections for the set of preselected temperatures are then interpolated for the problem-dependent temperature. Negative buckling algorithms have been implemented in addition to a real B: one with the positive imaginary B and the other with the negative imaginary B. Previously, only the positive and real B of cosine spatial shape was allowed. The mixed use of three different modes of buckling in the broad group wise input is implemented. All resonances are Doppler broadened by the method called "kernel broadening" as practiced in NJOY, thus eliminating the need to evaluate Doppler line functions (ψ and χ) previously calculated in the SLBW treatment. The GAM-1 resolved-resonance calculation routine,[13] a fast alternative to the much more accurate but time consuming Nordheim numerical method, was scrapped since speed is no longer a factor. Many of the INCITE routines were removed or combined with PHROG due to the unified energy scheme. A 1-D discrete-ordinate transport code, ANISN-PC,[14] is also incorporated into COMBINE7.0 to reflect one-dimensional (1-D) transport correction. The 167 fine-group constants generated by COMBINE for multiregions via stack cases are fed into ANISN to calculate regionwise spectra, which are used in the COMBINE to generate the regionwise broad group constants. The detail of ANISN code will be deferred to its manual. Figure 1 shows the COMBINE7.0 implementation scheme.
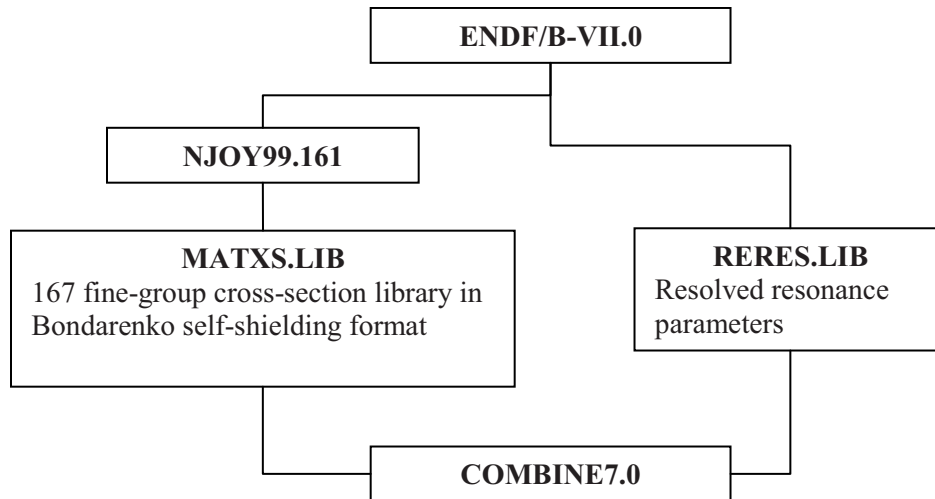
Figure 1. COMBINE7.0 implementation scheme.

ENDF/B-VII.0 nuclear data was released in December 2006 using the same ENDF-6 format.[1] The cross-section database is now derived entirely from ENDF/B-VII.0 nuclear data with the exception of Zr element cross-section data, which is based on ENF/B-VI.8 nuclear data. The NJOY99.259 version[15] was used to generate a 167 fine-group cross-section library, MATXS.LIB, in MATXS format (Bondarenko format) on sets of background cross sections and temperatures including thermal scattering cross sections. This cross-section library includes damage, heating, kerma, and gas production cross sections in addition to those vector and matrix cross sections required for transport calculations. Only those materials designated by ENDF/B File 7 formats as moderators and included in NJOY99.259 contain thermal S(α,β) scattering matrices. The nonmoderating materials in the library possess free thermal scattering matrices. A separate resolved resonance library, RERES.LIB, was also created that includes formats in SLBW, MLBW, R-M, and no resonance, extracting all resolved resonance parameters directly from ENDF/B-VII.0 nuclear data files. Along with the cross section library in Bondarenko format and the resolved resonance data library, the upgraded COMBINE version is now called COMBINE7.0.

1.1 COMBINE7.0 Code Abstract

1. **Program Identification:** COMBINE7.0

2. **Description of Problem:** COMBINE7.0 is a FORTRAN 90 computer code that generates multigroup neutron constants for use in the deterministic diffusion and transport theory neutronics analysis. The cross-section database used by COMBINE7.0 is derived from ENDF/B-VII.0. The neutron energy range covered is from 20 MeV to 1.0E-5 eV. The equations solved for energy dependent neutron spectrum are the B-3 or B-1 approximations to the transport equation. It is also capable of performing a 1D discrete-coordinates transport calculation for multiregions to generate regionwise broad group constants.

3. **Method of Solution:** The energy range is broken into 167 fine groups for the spectrum calculation. The resulting matrix of flux equations is then solved using standard numerical techniques to obtain the spectral weight function for generation of group-averaged constants. An alternate resolved resonance shielding of the fine-mesh cross section data is performed using the Nordheim method. An option to treat thermal self shielding using the ABH method is provided. User-defined self-shielding factors (from an auxiliary transport code such as ANISN/PC) may be entered. Calculated cross sections may be issued in any of several standard formats.

4. **Related Material:** A MATXS library file and a resolved resonance parameter library file are provided with the code package in ASCII format. Processors to convert the MATXS file to the required binary format or to convert the binary file to the ASCII file are provided.

cv700.f90:   COMBINE-7 Cycle 0 Fortran 90 source program.

                It requires matxs.lib and reres.lib to run a problem.

matxs.asc: 167 fine-group cross section library in ascii format

matxs.lib: 167 fine-group cross section library in binary format

reres.lib: resolved resonance library in ascii format

matxscv.f: Fortran program to convert matxs.asc (ascii file) to matxs.lib (binary file)

matxsca.f: Fortran program to convert matxs.lib to matxs.asc

anisn.pdf: ANISN/PC Manual (pdf file).

5. **Restrictions:** COMBINE7.0 is written to function properly on 32-bit word length machine. Accuracy to four or five decimal places in the computed spectrum and cross sections may be expected.

6. **Computers:** COMBINE7.0 is written in standard FORTRAN with the objective of total machine independence. The program has been successfully compiled by the Intel Visual Fortran Compiler (Version 10) and by the Lahey/Fujitsu Fortran compiler (LF95) on the Windows 32-bit platform.

7. **Run Time:** Variable from a few seconds to several minutes on PC-class hardware, depending primarily on the number and type of resonance self-shielding calculations required for a particular case.

8. **Programming Language:** Standard FORTRAN 90.

9. **Operating System:** COMBINE7.0 has successfully functioned under Windows and Linux operating systems.

10. **Machine Requirements:** As stated in item 6, Computers.

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2. THEORETICAL FOUNDATIONS

2.1 Derivation of BN Equations

The equations solved by COMBINE are the energy-dependent B_1 or B_3 spherical harmonic approximations to the transport equation originally developed by D. S. Selengut.[16] A derivation of the B_N spherical harmonics equations is straightforward, but rather tedious because of the complicated expansion integrals. The physical model is a homogeneous, critical, 1-D bare slab core. As such, the time-independent, energy dependent, Boltzmann neutron transport equation in plane geometry may be written

$$\mu \frac{\partial \Phi(x,\mu,E)}{\partial x} + \Sigma_t(x,E)\Phi(x,\mu,E) = \iint \Sigma_s(x;\boldsymbol{\Omega}',E'\to\boldsymbol{\Omega},E)\Phi(x,\mu',E')d\boldsymbol{\Omega}'dE' + Q(x,\mu,E) \tag{1}$$

where: $\Phi(x,E,\mu)$ is the neutron flux in the direction $\mu = \cos\theta$ relative to the 1-D x axis of the slab at energy E and position x and $\boldsymbol{\Omega}$ and $\boldsymbol{\Omega}'$ are the azimuthal angles associated with μ and μ', respectively; Σ_t is the total cross section; and $\Sigma_s(x;\boldsymbol{\Omega}',E'\to\boldsymbol{\Omega},E)$ is the neutron transfer cross section, including the multiplicity of neutrons emitted in each reaction event. Q represents the independent (or extraneous) neutron sources that are not dependent on the neutron density of the system. All cross sections are macroscopic here. It will be assumed that the angular variation of the transfer cross section, Σ_s, depends only on the scattering angle, $\mu_0 = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}'$. Then Σ_s may be expanded in a set of Legendre polynomials of μ_0; thus,

$$\Sigma_s(x;\boldsymbol{\Omega}',E'\to\boldsymbol{\Omega},E) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\Sigma_{sl}(x;E'\to E)P_l(\mu_0), \tag{2}$$

where the expansion coefficients $\Sigma_{sl}(x;E'\to E)$ are given by

$$\Sigma_{sl}(x;E'\to E) = 2\pi \int_{-1}^{1} \Sigma_s(x;E'\to E,\mu)P_l(\mu)d\mu. \tag{3}$$

If the expansion of Equation (3) is inserted into Equation (1), use of the addition theorem for Legendre polynomials and integration over azimuthal angles gives

$$\mu \frac{\partial \Phi(x,\mu,E)}{\partial x} + \Sigma_t(x,E)\Phi(x,\mu,E) = \sum_{l=0}^{\infty} \frac{2l+1}{2}P_l(\mu)\int_{E'}\Sigma_s(x,E'\to E)\int_{-1}^{1}\Phi(x;\mu',E')P_l(\mu')d\mu'dE' + Q(x,\mu,E). \tag{4}$$

The basis of the B_N method, as a means of estimating within-group neutron fluxes, is to assume the spatial distribution to be independent of neutron energy in plane geometry,

$$\Phi(x,\mu,E) = e^{-iBx}\psi(B,\mu,E), \tag{5}$$

where only the real part of e^{-iBx} satisfies the spatial boundary conditions for the scalar flux. The complex form of the spatial dependence is necessary for the equations to remain homogeneous. In Equation (5) the spatial dependence of the flux is eliminated by assuming that the solution is separable in (E,μ) and x and characterizing the spatial dependence of each of the variables by a simple buckling mode. If Equation (5) is inserted into the neutron transport Equation (4) with $Q(x,\mu,E)$ replaced by an isotropic fission source, $\frac{1}{2}\chi(E)e^{-iBx}$, and the transfer cross section is now designated as Σ_{sl} signifying the absence of fission contribution, the result is

$$\Sigma_t(E)(1 - \frac{iB\mu}{\Sigma_t})\psi(B,\mu,E)$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int \Sigma_{sl}(E' \to E) \int_{-1}^{1} \psi(B,\mu',E') P_l(\mu') d\mu' dE' + \frac{1}{2}\chi(E).$$

(6)

The neutron source is assumed to have the same spatial dependence as the flux. This assumption is also necessary in order for the equations to remain homogeneous. The source term, $\frac{1}{2}\chi(E)$, in Equation (6) is the result of Legendre polynomial expansion and truncation to the first term, assuming the fission source to be isotropic in lab coordinates. It is also noted that independent (or extraneous) neutron sources, which are not dependent on the neutron density of the system, are not included in this equation. Equation (6) could be multiplied by $P_n(\mu)$ and integrated over μ from -1 to 1 to obtain equations satisfied by the Legendre components of $\psi(B,\mu,E)$. More rapid convergence of the expansion is achieved, however, when equation (6) is divided by $\Sigma_t(1 - iB\mu/\Sigma_t)$, multiplied by $P_n(\mu)$, and then integrated to obtain, for $n = 0,1,2...$,

$$\phi_n(B,E)$$

$$= \sum_{l=0}^{\infty} (2l+1) \frac{A_{nl}(B,E)}{\Sigma_t(E)} \int \Sigma_{sl}(E' \to E) \phi_l(B,E') dE' + \frac{A_{n0}(B,E)}{\Sigma_t(E)} \chi(E),$$

(7)

using the following definitions:

$$(i)^n \phi_n(B,E) \equiv \int_{-1}^{1} \psi(B,\mu,E) P_n(\mu) d\mu. \text{ when } B \text{ is real,}$$

(8)

$$\phi_n(B,E) \equiv \int_{-1}^{1} \psi(B,\mu,E) P_n(\mu) d\mu. \text{ when } B \text{ is imaginary (B = \pm iC, where C is real),}$$

(9)

$$A_{nl}(B,E) \equiv \frac{(i)^{l-n}}{2} \int_{-1}^{1} \frac{P_n(\mu) P_l(\mu)}{1 - \frac{iB\mu}{\Sigma_t(E)}} d\mu$$

when B is real,

(10)

$$A_{nl}(B,E) \equiv \frac{1}{2} \int_{-1}^{1} \frac{P_n(\mu) P_l(\mu)}{1 - \frac{iB\mu}{\Sigma_t(E)}} d\mu$$

when B is imaginary.

(11)

When n = 0, for example, the value $P_0(\mu)$ is 1; hence, it follows from Equation (8) that $\Phi_0(B,E)$ is simply the total flux at E.

From Equations (10) and (11), the following symmetry and recursion relations can be derived

$$(i)^{n-l} A_{nl} = (i)^{l-n} A_{ln} \text{ when } B \text{ is real,}$$

(12)

$$A_{nl} = A_{ln} \text{ when } B \text{ is imaginary,}$$

(13)

$$\frac{1}{B/\Sigma_t}(2l+1)A_{nl} - (l+1)A_{n,l+1} + l \cdot A_{n,l-1} = \frac{\delta_{nl}}{B/\Sigma_t} \text{ when } B \text{ is real,}$$

(14)

$$\frac{1}{C\!\!\!\big/\!\Sigma_t}(2l+1)A_{nl}+(l+1)A_{n,l+1}+l\cdot A_{n,l-1}=\frac{\delta_{nl}}{C\!\!\!\big/\!\Sigma_t}\quad\text{when B = iC and C is real,}\tag{15}$$

$$\frac{1}{C\!\!\!\big/\!\Sigma_t}(2l+1)A_{nl}-(l+1)A_{n,l+1}-l\cdot A_{n,l-1}=\frac{\delta_{nl}}{C\!\!\!\big/\!\Sigma_t}\quad\text{when B = -iC and C is real.}\tag{16}$$

where δ_{nl} is the Kronecker delta.

Now, all of the Φ_n in Equation (7) is real quantity. l is the limit for the Legendre expansion of the differential scattering cross section; the expansion is truncated at $l+1$. However, l does not determine the order of the B_N equations. The integral in Equation (7) may be solved to any order n independent of the value of l. As n is increased beyond l, no particular advantage is gained in a spectrum code like COMBINE because the ultimate purpose of the solution fluxes is to collapse the cross sections to a few group libraries for spatial transport codes. For $n > l$ there are no cross sections in the library because the elastic scattering matrix was truncated at $l+1$. Therefore, there is no reason to include higher order fluxes than $n = 3$ in the B_3 solution. The same argument pertains to the B_1 approximation; in this case n is truncated at 1.

The coefficients, A_{nl}, will become a function of $\alpha = B/\Sigma_t$ and $A_{00}=\beta=\dfrac{\tan^{-1}\alpha}{\alpha}$ when B is real or

$\alpha = C/\Sigma_t$ and $A_{00}=\beta=\dfrac{\tanh^{-1}\alpha}{\alpha}$ when B = ±iC with a real C.

2.1.1 B-3 Approximation

Evaluation of Equation (10) for the B_3 approximation, limiting l and n to 3, is straightforward but rather tedious for the higher order coefficients.

$$A_{00}=\beta=\frac{\tan^{-1}\alpha}{\alpha}$$

$$A_{01}=-\frac{1-\beta}{\alpha}$$

$$A_{02}=-\frac{3}{2}\frac{(1-\beta)}{\alpha^2}+\frac{\beta}{2}$$

$$A_{11}=-\frac{1-\beta}{\alpha^2}$$

$$A_{12}=-\frac{3}{2}\frac{(1-\beta)}{\alpha^3}-\frac{\beta}{2\alpha}$$

$$A_{22}=\frac{1}{4\alpha}\left[\left(\frac{9}{\alpha^3}+\frac{6}{\alpha}+\alpha\right)\beta-\frac{3}{\alpha}-\frac{9}{\alpha^3}\right]$$

$$A_{03}=\frac{1}{2\alpha}\left[\left(\frac{5}{\alpha^2}+3\right)\beta-\frac{4}{3}-\frac{5}{\alpha^2}\right]$$

$$A_{13}=\frac{1}{2\alpha^2}\left[\left(\frac{5}{\alpha^2}+3\right)\beta-\frac{4}{3}-\frac{5}{\alpha^2}\right]$$

$$A_{23} = -\frac{1}{4\alpha}\left[\frac{15}{\alpha^4} + \frac{9}{\alpha^2} + \frac{4}{3} - \left(\frac{15}{\alpha^4} + \frac{14}{\alpha^2} + 3\right)\beta\right]$$

$$A_{33} = -\frac{1}{4\alpha^2}\left[\frac{25}{\alpha^4} + \frac{65}{3\alpha^2} + 4 - \left(\frac{25}{\alpha^4} + \frac{30}{\alpha^2} + 9\right)\beta\right] \tag{17}$$

Evaluation of Equation (11) with B = iC results in

$$A_{00} = \beta = \frac{\tanh^{-1}\alpha}{\alpha}$$

$$A_{01} = \frac{1-\beta}{\alpha}$$

$$A_{02} = -\frac{3}{2}\frac{(1-\beta)}{\alpha^2} - \frac{\beta}{2}$$

$$A_{11} = -\frac{1-\beta}{\alpha^2}$$

$$A_{12} = \frac{3}{2}\frac{(1-\beta)}{\alpha^3} + \frac{\beta}{2\alpha}$$

$$A_{22} = \frac{1}{4\alpha}\left[\left(\frac{9}{\alpha^3} - \frac{6}{\alpha} + \alpha\right)\beta + \frac{3}{\alpha} - \frac{9}{\alpha^3}\right]$$

$$A_{03} = -\frac{1}{2\alpha}\left[\left(\frac{5}{\alpha^2} - 3\right)\beta + \frac{4}{3} - \frac{5}{\alpha^2}\right]$$

$$A_{13} = \frac{1}{2\alpha^2}\left[\left(\frac{5}{\alpha^2} - 3\right)\beta + \frac{4}{3} - \frac{5}{\alpha^2}\right]$$

$$A_{23} = \frac{1}{4\alpha}\left[\frac{15}{\alpha^4} - \frac{9}{\alpha^2} + \frac{4}{3} - \left(\frac{15}{\alpha^4} - \frac{14}{\alpha^2} + 3\right)\beta\right]$$

$$A_{33} = -\frac{1}{4\alpha^2}\left[\frac{25}{\alpha^4} - \frac{65}{3\alpha^2} + 4 - \left(\frac{25}{\alpha^4} - \frac{30}{\alpha^2} + 9\right)\beta\right] \tag{18}$$

Evaluation of Equation (11) with B = -iC results in

$$A_{00} = \beta = \frac{\tanh^{-1}\alpha}{\alpha}$$

$$A_{01} = \frac{\beta - 1}{\alpha}$$

$$A_{02} = -\frac{3}{2}\frac{(1-\beta)}{\alpha^2} - \frac{\beta}{2}$$

$$A_{11} = \frac{\beta - 1}{\alpha^2}$$

$$A_{12} = \frac{3}{2}\frac{(\beta-1)}{\alpha^3} - \frac{\beta}{2\alpha}$$

$$A_{22} = \frac{1}{4\alpha}\left[\left(\frac{9}{\alpha^3} - \frac{6}{\alpha} + \alpha\right)\beta + \frac{3}{\alpha} - \frac{9}{\alpha^3}\right]$$

$$A_{03} = -\frac{1}{2\alpha}\left[\left(\frac{5}{\alpha^2} - 3\right)\beta - \frac{4}{3} + \frac{5}{\alpha^2}\right]$$

$$A_{13} = \frac{1}{2\alpha^2}\left[\left(\frac{5}{\alpha^2} - 3\right)\beta + \frac{4}{3} - \frac{5}{\alpha^2}\right]$$

$$A_{23} = \frac{1}{4\alpha}\left[-\frac{15}{\alpha^4} + \frac{9}{\alpha^2} - \frac{4}{3} + \left(\frac{15}{\alpha^4} - \frac{14}{\alpha^2} + 3\right)\beta\right]$$

$$A_{33} = -\frac{1}{4\alpha^2}\left[\frac{25}{\alpha^4} - \frac{65}{3\alpha^2} + 4 - \left(\frac{25}{\alpha^4} - \frac{30}{\alpha^2} + 9\right)\beta\right] \tag{19}$$

Thus, using the coefficients defined by Equation (17), (18), and (19), Equation (7) defines the B_3 fluxes, which are all real. When B is real, the spatial distribution is of cosine(Bx), where B^2 is the geometric buckling of the fundamental mode of the critical homogeneous geometry. When $B = iC$ with a real constant C, the spatial distribution is of positive exponential form with the negative buckling. In this case, there is a neutron leakage into the region, i.e., a negative leakage, which might be useful under certain circumstances. When $B = -iC$ with a real constant C, the spatial distribution is of negative exponential form with the negative buckling and the solution would behave like the case with the positive buckling. In the COMBINE7.0 coding, the series expansions of $\tan^{-1}\alpha$ and $\tanh^{-1}\alpha$ are utilized to calculate these coefficients. The fundamental limitation of the cases with the negative buckling is in the fact that solutions involve a hyperbolic tangent, $\tanh^{-1}(B/\Sigma_t)$. As can be seen in

$$\tanh^{-1}(B/\Sigma_t) = \frac{1}{2}\log\left[(1+B/\Sigma_t)/(1-B/\Sigma_t)\right],$$

B/Σ_t should be less than 1. Normally, B/Σ_t is much less than 1; however, it can be reset to a value less than 1 (0.8, e.g.) to avoid divergence when it is large.

The energy dependence of Equation (7) is approximated by a 167 fine group representation, spanning the energy range from 20 MeV to 1.0E-5 eV, for solution of the neutron spectrum. Integrating Equation (7) over the group energy interval, i.e., $E_g \leq E \leq E_{g-1}$ and truncating to L+1 terms generates

$$\phi_n^g$$

$$= \sum_{l=0}^{L} (2l+1) \frac{A_{nl}^g}{\Sigma_t^g} \sum_{g'=1}^{G} \Sigma_{sl}^{g' \to g} \phi_l^{g'} \frac{\Delta g'}{\Delta g} + \frac{A_{n0}^g}{\Sigma_t^g} \frac{\chi^g}{\Delta g} \tag{20}$$

where

$$\phi_n^g = \int_{E_g}^{E_{g-1}} \phi_n(E) \frac{dE}{E} / \Delta g$$

$$\Delta_g = \int_{E_g}^{E_{g-1}} \frac{dE}{E}$$

The maximum group number is designated as G in Equation (20). It is noted that the fluxes are now expressed as per-unit energy in lethargy coordinates. Equation (20) includes neutrons scattered down from all higher energy groups. It also includes neutrons scattered up from all lower energy groups if thermal upscattering occurs.

The B_3 solution to Equation (20) is given by the following matrix equation for each energy group g.

$$\left[I - C_g \right] \Phi_g = R_g \tag{21}$$

$$\Phi_g = \left[\Phi_0^g, \Phi_1^g, \Phi_2^g, \Phi_3^g \right]. \tag{22}$$

$$C_{nl}^g = (2l+1) \frac{A_{nl}^g}{\Sigma_t^g} \Sigma_{sl}^{g \to g} \tag{23}$$

where I is the four-rowed unit matrix, C_g is the matrix with 4 rows and 4 columns, and n,l are the row and column index, respectively, for C_g in Equation (21).

$$R_n^g = \frac{A_{n0}^g}{\Sigma_t^g} \frac{\chi^g}{\Delta g} + \sum_{l=0}^{3} (2l+1) \frac{A_{nl}^g}{\Sigma_t^g} \sum_{g'=1, g' \neq g}^{G} \Sigma_{sl}^{g' \to g} \Phi_l^{g'} \frac{\Delta g'}{\Delta g} \tag{24}$$

$$R_g = \left[R_0^g, R_1^g, R_2^g, R_3^g \right]. \tag{25}$$

When there is no thermal upscattering, Equation (21) is solved by Gauss elimination, sweeping from the highest energy to the lowest energy. When the thermal upscattering is present, it is solved by the combination of Gauss elimination and Gauss-Seidel iterative scheme. In this case, the thermal upscattering terms will be included, initially using assumed flux guess.

The fission source, χ, can be chosen from a fissile/fissionable isotope or calculated from the steady-state and fission rate weighted source spectrum. The steady-state fission spectrum for an isotope, i, is defined by

$$\chi_{i,g}^{SS} = \frac{\sum_{g'} \sigma_{f,g' \to g} \Phi_{g'} + \chi_g^D \sum_{g'} v_{g'}^D \sigma_{f,g'} \Phi_{g'}}{\sum_{g} \sum_{g'} \sigma_{f,g' \to g} \Phi_{g'} + \sum_{g} \chi_g^D \sum_{g'} v_{g'}^D \sigma_{f,g'} \Phi_{g'}}. \tag{26}$$

The fission rate weighted spectrum is then

$$\chi_g = \frac{\sum_i \chi_{i,g}^{SS} \sum_{g'} v_{tot,g'}^i N_i \sigma_{f,g}^i \Phi_{g'}}{\sum_i \sum_{g'} v_{tot,g'}^i N_i \sigma_{f,g'}^i \Phi_{g'}} .$$

(27)

The flux as defined in Equation (41) and included in the cross section library is initially used in Equation (27) and then the B_N spectrum calculated flux when once more spectrum calculation is performed.

2.1.2   B-1 Approximation

The B_1 equations can be the degenerate forms of B_3. Instead, B_1 equations with real B for instance are derived from Equation (7), emphasizing the physical approximations

$$\phi_0(B,E)$$
$$= \frac{\beta}{\Sigma_t(E)} \int T_{S0}(E' \rightarrow E)\phi_0(B,E)dE' + 3\frac{(\beta-1)}{\alpha\Sigma_t} \int T_{S1}(E' \rightarrow E)\phi_1(B,E)dE' + \frac{\beta}{\Sigma_t}\chi(E)$$

(28)

$$\phi_1(B,E)$$
$$= -\frac{(\beta-1)}{\alpha\Sigma_t(E)} \int \Sigma_{S0}(E' \rightarrow E)\phi_0(B,E)dE' + 3\frac{(1-\beta)}{\alpha^2\Sigma_t(E)} \int \Sigma_{S1}(E' \rightarrow E)\phi_1(B,E)dE' - \frac{(\beta-1)}{\alpha\Sigma_t(E)}\chi(E)$$

(29)

Solve Equations (28) and (29) for ϕ_0 and ϕ_1 to obtain

$$B\Phi_1 + \Sigma_t\Phi_0 = \int_{E'} \Sigma_{SO}(E' \rightarrow E)\Phi_0(E')dE' + \chi(E),$$

(30)

$$\gamma(E)\Sigma_t(E)\Phi_1(E) - \frac{B}{3}\Phi_0(E) = \int_{E'} \Sigma_{s1}(E' \rightarrow E)\Phi_1(E')dE'$$

(31)

where

$$\gamma(E) = \frac{1}{3}\frac{\beta\alpha^2}{(1-\beta)}.$$

$\Phi_0(E)$ and $\Phi_1(E)$ are interpreted as the energy-dependent flux and current, respectively. By examining Equations (30) and (31), it is seen that the B_1 approximation differs from the P_1 approximation by the factor $\gamma(E)$ in Equation (31). If $\gamma(E)$ is set to equal to 1.0, Equations (30) and (31) become the continuity equations for the P_1 approximation. The factor $\gamma(E)$ tends to improve the B_1 estimation of the energy-dependent transport current, $\Phi_1(E),$ for small homogeneous system.[16]

Similarly, for B = -iC

$$-C\Phi_1 + \Sigma_t\Phi_0 = \int_{E'} \Sigma_{SO}(E' \rightarrow E)\Phi_0(E')dE' + \chi(E),$$

(32)

$$-\gamma(E)\Sigma_t(E)\Phi_1(E) - \frac{C}{3}\Phi_0(E) = \int_{E'} \Sigma_{s1}(E' \rightarrow E)\Phi_1(E')dE'$$

(33)

For B = iC

$$C\Phi_1 + \Sigma_t\Phi_0 = \int_{E'} \Sigma_{SO}(E' \rightarrow E)\Phi_0(E')dE' + \chi(E),$$

(34)

$$-\gamma(E)\Sigma_t(E)\Phi_1(E) + \frac{C}{3}\Phi_0(E) = \int_{E'}\Sigma_{s1}(E' \to E)\Phi_1(E')dE' \tag{35}$$

Equations (30) and (31) in multigroup from reduce to

$$B\Phi_1^g + \Sigma_t^g\,\Phi_0^g = \sum_{g'=1}^{G}\Sigma_{s0}^{g'\to g}\,\Phi_0^{g'}\,\frac{\Delta g'}{\Delta g} + \frac{\chi^g}{\Delta g} \tag{36}$$

and

$$\gamma^g\,\Sigma_t^g\,\Phi_1^g - \frac{B}{3}\Phi_0^g = \sum_{g'=1}^{G}\Sigma_{s1}^{g'\to g}\Phi_1^g\,\frac{\Delta g'}{\Delta g}\;. \tag{37}$$

Equations similar to (36) and (37) are derived for imaginary B from Equations (32) through (35) with variations of sign. These equations are solved simultaneously as

$$\Phi_0^g = \frac{R_0^g(\gamma^g\,\Sigma_t^g - \Sigma_{s1}^{g\to g}) - BR_1^g}{(\Sigma_t^g - \Sigma_{s0}^{g\to g})\,(\gamma^g\,\Sigma_t^g - \Sigma_{s1}^{g\to g}) + \dfrac{B^2}{3}} \tag{38}$$

$$\Phi_1^g = \frac{R_1^g + \dfrac{B}{3}\Phi_0^g}{\gamma^g\,\Sigma_t^g - \Sigma_{s1}^{g\to g}} \tag{39}$$

where

$$R_0^g = \sum_{g'=1,g'\neq g}^{G}\Sigma_{s0}^{g'\to g}\Phi_0^{g'}\,\frac{\Delta g'}{\Delta g} + \frac{\chi^g}{\Delta g}\ \text{ and }\ R_1^g = \sum_{g'=1,g'\neq g}^{G}\Sigma_{s1}^{g'\to g}\Phi_1^{g'}\,\frac{\Delta g'}{\Delta g}$$

When upscattering is present, Gauss-Seidel iterative scheme is used.

2.1.3   Convergence on Gauss-Seidel Iterative Scheme

The calculation will be converged when the following equations are satisfied at all energy points.

$$\frac{\left|\phi_i^{(m+1)} - \phi_i^{(m)}\right|}{\phi_i^{(m+1)}} < \varepsilon \text{ and } \frac{\left|J_i^{(m+1)} - J_i^{(m)}\right|}{J_i^{(m+1)}} < \varepsilon,$$

where ε is the user input convergence criteria. The results are then normalized to have one total scalar flux.

2.2   Bondarenko Method

The multigroup approximation requires the groupwise cross sections and the energy texture is necessarily coarse with respect to the resonance structure in many materials. The resonance results in self-shielding effect. The magnitude of this self-shielding effect is in general a complicated function of the geometry and composition of the system. However, it has been found that a simple model called the Bondarenko Method[8] or Background Cross Section Method[17] does a surprisingly good job of representing the effects for many applications.[9] This method was adopted in the NJOY's GROUPR and MATXSR modules and the TRANSX code.[10] COMBINE7.0 followed those steps taken in the NJOY and TRANSX codes. The flux is assumed to vary inversely as the total macroscopic cross section. In the Bondarenko model, the narrow resonance (NR) approximation and the B_N approximation for large systems are invoked.[9] The model flux for the group averages for isotope i is written as

$$\Phi_l^i(E) = \frac{C(E)}{[\sigma_0^i + \sigma_t^i(E)]^{l+1}} \tag{40}$$

where $C(E)$ is the smooth part of the shape of the flux, $\sigma_t^i(E)$ is the microscopic total cross section for isotope i, and σ_0^i is called the background cross section (it represents the effects of all the other isotopes). The effect of the total cross section in the denominator is to put a dip in the flux for each peak in the cross section, and σ_0^i controls the relative size of the dip. A resonance material in a dilute mixture or in small pieces does not disturb a smooth flux very much by it presence—this is called the infinitely dilute case. When σ_0^i approaches a very large number, it becomes an infinitely dilute case. The l dependence shown here is appropriate for a large system with nearly isotropic scattering (the B_0 approximation), and it was used when the MATXS file was generated from NJOY.

The multigroup form of this model flux is

$$\Phi_{lg}^i = \frac{C_g}{\left[\sigma_{0,g}^i + \sigma_{t,g}^i\right]^{l+1}} . \tag{41}$$

The resonance absorption changes with the temperature due to Doppler broadening of the resonances. In order to take into account the effect of Doppler broadening, the basic cross sections in the resonance region must be adjusted appropriately for the broadening before they are used in computing group constants.

The Bondarenko method is basically an "infinite medium" method that parameterizes cross sections for a nuclide as a function of temperature, T, and the "background dilution" cross section, σ_0, of all other nuclides mixed with the nuclide. Simplistically, given the temperature and background dilution cross-section values, one determines self-shielded cross sections by interpolating in tables. Since self-shielding causes the "background dilution" values that a nuclide sets to change, an iterative procedure involving all nuclides is used. The geometric lump effect when present is accounted for by augmenting the background cross section.

For a homogeneous mixture, the appropriate background cross section is

$$\sigma_{0,g}^i = \frac{1}{N_i} \cdot \sum_{j \neq i} N_j \cdot \sigma_{t,g}^j(\sigma_{0,g}^i) \tag{42}$$

Where N is the number density for the isotope and $\sigma_{t,g}$ is the self-shielded total cross section of an energy group g. Because $\sigma_{t,g}$ depends on $\sigma_{0,g}$, finding $\sigma_{0,g}$ is an iterative process. For a mixture of resonance materials, interference between resonances in different materials is handled in an average sense only.

For a lump of resonance material embedded in a large moderating region, escapes from the lump also increase the background cross section. To account for this, the $\sigma_{0,g}$ value is augmented by an escape cross section

$$\sigma_{e,g}^i = \frac{1}{N_i \bar{l}} \tag{43}$$

where $\bar{l}$ is the mean chord length of lump given by

$$\bar{l} = \frac{4V}{S} \tag{44}$$

and where V and S are the volume and surface area of the lump. Multizone situations, such as reactor lattices, are accounted for by the use of Dancoff factors, which, in effect, modify the escape probability and, hence, the value of σ_e. The mean chord length $\bar{l}$ can be adjusted away from the geometric value of Equation (44) to compensate for the presence of other lumps (Dancoff correction) or for shortcoming in the escape probability model used to obtain Eq. (43). In the rational approximation, the Dancoff correction is equivalent to increasing the mean chord length, $\bar{l}$, by the factor $1/(1-c)$ or equivalently decreasing the surface area of lump by $1-c$ as in

$$\sigma_{e,g}^i = \frac{1}{N_i \cdot \bar{l} \cdot \dfrac{1}{(1-c)}} \tag{45}$$

when Bell corrections are applied

$$\sigma_{e,g}^i = \frac{1}{N_i \cdot \bar{l}} \cdot \frac{b_1 \cdot (1-c)}{1 + (b_2 - 1) \cdot c} \tag{46}$$

where b1 and b2 are called Bell corrections. When b1 = b2, the constant is usually called the Levine factor and Equation (46) becomes

$$\sigma_{e,g}^i = \frac{1}{N_i \cdot \bar{l}} \cdot \frac{1}{\dfrac{1}{b} + \dfrac{c}{1-c}} \tag{47}$$

where

$\quad b \quad = 1.26$ for the slab geometry

$\qquad = 1.35$ for the cylindrical geometry

$\qquad = 1.30$ for the spherical geometry.

The so-called "Levine factors," b, are approximate geometry dependent factors that are approximately correct for inaccuracies in the Rational Approximation.

When a double heterogeneity occurs due to fuel grains present within the macroscopic fuel lump, the Dancoff factor c' specifies the mutual shielding between these grains, independent of c for the lumps themselves. To better account for the double heterogeneity due to fuel grains present within the macroscopic fuel lump, a correction has been made to the escape probability and given by Stamatelatos and LaBauve[18] as

$$\sigma_{e,g}^i = \frac{1}{N_i \left[\bar{l} \cdot \left(\dfrac{1}{b} + \dfrac{c}{1-c} \right) + \bar{l}_G \left(\dfrac{1}{a} + \dfrac{c'}{1-c'} \right) \right]} \tag{48}$$

where

$\quad \bar{l}_G \quad =$ the average chord length of a single isolated spherical fuel grain

$\quad c' \quad =$ the Dancoff factor for fuel grains

$\quad A \quad = 1.77$, the Levine factor for spherical grains.

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The following equation for the background cross section has been applied

$$\sigma_{0,g}^{i} = \sigma_{e,g}^{i} + \frac{\sum_{i \neq j} N_j \cdot \sigma_{t,g}^{j} (\sigma_{0,g}^{j})}{N_i} \quad .$$ (49)

2.2.1 Fine-Group Cross Section Generation in Bondarenko Format

In COMBINE7.0, a 167 fine group structure is used and the multigroup cross section constants are generated in this fine group structure to be used in the B_N solution.

The NJOY99.259 version[15] was used to generate a 167 fine-group cross-section library, MATXS.LIB, in MATXS format (Bondarenko format) on sets of background cross sections and temperatures including thermal scattering cross sections. For C(E) in Equation (40), an NJOY built-in spectrum, Thermal--1/E--Fast Reactor--Fission + Fusion, is used. The equations providing the fundamental definitions in NJOY for the multigroup cross sections and the group-to-group matrix are

$$\sigma_{t,l,g} = \frac{\int_g \sigma_t(E)\phi_l(E)dE}{\int_g \phi_l(E)dE},$$ (50)

$$\sigma_{x,g} = \frac{\int_g \sigma_x(E)\phi_0(E)dE}{\int_g \phi_0(E)dE},$$ (51)

$$\sigma_{X,l,g' \to g} = \frac{\int_g dE \int_{g'} dE' \sigma_{Xl}(E' \to E)\phi_l(E)}{\int_g \phi_l(E)dE} \quad .$$ (52)

The energy-dependent cross-section database is now derived entirely from ENDF/B-VII.0 nuclear data with the exception of Zr element cross-section data, which is based on ENF/B-VI.8 nuclear data. All materials have either S(α,β) or free thermal scattering matrices.

2.2.2 Bondarenko Self-Shielding Interpolation

Bondarenko self-shielding is performed in COMBINE7.0 by background cross section and temperature interpolation. The interpolation is first performed for the background cross sections at each temperature. The generated cross sections for the set of preselected temperatures are then interpolated for the problem-dependent temperature. In the background cross-section interpolation, a log-log N^{th} order for the vector cross sections, and log-linear N^{th} order Lagrangean schemes are employed with a variation to the first order for the extremely high or low problem-dependent background cross section. The temperature interpolation uses a log-log N^{th} order Lagrangean scheme. Iteration is necessary to arrive at the correct background cross sections. Three iterations are performed for all isotopes. The first iteration is based on the infinite dilution of the rest isotopes for total cross sections. The accuracy, convergence, and stability of these schemes have been sufficiently tested and are satisfactory.

2.3 Resonance Region

The material cross-section libraries supplied for each material have complete multigroup cross sections based on Bondarenko method. The weakness of the Bondarenko model occurs for thermal reactor analysis in the "epithermal" energy region from about 4 eV to around 200 or 300 eV.[10] In this region, the resonances are no longer narrow, and the flux shape given by Equation (40) is no longer sufficiently accurate. For those materials where resolved resonance parameters are present via RERES.LIB, a Nordheim numerical solution[11] is applied as an option. Before B_1 or B_3 Equations are solved, the resonance parameters in the material libraries must be converted into average, self-shielded, temperature dependent, groupwise cross sections.

2.3.1 Resolved Resonances—Nordheim Numerical Method

The balance equation for the collision density in a homogeneous mixture of moderators and resonance absorbers in an infinite medium is[19]

$$F(E) = \phi(E)\Sigma_t(E) = \sum_k \int_E^{E/\alpha_k} \frac{\phi(E')\Sigma_s^k(E')dE'}{(1-\alpha_k)E'} \tag{53}$$

where

$\phi(E)$ =   scalar neutron flux

Σ_t =   total macroscopic cross section

Σ_s^k = $N_k\sigma_{sk}$ = macroscopic scattering cross section for material k

N_k =   atomic density of material k

σ_k =   microscopic cross section of material k

α_k = $\left(\dfrac{A_k-1}{A_k+1}\right)^2$, A_k = ratio of isotopic mass to mass of the neutron for material k

$F(E)$ =   collision density at energy E.

The right-hand side of Equation (53) requires a different integration limit for each moderator k. The flux $\phi(E)$ at each resolved resonance undergoes a severe depression at each strongly absorbing resonance. One or many resonances may fall within any given COMBINE multigroup. The average, self-shielded, absorption integral in each multigroup g within the resonance range is then given by

$$I_{ag}^k = \int_{Eg}^{E_{g+1}} \phi(E)\sigma_c^k(E)dE \tag{54}$$

where $\phi(E)$ is the solution of Equation (53) over the energy interval for the multigroup and σ_c is the capture cross section. Equation (53) is solved in lethargy space where

du   = $-\dfrac{dE}{E}$

dE   =   -Edu

E   = E_1e^{-u} .

Therefore, dE   = $E_1e^{-u}du$.

Equation (55) is transformed to[11]

$$I_{cg}^k = E_1 \int_{u_{g-1}}^{u_g} \phi\left[E(u)\right] \sigma_c^k\left[E(u)\right] e^{-u} du$$

$$I_{cg}^k = E_1 \int_{u_{g-1}}^{u_g} F\left[u(E)\right] \frac{\sigma_c^k(u)e^{-u}}{\Sigma_t(u)} du \tag{55}$$

where F[u(E)] is the collision density per unit energy in lethargy coordinates. The mixed lethargy-energy form of Equation (55) results from the fact that the integration is performed on a lethargy mesh, but the resonance cross sections are calculated in energy space because the cross sections are not easily transformed to lethargy coordinates. Equations similar to Equation (55) may be written for the fission and elastic scattering integrals using $\sigma_f^k(u)$ or $\sigma_s^k(u)$ in place of $\sigma_c^k(u)$.

If absorption occurs in an isolated lump surrounded by an infinite sea of moderators, the introduction of the lump escape probability[20] $P_0(\bar{l}, \Sigma_t)$, is given in terms of the average chord length of the lump, $\bar{l}$. This enables Equation (53) to be modified to closely approximate the heterogeneous absorption rate in the lump-moderator assembly. The collision density in the lump now consists of two distinct types of events:

1. Those neutrons that have had their last collision in the lump, which is given by the right-hand side of Equation (53) multiplied by the probability of colliding in the lump, $\left[1 - P_0(\bar{l}, \Sigma_t)\right]$, times V_F, the volume of the fuel lump.

2. Those neutrons that stream into the lump at lethargy u(E) from outside the lump, multiplied by the moderator escape probability[20] $P_M(\bar{l}, \Sigma_t)$, times the volume of the external moderator, V_M, contained in a unit cell.

$$V_F F(u) = V_F\left[1 - P_0(\bar{l}, \Sigma_t)\right] \sum_k \frac{1}{1-\alpha_k} \int_{u-\varepsilon_k}^u F(u') \frac{\Sigma_s^k(u')}{\Sigma_t(u')} du' + V_M P_M \phi_M(u) \Sigma_M(u) \tag{56}$$

where

$$\varepsilon_k = \ln\left(\frac{1}{\alpha_k}\right)$$

and $\phi_M(u)$ is the average, asymptotic, equilibrium neutron flux in the moderator residing outside the lump. The normalization of Equation (56) is arbitrary, since the point wise collision density F(u) will only be used to obtain average cross sections over the multigroups in the resolved resonance range. $\phi\left[u(E)\right]$ is set equal to 1/E in the region outside the lump, i.e., $\phi_{asym}\left[u(E)\right] = e^u / E_1$.

The moderator terms in Equation (56) may be removed by means of the reciprocity relation[9]

$$P_M V_M \Sigma_M = P_F V_F \Sigma_{tF} \tag{57}$$

Equation (56) then becomes

$$F(u) = (1 - P_0) \sum_{k-1}^7 \frac{1}{1-\alpha_k} \int_{u-\varepsilon_k}^u F(u') \frac{\sigma_s^k(u')}{\sigma_t(u')} du' + P_0 \sigma_t(u) \frac{e^u}{E_1} \tag{58}$$

where σ_s^k and σ_t are given by Equations (62) and (63), expressed in terms of the scattering per absorber atom.

$$P_0 = P_0(\bar{l}, \Sigma_t) \tag{59}$$

where

$$\bar{l} = \bar{l}_0 = \frac{4V}{S}, \text{ single isolated lump}$$

$$\frac{V}{S} = \text{ratio of volume of the absorber lump to the surface area}$$

$$= 1/2 \times \text{half thickness—plate geometry}$$

$$= 1/2 \times \text{radius—cylindrical geometry}$$

$$= 1/3 \times \text{radius—spherical geometry}$$

The escape probability P_0 is tabulated[11] for single isolated lumps. When a Dancoff factor C is incorporated to represent the mutual shielding in a repetitive array,[21] the escape probability P_0 is modified to be[11,22]

$$P = \frac{GP_0(1-C)}{\left[1 - (1 - \bar{l}\Sigma_t P_0)C\right]} \tag{60}$$

where P_0 in Equation (60) is the escape probability for a single isolated lump, P represents the mutually shielded value, C is the Dancoff Ginsberg correction factor for a regular array of lumps, and G is a double heterogeneity correction for the self-shielding of fuel grains within the absorber lump[23]

$$G = \left[1 + \sum_t \bar{l}_G \left(\frac{1}{a} + \frac{C'}{1 - C'}\right)\right]^{-1} \tag{61}$$

where

$\bar{l}_G = $ average chord length within a fuel grain, independent of $\bar{l}$, the average chord length in the lump

$C' = $ Dancoff factor for the fuel grains in the lump, independent of C

$a = $ 1.77—the Levine factor for spherical grains, A correction factor for the Wigner Rational Approximation for P_0, which is employed in deriving Equation (62).

When a double heterogeneity occurs due to fuel grains present within the macroscopic fuel lump, the Dancoff factor C' specifies the mutual shielding between these grains, independent of C for the lumps themselves.

In Equation (58), up to seven moderators are included for the down scatter source within the lump, the first always being the absorber atom itself. Three additional moderators and three additional admixed resonance absorbers with different masses can also be included.[3] This limit is felt to be sufficient for almost any fuel pin one would encounter in practice.

The cross sections in Equation (58) are evaluated relative to the number of absorber atoms as in

$$\sigma_s^k = \frac{\sum_s^k}{N_a} \tag{62}$$

where

N_a = atom density of the absorber atom in the lump.

$$\sigma_t = \sigma_a + \sigma_s + \sigma_m^1 + \sigma_m^2 + \sigma_m^3 + \sigma_a^1 + \sigma_s^1 + \sigma_a^2 + \sigma_s^2 + \sigma_a^3 + \sigma_s^3 \tag{63}$$

where: σ_s is the resonance scattering of the absorber atom itself; σ_m^i represents the three moderator's scattering cross sections per absorber atom; σ_a^i represents the three admixed absorber's absorption cross sections per absorber atom; and σ_s^i represents the three admixed absorber's scattering cross sections per absorber atom. The absorption cross section of the three additional moderators is assumed to be very small compared with the principal absorber or the admixed absorbers.

Equation (58) has proven itself to be remarkably accurate in many applications. A number of unique approximations are used in deriving Equation (58), the most important of which is the "flat flux assumption."[24] The spatial dependence of the flux across the lump has been subsumed into the escape probability P_0, which permits the elimination of the spatial dependence of the flux in Equation (58). P_0 is evaluated as a function of energy only. The approximation which makes this possible is that at each energy, the escape probability is evaluated as if only the average flat flux in the lump were known relative to the asymptotic flat flux existing outside the lump. The escape probability P_0 under the flat flux approximation is then given by[24]

$$P_0 \approx \frac{\bar{\phi}_{lump}}{\bar{\phi}_{asym}} \tag{64}$$

If an average flat flux can be assumed in the lump, the escape probability absorbs the spatial dependence in Equation (58). $P_0(\bar{l}, \Sigma_t)$ is evaluated at each energy across the resonance since $\Sigma_t(E)$ is a strong function of energy at resonance. Equation (64) is a truly remarkable result that makes possible a separate two-stage solution to a difficult problem; the first stage being the calculation of the escape probability P_0.[11] Equation (58) is solved numerically on a very fine energy mesh across each lethargy group where one or more resonances may reside.

2.3.2   Doppler Broadening of Resolved Resonance Parameters

Subroutines adopted from the NJOY code and incorporated in COMBINE7.0 numerically Doppler broaden the SLBW, MLBW, and R-M format resonance parameters by the kernel broadening method.[25] The subroutines were verified by kernel broadening the SLBW option and comparing with that using the ψ-χ function that was used in the previous COMBINE versions. At each mesh point the capture, fission, and elastic cross sections are calculated, accumulating contributions from all the resonances in the same resonance range. Figure 2 shows the Doppler broadened cross section as an example.
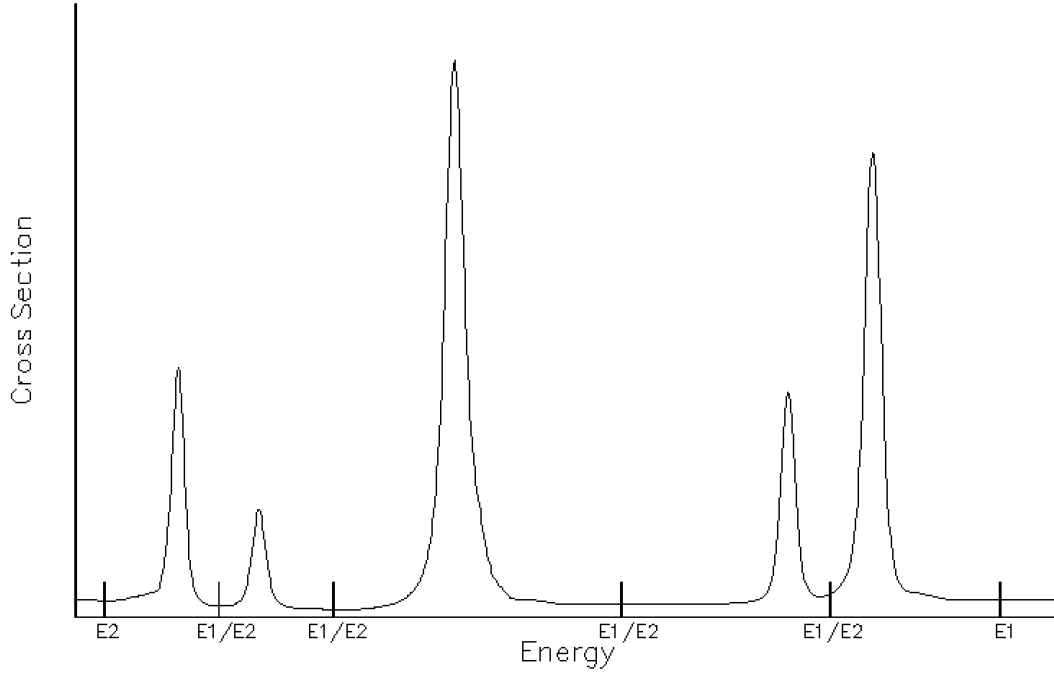
Figure 2. An example of Doppler broadened resonance cross sections.

2.3.3 Determination of E_1 /E_2 and the Number of Meshes for a Resonance

The first energy, E_1, corresponds to the first fine group energy boundary encountered just below the upper limit of the highest resolved resonance energy range. It can be the user input at any fine group energy boundary lower than that. The next E_1 (or E_2) is at the midpoint between the next two neighboring resonances, and so on. The lowest E_2 is also adjusted to correspond to the fine group energy boundary. For each resonance, a resonance integration interval is formed by E_1 and E_2. Considering an equal lethargy interval solution, a mesh size and the number of mesh intervals within the resonance integration are calculated according to the following recipe, which was adopted from GAM-II code[22] and modified.

$$\mathrm{r} = 5.0 + 0.5\sqrt{K * 273.0 * E_0 / AWRI} / \Gamma \tag{65}$$

$$\varepsilon = 1.0 / [AWR * \mathrm{int}\{0.5 * r * \sqrt{1.0 / (K * 273.0 * AWRI)} * |E_0| + 1.0\} * \mathrm{fmult}] \tag{66}$$

$$\mathrm{mesh} = \frac{\log(E_1 / E_2)}{\varepsilon} \tag{67}$$

where: mesh is the number of mesh intervals, K is the Boltzmann constant = 8.6173e-5 eV/K, the constant 273.0 defines the mesh reference temperature T_0, AWRI is the ratio of mass of a particular isotope to that of a neutron, Γ is the total resonance width, E_1 and E_2 are the high and low energy boundaries of the integration for a resonance, E_0 is the resonance energy, and fmult is the user input control parameter to make mesh coarse or finer (default= 1.0).

The number of mesh intervals is then made to be an even number so that the total number of mesh points become odd for Simpson's integration. The last mesh point of the previous resonance integration interval corresponds to the first mesh point of the present resonance integration interval, and so on. The lethargy mesh is generated independently for each resonance from midpoint to midpoint between resonances; therefore, the mesh spacing from resonance to resonance varies. The highest E1 and lowest E2 can be controlled by user input, other than the default values set in "reres.lib" and adjusted to the group boundaries in the code. The maximum allowable number of mesh intervals in a resonance

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integration interval is coded to be 1400. When the admixed resonance absorbers are present, the Doppler broadened cross sections are generated over these mesh points.

2.3.4　Absorber Narrow Resonance- Moderator Asymptotic Flux Approximation

In the Narrow Resonance (NR) approximation, the resonances are so narrow that all moderators, including the absorber, can scatter past the resonance. The scattering cross section over most of this range is essentially just that for potential scattering σ_p. The integral term in Equation (56) becomes

$$\frac{1}{1-\alpha_k}\int_{u-\varepsilon_k}^{u} F(u')\frac{\sigma_s^k(u')}{\sigma_t(u')}du' = \frac{\sigma_p^k}{1-\alpha_k}\cdot\int_{u-\varepsilon_k}^{u}\phi(u')du' = \frac{\sigma_p^k}{1-\alpha}\cdot\int_{u-\varepsilon_k}^{u}\frac{e^{u'}}{E_1}du' = \sigma_p^k\frac{e^u}{E_1},\tag{68}$$

when the asymptotic flux, $\phi_{asym}\big[u(E)\big] = e^u/E_1 = w(u)$, is applied.

The criteria to determine this approximation is when $\ln(\frac{E_i}{\alpha E_i})/\varepsilon \leq 1001$.

In the thermal energy range, $E \leq 5kT$, the flux shape is rather Maxwellian than e^u/E_1,[26]

$$\phi_{asym}\big[u(E)\big] = 5.936526/(kT)^2 \cdot E_1 e^{-u} e^{-\frac{E_1 e^{-u}}{kT}} = w(u)\ .\tag{69}$$

2.3.5　Self-Shielding Elastic Scattering Transfer Matrix

The solution of Equation (20) or (38) and (39) requires the self-shielded resolved resonance contributions to the elastic scatter matrix for the Legendre moments through L = 3 or L = 1, respectively. Departing from the previous versions, a simple normalization scheme is employed for this, utilizing the already available transfer matrix from Bondarenko self-shielded transfer matrix,

$$\sigma_{s,g'\to g}^l = (\sigma_{s,g'\to g}^l)_{Bondarenko}\cdot\frac{(\sigma_{s,g'}^0)_{Nordheim}}{(\sigma_{s,g'}^0)_{Bondarenko}}\ .\tag{70}$$

2.3.6　Numerical Integration with Simpson's Rule

Combining the integral form, absorber narrow resonance-moderator asymptotic flux approximation, and the thermal upscattering term, the numerical integration is expressed as

$$F(u) = \left\{1-(1-P(u))\frac{\varepsilon}{3\sigma_t(u)}\left[(\delta(N_0)\frac{\sigma_{s0}(u)}{\alpha_0}+\sum_i^3\delta(N_{a_i})\frac{\sigma_{sa_i}(u)}{\alpha_{a_i}}+\sum_j^3\delta(N_{m_j})\frac{\sigma_{sm_j}(u)}{\alpha_{m_j}})\right]\right\}^{-1}\cdot$$

$$\left\{\begin{array}{l}(1-P(u))\varepsilon\left[\begin{array}{l}\dfrac{\delta(N_0)}{3\alpha_0}\overset{u-\varepsilon}{\underset{u-n\varepsilon}{I}}F(u')\dfrac{\sigma_{so}(u')}{\sigma_t(u')}+\sum_i^3\dfrac{\delta(N_{a_i})}{3\alpha_{a_i}}\overset{u-\varepsilon}{\underset{u-n\varepsilon}{I}}F(u')\dfrac{\sigma_{sa_i}(u')}{\sigma_t(u')}+\sum_j^3\dfrac{\delta(N_{m_j})}{3\alpha_{a_i}}\overset{u-\varepsilon}{\underset{u-n\varepsilon}{I}}F(u')\dfrac{\sigma_{sm_j}(u')}{\sigma_t(u')}\\[2mm]+\delta(up)\sum_{g'}F_{g'}\dfrac{\sigma_{sg'\to g}^{upsct}}{\sigma_{tg'}}\dfrac{\Delta g'}{\Delta g}\end{array}\right]\\[4mm]+\left[(1-P(u))(\delta(NR)\sigma_{p_0}+\sum_i^3\delta(A_{a_i})\sigma_{pa_i}+\sum_j^3\delta(A_{m_j})\sigma_{pm_j}+P(u)\sigma_t(u)\right]w(u)\end{array}\right\}\tag{71}$$

where $\delta\,(N_x)$ means Nordheim integral treatment application for the resonance absorber, admixed resonance absorbers, admixed moderators, $\delta\,(NR)$, $\delta\,(A_a)$, $\delta\,(A_m)$ means application of absorber

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narrow resonance-moderator asymptotic flux approximation instead of Nordheim integral treatment, δ (up) means application of upscattering when thermal upscattering is present

$$\int_{u-n\varepsilon}^{u-\varepsilon} F(u')\frac{\sigma_s(u')}{\sigma_t(u')} = 2\sum_{i=1}^{2}(3-i)\sum_{j=1}^{\frac{n}{2}-i+1} F\left[u-(2j+i-2)\varepsilon\right]\frac{\sigma_s\left[u-(2j+i-2)\varepsilon\right]}{\sigma_t\left[u-(2j+i-2)\varepsilon\right]}$$
$$+ F(u-\varepsilon n)\frac{\sigma_s(u-\varepsilon n)}{\sigma_t(u-\varepsilon n)} \tag{72}$$

is the Simpson's rule integration.

When thermal upscattering is present, iteration is needed. Since the convergence is rapid when the available flux in the code is utilized, only once more iteration is performed.

2.3.7   Group Averaging

Two options are available for converting the resonance integrals in Equation (53) into average multigroup cross sections, depending on whether one desires averages over the whole cell or just over the absorber lump. The average cross section is defined by

$$\overline{\sigma}_{xg} = \frac{E_1\int_{u_{i-1}}^{u_i} F(u)\frac{\sigma_x(u)}{\sigma_t(u)}e^{-u}du}{E_1\int_{u_{i-1}}^{u_i}\phi(u)e^{-u}du} \tag{73}$$

where σ_x is the reaction cross section being averaged, F(u) is given by Equation (58), and σ_t is given by Equation (63). The reaction cross section is averaged over the absorber lump flux,

$\phi(u) = F(u)/\sigma_t(u) = $ lump flux

After obtaining capture/fission and scattering cross sections from Nordheim treatment, these cross sections overwrite the previous cross sections.

2.3.8   Dancoff-Ginsburg Correction Factor Calculation

Computation of the Dancoff factor C for arbitrary shapes and spacing of lumps is very difficult. Most accurate determinations have been performed for regular arrays of cylindrical fuel pins. An external code like SUPERDAN can provide Dancoff factors.[27] One option in COMBINE is an exact calculation described below. In the event that a precise calculation is not possible due to geometric irregularity or nonavailability, Bell offers an approximate formula based on the most general assumptions, which can be used as a last resort. Bell's formula can be written as[28]

$$C \approx \frac{\lambda_1}{\frac{4V_1}{S_a}+\lambda_1} \tag{74}$$

where

S_a = surface area of the absorbing lump

V_1 = the average external moderator volume per absorber lump

λ_1 = the external moderator mean-free-path in the same units as V_1 and S_a.

Equation (74) is deceptive in its simplicity considering the exact definition in Equation (75). It is exact in the limits of very large or very small lumps. The Rational Approximation for P_o has been used in deriving Equation (74) along with other assumptions, so it should be used only as a first order

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approximation when no other method is available. Equation (74) can be used with any regular or irregular geometry and is independent of geometric details other than average values of V_1 and S_a. A precise calculation of C for cylindrical pins is included in COMBINE and is described below.

The cylindrical pin Dancoff correction is computed in COMBINE following the methods of Gelling and Sauer.[29] This correction may be calculated for an infinite lattice composed of cylindrical pins in either a rectangle or a hexagon. Pins are assumed to be black to resonance-energy neutrons.

The Dancoff correction is defined as:[24]

$$C = \frac{\int dS \int \vec{n} \cdot \vec{\Omega} \exp\left[-\Sigma l(\vec{s},\vec{\Omega})\right] d\Omega}{\int dS \int \vec{n} \cdot \vec{\Omega} \, d\Omega} \tag{75}$$

where $l(\vec{s},\vec{\Omega})$ is a chord that extends from the lump surface element dS in the direction $\vec{\Omega}$ through the moderator to the point of intersection with a neighboring lump. Σ is the cross section for removal of neutrons from the energy range of the resonance and is the normal to the lump surface element.

In the case of a lattice composed of cylindrical pins, the Dancoff correction may be expressed as

$$C = \frac{4}{\pi} \int_0^{2\pi} \frac{d\rho}{2} \int_{-1}^{1} \frac{d\xi}{2} K_{i3}\left[\Sigma R_0 \cdot S\right] \quad . \tag{76}$$

The parameters are defined in Figure 3, and

$$K_{i3} = \int_0^\infty \exp\left[-x\cosh(u)\right]\cosh^{-3} u \, du \tag{77}$$

is the Bickley function of the third order.
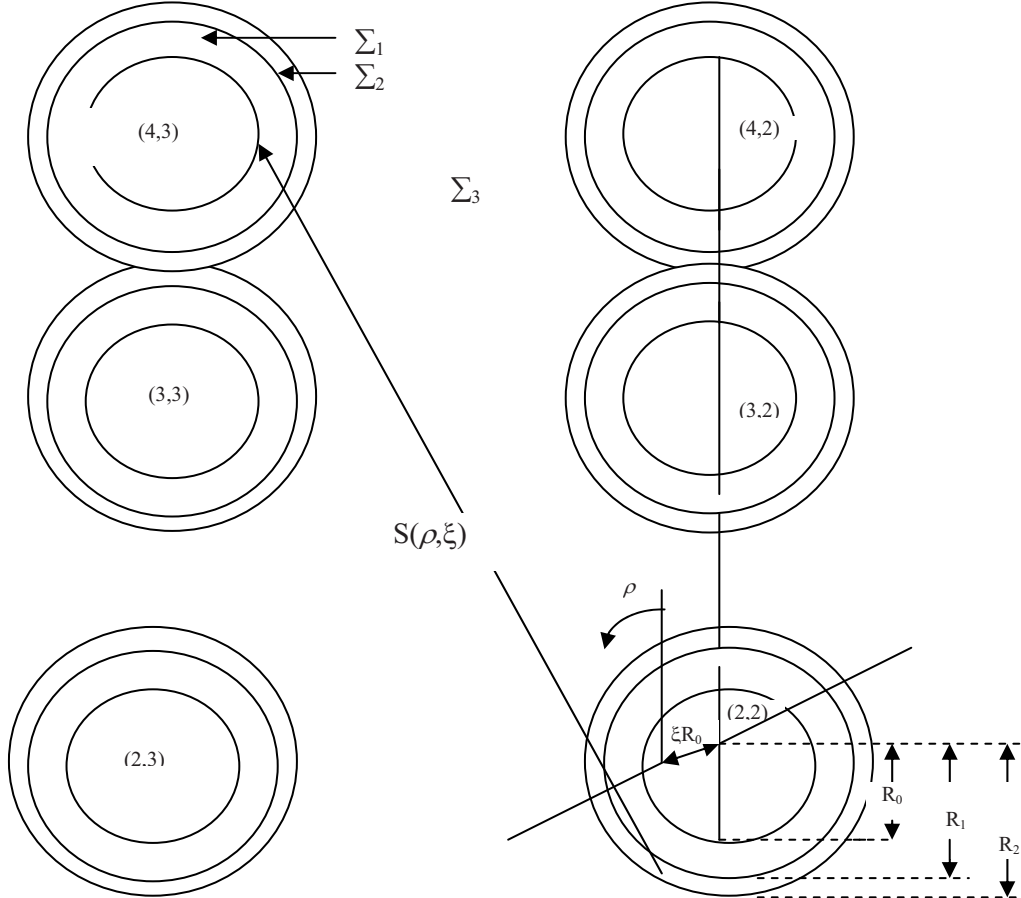
Figure 3. Parameters of the rectangular cell.

The two-dimensional lattice is represented exactly for a pin surrounded by up to four annular moderating regions and an external moderator. A library of pin configurations is contained within the code. A pin location is specified by the row n and the column m, where m and n are in units of pitch.

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Heterogeneity of the moderating region is accounted for by defining the argument of the Bickley function[29] as

$$\sum R_0 \cdot S = R_0 \sum_{i=1}^{N} \Sigma_i \, S_i \tag{78}$$

where s_i is the length of the chord through region i, having total cross section Σ_i.

The integral in Equation (76) is evaluated using the trapezoidal approximation. Because of symmetry, the upper limit is taken as $\pi/4$ for a rectangular lattice and $\pi/6$ for a hexagonal lattice. The integral over ρ is evaluated by using 20 equal angular intervals, and for each value of ρ the integral over ξ is evaluated by using 100 increments of equal length. For each set of (ρ,ξ) values, the length of the chord S_i through each region is calculated and the Bickely function is evaluated by the approximation

$$K_{i3}(x) = \frac{e^{-x}}{(0.6366198x + 1.6211389)^{1/2}} \cdot \frac{x^2 + 6.399407x + 5.066719}{x^2 + 6.766116x + 5.066719} \, . \tag{79}$$

This approximation yields values of $k_{i3}(x)$ to an accuracy of $\pm\, 0.05\%$.

2.4   Computation of Thermal Disadvantage Factors

The absorber lump appears black to neutrons at the peak resonance cross sections. For neutrons at thermal energies, the same lump is more than grey. As a consequence, corrections for thermal scattering are much more important. Amouyal and Benoist[30] have developed integral transport theory for the calculation of thermal disadvantage factors in grey absorber lumps. Strawbridge[31] has modified this theory to include a third clad region. The three region cell equations for the point wise disadvantage factors W_i in a cylindrical cell are,[30]

$$\frac{W(R_0)}{W_0} = 1 + \frac{\Sigma_{a0}(E)}{\Sigma_{t0}(E)}\left[\frac{1 - P_e}{P_e} - R_0\,\Sigma_{t0}(E)\right] \quad \text{x} \quad \left\{1 + \alpha\frac{\Sigma_{s0}(E)}{\Sigma_{t0}(E)} + \beta\left[\frac{\Sigma_{s0}(E)}{\Sigma_{t0}(E)}\right]\right\} \tag{80}$$

where

$\quad W_o \quad = \quad$ average energy dependent disadvantage factor in the cylindrical absorber rod

$\quad W(R_o) \quad = \quad$ energy dependent disadvantage factor at the surface of the absorber rod between the rod and the clad

$\quad \Sigma_{a0}(E) \quad = \quad$ absorption cross section in the absorber rod

$\quad \Sigma_{t0}(E) \quad = \quad$ total cross section in the absorber rod

$\quad \Sigma_{s0}(E) \quad = \quad$ scattering cross section in the absorber rod

$\quad R_0 \quad = \quad$ radius of the absorber rod

$\quad P_e \quad = \quad P_e\left[\bar{l}_o, \Sigma_{t0}^*(E)\right] = $ the first flight escape probability in a cylindrical absorber rod at energy E

where

$$\bar{l}_0 \quad = \quad 2\,R_o$$

$\alpha, \beta \quad = \quad$ tabulated empirical factors to correct the first flight escape probability P_e for the effects of scattering within the absorber rod.

Equation (80) resulted from considerations by A/B (Amouyal/Benoist) to adjust the first flight escape probability P_e (correct for a black pin) for the effects of scattering in a grey pin. The basis A/B thermal equation suppressing energy dependence, is

$$\frac{W(R_0)}{W_0} = \frac{1}{P_s(\bar{l}_0, \Sigma_{t0})} - R_0\,\Sigma_{a0} \tag{81}$$

where P_s is the escape probability for a single grey pin corrected for multiple scattering within the pin.

$$P_s\left(\bar{l}_0, \Sigma_{t0}\right) = \left(1 + \frac{\Sigma_{a0}}{\Sigma_{t0}}\left\{A\left[1 + \alpha\,\frac{\Sigma_{s0}}{\Sigma_{t0}} + \beta\left(\frac{\Sigma_{s0}}{\Sigma_{t0}}\right)^2\right] + R_{0\Sigma_{t0}}\right\}\right)^{-1} \tag{82}$$

where

$$A = \frac{1 - P_e}{P_e} - R_0\,\Sigma_{t0}$$

$P_e\left[\bar{l}_o, \Sigma_t(E)\right]$ is obtained from the tabular lookup used for resolved resonances.

When Equation (82) is substituted into Equation (81) we obtain Equation (80). For a black pin, $\Sigma_s = 0$ and Equation (81) can be reduced to Wigner's Rational Approximation using the flat flux assumption.

$$\frac{W(R_0)}{W_0} = \frac{1}{P_0(\bar{l}_0, \Sigma_{a0})} - R_0\,\Sigma_{a0} = \frac{W_1}{W_0} - R_0\,\Sigma_{a0}$$

where $\dfrac{1}{P_0} \approx \dfrac{W_1}{W_0}$ and W_1 is the asymptotic average flux in the moderator region outside the black absorber rod. Since the flat flux assumption implies a discontinuity in the flux at the boundary

$$W(R_0) = \frac{W_1 + W_0}{2}$$

$$\frac{W_1 + W_0}{2W_0} + R_0\,\Sigma_{a0} = \frac{1}{P_0}$$

$$\frac{W_1}{W_0} + 1 + 2R_0\Sigma_{a0} = \frac{2}{P_0}$$

$$P_0 = \frac{1}{1 + \bar{l}_0\,\Sigma_{a0}} \equiv \text{Rational Approximation,}$$

which is the Wigner's Rational Approximation equation when Σ_{a0} replaces Σ_{t0}. The ABH[30] equation for the external moderator Region 1, with absorption in the moderator included and an additional clad Region 2 separating the absorber and moderator, is

$$\frac{W_1}{W_0} = \frac{W(R_0)}{W_0} + \frac{\Delta W_2}{W_0} + \frac{3}{2} R_0^2 \Sigma_{a0} \left[1 + \frac{V_2}{V_0} \frac{\Sigma_{a2}}{\Sigma_{a0}} \frac{W_2}{W_0} \right] F \tag{83}$$

where

$$F = G \Sigma_{t1} + \frac{1}{R_2} \left(\lambda_1 - \frac{2}{3} \right)$$

$$G = \frac{R_1^2}{R_1^2 - R_2^2} \left[\frac{R_1^2}{R_1^2 - R_2^2} \ln\left(\frac{R_1}{R_2} \right) - \frac{3}{4} + \frac{R_2^2}{4 R_1^2} \right]$$

$$\lambda_1 = 0.710446 \left[\frac{1 + 1.5207587 \frac{3 D_1}{2 R_1}}{1 + 0.8103127 \frac{3 D_1}{2 R_1}} \right]$$ (the extrapolation length for the inner surface of the moderator

region)[32]

W$_1$ = disadvantage weight for the external moderator region

W$_2$ = disadvantage weight for the clad region

Σ_{t1} = the total cross section in the moderator region

Σ_{a2} = the absorption cross section in the clad region

R$_2$ = the outer radius of the clad region

R$_1$ = the outer radius of the moderator region

D$_1$ = the diffusion coefficient in the moderator region.

The equation for the clad disadvantage factor W$_2$ is

$$\frac{W_2}{W_0} = \frac{W(R_0)}{W_0} + \frac{\Delta W_2}{2 W_0} \tag{84}$$

where

$$\frac{\Delta W_2}{2} = \text{average incremental rise in the flux across the clad region.}$$

This can be obtained from simple diffusion theory by balancing the volume absorption rate in the absorbing rod to the diffusion current entering the rod,

$$W_0 \Sigma_{a0} V_0 = D_2 \frac{\Delta W_2}{\Delta R}\bigg|_{R_0} 2\pi R_0$$

$$\frac{\Delta W_2}{W_0} = \frac{\Sigma_{a0} \pi R_0^2 (R_2 - R_0)}{2\pi R_0 D_2}$$

$$\frac{\Delta W_2}{2 W_0} = \frac{\Sigma_{a0} R_0 (R_2 - R_0)}{4 D_2} \tag{85}$$

where D$_2$ is the diffusion coefficient in the clad region.

The weights W_0, W_1, and W_2 are normalized at each energy group as

$$W_0 VF_0 + W_2 VF_2 + W_1 VF_1 = 1 \tag{86}$$

where VF_0, VF_2, and VF_1 are the volume fractions of the absorber, clad and moderator regions, respectively.

Dividing Equation (86) by W_0, we have

$$\frac{1}{W_0} = VF_0 + \left[\frac{W_2}{W_0}\right] VF_2 + \left[\frac{W_1}{W_0}\right] VF_1 . \tag{87}$$

When Equations (80), (84), and (85) are solved for W_2/W_0, and Equation (83) is solved for W_1/W_0, Equation (87) is solved for W_0. Then

$$W_2 = \left(\frac{W_2}{W_0}\right) W_0 \tag{88}$$

$$W_1 = \left(\frac{W_1}{W_0}\right) W_0 . \tag{89}$$

2.4.1 Slab Geometry Disadvantage Weights

The equations for plate type geometry are taken from Theys[33] and are similar, but differ due to the difference in divergence.

$$\frac{W(X_0)}{W_0} = 1 + \frac{\Sigma_{a0}}{\Sigma_{t0}} A \left[1 + \alpha \frac{\Sigma_{s0}}{\Sigma_{t0}} + \beta \left[\frac{\Sigma_{s0}}{\Sigma_{t0}}\right]^2 \right] \tag{90}$$

where

$$A = \frac{1 - P_e}{P_e} - 2 X_0 \Sigma_{t0}$$

$$\frac{W_1}{W_0} = \frac{W(X_0)}{W_0} + \frac{\Delta W_2}{W_0} + \Sigma_{a0} X_0 \left[\Sigma_1^*(X_1 - X_2) + 3\lambda_1 - 2 \right]$$

$$\frac{\Delta W_2}{W_0} = \frac{\Sigma_{a0} X_0 (X_2 - X_0)}{2 D_2}$$

$$\frac{W_2}{W_0} = \frac{W(X_0)}{W_0} + \frac{\Delta W_2}{2 W_0}$$

where $\lambda_1 = 0.710446$ is the extrapolation length for the inner surface of the moderator region and Σ_1^* is the moderator region transport cross section. X_0, X_1, and X_2 plate geometry dimensions and all other quantities are defined as in the corresponding cylindrical geometry equations. Equations (86) to (89) are then solved for the disadvantage weights.

2.4.1.1 Self-Shielding Factors

Disadvantage factor weighted self-shielding factors SSF (ISO,g) are calculated at each energy group g for every isotope ISO in the 3 region cell.

$$SSF(ISO,g) \; = \; \frac{\sum\limits_{j=1}^{3} W_j^g VF_j N_j^{ISO}}{DENS(ISO)} \tag{91}$$

where

$$DENS(ISO) \; = \; \sum\limits_{j=1}^{3} VF_j N_j^{ISO} \tag{92}$$

VF_j = volume fraction of the j region in the cell

N_j^{ISO} = the isotopic density in each region of the cell.

The self-shielding factors SSF(ISO,g) are printed to the output. Effective cell-average microscopic cross sections of reaction type x at each mesh point are obtained from

$$\left\langle \sigma_{x,g}^{ISO} \right\rangle = SSF(ISO,g)\sigma_{x,g}^{ISO} \quad . \tag{93}$$

The fine group cross sections in the thermal energy range (1.0e-5—5.0435 eV) are replaced by those self-shielded with the ABH method in the three region geometry when this option is requested.

2.5   Age Equations

An option to perform an age calculation utilizing a moments method, which was available in the GAM-1 code, has been retained in COMBINE. The derivation of this method is described in Reference 13 and has been omitted here. However, the final equations solved for the age are briefly described below. In multigroup form, the *ith* group moment equations for $\phi_{00_i}, \phi_{11_i}, and\ \phi_{20_i}$ are

$$\Sigma_{t_i} \phi_{00_i} = \sum\limits_{j=l}^{i} (\Sigma_{s0 j\to i} + \Sigma_{inj\to i} + 2\Sigma_{n,2nj\to i})\phi_{00_j}\Delta_j + S_i \tag{94}$$

$$\Sigma_{t_i} \phi_{11_i} = \sum\limits_{j=l}^{i} \Sigma_{slj\to i} + \phi_{11_j}\Delta_j + \phi_{00_i} \tag{95}$$

$$\Sigma_{t_i} \phi_{20_i} = \sum\limits_{j=l}^{i} (\Sigma_{s0 j\to i} + \Sigma_{inj\to i} + 2\Sigma_{n,2nj\to i})\phi_{20_j}\Delta_j + \frac{\phi_{11i}}{3} \tag{96}$$

where all cross section definitions are the same as those described previously for the B-1 solution. Solving each moment equation for the *ith* group we have the final solution equations:

$$\phi_{00_i} = \frac{\Sigma_{t_i} \phi_{00_i} = \sum\limits_{j=1}^{i} (\Sigma_{s0 j\to i} + \Sigma_{inj\to i} + 2\Sigma_{n,2nj\to i})\phi_{00_j}\Delta_j + S_i}{\sum\limits_{j=i+1}^{NOG} (\Sigma_{s0_{i\to j}} + \Sigma_{in_{i\to j}} + 2\Sigma_{n,2n_{i\to j}})\Delta_j - \Sigma_{n,2n_{i\to i}}\Delta_i} \tag{97}$$

$$\phi_{11_i} = \frac{\phi_{00_i} + \sum\limits_{j=1}^{i+1} \Sigma_{slj\to i} + \Sigma_{in_{j\to i}}\phi_{11_j}\Delta_j}{\Sigma_{ti} - \Sigma_{sI_{i\to i}}\Delta_i} \tag{98}$$

$$\phi_{20_i} = \frac{\dfrac{\phi_{11_i}}{3} + \sum_{j=1}^{i-1}(\Sigma_{s0\,j\to i} + \Sigma_{in_j\to i} + 2\Sigma_{n,2n_j\to i})\phi_{20_j}\Delta_j}{\sum_{j=i+1}^{NOG}(\Sigma_{s0_i\to j} + \Sigma_{in_{i\to j}} + 2\Sigma_{n,2n_{i\to j}})\Delta_j - \Sigma_{n,2n_{i\to i}}\Delta_i} \qquad (99)$$

$$\tau_i = \frac{\phi_{20_i}}{\phi_{00_i}} = \text{age to group i.} \qquad (100)$$

2.6 Transport Approximations

The difference between the S_N and P_N require[10]

$$\sigma_{lg'\to g}^{SN} = \sigma_{lg'\to g}^{PN} \quad \text{for } g' \neq g \qquad (101)$$

and

$$\sigma_{lg\to g}^{SN} = \sigma_{lg\to g}^{PN} - \sigma_{ltg}^{PN} + \sigma_{g}^{SN} \qquad (102)$$

where σ_{g}^{SN} is not determined. The choice of σ_{g}^{SN} gives rise to a "transport approximation" and various recipes are in use:

- Consistent-P approximation is

$$\sigma_{\ell g\to g}^{SN} = \sigma_{\ell g\to g}^{PN} - (\sigma_{\ell tg}^{PN} - \sigma_{otg}^{PN}) \qquad (103)$$

- Inconsistent-P approximation is

$$\sigma_{\ell g\to g}^{SN} = \sigma_{\ell g\to g}^{PN} - (\sigma_{\ell tg}^{PN} - \sigma_{N+1tg}^{PN}) \qquad (104)$$

- Diagonal transport approximation

$$\sigma^{SN}_{\ell g \to g} = \sigma^{PN}_{\ell g \to g} - (\sigma^{PN}_{\ell tg} - \sigma^{PN}_{N+1tg} + \sigma^{PN}_{N+1g \to g}) \tag{105}$$

- Bell-Hansen Sandmeier or extended transport approximation

$$\sigma^{SN}_{\ell g \to g} = \sigma^{PN}_{\ell g \to g} - (\sigma^{PN}_{\ell tg} - \sigma^{PN}_{N+1tg} + \sum_{g'} \sigma^{PN}_{N+1g \to g'}) \tag{106}$$

When the P_N to S_N correction is requested in the COMBINE7.0 input, the average of the above approximations is used for B-1 calculation but only the consistent-P approximation is used for B-3 calculation.

3.   USER'S GUIDE

3.1   Derivation of Diffusion Coefficient and Transport Cross Section

Although it is not evident from a cursory examination of B-1 equations, the mathematical structure of the system of equations resulting in Equations (30) and (31) is predetermined by the assumptions embodied in Equation (5). The assumptions, mathematically valid for a bare critical system satisfying simple diffusion boundary conditions, are characteristic of the broad generalities leading to the so-called First Fundamental Theorem of Reactor Theory.[18] The usual approach to the B-N energy-dependent equations involves taking the Fourier transform of the steady-state transport equation for a slab, with the implication that diffusion boundary conditions are somehow applicable to any order N.

The conceptual difficulty with this approach is that the resultant equations obscure any direct relationship between the spatial and energy dependence of the variables, unless the resultant equations are first subjected to Fourier inversion. Such a relationship is required to derive a rigorous definition of the energy-dependent diffusion coefficient by means of Fick's law. The procedure of deriving the B-1 equations by use of Equation (5) and diffusion theory boundary conditions for the scalar flux enables one to accomplish this end in a straightforward way.

Equation (5) establishes the desired relationship between the variables subject to the boundary conditions at the extrapolated boundary of the slab. Only the real part of e^{-iBx} satisfies the boundary conditions for the spatially dependent scalar flux. The scalar flux is obtained from Equations (5), (8), and (9) in the conventional manner.

$$\Phi(x,\mu,E) = e^{-iBx}\psi(B,\mu,E)$$

$$\Phi_0(x,E) = \int_{-1}^{1}\Phi(x,\mu,E)d\mu = e^{-iBx}\int_{-1}^{1}\psi(B,\mu,E)d\mu = e^{-iBx}\phi_0(B,E) \tag{107}$$

From Fick's law, we obtain the relationship between the scalar flux and current

$$\vec{J}(x,E) = -D(E)\vec{\nabla}\Phi_0(x,E) = -\vec{k}D(E)\frac{d}{dx}\Phi_0(x,E) = D(E)B\phi_0(B,E)i\vec{k}e^{-iBx}. \tag{108}$$

where $\vec{k}$ is the unit vector in the x direction.

Therefore, $\vec{J}(x,E)$ is also separable in space and energy, a result consistent with Equation (5).

$$\therefore \ \vec{J}(x,E) = J(B,E)i\vec{k}\ e^{-iBx} \tag{109}$$

where $J(B,E) = D(E)B\phi_0(B,E)$. \tag{110}

It has been pointed out that Equation (110) does not give a clear-cut relationship between J(E) and $\phi_1(E)$ in Equations (30) and (31) since Fick's law is perfectly general. An alternate method of obtaining Equation (110) will be given, which helps clear up any ambiguity that may exist. Using the same assumptions and utilizing Equations (5), (8), and (9), we have

$$\vec{J}^*(x,E) = \vec{k}\int_{-1}^{1}\mu\Phi(x,\mu,E)d\mu = \vec{k}\int_{-1}^{1}\mu e^{-iBx}\psi(B,\mu,E)d\mu = i\ \vec{k}\phi_1(B,E)e^{-iBx} \text{ when B is real,}$$

$$= \vec{k}\ \phi_1(B,E)e^{-iBx} \text{ when B is imaginary.}$$

Introducing Fick's law without reference to the scalar flux boundary conditions we have

$$\vec{J}^*(x,E) = -D(E)\vec{\nabla}\Phi_0(x,E) = D(E)B\phi_0(B,E)i\,\vec{k}e^{-iBx} \quad .$$

Now equate $\vec{J}^*(x,E)$ from the two preceding equations to obtain a result similar to Equation (110) as

$$\vec{J}^*(x,E) = \phi_1(B,E)i\,\vec{k}e^{-iBx} = D(E)B\phi_0(B,E)i\,\vec{k}e^{-iBx} \text{ when B is real,}$$

$$= \phi_1(B,E)\vec{k}e^{-iBx} = D(E)B\phi_0(B,E)i\,\vec{k}e^{-iBx} \text{ when B is imaginary;}$$

$$\therefore \vec{J}(B,E) = \phi_1(B,E) = D(E)B\phi_0(B,E) \text{ when B is real,}$$

$$= iD(E)B\phi_0(B,E) \text{ when B is imaginary.} \tag{111}$$

From Equation (107), $D(E)$ is defined as

$$D(E) = \frac{\phi_1(B,E)}{B\phi_0(B,E)} \text{ when B is real,}$$

$$= \frac{\phi_1(B,E)}{iB\phi_0(B,E)} \text{ when B is imaginary.} \tag{112}$$

Equation (112) gives an unambiguous definition of the diffusion coefficient within the framework of the B-1 equations for a bare slab. The definition of the B-1 transport cross section at energy E in the domain of Fick's law is

$$\Sigma_{tr}(E) = \frac{1}{3D(E)} = \frac{B\,\phi_0(B,E)}{3\phi_1(B,E)} \text{ when B is real,}$$

$$\Sigma_{tr}(E) = \frac{1}{3D(E)} = \frac{iB\,\phi_0(B,E)}{3\phi_1(B,E)} \text{ when B is imaginary.} \tag{113}$$

In order to use Equation (113), the current from the solution run needs to be nonzero. Thus, when a zero buckling is input to the code, neither the diffusion coefficient nor the transport cross section is calculated. This situation corresponds to an infinite medium problem for which there is no net neutron current flow. If a diffusion coefficient is desired for a near infinite medium situation, a small but finite buckling input to the code will produce the desired results.

3.2   Summary Edits for Broad Group Constants

The equations for calculating the average cross sections are presented in this section in as complete a manners practical. This should facilitate the proper use of the average cross sections generated by the spectrum code.[3,4]

The COMBINE spectrum, cross-section library tape contains data tabulated for 167 fine lethargy groups. In a normal spectrum problem, the data are coalesced into a broad group structure, specified by the user, containing one or more fine groups per broad group. The coalescing is performed by utilizing 167 fine group fluxes and/or currents as the weighting functions. These energy dependent fluxes and currents may either be calculated for a particular reactor system or taken from an immediately preceding problem. The latter type of calculation is referred to as a cell calculation. The output from a spectrum problem normally includes average macroscopic cross-section data and may include average microscopic data for each material in the macroscopic calculation, if desired. As an alternative to the normal output, the user may request the calculation of macroscopic effective diffusion theory constants (blackness theory) in lieu of the normal cross section output.

Figure 4 illustrates the notation used in describing the average cross-section data and the relation of the fine-group data to the broad-group data generated in a spectrum problem. In Figure 4, broad group G contains the fine groups I through I+N and all averages for broad group G are performed over this range of fine groups.

In the notation used above, NOG refers to the number of fine groups and NOAG refers to the number of broad groups.

Fine Groups	1	2	3	· · ·	I-1	I	I+1	· · · ·	I+N-1	I+N	I+N+1	· · ·	K-1	K	K+1	· ·	K+N-1	K+N	K+N+1	· ·	NOG-1	NOG

Broad Groups	1	· ·	G	· · ·	G'	NOAG

Figure 4. Spectrum group structure.

The average cross sections are determined by the familiar relation

$$\overline{\Sigma} = \frac{\int_E \Sigma(E)w(E)dE}{\int_E w(E)dE} \tag{114}$$

where $\overline{\Sigma}$ represents the energy dependent cross section $\Sigma(E)$, and $w(E)$ is the energy dependent weighting function, normally either the fluxes or the currents. In the actual calculation, the continuous functions of the cross section and weighting parameter are represented by 167 fine group average values associated with a lethargy width, Δ_i. Thus,

$$\overline{\Sigma} = \frac{\sum_i \Sigma_i w_i \Delta_i}{\sum_i w_i \Delta_i} \quad . \tag{115}$$

In all cases, the integrations are performed utilizing the trapezoidal rule.

3.2.1   Average Macroscopic Cross Sections

The macroscopic cross-section data generated by the COMBINE7.0 code is described below in considerable detail to facilitate its proper use. In all cases, the average quantity has been defined for the broad group G where $\Sigma_i (cm^{-1}) = \sum_{k=1}^{NOI} N_k \sigma_i^k =>$ macroscopic cross section for i^{th} fine group of a system containing NOI materials

where N_k and σ_i^k are the atom density (# of atoms $\times 10^{-24}$ per cubic centimeter) and microscopic cross section (barns/atom), respectively, for the kth material and

Δ_i => lethargy width of fine group i

ϕ_i => average scalar flux in fine group i

J_i => average current (P_i flux) in fine group i

ψ_i => average P_2 flux for group i

χ_i => average P_3 flux for group i

$\overline{\Sigma}_{x_G}$ => average cross section for broad group G for a particular reaction denoted by x

ϕ_G => integrated scalar flux for group G

J_G => integrated current (P_1 flux) for group G

ψ_G => integrated P_2 flux for group G

χ_G => integrated P_3 flux for group G.

The integrated fluxes for broad group G are calculated as

$$\Phi_G = \sum_{i=I}^{i+N} \phi_i \Delta_i \tag{116}$$

$$J_G = \sum_{i=I}^{i+N} J_i \Delta_i \tag{117}$$

$$\psi_G = \sum_{i=I}^{i+N} \psi_i \Delta_i \tag{118}$$

$$\chi_G = \sum_{i=I}^{i+N} \chi_i \Delta_i \tag{119}$$

Average absorption cross section

$$\overline{\Sigma}_{a_G} = \frac{\sum_{i=I}^{I+N} \Sigma_{a_i} \phi_i \Delta_i}{\Phi_G} \tag{120}$$

Average fission cross section

$$\overline{\Sigma}_f = \frac{\sum_{i=I}^{I+N} \Sigma_{f_i} \phi_i \Delta_i}{\Phi_G} \tag{121}$$

Average number of neutrons per fission times the fission cross section

$$v\overline{\Sigma}_f = \frac{\sum_{i=I}^{I+N} v_i \Sigma_{f_i} \phi_i \Delta_i}{\Phi_G} \tag{122}$$

Average number of neutrons produced per fission

$$\bar{\nu}_G = \frac{\overline{\nu \Sigma}_{f_G}}{\overline{\Sigma}_{f_G}} \tag{123}$$

Average capture cross section

$$\overline{\overline{\Sigma}}_{c_G} = \overline{\overline{\Sigma}}_{a_G} - \overline{\overline{\Sigma}}_{f_G} \tag{124}$$

Average elastic, inelastic,(n,2n), (n,3n), or (n,4n) cross section for isotropic transfer from group G to G

$$\overline{\overline{\Sigma}}_{x_{G \to G'}} = \frac{\displaystyle\sum_{i=I}^{I+N} \sum_{k=K}^{K+N} \Sigma_{x_{i \to k}} \phi_i \Delta_i}{\Phi_G} \qquad x_{i \to k} = \begin{cases} s_0 \ (elastic) \\ in \ (inelastic) \\ n, 2n \ reactions \\ n, 3n \ reactions \\ n, 4n \ reactions \end{cases} \tag{125}$$

Average linearly anisotropic component of elastic or inelastic transfer cross section from group G to G′

$$\overline{\overline{\Sigma}}_{x1_{G \to G'}} = \frac{\displaystyle\sum_{i=I}^{I+N} \sum_{k=K}^{K+N} \Sigma_{x_{i \to k}} J_i \Delta_i}{J_G} \qquad x_{i \to k} = \begin{cases} s_i \ (elastic) \\ in \ (inelastic) \end{cases} \tag{126}$$

Average P₂ component of the elastic transfer cross section from group G to G

$$\overline{\overline{\Sigma}}_{s2_{G \to G'}} = \frac{\displaystyle\sum_{i=I}^{I+N} \sum_{k=K}^{K+N} \Sigma_{2_{i \to k}} \psi_i \Delta_i}{\psi_G} \tag{127}$$

Average P₃ component of the elastic transfer cross section from group G to G

$$\overline{\overline{\Sigma}}_{s3_{G \to G'}} = \frac{\displaystyle\sum_{i=I}^{I+N} \sum_{k=K}^{K+N} \Sigma_{3_{i \to k}} \chi_i \Delta_i}{\chi_G} \tag{128}$$

Average total transfer cross section for transfer from group G to G

$$\overline{\overline{\Sigma}}_{tt_{G \to G'}} = \overline{\overline{\Sigma}}_{s0_{G \to G'}} + \overline{\overline{\Sigma}}_{in_{G \to G'}} + 2\overline{\overline{\Sigma}}_{n,2n_{G \to G'}} + 3\overline{\overline{\Sigma}}_{n,3n_{G \to G'}} + 4\overline{\overline{\Sigma}}_{n,4n_{G \to G'}} \tag{129}$$

Average of isotropic elastic, inelastic, (n,2n), (n,3n), or (n,4n) total scattering cross section

$$\overline{\overline{\Sigma}}_{t_{xG}} = \sum_{G'=G}^{NOAG} \overline{\overline{\Sigma}}_{x_{G \to G'}} \qquad \chi_{G \to G'} = \begin{cases} s_0 \ (elastic) \\ in \ (inelastic) \\ n, 2n \ reactions \\ n, 3n \ reactions \\ n, 4n \ reactions \end{cases} \tag{130}$$

Average linearly anisotropic component of the elastic total scattering cross section

$$\overline{\overline{\Sigma}}_{t_{s1G}} = \sum_{G'=G}^{NOAG} \overline{\overline{\Sigma}}_{1_{G \to G'}} \tag{131}$$

Average out-scatter cross section

$$\overline{\overline{\Sigma}}_{out_G} = \sum_{G'=G+1}^{NOAG} \left[\overline{\overline{\Sigma}}_{s0_{G\to G'}} + \overline{\overline{\Sigma}}_{in_{G\to G'}} + \overline{\overline{\Sigma}}_{n,2n_{G\to G'}} + \overline{\overline{\Sigma}}_{n,3n_{G\to G'}} + \overline{\overline{\Sigma}}_{n,4n_{G\to G'}} \right] + \sum_{G'=G-\max up}^{G-1} \overline{\overline{\Sigma}}_{up_{G\to G'}} \tag{132}$$

Average removal cross section

$$\overline{\overline{\Sigma}}_{r_G} = \overline{\overline{\Sigma}}_{a_G} + \overline{\overline{\Sigma}}_{out_G} + \sum_{G'=G-\max up}^{G-1} \overline{\overline{\Sigma}}_{up_{G\to G'}} \tag{133}$$

Average total cross section

$$\overline{\overline{\Sigma}}_{t_G} = \overline{\overline{\Sigma}}_{a_G} + \overline{\overline{\Sigma}}_{s0_G} + \overline{\overline{\Sigma}}_{in_G} + \overline{\overline{\Sigma}}_{n,2n_G} + \overline{\overline{\Sigma}}_{n,3n_G} + \overline{\overline{\Sigma}}_{n,4n_G} \tag{134}$$

Integrated fission source

$$S_G = \sum_{i=I}^{I+N} S_i \tag{135}$$

Average inverse velocity

$$\left(\overline{1/v}\right)_G = \frac{\sum_{i=1}^{I+N} (1/v)_i \Phi_i \Delta_i}{\Phi_G} \tag{136}$$

Average diffusion coefficient (from Fick's law)

$$\overline{D}_G = \frac{J_G}{B\Phi_G} \tag{137}$$

Average transport cross section

$$\overline{\overline{\Sigma}}_{tr_G} = \frac{1}{3\overline{D}_G} = \frac{B\Phi_G}{3J_G} \tag{138}$$

If a cell calculation is performed—a spectrum obtained from a previous problem is used as a weighting function to generate average cross sections for another material—the diffusion coefficients and transport cross sections are defined in terms of cross sections of the material being averaged. An appropriate definition can be obtained from Equation (37). By first solving Equation (37) for $\frac{B}{3}\phi$, and

then dividing both sides by $J_i(\phi_1)$. We then have

$$\overline{\overline{\Sigma}}_{tr_{G_{cell}}} = \frac{\gamma^g \Sigma_t^g \Phi_1^g - \sum\limits_{g'=1}^{G} \Sigma_{s1}^{g' \to g} \Phi_1^g \dfrac{\Delta g'}{\Delta g}}{\Phi_1^g} \tag{139}$$

and

$$\overline{D}_{G_{cell}} = \frac{1}{3\overline{\overline{\Sigma}}_{tr_{G_{cell}}}} \quad . \tag{140}$$

In addition to the usual average cross-section data described above, some other miscellaneous cross-section data are calculated and printed out for the user. These quantities include the absorption and out-scatter cross sections for each broad group corrected for the (n,2n), (n,3n), and (n,4n) reaction. In the usual few group diffusion code the out-scatter cross section is generally used both as a removal term and a source term. However, the standard out-scatter term calculated by COMBINE accounts for the loss of one neutron by an (n,2n), (n,3n), or (n,4n) reaction in a particular broad group. Therefore, when this same term is used as a source term for the next group in a few group diffusion theory calculation of reactivity, it represents only one-half, one-third, or one-foruth of the actual source into that group from the (n,2n), (n,3n), or (n,4n) transfer reaction. Thus, in the corrected cross-section data, the out-scatter cross section is defined as

$$\overline{\Sigma}_{outG}^* = \sum\limits_{G'=G+1}^{NOAG} \left(\overline{\Sigma}_{s0_{G \to G'}} + \overline{\Sigma}_{in_{G \to G}} + 2\overline{\Sigma}_{n,2n_{G \to G'}} + 3\overline{\Sigma}_{n,3n_{G \to G'}} + 4\overline{\Sigma}_{n,3n_{G \to G'}} \right) + \sum\limits_{G'=G-\max up}^{G-1} \overline{\Sigma}_{up_{G \to G'}} \tag{141}$$

where now a corrected absorption term is defined as

$$\Sigma_{a_G}^* = \Sigma_{a_G} - \sum\limits_{G'=G}^{NOAG} \Sigma_{n,2n_{G \to G'}} - 2\sum\limits_{G'=G}^{NOAG} \Sigma_{n,3n_{G \to G'}} - 3\sum\limits_{G'=G}^{NOAG} \Sigma_{n,4n_{G \to G'}} \tag{142}$$

to conserve neutrons. The last term on the right-hand side of Equation (141) reflects the thermal outgoing upscattering.

3.2.2   Monoenergetic Transport Cross Section

The monoenergetic transport cross section offers an alternative to the Fick's law definition given by Equation (138) or (139) and has the redeeming feature that is always positive regardless of the shape of the spectrum. It is the classical value based on its definition from the one-energy transport equation.[9] For broad group G, the macroscopic value is

$$\overline{\Sigma}_{tr_G} = \overline{\overline{\Sigma}}_{t_G} - \Sigma_{t_{s1_G}} \tag{143}$$

Where the cross sections on the right-hand side are given by Equations (134) and (131).

3.2.3   Average Microscopic Cross Sections

The average microscopic cross sections are defined in a manner similar to the macroscopic cross sections. The main difference is the use of the microscopic cross section, σ, in the place of the macroscopic cross section, Σ. The one exception is the definition of a microscopic transport cross section. A unique definition of a microscopic transport cross section presents a conceptual difficulty in the same way that a microscopic diffusion coefficient would. The macroscopic values are extensive quantities resulting from some form of Fick's law, and there is no corresponding, physically meaningful relationship for microscopic values. Rather, it has become traditional to define a microscopic transport cross section

only in the metaphysical sense that "the whole is the sum of its assumed parts"; then from this, the macroscopic diffusion coefficient follows:

$$\bar{D}_G = \frac{1}{3\sum_k N_k \bar{\sigma}^k_{tr_G}} = \frac{1}{3\bar{\Sigma}_{tr_G}} \tag{144}$$

This being the case, the only thing required to define the microscopic transport cross section $\bar{\sigma}_{tr_G}$ in Equation (141) is a consistency relationship that will yield the proper macroscopic transport cross section for a particular mixture of materials as calculated by Equation (138). Any number of such consistency relationships could be defined and applied, as long as the macroscopic transport cross section in the denominator of Equation (143), computed from microscopic values, gives the same result as Equation (138).

One such equation that will yield the desired results is Equation (139), where Σ^* becomes the appropriate σ^k in each term of Equation (135). The broad microscopic transport cross section for the kth isotope is then given by

$$\bar{\sigma}^k_{tr_G} = \frac{\sum_{i=1}^{I+N} \gamma_i \sigma_{t_i} J_i \Delta_i - \sum_{G'=1}^{NOAG} \sigma_{s1_{G' \to G}} J_{G'}}{J_G} \tag{145}$$

A measure of the "arbitrariness" of this definition of the microscopic transport cross section is that it is entirely possible that the microscopic transport cross section as given by Equation (145) can be negative for one or several materials in the mixture, and yet, when multiplied by Nk and summed over all materials in the mixture, will yield the proper macroscopic transport cross section as given by Equation (138). This situation occurs when the mixture contains large amounts of a strong absorber and the resultant flux and current spectra are very hard. For moderating materials with a small absorption cross section, the second term in the numerator of Equation (145) can then be the leading term due to the high current weights given the transfer cross sections $\sigma_{s1_{G' \to G}}$ when G lies in the energy range of depressed flux and current at low energy. The resultant microscopic transport cross sections, even though negative, are consistent in the sense of Equation (143), since "consistency" is all that is required of them in the definition.

The same pathologic situation can occur for cell materials being averaged over the flux and current from another spectral problem. If the spectral problem contained a very strong absorber producing a very hard spectra and the cell material does not contain much absorption, the macroscopic transport cross section from Equation (134) can be negative in low-energy groups. In this case, the negative result could be interpreted as indicating that the homogenization for the cell material was not judiciously chosen.

3.2.4   Effective Diffusion Theory Constants (Blackness Theory)

Extensive use is made of diffusion theory in nuclear reactor design analysis; however, inherent in the diffusion theory approximation is its inadequacy in highly absorbing, low scattering regions such as control rods. Because many reactor systems include such regions, the blackness theory was developed to provide a convenient technique for handling these regions without recourse to a higher order transport solution. The approach is to treat the absorbing region as a fictitious diffusing medium of the same thickness but use blackness constants in the diffusion calculation, which yield more correct fluxes than could be obtained with the usual constants. The spectrum code incorporates an option to calculate blackness theory diffusion coefficients and absorption cross sections for use in highly absorbing regions of a system under study. The assumptions made in the development of the formulism used to calculate the

effective constants are that the absorbing region is a thin slab and the immediately surrounding regions can be adequately handled by diffusion theory methods. These effective constants incorporate factors to account for the mesh structure used to describe the region in a finite difference solution of the diffusion equation. A complete development of this theory can be found in Reference 34 and a review of its use may be found in References 35 and 36.

3.2.5   Mixed Number Density (MIND) Constants

An input option allows for the production of mixed number density (MND) constants[37] for one single broad group in the thermal spectrum. No multiple thermal group MND constants are defined. The constants are defined as

$$\Sigma_{MND} = \overline{\Sigma \mathbf{V}} = \frac{\int_0^{E_I} \Sigma(E)\phi_{SP}(E)dE}{\int_0^{E_1} \frac{1}{\mathbf{v}(E)}\phi_{SP}(E)dE} = \frac{\overline{(\Sigma)}_{SP}}{\left(\frac{1}{\mathbf{v}}\right)_{SP}} \tag{146}$$

where

Σ = the macroscopic absorption or fission cross section

$\phi_{SP}(E)$ = thermal flux spectrum solution

E_1 = upper energy of the single MND group

$\mathbf{v}(E)$ = velocity at energy E.

$$D_{MND} = \overline{D\mathbf{v}}_{max} = \frac{\int_0^{E_1} D(E)M(E)dE}{\int_0^{E_1} \frac{M(E)dE}{\mathbf{v}(E)}} = \frac{(\overline{D})_{max}}{\left(\frac{\overline{1}}{\mathbf{v}}\right)_{max}} \tag{147}$$

$$\Sigma_{tr}^{MND} = \frac{1}{3D_{MND}} \tag{148}$$

$$\sigma_{tr}^{MND} = \left(\frac{\overline{\sigma}_{tr}}{\mathbf{v}_{max}}\right) = \frac{\int_0^{E_1} \frac{M(E)dE}{\mathbf{V}(E)}}{\int_0^{E_1} \frac{M(E)dE}{\sigma_{tr}(E)}} = \frac{\left(\frac{\overline{1}}{\mathbf{v}}\right)_{max}}{\left(\frac{1}{\sigma_{tr}}\right)_{max}} \tag{149}$$

where "max" indicates averaging over a Maxwellian spectrum and M(E) = Maxwellian distribution at temperature T;

$$M(E)dE \frac{E[\exp(-E/kT)]}{(kT)^2}dE \tag{150}$$

where k is Boltzmann's constant and the average energy = 3/2kT and T corresponds to the ambient energy of the region.[35]

For each Σ in Equations (146) through (150) there is a corresponding microscopic σ calculated for the output files. σ_{tr} replaces D. There are also normalized MND constants defined as:

$$D^{NORM} = \frac{D_{MND}}{2.2 \times 10^5}$$

$$\Sigma_a^{NORM} = \frac{\Sigma_a^{MND}}{2.2 \times 10^5}$$

$$\Sigma_F^{NORM} = \frac{\Sigma_F^{MND}}{2.2 \times 10^5} \tag{151}$$

Normalized microscopic values are defined as:

$$\sigma_{tr}^{NORM} = (2.2 \times 10^5)\sigma_{tr}^{MND}$$

$$\sigma_a^{NORM} = \frac{\sigma_a^{MND}}{2.2 \times 10^5}$$

$$\sigma_F^{NORM} = \frac{\sigma_F^{MND}}{2.2 \times 10^5} \tag{152}$$

If the "unnormalized MND values" are used in a spatial diffusion calculation, the thermal flux will be values of neutron density. If normalized values are used, the thermal flux will be the 2200 meters/sec thermal flux. Summary data printed (and punched) will include MND values of

$$\Sigma_{tr}, D, \Sigma_a, \Sigma_F, \nu\Sigma_F, \sigma_{tr}, 1/3\sigma_{tr}, \sigma_a, \sigma_F, and\ \nu\sigma_F.$$

3.2.6   Multiplication Factors

Multiplication factors k_{inf} and k_{eff} are calculated for a COMBINE problem and printed after the broad group edits. k_{inf} is calculated as

$$k_{inf} = \frac{\sum\limits_{G=1}^{GG} \nu\Sigma_{f_G} \phi_G}{\sum\limits_{G=1}^{GG} \Sigma_{a_G} \phi_G} \tag{153}$$

where the numerator is the production rate of fission neutrons over the broad group spectra, the denominator is the absorption rate, and GG is the total number of broad groups. When $B = C$ or $B = -iC$ with a real constant C, then

$$k_{eff} = \frac{\sum\limits_{G=1}^{GG} \nu\Sigma_{f_G} \phi_G}{\sum\limits_{G=1}^{GG} \left(\Sigma_{a_G} + D_G C_G^2\right)\phi_G} \tag{154}$$

where D_G is the broad group diffusion coefficient and C_G^2 are the buckling coefficients specified in the floating point input data.

When $B = iC$,

$$k_{eff} = \frac{\displaystyle\sum_{G=1}^{GG} \nu \Sigma_{f_G} \phi_G}{\displaystyle\sum_{G=1}^{GG} \left(\Sigma_{a_G} - D_G C_G^2 \right) \phi_G} \qquad (155)$$

since there is a negative leakage. In this case k_{eff} exceeds k_{inf}.

4. COMBINE7.0 FILES DESCRIPTION

Logical Unit	Name/status	Format	Usage
401	matxs.lib	unformatted	Boondarenko based cross section library
402	reres.lib	formatted	Resolved resonance parameters library
403	combine.inp	formatted	COMBINE input
404	combine.out	formatted	COMBINE output
405	anisn.inp	formatted	ANISN input
406	anisn.out	formatted	ANISN output
430	combine.sig/ anisnc4.lib	formatted	Formerly nt4=4 in ANISN
437	combine.flx	formatted	Flux output
435	anisnc4.flux	formatted	Formerly 10 in ANISN
445	anisnc4.pun	formatted	Formerly 7 in ANISN
439	scratch	unformatted	temporary self shielded static cross sections, adum, generated in s.r spectrum
411–429	scratch	unformatted	temporary cross section files for cases to be 1-D transport (ANISN) corrected when ioned = 1, to be used in s.r. xscoal with ioned = 2.
431	scratch	Direct access	total cross sections for Bondarenko self shielding
432	scratch	unformatted	static (adum) cross section file for region 1 in ABH
433	scratch	unformatted	static (adum) cross section file for region 2 in ABH
434	scratch	unformatted	static (adum) cross section file for region 3 in ABH
436	scratch	unformatted	temporary flux and higher moments
438	scratch	unformatted	shielded bondarenko cross section file,adum, generated in s.r. bondar
440	scratch	unformatted	(sigaz(i),sigfz(i),sigsz(i),amu1(i),i=1,np) for the pricipal resonance absrober after doppler broadening
441	scratch	unformatted	temporary (sigaz(i),sigfz(i),sigsz(i),amu1(i),i=1,np) for the pricipal and admixed resonance absrobers before doppler broadening
442	scratch	unformatted	sa0,ss0,etc., and collision probability file for ABH
446	scratch	unformatted	(sigaz(i),sigfz(i),sigsz(i),amu1(i),i=1,np) for the first admixed resonance absrober after doppler broadening
447	scratch	unformatted	(sigaz(i),sigfz(i),sigsz(i),amu1(i),i=1,np) for the second admixed resonance absrober after broadening
448	scratch	unformatted	(sigaz(i),sigfz(i),sigsz(i),amu1(i),i=1,np) for the third resonance absrober after doppler broadening
443	scratch	formatted	formats and writes broad group output data in s.r. xscoal for post processing
444	scratch	unformatted	
450–499	scratch	unformatted	thermal matrix cross sections for isotopes used in both sr. bonche and bondar, is+449
407	scratch	unformatted	Formerly nt8=8 in ANISN
408	scratch	unformatted	Formerly nt9=9 in ANISN
409	scratch	unformatted	Formerly nt1=1 in ANISN
410	scratch	unformatted	Formerly ntt=2 in ANISN
449	scratch	unformatted	Formerly 3 in ANISN

5. COMBINE7.0 INUT STRUCTURE

Position	Name	Description of Data
Word 1	IONED	Type of problem to be performed
		0 Standard COMBINE problem.
		1 COMBINE/ANISN/COMBINE sequence.
		-1 ANISN only.
Word 2	NSTACK	Total number of stacked cases.

This is the first card in combine.inp, which is always required.

When IONED = 0, a standard COMBINE only is performed and the COMBINE input data as described in the next section follows.

When IONED = 1, a standard COMBINE calculation in the full 167 fine-group structure is performed, generating anisnc4.lib. An ANISN input file, 'anisn.inp' with the igm=167, is required. An ANISN calculation is performed to provide flux and moments back to COMBINE portion. The broad group (as specified in the input) cross section coalescing is performed in COMBINE portion, generating 'combine.sig'.

When IONED = -1, a standard ANISN calculation is performed, no more COMBINE input data is required. The files 'anisn.inp' and 'anisnc4.lib' are required.

6.   COMBINE7.0 INPUT DATA FILE ORGANIZATION

A problem consists of a title record, comment records (optional), data records, and a terminator record. A listing of the records is printed at the beginning of each problem. The order of the title, data, and comment records is unimportant except that only the last title record, or the last data record having a particular data record number, will be used.

When a format error is detected, a line containing a dollar sign ($) located under the character causing the error and a comment giving the column of the error is printed. An error flag is set such that input processing continues, but the problem will be aborted at the end of input processing.

1. **Title Record.** *A title record must be entered for each problem.* A title record is identified by an equal sign (=) as the first nonblank character. The title record is normally placed first in the problem.

2. **Comment Records.** An asterisk (*) or a dollar sign ($) appearing as the first nonblank character identifies the record as a comment record. Blank records are treated as comment records. The only processing of comment records is printing of contents. Comment records may be placed anywhere in the input file.

3. **Data Records.** The data records contain a varying number of fields, which may be integer, floating point, or alphanumeric. Blanks preceding and following fields are ignored.

    The first field on a data record is a record number that must be an unsigned integer. If the first field has an error or is not an integer, an error flat is set. Consequently, data on the record are not used and the record will be identified by the record number in the list of unused data records. After each record number and the accompanying data are read, the record number is compared to previously entered record numbers. If a matching record number is found, the data entered on the previous record are replaced by the data on the current record. If the record being processed contains only a record number, the record number and the data entered on the previous record are deleted. If a record causes replacement or deletion of data, a statement is printed indicating that the record is a replacement.

    A number field on a data record is started by either a digit (0 through 9), a sign (+ or -), or a decimal point (.). A comma or a blank (with one exception noted below) terminates a particular number field. The number field has a number part, and optionally, an exponent part. A number field without a decimal point or an exponent is an integer field; a number field with either a decimal point, an exponent, or both is a floating-point field. A floating-point field without a decimal point is assumed to have a decimal point immediately in front of the first digit. The exponent denotes the power of 10 to be applied to the number part of the field. The exponent part has an E and a sign (+ or -) followed by a number giving the power of 10. These rules for floating point numbers are identical to those for entering data in FORTRAN e or f format fields except that no blanks (one exception) are allowed between characters. Floating point data punched by FORTRAN programs can be read. To permit reading of floating point data, a blank following an E denoting an exponent is treated as a plus sign. Acceptable ways of entering floating-point numbers, all containing the quantity 12.45, are illustrated by six fields: 12.45, +12.45, 1245+2, 1.245+1, 1.245e1, and 1.245e+1.

4. **Terminator Records.** A record having a period as the first nonblank character is used as a terminator. Most previous input records are erased before the input to the next problem is processed. Therefore, each problem must contain a complete input data file sufficient for that type of problem. Also, the final problem is terminated by a period record.

5. **Data Record Summary.** A data record contains: the record number and a descriptive title of the data contained on the record; an explanation of any variable data input on this record; and the order of the data on the record, the variable name, and the input data requirements, where applicable. Any variable names beginning with the letters I, J, K, L, M, or N are of type INTEGER. Any variable names starting with another letter are of type REAL. After N words on a record, default values will be used for the rest. However, data items should not be skipped up to N words.

6.1 Title Record and Integer Data Records

6.1.1 Title Record

A title record must be present for each problem and is identified by an equal sign (=) as the first character on the record.

6.1.2 Problem Basic Control Information Record 1010101

This record is required for each problem. The first four words are always required.
(N words, $4 \leq N \leq 9$)

Position	Name	Description of Data
Word 1	NTYPE	Type of calculation to be performed.
		1— Standard B-1 flux approximation if LEG = 1, or Standard B-3 flux approximation if LEG = 3.
		2— Standard P-1 flux approximation if LEG = 1. $\gamma(E) = 1.0$ in Equation (16).
		4— Cell calculation; fluxes, from the preceding problem will be used for averaging cross sections. Currents will be recalculated from Equations (32) and (162) using the P-1 approximation with $\gamma(E) = 1.0$.
		6— Blackness calculation; fluxes from the preceding problem will be used to obtain effective diffusion theory cross sections.
Word 2	LEG	1— B-1 or P-1 calculation.
		3— B-3 calculation.
Word 3	NOI	Number of materials in the spectrum, cell or blackness calculation (1 < NOI < 50).
Word 4	NOUG	Total number of broad groups in the spectrum, cell or blackness calculation (1 < NOUG < 167).
Word 5	MICR	Microscopic cross section option (must be set to 1 if microscopic cross sections are to be output to the ASCII cross section file.
		0— No average microscopic data desired. (Default)
		1— Calculate average microscopic cross sections.
Word 6	MSTU	Source option.
		-1— Fission rate weighted spectrum will be used. If not specified or zero, the code set MSTU = -1. (Default)
		N— Fission spectrum of the material XX in the 10420XX card (N = XX).
		(If not specified or zero, the code sets MSTU=-1.)
		When rabs in 1043XXY /= 0, MSTU is reset to -1.
Word 7	MAXIT	Maximum number of iterations when up scattering is present. When 0, the code sets MAXIT = 500. The conversion iteration stops when satisfied either "CONV" or MAXIT criteria. When there is no up scattering, no iteration is needed.
Word 8	ICHET	0— No ABH thermal calculation is being requested. No 2XXXXXX records will be present. (Default)
		1— An ABH thermal calculation will be performed for rectangular geometry. Input is on 2XXXXXX records.
		2— Cylindrical ABH geometry.
		3— Spherical ABH geometry.
Word 9	ISN	Transport correction
		0— No transport correction (default)
		1— P_N to S_N correction desired.

Position	Name	Description of Data
Word 10	MAGE	Age calculation option.
		0— No age calculation desired. (Default)
		1— Age calculation desired.
Word 11	MNDFLG	0— No Mixed number density calculation. (Default)
		1— Mixed number density calculation. Requires 1490001 record.

6.1.3 Energy Group Structure Record 10102YY

This record is required for the first problem. YY specifies up to 20 continuation records.
(N words, $1 \leq N \leq 167$)

Position	Name	Description of Data
Word 1 to Word NOUG	NGP (I)	Broad energy group structure starting with the *upper limit* of the first broad group.
		($1 < I < 167$). See Table 1 following input description. The upper limit of broad group number 1 must be the fine group number 1 (corresponding to 20.0 MeV).
		$1 <$ number of broad groups < 167

Resonance Calculation Option Record 102010Y. This record is required only if Nordheim resonance calculations are to be performed for resonance materials. If this record is not present, NXSR = 0 for all materials.

Y specifies up to nine continuation records. (N words, $1 \leq N \leq 50$)

Position	Name	Description of Data
Word 1 to NOI	NXSR (I)	Resonance calculation option ($1 < I < 50$).
		0—Bondarenko self shielding treatment.
		1—Nordheim self shielding treatment (use only for those isotopes with iwr > 0, see Table 2).
		2—Average of Bondarenko and Nordheim treatments. Highly recommended for the case of LEU.

6.1.4   Macroscopic Interface File Option Record 1030101

This record is only required for each problem for which macroscopic cross-section data are to be output to the interface file, combine.sig. (N words, $2 \leq N \leq 5$)

Position	Name	Description of Data
Word 1	IPUN	Macroscopic interface file data option.
		0—No output macroscopic data desired
		1—Output the macroscopic cross sections to the ASCII cross-section file.
		2—Output the calculated energy-dependent fluxes in neutral ASCII format.
		3—Output both the macroscopic cross sections and the fluxes.
Word 2	MTLNO	Material number used to reference interface file macroscopic cross-section data.
		If MTL(I) < 900, isotope chi values will be added in the '5d' record of the ISOTXS format, having ICHI set to 1, regardless whether they are all 0.0.
Word 3	NCOP	Format flag for ASCII cross section output file.
		0—INL format. (Default)
		1—ANISN format. (Not working currently, to be fixed)
		2 CCCC ISOTOX format
		3—AMPX Working Library format suitable for KENO5A. (not working currently, to be fixed)
Word 4	IAD	Option parameter that will be placed in columns 2 and 3 of the title record accompanying the macroscopic data to indicate to the diffusion or transport theory codes how these data are to be used in updating a cross-section library file associated with these codes. (Used only with INL format).
		0—Completely replace material MTLNO on the library tape. (Default)
		1—Replace only those values on the library tape for material MTLNO which are entered on the interface records.
Word 5	IDIFF	Option parameter that will be placed in columns 4 and 5 of the title record accompanying the diffusion or transport theory codes indicating whether to use the values of the diffusion coefficients or transport cross sections. (Used only with INL format).
		0—Use the transport cross sections (Monoenergetic definition). (Default)
		1—Use the diffusion coefficients (Fick's law definition).

6.1.5   Microscopic Interface File Option Record 10302XX

These records are required only for those materials for which microscopic cross-section data are to be output to the interface file, combine.sig. The material number is indicated by XX ($1 \leq XX \leq NOI$) (N words, $2 \leq N \leq 4$). Also MICR on record 1010101 must be = 1.

Position	Name	Description of Data
Word 1	NPUN(I)	Microscopic interface file output option for material I.
		0—Do not output microscopic data for this material.
		1—Output self-shielded microscopic cross-section data.
Word 2	MTL(I)	Material number used to reference microscopic cross-section data for material I. This is used for INL and ISOTXS format output. For ANISN and AMPX format, the materials are output numbered in ascending order as processed. If MTL(I) < 900, isotope chi values will be added in the '5d' record of the ISOTXS format, having ICHI set to 1, regardless whether they are all 0.0.
Word 3	NAD(I)	Option parameter that will be placed in columns 2 and 3 of the title record accompanying the interface microscopic data for Material I to indicate to the diffusion or transport theory codes how these data are to be used in updating a cross-section library file associated with these codes. (Used only with INL format).
		0—Completely replace material MTL(I) on library file. (Default)
		1—Replace only those values on the library file for material MTL(I) that are entered on the records.
Word 4	NDIFF(I)	Option parameter that will be placed in columns 4 and 5 of the title record accompanying the interface microscopic data for material I to indicate to the diffusion or transport theory codes whether to use the values of either the transport cross section or the values of the quantity $1/(3\sigma tr)$.
		(Used only with INL format).
		0—Use the transport cross section (monoenergetic definition). (Default)
		1—Use the quantity $1/(3\sigma tr)$ (Fick's law definition).

6.2   Floating Point Data Records

6.2.1   General Floating Point Data Record 1041001

This record is required for each problem. (N words, $1 \leq N \leq 3$)

Position	Name	Description of Data
Word 1	BUCK	Constant buckling, cm-2 (B2 value must be nonzero and positive).
		-1.0—Read 14700YY and 14710YY records for broad group wise buckling and buck sign. Requires 14700YY and 14710YY records.
Word 2	BUCKSIGN	0.0—Exp (-iBx) spatial distribution, i.e., fundamental mode cosine shape. (Default)
		-1.0—Exp (-Bx) spatial distribution
		+1.0—Exp (+Bx) spatial distribution
		Applied when BUCK > 0.0.
Word 3	CONV	Convergence criteria for fluxes and currents or for renormalization factor. (If not specified or zero, the code sets CONV = 0.00001.)

6.2.2   Material Specification Record 10420XX

These records are required for each problem. The material number is indicated by XX $(1 \leq XX \leq NOI)$. (N words, $3 \leq N \leq 6$)

Position	Name	Description of Data
Word 1	BISO(I)	ENDF material identification number for Ith material. Optionally if negative, print out the Bondarenko self-shielded fine-group vector cross sections, including damage, heat, and kerma.
Word 2	TISO(I)	Temperature (K) for Ith material.
Word 3	DENS(I)	Homogeneous atom density × 10-24 of the Ith material. May not be zero. Set to a very small number to force an infinite dilution calculation.
Word 4	THERMS(I)	0.0—static thermal scattering (no upscattering). (Default)
		1.0—free gas thermal scattering (will include upscattering). (see Table 3)
		2.0—S(α,β) thermal scattering (will include upscattering). (see Table 3)
Word 5	EPFISS(I)	Total thermal energy yield/fission (w·sec/fiss). (Default = 0.0)
Word 6	SSFF(I)	Self-shielding factor flag for Ith material.
		0.0—no input of additional self-shielding factors. (Default)
		1.0—additional self-shielding factors input by broad group. The self-shielding factors are input on records 146XXYY. All cross sections already processed either by Bondarenko self-shielding treatment or by additional ABH or Nordeim treatment will be multiplied by these additional self-shielding factors. Care should be taken when this option is used.

6.2.3 Material Resonance Specification Record 1043XXY

These records are required only for those materials for which a resonance calculation is to be performed. XX indicates the material number where (1 < XX < NOI) and Y specifies up to 9 continuation records. These records are used for the Nordheim resonance treatment when NXSR = 1.0 and also for the heterogeneous effect in the Bondarenko treatment when NXSR = 0.0. (N words, 3 < N < 23)

Position	Name	Description of Data
Word 1	TEMP(I))	Temperature (K) of absorber lump.
Word 2	GEOM(I)	Geometry of absorber lump.
		0.0—Homogeneous medium. DENS(I) is atom density. (see 10420XX record)
		1.0—Slab Geometry heterogeneous.
		2.0—Cylindrical Geometry heterogeneous.
		3.0—Spherical Geometry heterogeneous.
Word 3	DZERO(I)	Heterogeneous absorber atom density in absorber lump x 10^{-24}. May not be zero. Set to a very small number to force an infinite dilution calculation.
Word 4	ABAR(I)	Lump dimension—radius of cylinder or sphere or thickness of slab in centimeters.
Word 5	CIN(I)	Dancoff-Ginsburg fuel lump correction factor or option flag. (If no shadowing, CIN = 0.0, also CIN is not used if IGEOM(I) = 0.)
		0.0 to 1.0—Value of the correction factor CIN which is to be read in.
		2.0—Calculate correction factor (cylinders only).
		3.0—Same as for "last material," which required a correction factor. (Caution: The user should exercise care in using this option.) "Last Material" here means preceding MATXS ID in the order on library file.
Word 6	ELZERO(I)	Double heterogeneity fuel lump spherical grain average chord length. See Equation (62) in text.
		$$\bar{l}_G = \frac{4V}{S} = \frac{4}{3}r \text{ cm}$$
Word 7	CZERO(I)	Double heterogeneity fuel lump grain Dancoff factor C_0. See Equations (43) and (99) in text. This is independent of CIN(I).
Word 8	S(I)	0.0—Use $\phi_{lump.}$ (Default)
Word 9	AMOD(I,1)	First admixed moderator ID. The XX in 10420XX record (not BISO). (Real)
Word 10	AMOD(I,2)	Second admixed moderator ID. The XX in 10420XX record. (Real)
Word 11	AMOD(I,3)	Third admixed moderator ID. The XX in 10420XX record. (Real)
Word 12	ADENM(I,1)	Atomic density of the first admixed moderator, AMOD(I,1).
Word 13	ADENM(I,2)	Atomic density of the second admixed moderator, AMOD(I,2).
Word 15	RABS(I,1)	First admixed resonance absorber ID. The XX in 10420XX record (not BISO). (Real)
Word 16	RABS(I,2)	Second admixed resonance absorber ID. The XX in 10420XX record. (Real)
Word 17	RABS(I,3)	Third admixed resonance absorber ID. The XX in 10420XX record. (Real)
Word 18	ADENABS(I,1)	Atomic density of the first admixed resonance absorber, RABS(I,1).
Word 19	ADENABS(I,2)	Atomic density of the second admixed resonance absorber, RABS(I,2).
Word 20	ADENABS(I,3)	Atomic density of the third admixed resonance absorber, RABS(I,3).
Word 21	RTYPE1(I)	= 0.0—All waves available in RERES.LIB. (Default)
		> 0.0—s-wave only.
Word 22	RTYPE2(I)	= 0.0—Use E_{high} as in the RERES.LIB. (Default)
		> 0.0—Reset E_{high} to RTYPE2(I).

Position	Name	Description of Data
Word 23	RTYPE3(I)	= 0.0—Use Elow as in the RERES.LIB. (Default, currently set to 0.0125 eV)
		> 0.0—Reset E_{low} to RTYPE3(I).
Word 24	RTYPE4(I)	> 10.0—NINT(RTYPE4(I)) is the minimum number of mesh points per resonance (Default, set to 10). Currently, the code sets the maximum number of mesh points per resonance to 1400.

6.2.4   Material Dancoff Specification Record 1044XXY

These records are required for all materials for which a fuel lump Dancoff calculation is to be performed. XX indicates the material number where $1 \leq XX \leq NOI$, and Y specifies up to nine continuation records. (N words, $8 \leq N \leq 12$)

Position	Name	Description of Data
Word 1	REG(I)	Number of nonabsorber regions in unit cell (REG(I) < 5).
Word 2	XK(I)	Lattice arrangement of cylindrical pins.
		1.0—Rectangular.
		2.0—Hexagonal.
Word 3	RADX(I,1)	Outer radius, in centimeters, of first nonabsorber region in unit cell, i.e., region immediately adjacent to absorber lump. ABAR(I) on record 10430IY is the radius of the absorber R_0 in Equations (77) and (79).
Word 4	RADX(I,2)	Outer radius of second nonabsorber region in unit cell.
Word 5	RADX(I,3)	Outer radius of third nonabsorber region in unit cell.
Word 6	RADX(I,4)	Outer radius of fourth nonabsorber region in unit cell.
Word 7	RADX(I,5)	Outer radius of fifth nonabsorber region in unit cell.
Word 9	SIG(I,2)	Macroscopic total cross section of second nonabsorber region in unit cell.
Word 10	SIG(I,3)	Macroscopic total cross section of third nonabsorber region in unit cell.
Word 11	SIG(I,4)	Macroscopic total cross section of fourth nonabsorber region in unit cell.
Word 12	SIG(I,5)	Macroscopic total cross section of fifth nonabsorber region in unit cell.

NOTE: The macroscopic total cross section in each nonabsorber region is the average macroscopic scattering plus absorption cross section in the resolved resonance range $\sum_l$ in Equation (88). The radius of the last nonabsorber region is the average radius of the unit cell based on the last moderator volume in the hexagonal or square lattice pitch.

6.2.5   Material General Resonance Data Record 10450XX

These records are required only for those materials for which the user desires to modify the standard resonance calculational procedure. XX indicates that material number where $1 \leq XX \leq NOI$. (N words, $1 \leq N \leq 3$).

Position	Name	Description of Data
Word 1	THERMUP(I)	0.0—No thermal upscattering in the Nordheim resonance treatment. (Default)
		1.0—Thermal upscattering in the Nordheim resolved resonance treatment.
Word 2	FMULT(I)	A factor which will multiply the recommended mesh spacing to obtain a coarse or finer mesh to use in performing the resolved resonance calculation. Default value is 1.0. If less than 1.0, less meshes are used. If greater than 1.0, more meshes are used. The maximum number of mesh intervals per resonance, however, is limited to 904. The minimum is 10.

Position	Name	Description of Data
Word 3	XLMT(I)	0.0—All resonances are used in constructing cross sections. (Default)
		X—The number of neighboring resonances in either direction to be considered. (Not recommended)

6.2.6 Material Self-Shielding Factor Records (146XXYY)

These records are required only for those materials if self-shielding factors are to be input, i.e., if SSFF(I) = 1.0 for material XX. NOUG values must be input. XX specifies the material number, where 1 < XX < NOI, and YY specifies up to 20 continuation records.

Position	Name	Description of Data
Word 1 to NOUG	SSFBG(J)	Self-shielding factors for material I (specified by XX) and broad group J, listed in consecutive order.
		(1 < J < NOUG)
		These data are necessary only for those materials that require self-shielding factors. Input self-shielding factors in the epithermal energy groups for materials with a resonance range will double self-shield resonance materials which are automatically self-shielded on records 1044XXY. Input self-shielding factors in this energy range should be 1.0 or an infinitely dilute resonance calculation should be performed to prevent double self-shielding of resonances (caveat emptor).

6.2.7 Broad Group Buckling Factor Records (14700YY)

This record is required only if broad group wise buckling is to be input, i.e., if buck ≤0.0 for the problem. NOUG nonzero and positive values must be input. YY specifies up to 20 continuation records. (NOUG words).

Position	Name	Description of Data
Word 1 to NOUG	BUCKBG(J)	Broad group wise buckling corresponding to 101020Y record. ($1 \leq J \leq$ NOUG) (must be nonzero and positive)

6.2.8 Broad Group Buckling Sign Records (14710YY)

This record is required only if broad group wise buckling is present in 14700YY record. NOUG values must be input. YY specifies up to 20 continuation records. (NOUG words).

Position	Name	Description of Data
Word 1 to NOUG	GBSIGN(J)	Broad group wise buckling sign corresponding to 14700YY record. ($1 \leq J \leq$ NOUG).
		0.0— exp (-iBx) spatial distribution, i.e., fundamental mode cosine shape.
		-1.0— exp (-Bx) spatial distribution
		+1.0— exp (+Bx) spatial distribution

6.2.9   Blackness calculation option Record (1480001)

This record is required if the blackness calculation has been requested on Record 1010101 (NTYPE = 6). (N words, $2 \leq N \leq 5$)

Position	Name	Description of Data
Word 1	TH	Thickness of highly absorbing region, in centimeters, for which a "Blackness theory" calculation of effective diffusion constants is desired.
Word 2	H	Width of mesh, in centimeters, used to describe the interior of a highly absorbing region in a diffusion theory calculation.
Word 3	CB	A quantity occurring in the blackness theory equations which can be approximated by $$3\left(\frac{\Sigma_{tr}}{\Sigma_t}\right)$$ where Σ_{tr} and Σ_t represent the transport and total cross sections, respectively, for the regions immediately surrounding the blackness region. (Default = 3.0, assuming $\frac{\Sigma_{tr}}{\Sigma_t}$ to be unity)
Word 4	AK1	First blackness coefficient. (usually set to 1.0). (Default = 1.0)
Word 5	AK2	Second blackness coefficient. (usually set to 1.0). (Default = 1.0)

6.2.10   MND calculation option Record (1490001)

If the MND option has been requested on Card 1010101 (MNDFLG = 1), MND constants will be printed out for D, Σ_a, Σ_f macro and σ_{tr}, σ_a, σ_f microscopic cross sections. No MND constants will be output in the ASCII file. The other cross sections that are output will not be MND constants. (N words, $2 \leq N \leq 2$)

Position	Name	Description of Data
Word 1	IENDMN (Integer)	Highest fine energy group included in MND calculation.
Word 2	TPMND	Temperature of Maxwellian spectrum for MND calculation.

NOTE: *The MND option can only be used for a single thermal group. No multithermal group MND option is defined.*

6.3   Mixed Integer and Floating Point Data Records

ABH input data on 2XXXXXX series records are only required if ICHET = 1 on the first input record.

6.3.1   ABH REGION DESCRIPTION RECORDS 2010401

This record is required for each problem if the ABH option is to be run. (4 words) See Equations (166) through (175) in the text.

Position	Name	Description of Data
Word 1	NREG	Number of regions in ABH calculation. NREG must be set to 3.)
Word 2	RAD(1)	Outer radius of region 1 (cm) (half thickness of fuel slab).
Word 3	RAD(2)	Outer radius of region 2 (cm) (cladding).
Word 4	RAD(3)	Outer radius of region 3 (cm) (moderator half thickness in slab geometry).

6.3.2   ABH Material Description for Each Region Record 2015XYY

These records are required for each problem if the ABH option is to be run. X specifies the region number, where $1 \leq X \leq 3$, and Y specifies up to 19 continuation records. Up to NOI materials may be specified per region (N words, $3 \leq N \leq 101$).

Position	Name	Description of Data
Word 1	NMAT	Number of materials in region specified by X (integer).
Word 2	IJSO(1,X)	First material identification number. The XX in 10420XX record.
Word 3	ADENS(1,X)	Heterogeneous atom density X 10^{-24} of the first material in region X.
Word 4	IJSO(2,X)	Second material identification number. The XX in 10420XX record.
Word 5	ADENS(2,X)	Heterogeneous atom density X 10^{-24} of the second material in region X.

NOTE 1: *In the event the problem requestor wishes to include materials in the ABH calculation with zero atom density to force the generation of thermal self-shielded microscopic cross sections, an arithmetic indefinite will occur. To overcome this defect, use a very small atom density, e.g., 10^{-15} for these materials.*

NOTE 2: *All materials included in the 10420XX cards (NOI materials) should be used in the 20105XY cards.*

6.4 Fine Energy Group Structure

Group Number	Upper Energy (eV)	Group Number	Upper Energy (eV)	Group Number	Upper Energy (eV)	Group Number	Upper Energy (eV)
1	2.0000E+07	43	9.6112E+02	85	1.1300E+00	127	3.5000E-01
2	1.6905E+07	44	7.4852E+02	86	1.1250E+00	128	3.4000E-01
3	1.4918E+07	45	5.8295E+02	87	1.1100E+00	129	3.3000E-01
4	1.3499E+07	46	4.5400E+02	88	1.0900E+00	130	3.2000E-01
5	1.1912E+07	47	3.5358E+02	89	1.0800E+00	131	3.1000E-01
6	1.0000E+07	48	2.7536E+02	90	1.0700E+00	132	3.0000E-01
7	7.7880E+06	49	2.1445E+02	91	1.0600E+00	133	2.9000E-01
8	6.0653E+06	50	1.6702E+02	92	1.0500E+00	134	2.8000E-01
9	4.7237E+06	51	1.3007E+02	93	1.0250E+00	135	2.7000E-01
10	3.6788E+06	52	1.0130E+02	94	1.0000E+00	136	2.6000E-01
11	2.8650E+06	53	7.8893E+01	95	9.9000E-01	137	2.5000E-01
12	2.2313E+06	54	6.1442E+01	96	9.8000E-01	138	2.4000E-01
13	1.7377E+06	55	4.7851E+01	97	9.7000E-01	139	2.3000E-01
14	1.3534E+06	56	3.7267E+01	98	9.5000E-01	140	2.2000E-01
15	1.0540E+06	57	2.9023E+01	99	9.3000E-01	141	2.0000E-01
16	8.2085E+05	58	2.2603E+01	100	9.1000E-01	142	1.8000E-01
17	6.3928E+05	59	1.7603E+01	101	8.9000E-01	143	1.6000E-01
18	4.9787E+05	60	1.3710E+01	102	8.7600E-01	144	1.4000E-01
19	3.8774E+05	61	1.0677E+01	103	8.5000E-01	145	1.2000E-01
20	3.0197E+05	62	8.3153E+00	104	8.0000E-01	146	1.0000E-01
21	2.3518E+05	63	6.4760E+00	105	7.5000E-01	147	9.5000E-02
22	1.8316E+05	64	5.0435E+00	106	7.0000E-01	148	9.0000E-02
23	1.4264E+05	65	3.9279E+00	107	6.8300E-01	149	8.5000E-02
24	1.1109E+05	66	3.0590E+00	108	6.5000E-01	150	8.0000E-02
25	8.6517E+04	67	2.3824E+00	109	6.2500E-01	151	7.5000E-02
26	6.7379E+04	68	2.3300E+00	110	6.0000E-01	152	7.0000E-02
27	5.2475E+04	69	2.2900E+00	111	5.9000E-01	153	6.5000E-02
28	4.0868E+04	70	2.2000E+00	112	5.7500E-01	154	6.0000E-02
29	3.1828E+04	71	2.1000E+00	113	5.5000E-01	155	5.0000E-02
30	2.4788E+04	72	2.0000E+00	114	5.3200E-01	156	4.0000E-02
31	1.9305E+04	73	1.9000E+00	115	5.0000E-01	157	3.0000E-02
32	1.5034E+04	74	1.8600E+00	116	4.9000E-01	158	2.5000E-02
33	1.1709E+04	75	1.7800E+00	117	4.8000E-01	159	2.0000E-02
34	9.1188E+03	76	1.7000E+00	118	4.7500E-01	160	1.5000E-02
35	7.1017E+03	77	1.6000E+00	119	4.7000E-01	161	1.0000E-02
36	5.5308E+03	78	1.5000E+00	120	4.6000E-01	162	8.0000E-03
37	4.3074E+03	79	1.4400E+00	121	4.5000E-01	163	7.0000E-03
38	3.3546E+03	80	1.3500E+00	122	4.3000E-01	164	5.0000E-03
39	2.6126E+03	81	1.3000E+00	123	4.2000E-01	165	4.0000E-03
40	2.0347E+03	82	1.2500E+00	124	4.1400E-01	166	2.0000E-03
41	1.5846E+03	83	1.2000E+00	125	3.8000E-01	167	1.0000E-03
42	1.2341E+03	84	1.1500E+00	126	3.6000E-01		1.0000E-05

6.5 Materials in the "MATXS" Fine Group Cross Section Library and the "RERES" Resolved Resonance Library

Element/ isotope	ENDF/B Material ID	Resolved Resonance in reres.lib*	Thermal Scattering**	Element/ Isotope	ENDF/B Material ID	Resolved Resonance in reres.lib	Thermal Scattering
H-1	125	0	H in H$_2$O, f	K-40	1928	0	f
H-1	126	0	H in ZrH	K-41	1931	2	f
H-1	127	0	H in Ch2	Ca-40	2025	2	f
H-2	128	0	D in D$_2$O, f	Ca-42	2031	2	f
H-3	131	0	f	Ca-43	2034	2	f
He-3	225	0	f	Ca-44	2037	2	f
He-4	228	0	f	Ca-46	2043	0	f
Li-6	325	0	f	Ca-48	2049	2	f
Li-7	328	0	f	Sc-45	2125	2	f
Be-9	425	0	Be-metal	Ti-46	2225	2	f
Be-9	426	0	Be in BeO	Ti-47	2228	2	f
B-10	525	0	f	Ti-48	2231	2	f
B-11	528	0	f	Ti-49	2234	2	f
C	600	0	graphite, f	Ti-50	2237	2	f
N-14	725	0	f	V	2300	5	f
N-15	728	0	f	Cr-50	2425	3	f
O-16	825	0	f	Cr-52	2431	3	f
O-16	826	0	O in BeO	Cr-53	2434	3	f
O-17	828	0	f	Cr-54	2437	3	f
F-19	925	0	f	Mn-55	2525	2	f
Na-22	1122	0	f	Fe-54	2625	3	f
Na-23	1125	2	f	Fe-56	2631	3	f
Mg-24	1225	0	f	Fe-57	2634	3	f
Mg-25	1228	0	f	Fe-58	2637	3	f
Mg-26	1231	0	f	Co-58	2722	2	f
Al-27	1325	3	f	Co-58m	2723	2	f
Si-28	1425	3	f	Co-59	2725	3	f
Si-29	1428	3	f	Ni-58	2825	3	f
Si-30	1431	3	f	Ni-59	2828	2	f
P-31	1525	0	f	Ni-60	2831	3	f
S-32	1625	2	f	Ni-61	2834	3	f
S-33	1628	2	f	Ni-62	2837	3	f
S-34	1631	2	f	Ni-64	2843	3	f
S-36	1637	0	f	Cu-63	2925	3	f
Cl-35	1725	0	f	Cu-65	2931	3	f
Cl-37	1731	0	f	Zn	3000	5	f
Ar-36	1825	2	f	Ga-69	3125	2	f
Ar-38	1831	2	f	Ga-71	3131	2	f
Ar-40	1837	3	f	Ge-70	3225	2	f
K-39	1925	2	f	Ge-72	3231	2	f
Ge-73	3234	2	f	Nb-95	4131	0	f
Ge-74	3237	2	f	Mo-92	4225	2	f
Ge-76	3243	2	f	Mo-94	4231	2	f
As-74	3322	2	f	Mo-95	4234	2	f
As-75	3325	2	f	Mo-96	4237	2	f
Se-74	3425	2	f	Mo-97	4240	2	f
Se-76	3431	2	f	Mo-98	4243	2	f

Element/ isotope	ENDF/B Material ID	Resolved Resonance in reres.lib*	Thermal Scattering**	Element/ Isotope	ENDF/B Material ID	Resolved Resonance in reres.lib	Thermal Scattering
Se-77	3434	2	f	Mo-99	4246	0	f
Se-78	3437	2	f	Mo-100	4249	2	f
Se-79	3440	0	f	Tc-99	4325	2	f
Se-80	3443	2	f	Ru-96	4425	0	f
Se-82	3449	2	f	Ru-98	4431	0	f
Br-79	3525	2	f	Ru-99	4434	2	f
Br-81	3531	2	f	Ru-100	4437	2	f
Kr-78	3625	2	f	Ru-101	4440	2	f
Kr-80	3631	2	f	Ru-102	4443	2	f
Kr-82	3637	0	f	Ru-103	4446	2	f
Kr-83	3640	2	f	Ru-104	4449	2	f
Kr-84	3643	2	f	Ru-105	4452	0	f
Kr-85	3646	2	f	Ru-106	4455	0	f
Kr-86	3649	2	f	Rh-103	4525	2	f
Rb-85	3725	2	f	Rh-105	4531	1	f
Rb-86	3728	2	f	Pd-102	4625	2	f
Rb-87	3731	2	f	Pd-104	4631	2	f
Sr-84	3825	2	f	Pd-105	4634	2	f
Sr-86	3831	2	f	Pd-106	4637	2	f
Sr-87	3834	2	f	Pd-107	4640	2	f
Sr-88	3837	2	f	Pd-108	4643	2	f
Sr-89	3840	0	f	Pd-110	4649	2	f
Sr-90	3843	0	f	Ag-107	4725	2	f
Y-89	3925	2	f	Ag-109	4731	2	f
Y-90	3928	2	f	Ag-110m	4735	2	f
Y-91	3931	0	f	Ag-111	4737	2	f
Zr	4000	5	Zr in ZrH	Cd-106	4825	2	f
Zr-90	4025	2	f	Cd-108	4831	2	f
Zr-91	4028	2	f	Cd-110	4837	2	f
Zr-92	4031	2	f	Cd-111	4840	2	f
Zr-93	4034	2	f	Cd-112	4843	2	f
Zr-94	4037	2	f	Cd-113	4846	2	f
Zr-95	4040	0	f	Cd-114	4849	2	f
Zr-96	4043	2	f	Cd-115m	4853	2	f
Nb-93	4125	1	f	Cd-116	4855	2	f
Nb-94	4128	2	f	In-113	4925	2	f
In-115	4931	2	f	Xe-132	5449	2	f
Sn-112	5025	2	f	Xe-133	5452	0	f
Sn-113	5028	2	f	Xe-134	5455	2	f
Sn-114	5031	2	f	Xe-135	5458	1	f
Sn-115	5034	2	f	Xe-136	5461	2	f
Sn-116	5037	2	f	Cs-133	5525	2	f
Sn-117	5040	2	f	Cs-134	5528	2	f
Sn-118	5043	2	f	Cs-135	5531	2	f
Sn-119	5046	2	f	Cs-136	5534	0	f
Sn-120	5049	2	f	Cs-137	5537	0	f
Sn-122	5055	2	f	Ba-130	5625	2	f
Sn-123	5058	0	f	Ba-132	5631	2	f
Sn-124	5061	2	f	Ba-133	5634	2	f
Sn-125	5064	2	f	Ba-134	5637	2	f

Element/ isotope	ENDF/B Material ID	Resolved Resonance in reres.lib[*]	Thermal Scattering[**]	Element/ Isotope	ENDF/B Material ID	Resolved Resonance in reres.lib	Thermal Scattering
Sn-126	5067	0	f	Ba-135	5640	2	f
Sb-121	5125	2	f	Ba-136	5643	2	f
Sb-123	5131	2	f	Ba-137	5646	2	f
Sb-124	5134	0	f	Ba-138	5649	2	f
Sb-125	5137	0	f	Ba-140	5655	2	f
Sb-126	5140	2	f	La-138	5725	2	f
Te-120	5225	0	f	La-139	5728	2	f
Te-122	5231	2	f	La-140	5731	2	f
Te-123	5234	2	f	Ce-136	5825	2	f
Te-124	5237	2	f	Ce-138	5831	2	f
Te-125	5240	2	f	Ce-139	5834	2	f
Te-126	5243	2	f	Ce-140	5837	2	f
Te-127m	5247	0	f	Ce-141	5840	2	f
Te-128	5249	2	f	Ce-142	5843	2	f
Te-129m	5253	0	f	Ce-143	5846	2	f
Te-130	5255	2	f	Ce-144	5849	0	f
Te-132	5261	2	f	Pr-141	5925	2	f
I-127	5325	2	f	Pr-142	5928	2	f
I-129	5331	2	f	Pr-143	5931	2	f
I-130	5334	2	f	Nd-142	6025	2	f
I-131	5337	0	f	Nd-143	6028	2	f
I-135	5349	0	f	Nd-144	6031	2	f
Xe-123	5422	0	f	Nd-145	6034	2	f
Xe-124	5425	2	f	Nd-146	6037	2	f
Xe-126	5431	2	f	Nd-147	6040	2	f
Xe-128	5437	2	f	Nd-148	6043	2	f
Xe-129	5440	2	f	Nd-150	6049	2	f
Xe-130	5443	2	f	Pm-147	6149	2	f
Xe-131	5446	2	f	Pm-148	6152	0	f
Pm-148m	6153	1	f	Er-170	6849	2	f
Pm-149	6155	0	f	Lu-175	7125	2	f
Pm-151	6161	2	f	Lu-176	7128	2	f
Sm-144	6225	2	f	Hf-174	7225	2	f
Sm-147	6234	2	f	Hf-176	7231	2	f
Sm-148	6237	2	f	Hf-177	7234	2	f
Sm-149	6240	2	f	Hf-178	7237	2	f
Sm-150	6243	2	f	Hf-179	7240	2	f
Sm-151	6246	2	f	Hf-180	7243	2	f
Sm-152	6249	2	f	Ta-181	7328	2	f
Sm-153	6252	2	f	Ta-182	7331	2	f
Sm-154	6255	2	f	W-182	7431	2	f
Eu-151	6325	2	f	W-183	7434	2	f
Eu-152	6328	2	f	W-184	7437	2	f
Eu-153	6331	2	f	W-186	7443	2	f
Eu-154	6334	2	f	Re-185	7525	2	f
Eu-155	6337	2	f	Re-187	7531	2	f
Eu-156	6340	2	f	Ir-191	7725	2	f
Eu-157	6343	2	f	Ir-193	7731	2	f
Gd-152	6425	3	f	Au-197	7925	2	f
Gd-153	6428	3	f	Hg-196	8025	2	f

Element/ isotope	ENDF/B Material ID	Resolved Resonance in reres.lib[*]	Thermal Scattering[**]	Element/ Isotope	ENDF/B Material ID	Resolved Resonance in reres.lib	Thermal Scattering
Gd-154	6431	3	f	Hg-198	8031	2	f
Gd-155	6434	3	f	Hg-199	8034	2	f
Gd-156	6437	3	f	Hg-200	8037	2	f
Gd-157	6440	3	f	Hg-201	8040	2	f
Gd-158	6443	3	f	Hg-202	8043	2	f
Gd-160	6449	3	f	Hg-204	8049	0	f
Tb-159	6525	2	f	Pb-204	8225	2	f
Tb-160	6528	3	f	Pb-206	8231	3	f
Dy-156	6625	2	f	Pb-207	8234	3	f
Dy-158	6631	2	f	Pb-208	8237	3	f
Dy-160	6637	2	f	Bi-209	8325	2	f
Dy-161	6640	2	f	Ra-223	8825	0	f
Dy-162	6643	2	f	Ra-224	8828	0	f
Dy-163	6646	2	f	Ra-225	8831	0	f
Dy-164	6649	2	f	Ra-226	8834	2	f
Ho-165	6725	2	f	Ac-225	8925	0	f
Ho-166m	6729	2	f	Ac-226	8928	0	f
Er-162	6825	2	f	Ac-227	8931	0	f
Er-164	6831	2	f	Th-227	9025	0	f
Er-166	6837	2	f	Th-228	9028	2	f
Er-167	6840	2	f	Th-229	9031	2	f
Er-168	6843	2	f	Th-230	9034	1	f
Th-232	9040	3	f	Pu-246	9458	0	f
Th-233	9043	0	f	Am-241	9543	1	f
Th-234	9046	0	f	Am-242	9546	2	f
Pa-231	9131	3	f	Am-42m	9547	2	f
Pa-232	9134	2	f	Am-243	9549	1	f
Pa-233	9137	3	f	Am-244	9552	0	f
U-232	9219	3	f	Am-44m	9553	0	f
U-233	9222	3	f	Cm-241	9628	0	f
U-234	9225	2	f	Cm-242	9631	1	f
U-235	9228	3	f	Cm-243	9634	1	f
U-236	9231	2	f	Cm-244	9637	2	f
U-237	9234	1	f	Cm-245	9640	2	f
U-238	9237	3	f	Cm-246	9643	2	f
U-239	9240	1	f	Cm-247	9646	1	f
U-240	9243	1	f	Cm-248	9649	1	f
U-241	9246	1	f	Cm-249	9652	2	f
Np-235	9340	0	f	Cm-250	9655	2	f
Np-236	9343	2	f	Bk-249	9752	2	f
Np-237	9346	2	f	Bk-250	9755	2	f
Np-238	9349	0	f	Cf-249	9852	2	f
Np-239	9352	0	f	Cf-250	9855	1	f
Pu-236	9428	2	f	Cf-251	9858	1	f
Pu-237	9431	0	f	Cf-252	9861	1	f
Pu-238	9434	1	f	Cf-253	9864	1	f
Pu-239	9437	3	f	Cf-254	9867	0	f
Pu-240	9440	2	f	Es-253	9913	1	f
Pu-241	9443	3	f	Es-254	9914	0	f
Pu-242	9446	1	f	Es-255	9915	0	f

Element/ isotope	ENDF/B Material ID	Resolved Resonance in reres.lib[*]	Thermal Scattering[**]	Element/ Isotope	ENDF/B Material ID	Resolved Resonance in reres.lib	Thermal Scattering
Pu-243	9449	1	f	Fm-255	9936	0	f
Pu-244	9452	1	f				

* Presence of resolved resonance parameters in the reres.lib.

iwr = 0: No resonance parameters, includes only awr and ap

1: Single-Level Breit-Wigner (SLBW) format

2: Multilevel Breit-Wigner (MLBW) format

3: Reich-Moore (R-M) format

4: multi-isotope SLBW format

5: multi-isotope MLBW format

** Cross sections are mostly processed at T=293, 900, 1300, and 2200 K and at σ_0 = 1.0e10e4, 1.0e2, 1.0 barns. For some important isotopes, cross sections are processed with up to 8 σ_0 values and as low as 0.01 barns. For those having the free (f)/S(α,β) thermal scattering cross sections, the temperatures are dictated by the ENF/B-VII.0. The maximum temperature for free or S(α,β) thermal scattering is

800 K for H-1 in H2O, 1200 K for H-1 in ZrH, 350 K for H-1 in CH2, 650 K for H-1 in D2O, 1200 K for Be, 1220 K for Be in BeO, 2000 K for graphite, 2200 K for O-16, 1200 K for O-16 in BeO, 1200 K for Zr in ZrH

6.6   MATXS.LIB File Description

```
----------------------------------------------------------------------
         file structure
             record type                        present if
             =============================      ===============
             file identification                always
             file control                       always
             set hollerith identification       always
             file data                          always
  *************(repeat for all particles)
  *          group structures                   always
  *************
  *************(repeat for all materials)
  *          material control                   always
  *
  * ***********(repeat for all submaterials)
  * *          vector control                   n1db.gt.0
  * *
  * * *********(repeat for all vector blocks)
  * * *        vector block                     n1db.gt.0
  * * *********
  * *
  * * *********(repeat for all matrix blocks)
  * * *        matrix control                   n2d.gt.0
  * * *
  * * * *******(repeat for all sub-blocks)
  * * * *    matrix sub-block                   n2d.gt.0
  * * * *******
  * * *
  * * *        constant sub-block               jconst.gt.0
  * * *
  *************
----------------------------------------------------------------------
----------------------------------------------------------------------
         file identification
  hname,(huse(i),i=1,2),ivers
  1+3*mult
  format(4h 0v ,a8,1h*,2a8,1h*,i6)
  hname         hollerith file name  - matxs - (a8)
  huse          hollerith user identifiation   (a8)
  ivers         file version number
  mult          double precision parameter
                     1- a8 word is single word
                     2- a8 word is double precision word
----------------------------------------------------------------------
----------------------------------------------------------------------
         file control
  npart,ntype,nholl,nmat,maxw,length
  format(6h 1d   ,6i6)
  npart       number of particles for which group
                  structures are given
  ntype       number of data types present in set
  nholl       number of words in set hollerith
                  identification record
  nmat        number of materials on file
```

```
    maxw         maximum record size for sub-blocking
    length       length of file
----------------------------------------------------------------------
----------------------------------------------------------------------
          set hollerith identification
    (hsetid(i),i=1,nholl)
    format(4h 2d /(9a8))
    hsetid       hollerith identification of set (a8)
                 (to be edited out 72 characters per line)
----------------------------------------------------------------------
----------------------------------------------------------------------
          file data
    (hprt(j),j=1,npart),(htype(k),k=1,ntype),(hmatn(i),i=1,nmat),
   1(ngrp(j),j=1,npart),(jinp(k),k=1,ntype,(joutp(k),k=1,ntype),
   2(nsubm(i)i=1,nmat),(locm(i),i=1,nmat)
    format(4h 3d ,4x,8a8/(9a8))    hprt,htype,hmatn
    format(12i6)                   ngrp,jinp,joutp,nsubm,locm
    hprt(j)      hollerith identification for particle j
                     n          neutron
                     g          gamma
                     p          proton
                     d          deuteron
                     t          triton
                     h          he-3 nucleus
                     a          alpha (he-4 nucleus)
                     b          beta
                     r          residual or recoil
                                (heavier than alpha)
    htype(k)      hollerith identification for data type k
                     nscat      neutron scattering
                     ng         neutron induced gamma production
                     gscat      gamma scattering (atomic)
                     gg         gamma scattering (photonuclear)
                     pn         proton induced neutron production
                       .           .
                       .           .
                       .           .
                     dkn        delayed neutron data
                     dkhg       decay heat and gamma data
                     dkb        decay beta data
    hmatn(i)     hollerith identification for material i
    ngrp(j)       number of energy groups for particle j
    jinp(k)      type of incident particle associated with
                   data type k.  for dk data types, jinp is 0.
    joutp(k)     type of outgoing particle associated with
                   data type k
    nsubm(i)     number of submaterials for material i
    locm(i)      location of material i
----------------------------------------------------------------------
----------------------------------------------------------------------
          group structure
    (gpb(i),i=1,ngr),emin
    ngr=ngrp(j)
    format(4h 4d ,8x,1p,5e12.5/(6e12.5))
    gpb(i)       maximum energy bound for group i for particle j
    emin         minimum energy bound for particle j
----------------------------------------------------------------------
```

```
      -----------------------------------------------------------------
           material control
      hmat,amass,(temp(i),sigz(i),itype(i),n1d(i),n2d(i),
     1locs(i),i=1,nsubm)
      format(4h 5d ,a8,1p,2e12.5/(2e12.5,5i6))
      hmat        hollerith material identifier
      amass       atomic weight ratio
      temp        ambient temperature or other parameters for
                      submaterial i
      sigz        dilution factor or other parameters for
                      submaterial i
      itype       data type for submaterial i
      n1d         number of vectors for submaterial i
      n2d         number of matrix blocks for submaterial i
      locs        location of submaterial i
      -----------------------------------------------------------------
      -----------------------------------------------------------------
           vector control
      (hvps(i),i=1,n1d),(nfg(i),i=1,n1d),(nlg(i),i=1,n1d)
      format(4h 6d ,4x,8a8/(9a8))        hvps
      format(12i6)                       iblk,nfg,nlg
      hvps(i)     hollerith identifier of vector
                      nelas      neutron elastic scattering
                      n2n        (n,2n)
                      nnf        second chance fission
                      gabs       gamma absorption
                      p2n        protons in, 2 neutrons out
                        .            .
                        .            .
                        .            .
      nfg(i)      number of first group in band for vector i
      nlg(i)      number of last group in band for vector i
      -----------------------------------------------------------------
      -----------------------------------------------------------------
           vector block
      (vps(i),i=1,kmax)
      kmax=sum over group band for each vector in block j
      format(4h 7d ,8x,1p,5e12.5/(6e12.5))
      vps(i)      data for group bands for vectors in block j.
                  block size is determined by taking all the group
                  bands that have a total length less than or equal
                  to maxw.
      -----------------------------------------------------------------
      -----------------------------------------------------------------
          scattering matrix control
      hmtx,lord,jconst,
     1(jband(l),l=1,noutg(k)),(ijj(l),l=1,noutg(k))
      mult+2+2*noutg(k)
      format(4h 8d ,4x,a8/(12i6))        hmtx,lord,jconst,
                                         jband,ijj
      hmtx        hollerith identification of block
      lord        number of orders present
      jconst      number of groups with constant spectrum
      jband(l)    bandwidth for group l
      ijj(l)      lowest group in band for group l
      -----------------------------------------------------------------
      -----------------------------------------------------------------
```

```
            scattering sub-block
      (scat(k),k=1,kmax)
      kmax=lord times the sum over all jband in the group range of
             this sub-block
      format(4h 9d ,8x,1p,5e12.5/(6e12.5))
      scat(k)      matrix data given as bands of elements for initial
                   groups that lead to each final group.  the order
                   of the elements is as follows:  band for p0 of
                   group i, band for p1 of group i, ... , band for p0
                   of group i+1, band for p1 of group i+1, etc.  the
                   groups in each band are given in descending order.
                   the size of each sub-block is determined by the
                   total length of a group of bands that is less than
                   or equal to maxw.
                   if jconst.gt.0, the contributions from the jconst
                   low-energy groups are given separately.
-----------------------------------------------------------------------
-----------------------------------------------------------------------
            constant sub-block
      (spec(l),l=1,noutg(k)),(prod(l),l=l1,ning(k))
      l1=ning(k)-jconst+1
      noutg(k)+jconst
      format(4h10d ,8x,1p,5e12.5/(6e12.5))
      spec         normalized spectrum of final particles for initial
                   particles in groups l1 to ning(k)
      prod         production cross section (e.g., nu*sigf) for
                   initial groups l1 through ning(k)
          this option is normally used for the energy-independent
          neutron and photon spectra from fission and radiative
          capture usually seen at low energies.
-----------------------------------------------------------------------
```

6.7 Description of Resolved Resonance Library (reres.lib) Format

Card: title
 For a material
  Card: aid,iwr,awr,ap,elow,ehigh,nernis,mat (A10,I1,4E11.6,I11,I4)
   If 1 ≤ iwr ≤ 3
    For j=1,nernis
     Card: elt,eht,spi,ap,nls,naps,mat (4E11.6,2I11,I4)
      For l=1,nls
       Card: nrj,qx,lrx,mat (I11,E11.6,I11,33X,I4)
        For i=1,nrj
         Card: er,aj,gn,gg,gf,gt,mat (6E11.6,I4)
   If iwr ≥4
    Card: elt,eht,mat (2E11.6,44X,I4)
     For j=1,nernis
      Card: awri,abn,naps,spi,ap,nls,mat (2E11.6,I11,2E11.6,I11,I4)
     For l=1,max(nls)
      Card: nrj,qx,lrx,mat (I11,E11.6,I11,33X,I4)
        For i=1,nrj
         Card: igf,er,aj,gn,gg,gt,mat (I11,5E11.6,I4)
 Repeat for materials

aid	material identification.
iwr	l for sigle-level Breit-Wigner (SLBW), 2 for multilevel Breit-Wigner (MLBW), 3 for Reich-Moore, 4 for multiisotope SLBW, 5 for multiisotope MLBW.
awr	ratio of the material mass to that of a neutron.
ap	scattering radius in units of 10^{-12} cm.
elow	lower limit for the whole resolved resonance energy range (same as in ENDF/B-VII.0).
ehigh	upper limit for the whole resolved resonance energy range (same as in ENDFB-VII.0.
nernis*	number of energy ranges for iwr=1, 2, 3 or number of isotopes for iwr=4, 5.
mat	ENDF/B-VII material identification number.
elt	lower limit for an energy range (adjusted for COMBINE7, differing from elow: see reres.lib).
eht	upper limit for an energy range.
nls	number of *l*-values (neutron orbital angular momentum).
naps	flag controlling the use of the two radii.
nrj	number of resolved resonances for a given l-value.
qx	Q-value to be added to the incident particle's center of-mass energy to determine the channel energy.
lrx	flag indicating whether this energy range contains a competitive width.
er	resonance energy.
aj	floating point value of J (the spin, or total angular momentum of the resonance).
gn	neutron width, Γ_n, evaluated at the resonance energy, er.
gg	radiation width, , Γ_g.
gf	fission width, , Γ_f (Γ_{fa} for R-M).
gt	resonance total width (Γ_{fb} for R-M).
awri	ratio of the mass of a particular isotope to that of a neutron
abn	the abundance of an isotope in the material
igf	isotope index

---

* All have only one energy range except Pu-239 which has three energy ranges.

6.8   Cross section and constants internal record

The data in the internal master cross section library consist of alphanumeric, integer, and floating point records. The alphanumeric records are used for identification purposes, the integer data for the most part indicate the number and types of records to be read, and the floating point records make up the actual cross-section data.

The initial data records on the tape are used for identification and to indicate the number of materails, fission spectra and energy groups in the library. Subsequent records describe the cross-section data, with similar types of data records being repeated for each material until all materials have been described. The materails are always arranged in the library so that the identification numbers are in ascending order. The cross-section data records I the library have been condensed as much as feasible to reduce the processing time. Therefore, the length and number of data records present for a particular material depend on the amount of data required to describe the pertinent cross sections. The minimum number of records in the library for any material is two and the maximum is four.

A detailed description of the arrangement of the data within the library, including the mnemonic names and meanings of the data in the order of their occurrences in the library is found below. The cross-section data records for each material are arranged as shown below and are repeated for each material.

6.8.1   First Data Record for Material k

Mnemonic Name	Description or Function of Data
BISO(IS)	Material number
LTOT	Integer indicating the total number of words of data contained in the cross-section vector ADUM
IWA	Absorption reaction flag.
	If IWA = 1, absorption cross sections are present.
IWF	Fission reaction flag.
	If IWF = 1, fission cross sections and the values of the average number of neutrons per fission are present. If IWA = 0, IWA is ignored.
IWS	=> No elastic scattering transfer matrices present
	1 => Elastic scattering transfer matrices present
LOL(L)	Number of cross-section values in List L.
	L = 1 => inelastic transfer matrix is present if $\lvert LOL1 \rvert$ = 1.
	L = 2 => N,2N transfer matrix is present if $\lvert LOL2 \rvert$ = 1.
	L = 3 => P_0 and P_1 elastic transfer matrix is present if $\lvert LOL3 \rvert$ = 1.
	L = 4 => P_2 and P_3 elastic transfer matrix is present if $\lvert LOL4 \rvert$ = 1.
	L = 5 => P_0, N, 3N transfer matrix is present if $\lvert LOL5 \rvert$ = 1.
	L = 6 => P_0, N, 4N transfer matrix is present if $\lvert LOL6 \rvert$ = 1.

NOTE: *LOL(1) and LOL(2) negative implies P_1 inelastic or P_1, N,2N matrices are also present in addition to P_0 matrices. In either case, P_1 matrix follows directly behind the P_0 matrix. The length of either matrix is $\lvert LOL(1) \rvert$ or*

$\lvert LOL(2) \rvert$. LA and LD vectors apply to both P_0 and P_1 matrices in both cases. Only P_0, N,3N and N,4N cross sections are allowed.

| LA(L) | Number of fine groups *scattered from* in list L, starting with the first fine group, i.e., number of the highest fine group for which scattering reaction of type I is present (threshold group). |

Mnemonic Name	Description or Function of Data
LD(L)	Maximum number of fine groups scattered to in list L, i.e., the maximum number of groups downscattered (this value is constant for all groups in which a scattering reaction is tabulated for a particular material).
AW(IS)	The atomic weight ratio of this material.

6.8.2   Second Data Record for Material k

Mnemonic Name	Description or Function of Data
ADUM(I) (I = 1,LTOT)	Vector containing the complete set of microscopic cross sections and values of neutrons produced per fission for material k. All scattering matrices are in this vector.
	The cross section values, if present, are contained in the vector in the following order:
	If IWA = 1, the first MAXG (the number of groups used) values are the absorption cross sections starting with group 1.
	If IWA = 1, and IWF = 1, the next MAXG values are the fission cross sections followed by MAXG values of neutrons produced per fission.
	If IWF = 1, the next MAXG values are the fluxes from MATXS.LIB followed by MAXG chi values (fission spectrum) for this material.
	If $|\text{LOL1}| = 1$, the next LOL(1) values are the P0 inelastic cross sections for transfer from group I to group J. The list starts with I = 1 and contains the values for J ranging from 1 to LD(1) + 1. Then the values for I = 2 with J ranging from 2 to LD(1) + 2 are next, etc. until I = LA(1).
	There are LD(1) + 1 values listed for each I, as long as LD(1) + I ≤MAXG. When LD(1) + I > MAXG then only MAXG + 1 - I values are listed for I.
	If LOL1 = -1, the next LOL(1) values are the P1 inelastic cross sections for transfer from group I to group J. The structure of this list is identical to 4.
	If $|\text{LOL2}| = 1$, next LOL(2) values are the P0 (n,2n) cross sections for transfer from group I to group J. The list is ordered as above for the inelastic data.
	If LOL2 = -1, the next LOL(2) values are the P1 (n,2n) cross sections for transfer from group I to group J. The structure of this list is identical to 6.
	If LOL3 = 1, the next LOL(3) values are the isotropic elastic scattering cross sections for transfer from group I to group J followed by the same number of values for the linearly anisotropic component of the elastic scattering cross sections from group I to group J.
	If LOL4 = 1, the next LOL(4) values are the P2 components of the elastic scattering cross sections for transfer from group I to J followed by the P3 components from group I to group J.
	If LOL5 = 1, the next LOL(5) values are the P0 (n,3n) cross sections for transfer from group I to group J. The list is ordered as above for the inelastic data. There is no P1 (n,3n) matrix.
	If LOL6 = 1, the next LOL(6) values are the P0 (n,4n) cross sections for transfer from group I to group J. The list is ordered as above for the inelastic data. There is no P1 (n,4n) matrix.

6.9 Thermal *S(α,β)* and Free Scattering Cross Section Internal Record

itfile = 449 + is
l = group scattered from
jj=group scattered to
ljj=(l-1)*maxg+jj
write (itfile) l,jj,therm0(ljj),therm1(ljj),therm2(ljj),therm3(ljj)
where

$1 \leq is \leq noi$ (noi = number of materials in the problem),
$65 \leq l \leq 167$ (fine groups in the thermal energy range),
$65 \leq jj \leq 167$ (fine groups in the thermal energy range),

7. PROGRAMMER'S GUIDE

COMBINE7.0 is written in FORTRAN 90 and is currently compiled using the Intel Visual Fortran compiler or the Lahey/Fujitsu (LF95) Fortran compiler on the Windows 32 platform. The Intel Visual Fortran compiler provides the faster run time. The source code is heavily commented to explain subroutine functions, data structures, etc. This section provides a short description of each subroutine and shows the overlay structure.

7.1   Flow Diagram

```
combine7†  ──  cpu_time

                  headlin

                  main  ────────  uninpin  ──

                  tail            unifs  ──

                  modules         pstpro  ──

                  Block data      anisn#
```
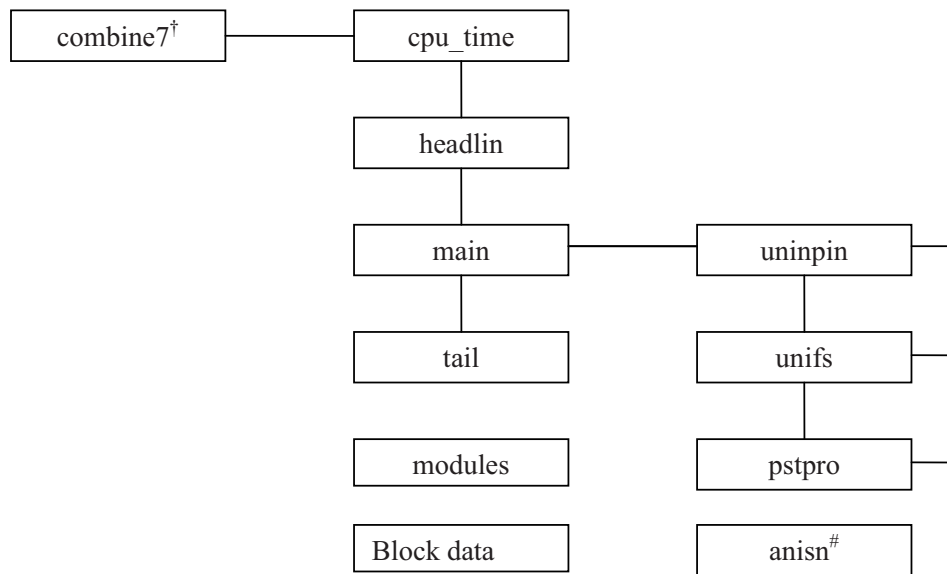
```
--  uninpin -  inp      -    inppck
                         -    inpw
                         -    inpcvi  -   inpalf
                         -    inpalf
            -  unindat -    uninin
                         -    inp2     -   iinkw
                                       -   inpmod  -   inpupk
                         -    endck
                         -    iinkw
                         -    jinkw
                         -    jnp2     -   jinkw
                                       -   jnpmod  -   jnpupk
                         -    err
                         -    unchet  -   jinkw
                                       -   jnp2     -   jinkw
                                                    -   jnpmod  -   jnpupk
```

```
--   unifs    -    spectrum-    mascot  -    output
                          -      bondar  -    lethrg
                                         -    ginsburg-    dancof
                                         -    skipr
                                         -    totcs    -    skipr
                                         -    bonsig0
                 -    lethrg
                 -    nordheim-    reslib
                                  -    grid
                                  -    cross1  -    facts
                                               -    facphi
                                  -    cross2  -    facts
                                               -    facphi
                                  -    cross3  -    facts
                                               -    facphi
                                               -    frobns  -    thrinv
                                                            -    abcmat
                                  -    tbroad  -    movpanl
                                               -    broadn  -    bsigma  -    hunky  -    funky
                                                                                      -    hnabb[*]
                                                                         -    funky
                                  -    admabs  -    reslib
                                               -    cross1  -    facts
                                                            -    facphi
                                               -    cross2  -    facts
                                                            -    facphi
                                               -    cross3  -    facts
                                                            -    facphi
                                                            -    frobns  -    thrinv
                                                                         -    abcmat
                                               -    tbroad  -    movpanl
                                                            -    broadn  -    bsigma  -    hunky -    funky
                                                                                                -    hnabb[*]
                                                                                     -    funky
                                  -    resol   -    newbv   -    interp
                                               -    escape  -    newcyl
                                                            -    newslb
                                               -    trapz
                                               -    samps[*]
                                               -    semps[*]
                                               -    somps[*]
                                               -    sumps[*]
                                               -    svmps[*]
                                               -    swmps[*]
                                               -    sxmps[*]
                                               -    prnres
                 -    chetxs
                 -    chetah  -    getche  -    bonche  -    lethrg
                                                       -    skipr
                                                       -    totcs    -    skipr
                                                       -    bonsig0
                                                       -    unpakk
                               -    eprob   -    escap   -    newcy
                                                        -    newsl
                               -    benwa1  -    intrp
                               -    benwa2  -    intrp
```

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```
                         -    flux    -    bone
                                      -    bthree   -    eval
                                                    -    solv
                                      -    age
                                      -    blknes
        -  xscoal        -    coalesc
                         -    mnd      -    maxwel
                         -    punch
                         -    prtscat
                         -    unpakk
--   pstpro   -   stran  -    contrl   -    updn
                                       -    writhd
                                       -    writhk
                                       -    mapss
                                       -    amatin
                                       -    mapsa    -    writfl
                                       -    mapsi
                                       -    mapdr
                                       -    mapsk
```

_____

Note 1:   † indicates   "program",

         *"function",

         otherwise,   "subroutine".

         # see ANISN manual.

Note 2:   SR.QUIT is used at several places to close temporary files and terminate execution.

An intricsi subroutine, "exit" is used to terminate execution, close all files, and return control to the operating system.

7.2   Summary of Contents of Subroutines

7.2.1   Program COMBINE7.0 and Supporting Subroutines

Overall control of COMBINE7.0 is maintained in PROGRAM COMBINE7.0. It controls the flow of the overall program. COMBINE7.0 calls SR.MAIN to read and digest all of the input data, perform spectrum calculation, and process the cross-section output data into the user-specified final format. It also calls the date and time subroutines to produce the banner information printed at the beginning and end of the printed output.

SR. ABCMAT

Routine to do a matrix multiplication. Called from sr.frobns.

SR. ADMABS

Generates cross sections from the admixed absorber resonances.

SR.AGE

AGE calculates moments and Fermi age from the second moment when an age calculation is requested. These are Equations (137) through (143) in the text.

SR.AMATIN

Processes the neutral internal cross-section file prior to reformatting.

SR.BENWA1

BENWA1 calculates thermal disadvantage factors at each energy point for slab geometry. The slab geometry equations are Equations (172) to (176) in the text. The weights are then used in SR.CHETXS to calculate self-shielding factors for each material in the three region slab geometry cell described in the input data. BENWA1 is called from SR.CHETAH.

SR.BENWA2

BENWA2 calculates thermal disadvantage factors at each energy point for cylindrical geometry. The cylindrical geometry equations are Equations (166) to (175) in the text. The weights are then used in SR.CHETXS to calculate self-shielding factors for each material in the three region, cylindrical geometry cell described in the input data. BENWA2 is called from SR.CHETAH.

BLOCK DATA BLK1

Collision Probabilities from case and Placzek pin locations for dancoff calculation.

SR.BLKNES

BLKNES calculates thermal blackness coefficients for diffusion theory codes. BLKNES is called from SR.FLUX.

SR.BONCHE

Returns Bondarenko shielded cross sections. This routine is used when ABH calculation is requested.

SR.BONDAR

Bondarenko self-shields and transfers all requested library material cross sections to the file unit 419. The file unit 419 is then library file with no additional material to be processed in SR. SPECTRUM.

SR.BONE

BONE solves the B-1 or P-1 groupwise fast spectrum equations by substitution. The solution proceeds from group 1 through group 167 with the thermal upscattering iterations. These are Equations (33) and (34) in the text. The 167 group isotropic neutron flux and current are returned. BONE is called from SR.FLUX.

SR.BONSIG0

Calculates the groupwise Bondarenko background cross sections for the Bondarenko self shielding. Includes the heterogeneous component.

SR. BROADN

Doppler broaden the resolved resonance cross sections.

SR.BSIGMA

A part of Doppler broadening algorithm. Called from SR.BROADN.

SR.BTHREE

BTHREE solves the B-3 groupwise fast spectrum equations by the Gauss-Seidel iteration. These are Equations

(26) through (30) in the text. The groupwise solution proceeds from group 1 through group 167 with the thrmal upscattering iteration. Four Legendre moments for the B-3 fluxes are returned for each microgroup. BTHREE is called from SR.FLUX.

SR.CHETAH

Controls the calculation of thermal disadvantage factors when ABH calculation is requested. The actual disadvantage factors are calculated in SR.BENWA1 for the slab geometry and SR.BENWA2 for the cylindrical geometry. CHETAH is called from SR.SPECTRUM.

SR.CHETAH

CHETAH controls the calculation of the thermal disadvantage factors when an ABH calculation is requested in the input. The actual disadvantage factors are calculated in SR.BENWA1 for slab geometry and SR.BENWA2 for cylindrical geometry.

SR.CHETXS

Corrects cross section in the thermal energy range by ABH's thermal disadvantage factors and substitute microscopic cross sections. Apply only to absorption, fission, and elastic cross section since inelastic, (n,xn) occur at epithermal energy range.

SR.COALSEC

COALSEC calculates the broad group fluxes, currents, and cross sections from the fast spectrum flux/current weighted values. It is called to calculate both macroscopic and microscopic values based on Equations (236) through (266) in the text. COALSEC is called from SR.XSCOAL.

SR.CONTRL

Controller for final formatting of the ASCII cross-section output file.

SR.CROSS1

CROSS1 calculates the single level Breit-Wigner resolved resonance cross sections on energy mesh generated in SR.GRID. Doppler-broadening occurs in SR.TBORAD.

SR.CROSS2

CROSS2 calculates the multi level Breit-Wigner resolved resonance cross sections on energy mesh generated in SR.GRID. Doppler-broadening occurs in SR.TBORAD.

SR.CROSS3

CROSS3 calculates the Reich-Moore resolved resonance cross sections on energy mesh generated in SR.GRID. Doppler-broadening occurs in SR.TBORAD.

SR.DANCOF

DANCOF calculates the Dancoff-Ginsburg factor C for a set of square lattice or hexagonal lattice pins in regular arrays depending upon the type of lattice requested in the input. The factor C(I) for the I resonance material is returned for each calculation. The calculation is for Equations (86) through (88) in the text. DANCOFF is called from SR.GINSBURG.

SR.ENDCK

ENDCK prints an error message when errors are detected on an input card.

SR.EPROB

Calls SR.ESCAP to calculate the escape probability, P_0, for the cell thermal disadvantage factor calculation. The same capture probability tables are used that were constructed for the resolved resonance calculation in the fast spectrum code. EPROB is called from SR.CHETAH.

SR.ERR

ERR prints an error message indicating which items on a given input card are in error.

SR.ESCAP

Copy of SR.ESCAPE. Computes the escape probability, P_0, to be used in the ABH solution. Used for overlay efficiency. Called from SR.EPROB.

SR.ESCAPE

ESCAPE calculates the heterogeneous lump escape probability, P_0, used in Equation (40) for the solution of the resolved resonance collision density. ESCAPE calls SR.NEWCYL or SR.NEWSLB for table lookup values of cylindrical or slab geometries respectively. ESCAPE returns P_0 the escape probability and is called from SR.RESOL.

SR.EVAL

EVAL evaluates the B-3 coefficients A_{ij} in Equations (24). EVAL is called from SR.BTHREE.

SR.FACPHI

Calculate phase shift for the resonance calculation. Called from SR.CROSS1, CROSS2, and CROSS3.

SR.FACTS

Calculates penetration and shift factors for the resonance calculation. Called from SR.CROSS1, CROSS2, and CROSS3.

SR.FLUX

Calls SR.BONE, BTHREE, AGE, and BLKNES for the B-1 spectrum, B-3 spectrum, age, and blakness calculation, respectively.

SR.FROBNS

Inverts a complex matrix. Called from SR.CROSS3.

SR.FUNKY

Designed to define functions that appear in Doppler broadening calculations.

SR.GETCHE

GETCHE reads thermal cross-section data for each material in the three regions, cell disadvantage factor calculation. It is called by CHETAH once for each region in the cell. Macroscopic cross sections are accumulated in each region for use in the disadvantage factor calculation.

SR.GINSBURG

A drive subroutine for Dancoff-Ginsburg factor calculaton.

SR.GRID

GRID calculates a discrete lethargy mesh in energy space which is used in SR.CROSS1, CROSS2, and CROSS3 to calculate the resonance cross sections used in solving Equation (40) for the collision density and Equation (56) for the resonance integrals in the resolved resonance range. The lethargy mesh is generated independently for each resonance from midpoint to midpoint between resonances. The mesh interval is directly proportional to the resonance width and inversely proportional to the resonance energy. A maximum of 900 uniform mesh intervals are permitted for each resolved resonance. However, the mesh spacing from resonance to adjacent resonance varies with gamma, the width of each resonance. The mesh spacing may be controlled by the input parameters FMULT and XLMT defined in the input instructions. The default values, however, produce optimum results. The mesh is therefore non-uniform across the series of resonance levels upstream from any given mesh point in order to calculate scatter-in sources when solving Equation (40). GRID is called from SR.NORDHEIM.

SR.HEADLIN

Prints banner page. Calls date and time.

FUNCTION.HNABB

Calculates hn(a,b) for b $>=$ a by a direct Taylor series expansion of the defining integral. Used in Doppler broadening calculation.

SR.HUNKY

This routine is designed to define functions that appear in Doppler broadening calculations.

SR.INP

Driver for the free format input package. Sets up an array of input data and a table of pointers to the data to allow free field input processing. Supervises subroutines INPALF, INPCVI, INPPCK, INPW. See the extensive comments in these subroutines for details.

SR.INP2

Routine to transfer data from input card buffer to designated storage area in core. Supervises subroutines IINKW, INPMOD/INPUPK. See the extensive comments in these subroutines for details.

SR.INTERP

INTERP is called from SR.NEWBV which is called by SR.RESOL for the resolved resonance numerical solution. NEWBV is called by RESOL to set new back values for the scatter-in source on the right-hand side of Equation (40). INTERP is called by NEWBV to interpolate from old back values to the new back value mesh.

SR.INTRP

INTRP linearly interpolates the dependent variable XY from the input table X,Y, from the argument XX. INTRP is called from SR.BENWA1 and SR.BENWA2.

SR.JNP2

Copy of SR.INP2. Supervises subroutine JINKW, JNPMOD/JNPUPK. Used for overlay efficiency.

SR.LETHRG

LETHRG calculates broad group energy boundaries and lethargy widths from the input cut point. LETHRG is called from SR.BONDAR.

SR.MAIN

Calls SR.UNINPIN for input data processing.
Calls SR.UNIFS for spectrum calculation.
Calls SR.PSTPRO for cross section post processing.

SR.MAPDR

Generate directory record for AMPX material.

SR.MAPSA

Maps cross sections into ANISN 14** format.

SR.MAPSI

Maps cross sections into CCCC ISOTXS format.

SR.MAPSK

Maps INL format data into KENO5A working library format and write.

SR.MAPSS

Maps cross sections into INL format.

SR.MAXWEL

MAXWEL generates a 101 point Maxwellian thermal flux spectrum at the input temperature requested to be used in the MND calculation of MND thermal constants. These are Equations (226) to (232) in the text. MAXWEL is called from SR.MND.

SR.MND

MND calculates Mixed Number Density constants when requested in the input. These are given in Equations (226) to (232) in the text. MND constants may only be calculated for a single thermal energy group. The MND constants are then printed for scrutiny by the user. MND is called from SR.'s MICRO and INMN3.

SR.MOVPANL

Move panel for Doppler broadening. Called from SR.TBROAD.

SR.NEWBV

NEWBV is called by SR.RESOL to calculate a set of new back values for the scatter-in source on the right-hand side of Equation (40). New back values are required because a new uniform mesh is required for Simpson's rule integration of the right-hand side of Equation (40) for the scatter-in source. SR.INTERP is called by NEWBV to interpolate to the new uniform mesh from old back values on the old non-uniform mesh generated for the cross-section calculation in SR.CROSS.

SR.NEWCY

Copy of SR.NEWCYL. Used for overlay efficiency.

SR.NEWCYL

NEWCYL is called by SR.ESCAPE to do the tabular interpolation for the capture probability P_c for cylindrical pins. The escape probability $P_0=1-P_c$.

SR.NEWSL

Copy of SR.NEWSLB. Used for overlay efficiency.

SR.NEWSLB

NEWSLB is called by SR.ESCAPE to do the tabular interpolation for the capture probability P_c for slab geometry. The escape probability $P_0=1-P_c$.

SR.NORDHEIM

Drive routine for Nordeim integral treatment for resonance integrals.

SR.OUTPUT

Writes out most of the data input.

SR.PRNRES

PRNRES prints the results of the resolved resonance calculations by fine group. PRNRES is called from SR.NORDHEIM.

SR.PRTSCAT

PRTSCAT prints out the broad group scattering matrices for both macroscopic and microscopic cross-section data. PRTSCAT is called from SR.XSCOAL.

SR.PSTPRO

Controlled for ASCII flux and cross-section output file post processing.

SR.PUNCH

PUNCH formats and writes the device-specified broad group output data. PUNCH is called from SR.XSCOAL.

SR.QUIT

Exit subroutine. Closes files and terminates program.

SR.MASCOT

Initializes macroscopic scattering cross sections and calls SR.OUTPUT. Called from SR.SPECTRUM.

SR.RESLIB

Read resolve resonance parameters from the "reres.lib" file. Reverse the order from high to low energy.

SR.RESOL

RESOL performs the calculation of the resolved resonance integrals by means of the Nordheim numerical solution. It calls SR.CROSS to generate the Doppler-broadened cross sections from the resolved resonance parameters. It solves Equation (4) at each fine lethargy mesh point for the collision density. It constructs resonance integrals from Equation (56). Shielding of the elastic scattering matrices is performed using Equations (76) through (86) in the text. SR.PRNRES is then called to print the results of the resonance calculations at the completion of the unresolved resonance calculation. RESOL is called from SR.NORDHEIM.

FUNCTION SAMPS

SAMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the principal resonance absorber by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SAMPS is called from SR.RESOL.

FUNCTIOM SEMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the first input moderator by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

SR.SKIPR

Skip forward or backward on a coded or blocked binary tape. Works on the binary "matxs.lib."

SR.SOLV

SOLV solves the B-3 Equation (26) by means of block Gauss elimination one group a time from high to low in energy. SOLV is called from SR.BTHREE.

FUNCTIOM SOMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the second input moderator by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

SR.SPECTRUM

Drives spectrum calculation by first generating the required fine group cross sections and then calculating spectrum.

SR.STRAN

Driver for reformatting the ASCII cross-section output file from internal format to the user-requested final format. Sets up storage, etc.

FUNCTIOM SUMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the third input moderator by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

FUNCTIOM SVMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the first input admixed

resonance absorber by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

FUNCTIOM SWMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the second input admixed resoanance absorber by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

FUNCTIOM SXMPS

SEMPS integrates the scatter-in source term on the right-hand side of Equation (40) for the third input admixed resonance absorber by means of Simpson's rule. The integration is over the back-value mesh generated in SR.NEWBV. SEMPS is called from SR.RESOL.

SR.TAIL

Prints final banner. Print date, time, and elapsed run time.

SR.TBROAD

Manages the paging of cross section data for Doppler broadening.

SR.THRINV

Inverts symmetric matrix. Called from SR.FROBNS.

SR.TOTCS

Read total cross section from vector blocks in "matxs.lib" for all sibmaterials and save on direct access file, 'is' unit.

SR.TRAPZ

TRAPZ performs a trapezoidal integration of seven dependent variables from SR.RESOL over uniform mesh for one energy group in the resolved resonance range. The seven integrals are returned. TRAPZ is called from SR.RESOL.

SR.UNCHET

UNCHET reads and prints the three region ABH disadvantage factor input data on the 2000000 series cards in the input description. UNCHET is called from SR.UNINDAT only when an ABH disadvantage factor calculation is requested.

SR.UNIFS

Calls SR.SPECTRUM, which drives the spectrum calculation. Also calls SR.XSCOAL, which drives the cross section coalescing.

SR.UNINDAT

UNINDAT reads the input integer data cards in the 1000000 series and maps the input data onto modules. The data are then checked for range errors and any errors are printed. UNINDAT is called from SR.UNINPIN.

SR.UNININ

UNININ initializes the input integer data arrays before the entry of change case data. This preserves unchanged values from the previous problem. UNININ is called from SR.UNINDAT.

SR.UNINPIN

UNINPIN controls the reading of all input data on 1000000 series cards using INP subroutines. SR.UNINDAT is called to map input data which is read onto modules. UNINPIN is called form PROGRAM COMBINE7.

SR.UNPAKK

Takes the cross section data present in the ADUM array read from unit 404(????) and packs them into the local variables. UNPAKK is called from SR.GETCHE and SR.XSCOAL.

SR.UPDN

Find the largest upscatter distance, largest downscatter distance, count total number of materials in the file, and manufacture an ISOTXS 6-character name for each material.

SR.WRITFL

Utility for writing ANISN, free form, ASCII input using repeats and fills as appropriate.

SR.WRITHD

Writes header information if ISOTXS cross-section output is specified.

SR.WRITHK

Writes header for KENO5 fromat.

SR.XSCOAL
Drives the coalescing option.

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APPENDIX A

INL CROSS-SECTION FORMAT DESCRIPTION

Appendix A
INL Cross-Section Format Description

The internal INEL format is based on a word-addressable card image file structure. The following tables describe this structure. A nonzero value in column 1 of a data record for a material signifies the end of data for that material The scatter matrices do not have the 2L + 1 term multiplied into them.

Table A-1. The library material title record summary.

Information or Mnemonic Name of Data	Record Columns	Description or Function
IAD	2-3	A nonzero value means update rather than replace or add this material to the library file.
IDIFF	4-5	A nonzero value means the SIGMU(J,IM) values are computed from the input D(J,IM) values instead of read directly.
MTLNO (or LM)	6-8	Library material identifying number.
IENPF	9-10	Controls how the energy per fission values are input:
		$0, \varepsilon_j^m = $ EPFISS,
		$1, \varepsilon_j^m = \varepsilon_1^m,$
		$2, \varepsilon_j^m$ as input, where m = MTLNO.
	11-12	Must be blank.
Any Hollerith characters	13-72	Library material title information.

Table A-2. The library material floating point data summary.

Index 1 Card Cols. 2-3	Index 2 Card Cols. 4-5	Index 3 Card Cols. 6-8	Index 4 Card Cols. 9-10	Mnemonic Name of Data	Description or Function of Data (index which increases as more data words are added across a card is enclosed in parenthesis)
1	LM	J	1	DC(J,LM)	Diffusion coefficient for group J of library material LM (when IDIFF = 1 on the title card). (J)
1	LM	J	2	SIGA(J,LM)	Absorption cross section for group J of library material LM. (J)
1	LM	J	3	SIGNU(J,LM)	Neutron per fission times fission cross section for group J of library material LM ($\upsilon\sum_f$).
1	LM	J	4	SIGFIS(J,LM)	Fission cross section for group J of library material LM. (J)
1	LM	J	5	ENERGY(J;LM)	Energy per fission for group J of library material LM. (J)
3	LM	J	K	TRMAT(J,K)	General scattering transfer cross sections $\sum_{s0}$, from group J to group K for library material m $\equiv$ LM (K may be less than, equal to, or greater than J). (K)
4	LM	J	0	SIGMU(J,LM)	Transport cross section σ_{uj}^m for group j = J of library material m $\equiv$ LM (used in group j = J for mixing the macroscopic cross section, $\sum_{uj}^m$, from which the macroscopic diffusion coefficient, D_j^m, for macroscopic material m is computed). This input data is used only if IDIFF = 0 or blank on the title card.(J)
6	LM	J	K	TRMAT1(J,K)	Same as INDEX1 = 3 for values of $\sum_{s1}^m$ (K)
7	LM	J	K	TRMAT2(J,K)	Same as INDEX1 = 3 for values of $\sum_{s2}^m$ (K)
8	LM	J	K	TRMAT3(J,K)	Same as INDEX1 = 3 for values of $\sum_{s3}^m$ (K)

APPENDIX B

ANISN CROSS-SECTION FORMAT DESCRIPTION

Appendix B
ANISN Cross-Section Format Description

If the ANISN output format is selected, all cross sections are output in the standard ANISN card image 14** format (see Reference B-1 for details). The absorption, nu-sigma-fission, and total cross sections are always present regardless of the scattering order of the material or the current group number. For scattering orders beyond

e = 0, the absorption, nu-sigma-fission, and total cross sections are 0.0.

The upscatter cross sections are present only when (HIS-IHT) is greater than 1. If they are present, there are NUS = (HIS - IHT - 1) locations present for every group and for every scattering order (material). This includes the physically nonexistent quantities such as σ upscattering from group (IGM + NUS) to the lowest energy group IGM. In this way, the number of upscatter cross sections for each group in the cross-section table remains constant. The cross-section arrangement is summarized in Table B-1.

Table B-1. Cross-section arrangement.

Cross Section	Group	Position Description
σ absorption	g	
υσ fission	g	
σ total or σ transport	g	IHT
σ upscatter	(g + NUS)→g	
•	•	
•	•	
•	•	
σ upscatter	(g + 1)→g	IHS
σ self-scatter	g→g	
σ downscatter	(g - 1)→g	
•	•	
•	•	
•	•	
σ downscatter	(g - NDS)→g	IHM
σ upscatter (code calculated)	From g	IHP = IHM + 1

Finally, it should be noted that the higher-order scattering materials are output by COMBINE/PC without the $(2\ell + 1)$ term premultiplied into them.

B. REFERENCE

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APPENDIX C

CCCC INTERFACE FILE FORMATS AND CONVENTIONS

Appendix C
CCCC Interface File Formats and Conventions[a]

ISOTXS—Nuclide (Isotope) Ordered, Multigroup Neutron Cross-Sections

The changes in ISOTXS-IV relative to ISOTXS-III are in the main part, clarifications of ambiguities present in the latter. The changes reflected in Version IV are:

- If scattering bandwidth, JBAND(J,N), is zero, no scatter data are present in block N. (see 4D record.)

- The position of self-(or within-group-) scatter must liewithin the scattering bandwidth unless the bandwidth is zero, i.e.,

  I < IJJ(J,N) < JBAND(J,N) if JBAND(J,N) ≠0.

- (See 4D record.)

- The Legendre expansion coefficient factor $(2\rho + 1)$ is not included in the P ρ weighted transport and total cross sections. (See 5D record.)

- The n,2n principal cross section (see 5D record) is clarified as the n,2n reaction cross section while the n,2n scatter matrix terms are clarified (see 4D record NOTE) as emission (productin) based, i.e.,

$$\sigma_{n,2n(g)} = 0.5 \sum_{g'} \sigma_{n,2n}(g \to g') \tag{C-1}$$

In addition, the following is included to clarify the meaning of the vectors IDSCT(N) and LORD(N) contained in the ISOTOPE CONTROL AND GROUP-INDEPENDENT DATA (4D) record and to remove an ambiguity in the subblocking of scattering data.

IDSCT(N) specifies the identity and ordering of scattering data blocks, and LORD(N) specifies the number of Legendre orders contained in each block. Each block of scattering may be subblocked into NSBLOCK records (subblocks) where NSBLOCK is found on the FILE CONTROL (ID) record. With the single exception below, sub-blocking shall not be used (NSBLOCK > 1) if the individual blocks defined by IDSCT and LORD contain more than one Legendre order of scattering. The single exception is that subblocking may be used with more than one Legendre order per record (subblock) only if each record (subblock) contains data for a single "scattered-into" group.

Finally, the following information is reproduced from the Version III specifications for the sake of completeness.

The P ρ weighted transport and total cross sections can be defined[b] as

$$\sigma_{n,22,(g)} = 0.5 \sum_{g'} \sigma_{n,2n}(g \to g') \quad \rho = 1, \ldots, LTRN , \tag{C-2}$$

and

---

a. Extracted from LA-6941-MS, Standard Interface Files and Procedures for Reactor Physics Codes Version IV by R. Douglas O'Dell.

b. Other definitions of the P ρ weighted transport cross section are also possible.

The P ρ weighted scattering cross sections given in the scattering blocks are defined as

$$\sigma_{t\rho}^{g} \equiv \frac{\int_{g} \sigma_{\rho}(E)dE}{\int_{g} \sigma_{\rho}(E)dE} \quad \rho = 0,1,\ldots,\text{LTOT-1} \quad . \tag{C-3}$$

$$\sigma_{s\rho}(g \to g') \equiv \frac{\int_{g} \int_{g} \sigma_{s\rho}(E \to E')\sigma_{\rho}(E)dE'dE}{\int_{g} \sigma_{\rho}(E)dE} \tag{C-4}$$

```
C********************************************************************************
C   REVISED 11/30/76          -
C                    -
CF       ISOTXS-IV            -
CE       MICROSCOPIC GROUP NEUTRON CROSS SECTIONS            -
C               -
CN  THIS FILE PROVIDES A BASIC BROAD GROUP         -
CN  LIBRARY, ORDERED BY ISOTOPE           -
CN  FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES        -
CN  ONLY       -
C               -
C********************************************************************************
C-------------------------------------------------------------------------------------------------------------------
CS      FILE STRUCTURE            -
CS               -
CS        RECORD TYPE    PRESENT IF            -
CS        ================================= ============            -
CS        FILE IDENTIFICATION        ALWAYS            -
CS        FILE CONTROL   ALWAYS            -
CS         FILE DATA        ALWAYS            -
CS         FILE-WIDE CHI DATA        ICHIST .GT. 1            -
CS               -
CS ************(REPEAT FOR ALL ISOTOPES)            -
CS *      ISOTOPE CONTROL AND GROUP         -
CS *        INDEPENDENT DATA        ALWAYS            -
CS *      PRINCIPAL CROSS SECTIONS     ALWAYS            -
CS *        ISOTOPE CHI DATA        ICHI .GT .1            -
CS *               -
CS *   **********(REPEAT TO NSCMAX CATTERING BLOCKS)            -
CS *  *    *******(REPEAT FROM 1 TO NSBLOK)            -
CS *  *  *    SCATTERING SUB-BLOCK        LORD (N) .GT .0            -
CS ************            -
C               -
C-------------------------------------------------------------------------------------------------------------------
```

```
C-------------------------------------------------------------------------------------------------------------------------------
CR       FILE IDENTIFICATION                      -
C                                                 -
CL  HNAME, (HUSE (I), I=1,2), IVERS               -
C                                                 -
CW 1+3*MULT=NUMBER OF WORDS                       -
C                                                 -
CB FORMAT (11H  OV  ISOTXS ,    1H*,              -
CB 12A6, 1H*, I6)                     -
C                                                 -
CD HNAME      HOLLERITH FILE NAME - ISOTXS - (A6)              -
CD HUSE (I)    HOLLERITH USER IDENTIFICATION (A6)              -
CD IVERS       FILE VERSION NUMBER                    -
CD MULT        DOUBLE PRECISION PARAMETER            -
CD      1 -  A6 WORD IS SINGLE WORD              -
CD      2 -  A6 WORD IS DOUBLE PRECISION WORD             -
C                                                 -
C-------------------------------------------------------------------------------------------------------------------------------
C-------------------------------------------------------------------------------------------------------------------------------
CR       FILE CONTROL     (1D RECORD)                  -
C                                                 -
CL  NGROUP, NISO, MAXUP, MAXDN, MAXORD, ICHIST, NSCMAX, NSBLOK              -
C                                                 -
CW 8 = NUMBER OF WORDS                 -
C                                                 -
CB FORMAT (4H  1D   ,8I6)             -
C                                                 -
CD NGROUP         NUMBER OF ENERGY GROUPS IN FILE             -
CD NISO    NUMBER OF ISOTOPES IN FILE         -
CD MAXUP         MAXIMUM NUMBER OF UPSCATTER GROUPS                 -
CD MAXDN         MAXIMUM NUMBER OF DOWNSCATTER GROUPS                  -
CD MAXORD        MAXIMUM SCATTERING ORDER (MAXIMUM VALUE OF              -
CD LEGENDRE EXPANSION INDEX USED IN FILE).             -
CD ICHIST FILE-WIDE FISSION SPECTRUM FLAG               -
CD ICHIST . EQ . 0,      NO FILE-WIDE SPECTRUM             -
CD ICHIST .EQ . 1,      FILE-WIDE CHI VECTOR           -
CD ICHIST .GT . 1,      FILE-WIDE CHI MATRIX           -
CD NSCMAX        MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA                 -
CD NSBLOK        SUBBLOCKING CONTROL FOR SCATTER MATRICES.  THE                -
CD         SCATTERING DATA ARE SUBBLOCKED INTO NSBLOK              -
CD         RECORDS (SUBBLOCKS) PER SCATTERING BLOCK.              -
C                                                 -
C-------------------------------------------------------------------------------------------------------------------------------
```

```
C---------------------------------------------------------------------------------------------------------------------
CR      FILE DATA (2D  RECORD)              -
C                                          -
CL   (HSETID (I) , I=1 , 12) , (HISONM (I) , I=1 , NISO) ,            -
CL  1(CHI(J) , J=1, , NGROUP) , (VEL (J) , J=1 , NGROUP)              -
CL  2(EMAX(J) , J=1 , NGROUP) , EMIN, (LOCA(I) , I=1 , NISO)               -
C                                          -
CW (NISO+12)*MULT+1+NISO                   -
CW +GROUP*(2+ICHIST*(2/(ICHIST+1)))=NUMBER OF WORDS               -
C                                          -
CB FORMAT  (4H 2D  , 1H*, 11A6, 1H*/       HSETID,HISONM           -
CB 11H* ,A6, 1H* ,9(1X,A6)/(10(10(1X,A6)))            -
CB FORMAT (   6E12.5)        CHI   (PRESENT IF  ICHIST  .EQ .1)            -
CB FORMAT (   6E12.5)        VEL, EMAX, EMIN          -
CB FORMAT (12I6) LOCA               -
C                                          -
CD HSETID (I)       HOLLERITH IDENTIFICATION OF FILE  (A6)            -
CD HISONM (I)       HOLLERITH ISOTOPE LABEL FOR ISOTOPE   I  (A6)             -
CD CHI (J)  FILE-WIDE FISSION SPECTRUM (PRESENT IF ICHIST. EQ .1)          -
CD VEL (J) MEAN NEUTRON VELOCITY IN GROUP  J  (CM/SEC)            -
CD EMAX (J)        MAXIMUM ENERGY BOUND OF GROUP J (EV)          -
CD EMIN   MINIMUM ENERGY BOUND OF SET (EV)               -
CD LOCA (I)        NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR          -
CD ISOTOPE  I.   LOCA (1) = 0             -
C                                          -
C---------------------------------------------------------------------------------------------------------------------
C---------------------------------------------------------------------------------------------------------------------
CR FILE-WIDE  CHI  DATA      (3D  RECORD)              -
C                                          -
CC      PRESENT  IF  ICHIST .GT .1         -
C                                          -
CL  ((CHI(K,J) , K=1 , ICHIST) , J=1 , NGROUP) , (ISSPEC (I=1 , NGROUP)            -
C                                          -
CW NGROUP*( ICHIST+1)=NUMBER  OF  WORDS               -
C                                          -
CB  FORMAT ( 4H  3D  ,  5E12.5/ (6E12.5)) CHI               -
CB  FORMAT ( 12I6)       ISSPEC                -
C                                          -
CD CHI (K , J)       FRACTION OF NEUTRONS EMITTED INTO ROUP J AS A              -
CD RESULT OF FISSION IN ANY GROUP, USING SPECTRUM K          -
CD ISSPEC ( I )      ISSPEC ( I ) =K  IMPLIES THAT SPECTRUM K IS USED              -
CD TO CALCULATE EMISSION SPECTRUMF ROM FISSION           -
CD IN GROUP I               -
C                                          -
C---------------------------------------------------------------------------------------------------------------------
```

```
C---------------------------------------------------------------------------------------------------
CR      ISOTOPE CONOTROL AND GROUP INDEPENDENT DATA   (4D RECORD)            -
C                                                      -
CL   HABSID, HIDENT, HMAT, AMASS, EFFISS, ECAPT, TEMP, SIGPOT, ADENS, KBR, ICHI,        -
CL 1IFIS, IALF, INP, IN2N, IND, INT, LTOT, LTRN, ISTRPD,          -
CL 2(IDSCT (N), N=1, NSCMAS), (LORD (N), N=1, NSCMAX),            -
CL 3((JBAND (J,N), J=1, NGROUP), N=1, NSCMAX),           -
CL 4((IJJ(J,N), J=1, NGROUP), N=1, NSCMAX)          -
C                                           -
CW 3*MULT+17+NSCMAX*(2*NGROUP+2) = NUMBER OF WORDS            -
C                                           -
CB   FORMAT (4H 4D ,3 (1X,A6)/    6E12.5/          -
CB 1(12I6))          -
C                                  -
CD HABSID         HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR ALL         -
CD VERSIONS OF THE SAME ISOTOPE IN FILE (A6)        -
CD HIDENT         IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA         -
CD CAME (E.G. ENDF/B)    (A6)              -
CD HMAT  ISOTOPE IDENTIFICATION (E.G. ENDF/B MAT NO.)(A6)          -
CD AMASS GRAM ATOMIC WEIGHT                -
CD EFISS   TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)         -
CD ECAPT  TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT)          -
CD TEMP   ISOTOPE TEMPERATURE (DEGREES KELVIN)           -
CD SIGPOT AVERAGE EFFECTIVE POTENTIAL SCATTERING IN          -
CD RESONANCE RANGE (BARNS/ATOM)            -
CD ADENS DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE           -
CD CROSS SECTIONS WERE GENERATED (A/BARN-CM)           -
CD KBR      ISOTOPE CLASSIFICATION          -
CD 0=UNDEFINED          -
CB 1=FISSILE          -
CB 2=FERTILE          -
CD 3=OTHER ACTINIDE           -
CD 4=FISSION PRODUCT           -
CD 5=STRUCTURE          -
CD 6=COOLANT          -
CD 7=CONTROL          -
CD ICHI     ISOTOPE FISSION SPECTRUM FLAG            -
CD ICHI.EQ.1,      USE FILE-WIDE CHI           -
CD ICHI.EQ.1,      ISOTOPE CHI VECTOR          -
CD ICHI.GT.1,      ISOTOPE CHI MATRIX          -
CD IFIS(N,F) CROSS SECTION FLAG         -
CD         IFIS =0, NO FISSION DATA IN PRINCIPAL CROSS          -
CD SECTION RECORD          -
CD =1, FISSION DATA PRESENT IN PRINCIPAL          -
CD CROSS SECTION RECORD          -
CD IALF    (N, ALPHA) CROSS SECTION FLAG           -
CB         SAME OPTIONS AS IFIS          -
CB INP (N, P) CROSS SECTION FLAG          -
CD         SAME OPTIONS AS IFIS          -
CD IN2N    (N, 2N) CROSS SECTION FLAG          -
CD         SAME OPTIONS AS IFIS          -
CD IND(N,D) CROSS SECTION FLAG          -
CD         SAME OPTIONS AS IFIS          -
CD INT(N, T) CROSS SECTION FLAG          -
CD         SAME OPTIONS AS IFIS          -
```

CD LTOT   NUMBER OF MOMENTS OF TOTAL CROSS SECTION PROVIDED   -
CD   IN PRINCIPAL CROSS SECTIONS RECORD   -
CD LTRN   NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION   -
CD   PROVIDED IN PRINCIPAL CROSS SECTIONS RECORD   -
CD ISTRPD NUMBER OF COORDINATE DIRECTIONS FOR WHICH   -
CD   COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS   -
CD   ARE GIVEN. IF ISTRPD = 0, NO COORDINATE DEPENDNET   -
CD   TRANSPORT CROSS SECTIONS ARE GIVEN.   -
CB IDSCT(N)   SCATTERING MATRIX TYPE IDENTIFICATION FOR   -
CB   SCATTERING BLOCK N. SIGNIFICANT ONLY IF   -
CD   LORD (N). GT.0   -
CD   IDSCT (N) =000 + NN, TOTAL SCATTERING, (SUM OF   -
CD ELASTIC, INELASTIC, AND N, 2N SCATTERING   -
CD MATRIX TERMS).   -
CD   =100 + NN, ELASTIC SCATTERING   -
CD   =200 + NN, INELASTIC SCATTERING   -
CD   =300 + NN, (N, 2N) SCATTERING,-----SEE   -
CD   NOTE BELOW   -
CD   WHERE NN IS THE LEGENDRE EXPANSION INDEX OF THE   -
CD   FIRST MATRIX IN BLOCK N   -
CD LORD (N)   NUMBER OF SCATTERING ORDERS IN BLOCK N. IF   -
CD   LORD (N) = 0, THIS BLOCK IS NOT PRESENT FOR THIS   -
CD   ISOTOPE. IF NN IS HE VALUE TKEN FROM   -
CD   IDSCT (N), THEN THE MATRICES IN THIS BLOCK   -
CD   HAVE LEGENDRE EXPANSION INDICES OF NN, NN+1,   -
CB   NN+2,…, NN+LORD (N) - 1   -
CB JBAND(J,N)   NUMBER OF GROUPS THAT SCATTER INTO GROUP J,   -
CD   INCLUDING SELF-SCATTER, IN SCATERING BLOCK N.   -
CD   IF JBAND (J,N) = 0, NO SCATTER DATA IS PRESENT IN   -
CD   BLOCK N   -
CD IJJ(J,N) POSITION OF IN-GROUP SCATTERING CROSS SECTION IN   -
CD   SCATTERING DATA FOR GROUP J, SCATTERING BLOCK   -
CD   N, COUNTED FROM THE FIRST WORD OF GROUP J DATA.   -
CD   IF JBAND (J,N). NE. 0 THEN IJJ(,N) MUST SATISFY   -
CD   THE RELATION 1.LE.IJJ (J,N).LE.JBAND (J,N)   -
C   -
CN   NOTE- FOR N,2N, SCATTER, THE MATRIX CONTAINS TERMS,   -
CN   SCAT (J TO G), WHICH ARE EMISSION (PRODUCTION)   -
CN   BASED, I.E., ARE DEFINED SUCH THAT MACROSCOPIC   -
CN   SCAT (J TO G) TIMES THE FLUX IN GROUP J GIVES   -
CN   THE RATE OF EMISSION (PRODUCTION) OF NEUTRONS   -
CN   INTO GROUP G.   -
C   -
C--

```
C----------------------------------------------------------------------------------------------------
CR  PRINCIPAL CROSS SECTIONS       (5D RECORD)              -
C    ((STRPL (J,L), J=1, NGROUP), L=1, LTRN),               -
CL  1((STOTPL (J,L), J=1, NGROUP), L=1, LTOT), (SNGAM(J), J=1, NGROUP),        -
CL  2(SFIS (J), J=1, NGROUP), (SNUTOT (J), J=1, NGROUP),          -
CL  3(CHISO (J), J=1, NGROUP), (SNALF (J), J=1, NGROUP),          -
CL  4(SNP (J), J=1, NGROUP), (SN2N (J), J=1, NGROUP),           -
CL  5(SND (J), J=1, NGROUP), (SNT (J), J=1, NGROUP)             -
CL  6((STRPD (J,I), J=1, NGROUP), I=1, ISTRPD)              -
C                                     -
CW  (1+LTRN+LTOT+IALF+INP+IN2N+IND+INT+ISTRPD+2*IFIS+              -
CW  ICHI* (2/(ICHI+1)))*NGROUP=NUMBER OF WORDS            -
C                                     -
CB   FORMAT (4H  5D  ,      5E12.5/(6E12.5)) LENGTH OF LIST AS ABOVE           -
C                                     -
CD  STRPL (J,L)        PL WEIGHTED TRANSPORT CROSS SECTION          -
CD  THE FIRST ELEMENT OF ARRAYY STRPL IS THE          -
CD  CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION          -
CD  THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1)         -
CD  IS NOT INCLUDED IN STRPL (J,L).            -
CD  SNGAM (J)         (N,GAMMA)           -
CD  SFIS (J)          (N,F)  (PRESENT IF IFIS.GT.0)        -
CD  SNUTOT (J)        TOTAL NEUTRON YIELD/FISSION(PRESENT IF IFIS.GT.0)       -
CD  CHISO (J)        ISOTOPE CHI      (PRESENT IF ICHI.EQ.1)        -
CD  SANLF (J)        (N, ALPHA)       (PRESENT IF IALF.GT.0)         -
CD  SNP (J)          (N,P)  (PRESENT IF INP.GT.0)        -
CD  SN2N (J)         (N, 2N)        (PRESENT IF IN2N.GT.0)    ----SEE       -
CD        NOTE BELOW----                  -
CD  SND (J)          (N,D)  (PRESENT IF IND.GT.0)        -
CD  SNT (J)          (N,T)  (PRESENT IF IND.GT.0)        -
CB  STRPD (J,I)        COORDINATE DIRECTION I TRANSPORT CROSS SECTION        -
CB  (PRESENT IF ISTRPD.GT.0)              -
C                                     -
CN       NOTE - THE PRINCIPAL N,2N CROSS SECTION SN2N(J)          -
CN  IS DEFINED AS THE N,2N CROSS SECTION SN2N(J)          -
CN  I.E., SUCH THAT MACROSCOPIC SN2N(J) TIMES THE          -
CN  FLUX IN GROUP J GIVES THE RATE AT WHICH N, 2N          -
CN  REACTIONS OCCUR IN GROUP J.  THUS, FOR N, 2N          -
CN  SCATTERING, SN2N (J) = 0.5*(SUM OF SCAT (J TO G)          -
CN  SUMMED OVER ALL G).               -
C                                     -
C----------------------------------------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------------------------------------------------------
CR  ISOTOPE CHI DATA      (6D RECORD)                    -
C                                              -
CC  PRESENT IF ICHI.GT.1                    -
C                                              -
CL  ((CHIISO(K,J),K=1,ICHI),J=1, NGROUP), (ISOPEC(I), I=1, NGROUP)        -
C                                              -
CW  NGROUP*(ICHI+1) = NUMBER OF WORDS                      -
C                                              -
CB  FORMAT (4H  6D  , 5E12.5))    CHIISO                  -
CB  FORMAT (12I6)     ISOPEC                    -
C                                              -
CD  CHIISO (K, J)     FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A          -
CD       RESULT OF FISSION IN ANY GROUP, USING SPECTRUM K          -
CD  ISOPEC (I)   ISOPEC (I) = K IMPLIES THAT SPECTRUM K IS USED            -
CD       TO CALCULATE EMISSION SPECTRUM ROM FISSION            -
CD       IN GROUP I                    -
C                                              -
C                                              -
C-----------------------------------------------------------------------------------------------------------------------
C-----------------------------------------------------------------------------------------------------------------------
CR           SCATTERING SUB-BLOCK  (7D RECORD)            -
C                                              -
CC       PRESENT IF LORD (N) .GT.0                -
C                                              -
CL  ((SCAT (K, L), K=1, KMAX), L=1, LORDN)                -
C                                              -
CC  KMAX=SUM OVER J OF JBAND (J,N) WITHIN THE J-GROUP RANGE OF THIS          -
CC     SUB-BLOCK. IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP          -
CC     RANGE CONTAINED WITHIN THIS SUB-BLOCK IS            -
CC     JL = (M-1)*((NGROUP-1)/NSBLOK + 1)+1 TO JU=MINO (NGROUP, JUP),          -
CC     WHERE JUP = M* ((NGROUP-1)/NSBLOK + 1).            -
C                                              -
CC  LORDN = LORD (N)                    -
CC  N IS THE INDEX FOR THE LOOP OVER NSCMAX (SEE FILE STRUCTURE)          -
C                                              -
CW  KMAX*LORDN = NUMBER OF WORDS            -
C                                              -
CB  FORMAT (4H  7D  ,    5E12.5))                -
C                                              -
CD  SCAT (K,L)      SCATTERING MATRIX OF SCATTERING ORDER L, FOR          -
CD       REACTION TYPE IDENTIFIED BY IDSCT (N) FOR THIS          -
CD       BLOCK. JBAND (J, N) VALUES FOR SCATTERING INTO          -
CD       GROUP J ARE STORED AT LOCATIONS K=SUM FROM 1          -
CD       TO (J-1) OF JBAND (J,N) PLUS 1 TO K-1+JBAND (J,N).          -
CD       THE SUM IS ZERO WHEN J=1.  J-TO-J SCATTER IS            -
CD       THE IJJ (J, N) -TH ENTRY IN THE RANGE JBAND (J, N).          -
CD       VALUES ARE STORED IN THE ORDER (J+JUP),          -
CD       (J + JUP - 1),…, (J + 1), J, (J - 1),…, (J - JDN),          -
CD       WHERE JUP = IJJ (J, N) - 1 AND JDN = JBAND (J, N) - IJJ (J, N)          -
C                                              -
C-----------------------------------------------------------------------------------------------------------------------
CEOF
```

APPENDIX D

VALIADTION OF COMBINE7.0 CRITICALITY SEQUENCES

Appendix D
Validation of COMBINE7.0 Criticality Sequences

Criticality validation calculations were performed as part of verification and validation of the code. The COMBINE7.0 criticality validation suite is a collection of 29 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments* (IHECB) [1] and/or *Cross Section Evaluation Working Group Benchmark Specifications* (CSEWG) [2]. The cases in the suite were selected to compass a variety of fissle materials in configurations that produce fast, intermediate, and thermal spectra, but were limited to those configurations which COMBINE7.0 calculation sequence, i.e., COMBINE7.0/ANISN, can afford, . Some independent MCNP [3] calculations were also performed, all based on ENDF/B-VII.0 nuclear data. The distribution of cases by fuel material and spectrum is shown in Table D.1, and a brief summary of each case is followed. The results are listed in Table D.2, D.3, D.4, and D.5 for the combination of B1 or B3 and Sn correction or no Sn correction. The experiment k_{eff} values have some uncertaites involved and estimated to be mostly with in 1.0000 ± 0.0050 [1]. The k_{eff} values from MCNP calculations are also included. The results show the sensitivity to the deterministic nature of the method and to the B_L approximation limited to L=1 or L=3. The results are very robust despite these limitations and are very comparable to the experiments or the MCNP results. A limited number of cases included the one-dimensional transport correction, showing a small improvement. Some sensitivity can be digested from these calculations. All the relevant input files are included in the code package.

Table D.1: Criticality Validation Suite

Spectrum		Fast		Intermediate	Thermal	
		Heavy	Light		Soution	
Geometry	Bare	Reflector	Refelctor	Any	Lattice of Fuel Pins in Water	Bare	Reflector
HEU	GODIVA	FLATTOP-25		HCI-004		ORNL-1, ORNL-2, ORNL-10, L-8, L-9	L-7, L-10
IEU	IEU-MF-03						
LEU					TRX1, TRX2, BAPL1, BAPL2, BAPL3		
^{233}U	JEZEBEL-23	UMF002-1, UMF002-2	UMF005-1, UMF005-2				
Pu	JEZEBEL, JEZEBEL-Pu	FLATTOP-PU		PCI-001		PNL-1, PNL-2, PNL-3, PNL-4	

GODIVA

This is a bare sphere of enriched uranium metal modeled as a homogeneous sphere of radius 8.741 cm with the composition shown in the following table (number densities are given in nuclides per barn-cm).

Isotope	Density
^{235}U	0.045000
^{238}U	0.002498
^{234}U	0.000492

FLATTOP-25

This is a spherical system consisting of a highly enriched uranium core in a thick natural uranium reflector. The core radius is 6.116 cm and the outer radius of the reflector is 24.13 cm. The compositions for the two regions (nuclides per bar-cm) are given in the following table.

Isotope	Core	Reflector
^{235}U	0.04449	0.00034
^{238}U	0.00270	0.04774
^{234}U	0.00049	

FLATTOP-PU

This is a spherical system consiting of a plutonium core in a thick natural uranium reflector. The radius of the core is 4.533 cm and the outer radius of the reflector is 24.13 cm. The compositions of the two regions are given in the following table.

Isotope	Core	Reflector
^{239}Pu	0.03674	
^{240}Pu	0.00186	
^{241}Pu	0.00012	
Ga	0.00138	
^{235}U		0.00034
^{238}U		0.04774

JEZEBEL

This is a bare sphere of plutonium modeled as a homogeneous sphere of radius 6.385 cm with the composition shown in the following table (all number of densities are given as nuclides per barn-cm).

Isotope	Density
^{239}Pu	0.037050
^{240}Pu	0.001751
^{241}Pu	0.000117
Ga	0.001375

JEZEBEL-23

This is a bare sphere of enriched ^{233}U metal (98.13%) with radius 5.983 cm and the composition shown in the following table (all number of densities are given as nuclides per barn-cm).

Isotope	Density
^{233}U	0.04671
^{234}U	0.00059
^{235}U	0.00001
^{238}U	0.00029

JEZEBEL-Pu

This is a bare sphere of enriched plutonium meta, containing 20.1% ^{240}Pu. It is modeled as a homogeneous sphere of radius 6.65985 cm with the composition shown in the following table (all number of densities are given as nuclides per barn-cm).

Isotope	Density
^{239}Pu	0.029946
^{240}Pu	0.007887
^{241}Pu	0.001203
^{242}Pu	0.000145
Ga	0.001372

U233-met-fast-002 (umf-002)

This is a spherical system consisting of a highly enriched ^{233}U surrounded by highly enriched ^{235}U.

- Case (1) The core radius is 5.0444 cm and the outer radius of the surrounding highly enriched ^{235}U is 6.2661 cm.
- Case (2) The core radius is 4.5999 cm and the outer radius of the surrounding highly enriched ^{235}U is 6.5887 cm.

Both critical experiments were performed at Los Alamos Scientific Laboratory.

The compositions for the two regions (nuclides per bar-cm) of these cases are given in the following table. Temperature is at 293 ^{0}K.

Isotope	Case 1	Case 2
^{233}U core		
^{233}U	4.7253×10^{-2}	4.7312×10^{-2}
^{234}U	5.2705×10^{-4}	5.2770×10^{-4}
^{238}U	3.2975×10^{-4}	3.3015×10^{-4}
^{235}U Surroundings		
^{235}U	4.4892×10^{-1}	4.4892×10^{-1}
^{238}U	3.2340×10^{-3}	3.2340×10^{-3}

U233-met-fast-005 (umf-005)

This is a spherical system consisting of a highly enriched ^{233}U, reflected by beryllium.

- Case (1) The core radius is 5.0444 cm and the outer radius of the reflector is 7.0891 cm.
- Case (2) The core radius is 4.5999 cm and the outer radius of the reflector is 8.7960 cm.

Both critical experiments were performed at Los Alamos Scientific Laboratory.

The compositions for the two regions (nuclides per bar-cm) of these cases are given in the following table. Temperature is at 293 ^{0}K.

Isotope	Case 1	Case 2
^{233}U core		
^{233}U	4.7253x10^{-2}	4.7312x10^{-2}
^{234}U	5.2705x10^{-4}	5.2770x10^{-4}
^{238}U	3.2975x10^{-4}	3.3015x10^{-4}
Beryllium Reflector		
Be	1.1984x10^{-1}	1.1984x10^{-1}
O	1.3776x10^{-3}	1.3776x10^{-3}

Pu-Comp-Inter-001 (PCI-001)

This is a k_∞ experiment at the HECTOR reactor (Winfrith, UK, 1960s): a graphite moderated plutonium oxide core (5% ^{240}Pu). The benchmark model is an infinite medium with a material composition appropriate to the interpolated boron/^{239}Pu ratio. It is modeled as a homogeneous infinite medium with the composition shown in the following table (all number of densities are given as nuclides per barn-cm).

Isotope	Density
^{239}Pu	2.7350x10^{-4}
^{240}Pu	1.5490x10^{-5}
^{241}Pu	1.0720x10^{-6}
^{242}Pu	5.8000x10^{-8}
^{1}H	1.0770x10^{-4}
^{10}B	1.0151x10^{-4}
^{11}B	4.0859x10^{-4}
C	7.0900x10^{-2}
^{16}O	2.7070x10^{-3}
^{40}Ca	8.0267x10^{-4}
^{42}Ca	5.3572x10^{-6}
^{43}Ca	1.1178x10^{-6}
^{44}Ca	1.7272x10^{-5}
^{46}Ca	3.3120x10^{-8}
^{48}Ca	1.5484x10^{-6}

HEU-Comp-Inter-004 (HCI-004)

This is a k_∞ experiment at the HECTOR reactor (Winfrith, UK, 1960s): a graphite moderated uranium oxide core. The benchmark model is an infinite medium with a material composition appropriate to the interpolated boron/^{235}U ratio. It is modeled as a homogeneous infinite medium with the composition shown in the following table (all number of densities are given as nuclides per barn-cm).

Isotope	Density
^{234}U	3.1200×10^{-6}
^{235}U	2.5020×10^{-4}
^{236}U	4.2670×10^{-7}
^{238}U	1.7190×10^{-5}
^{1}H	1.1260×10^{-4}
^{10}B	5.7849×10^{-5}
^{11}B	2.3285×10^{-4}
C	7.5650×10^{-2}
^{16}O	1.6500×10^{-2}
^{40}Ca	5.5227×10^{-4}
^{42}Ca	3.6860×10^{-6}
^{43}Ca	7.6909×10^{-7}
^{44}Ca	1.1884×10^{-5}
^{46}Ca	2.2788×10^{-8}
^{48}Ca	1.0653×10^{-6}

AQUEOUS THERML CRITICALS

Three unreflected spheres from the ORNL series were computed. These benchmarks contain ^{235}U in the form of uranyl nitrate dissolved in water. One of the devices was poisoned with boron. The CSEWG treatment for these criticals models them as bare spheres of the core solution corrected for the thin aluminum shells, nonspherical shape, fill tubes, and room retrun. Benchmarks ORNL-1 and ORNL-2 are of radius 34.595 cm, and ORNL-10 has a radius of 61.011 cm. The compositions specified for the CSEWG models are as follows.

Material	ORNL-1	ORNL-2	ORNL-10
^{10}B	0.0	1.0286×10^{-6}	0.0
H	0.066228	0.066148	0.066394
O	0.033736	0.033800	0.033592
N	1.869×10^{-4}	2.129×10^{-4}	1.116×10^{-4}
^{234}U	5.38×10^{-7}	6.31×10^{-7}	4.09×10^{-7}
^{235}U	4.8066×10^{-5}	5.6206×10^{-5}	3.6185×10^{-5}
^{236}U	1.38×10^{-7}	1.63×10^{-7}	2.20×10^{-7}
^{238}U	2.807×10^{-6}	3.281×10^{-6}	1.985×10^{-6}

In order to get a case with higher leakage, one additional sphere from the L series of uranyl fluoride assemblies was calculated. The L-7 assembly is modeled as an aluminum-clad sphere with radius of 11.5176 cm, respectively. The aluminum container has a thickness of 0.16, and the aluminum number density is taken to be 0.06025 per barn-cm. The number densities for the solution are given in the following table.

Material	L-7	L-8	L-9	L-10	L-11
H	0.0633680	0.0666144	0.066634	0.0647289	0.066722
O	0.0334713	0.0334357	0.0334344	0.034627	0.033473
F	0.0017873	0.00012855	0.0001027	0.0010983	0.00011249
^{234}U	8.7577×10^{-6}	7.327×10^{-7}	5.854×10^{-7}	5.3816×10^{-6}	5.5393×10^{-7}
^{235}U	8.32694×10^{-4}	5.99051×10^{-5}	4.7856×10^{-5}	5.11691×10^{-4}	5.2444×10^{-5}
^{236}U	4.2895×10^{-6}	0.0	0.0	2.6359×10^{-6}	2.8022×10^{-7}
^{238}U	4.78991×10^{-5}	3.638×10^{-6}	2.9063×10^{-6}	2.9340×10^{-5}	2.9675×10^{-6}

The L-7, L-10, and L-11 assembly has an additional 20.0 cm of water outside the aluminum shell (the number densities for the hydrogen and oxygen are .0666883 and .0333442 per bar-cm, respectively).

Four unreflected spheres of plutonium nitrate solution were also computed. The PNL-1 and PNL-2 benchmarks both have an effective radius of 19.509 cm. The isotopic compositions of the solutions are given in the following table.

Material	PNL-1	PNL-2
H	0.06563	0.05416
O	0.03456	0.03977
N	6.216×10^{-4}	4.720×10^{-3}
^{239}Pu	9.373×10^{-5}	4.141×10^{-4}
^{240}Pu	4.501×10^{-6}	1.988×10^{-5}

Similarly, the PNL-3 and PNL-4 benchmarks have an effective radius of 22.70 cm. The isotopic compositions of the solutions are given in the following table.

Material	PNL-1	PNL-2
H	0.06495	0.06041
O	0.03441	0.03712
N	7.394×10^{-4}	2.775×10^{-3}
Fe	1.294×10^{-6}	1.520×10^{-6}
^{239}Pu	5.395×10^{-5}	6.633×10^{-5}
^{240}Pu	2.355×10^{-6}	2.895×10^{-6}

LATTICE THERMAL CRITICALS

TRX LATTICES

The TRX lattices were a series using a triangular pattern of slightly-enriched metallic uranium rods in a water moderator. The CSEWG benchmarks model the unit cell with cylindrical geometry as given in the following table.

Region	Radius	Isotope	Density
Fuel	0.4915	^{235}U	6.253×10^{-4}
		^{238}U	4.7205×10^{-2}
Void	0.5042		
Clad	0.5753	Al	6.025×10^{-2}
Moderator	*	^{1}H	6.676×10^{-2}
		^{16}O	3.338×10^{-2}

The * in the table represents the outer radius of the moderator region, which varies between the two lattices analyzed here. The lattice spacings for TRX-1 and TRX-2 are 1.8060 cm and 2.1740 cm, respectively, which translate into radii of 0.9482 cm and 1.1414 cm, respectively.

The specifications in ENDF-202 sugest that these assemblies can be computed as infinite cylinders, and then a lekage correction can be applied using an homogenized B_l calculation with a total buckling of

$B^2 = 0.0057$ cm^{-2} for TRX-1 or $B^2 = 0.005469$ cm^{-2} for TRX-2. He physical height is approximately 136.98 cm with vacuum boundary conditions. TRX-1 contained 764 fuel rods. When circularized, this corresponds to an effective radius of 26.209 cm. The corresponding radius for TRX-2 is 27.441 cm. The water reflector was taken to have a thickness of about 30 cm with a vacuum boundary condition on its outer surface.

BAPL LATTICES

The BAPL lattices were a series using a triangular pattern of slightly-enriched uranium oxide rods in a water moderator. The CSEWG benchmarks model the unit cell with cylindrical geometry as given in the following table.

Region	Radius	Isotope	Density
Fuel	0.4684	^{235}U	3.112×10^{-4}
		^{238}U	2.3127×10^{-2}
		^{16}O	
Void	0.5042		
Clad	0.5753	Al	6.025×10^{-2}
Moderator	*	^{1}H	6.676×10^{-2}
		^{16}O	3.338×10^{-2}

The * in the table represents the outer radius of the moderator region, which varies between the three lattices analyzed here. The lattice spacings for BAPL-1, BAPL-2, and BAPL-3 are 1.5578, 1.6523, and 1.8057 cm, respectively, which translate into radii of 0.8178, 0.8675, and 0.9480 cm, respectively.

These three lattices can be calculated using the methods discussed above for the TRX lattices. The axial buckling is taken to be the same as for the TRX lattices; namely, 0.000526, giving a buckling height of 136.98 cm. The core radii can be calculated from the cell radii and the critical number of rods: 38.122 cm for BAPL-1 (2173 rods), 36.342 cm for BAPL-2 (1755-rods), and 37.623 cm for BAPL-3 (1575 rods).

Table D.2: Calculated keff eigenvalues against the measured keff =1.000 B1 and No Sn Transport Correction

| IHECB/CSEWG Benchmarks | mcnp | COMBINE7.0 | |
		Bondarenko Self shielding	Bondarenko + Nordheim self shielding
GODIVA (hmf-001)	1.00014(22)	0.99797	0.99797
FLATTOP-25 (hmf-028)	1.00275(24)	0.99900	0.99900
FLATTOP-Pu (pmf-006)	1.00067(25)	0.99325	0.99326
JEZEBEL (pmf-001 bare)	1.0001(20)	0.99612	0.99612
JEZEBEL-23 (umf-001)	1.00032(21)	0.99647	0.99647
JEZEBEL-Pu (pmf-002)	1.00025(20)	0.99665	0.99665
umf002-1	0.99891 (21)	0.99458/0.99408	0.99458/0.99408
umf002-2	1.00002 (21)	0.99542/0.99477	0.99542/0.99477
umf005-1	0.99396 (21)	0.98844/0.98801	0.98769/0.98801
umf005-2	0.99201 (23)	0.98201/0.98519	0.98201/0.98519
pci-001	1.01150(28)	1.00991	1.00497
hci-004	0.98781(24)	0.99223	0.98942
ORNL-1 (hst-013 Case 1)		0.99806	0.99794
ORNL-2 (hst-013 Case 2)		0.99717	0.99704
ORNL-10 (hst-032)		0.99133	0.99903
L-7 (hst009-3)		0.99835	0.99745
L-8		1.00495	1.00488
L-9		1.00292	1.00288
L-10		0.99573	0.99521
L-11 (hst012)		1.00021	1.00016
PNL-1		1.00765	1.00723
PNL-2		1.00446	1.00391
PNL-3		0.99398	0.99371
PNL-4		0.99976	0.99945
TRX1-r[*]	0.99908(29)	1.00196	0.99839
TRX2-r[**]	0.99908(28)	1.00044	1.00257
BAPL1-r[**]		1.00436	1.00367
BAPL2-r[**]		1.00136	1.00134
BAPL3-r[**]		1.00258	1.00271

Note: /1-D transport correction

Table D.3: Calculated keff eigenvalues against the measured keff =1.000 B1 and Sn Transport Correction

| IHECB/CSEWG Benchmarks | k_{eff} | | |
| | | COMBINE7.0 | |
	mcnp	Bondarenko Self shielding	Bondarenko + Nordheim self shielding
GODIVA (hmf-001)	1.00014(22)	1.000190	1.000190
FLATTOP-25 (hmf-028)	1.00275(24)	0.999517	0.999518
FLATTOP-Pu (pmf-006)	1.00067(25)	0.994095	0.994097
JEZEBEL (pmf-001 bare)	1.0001(20)	0.999222	0.999223
JEZEBEL-23 (umf-001)	1.00032(21)	0.999314	0.999314
JEZEBEL-Pu (pmf-002)	1.00025(20)	0.999826	0.999828
umf002-1	0.99891 (21)	0.99865/0.99815	0.998647/0.99815
umf002-2	1.00002 (21)	0.99999/0.99935	0.999991/0.99935
umf005-1	0.99396 (21)	0.99114/0.99113	0.990633/0.99113
umf005-2	0.99201 (23)	0.98479/0.98884	0.984780/0.98879
pci-001	1.01150(28)	1.00991	1.00497
hci-004	0.98781(24)	0.99223	0.98936
ORNL-1 (hst-013 Case 1)		0.99699	0.99685
ORNL-2 (hst-013 Case 2)		0.99610	0.99594
ORNL-10 (hst-032)		0.99848	0.99849
L-7 (hst009-3)		0.99712	0.99638
L-8		1.00374	1.00364
L-9		1.00190	1.00182
L-10		0.99446	0.99400
L-11 (hst012)		0.99914	0.99906
PNL-1		1.00610	1.00570
PNL-2		1.00218	1.00173
PNL-3		0.99247	0.99218
PNL-4		0.99795	0.99763
TRX1-r[*]	0.99908(29)	1.00035	0.99698
TRX2-r[**]	0.99908(28)	1.00307	1.00132
BAPL1-r[**]		1.00262	1.00207
BAPL2-r[**]		0.99974	0.99988
BAPL3-r[**]		1.00115	1.00142

Note: /1-D transport correction

Table D.4: Calculated keff eigenvalues against the measured keff =1.000 B3 and No Sn Transport Correction

IHECB/CSEWG Benchmarks	mcnp	k_{eff} COMBINE7.0 Bondarenko Self shielding	Bondarenko + Nordheim self shielding
GODIVA (hmf-001)	1.00014(22)	1.00273	1.00273
FLATTOP-25 (hmf-028)	1.00275(24)	1.00654	1.00633
FLATTOP-Pu (pmf-006)	1.00067(25)	1.00492	1.00486
JEZEBEL (pmf-001 bare)	1.0001(20)	1.00274	1.00274
JEZEBEL-23 (umf-001)	1.00032(21)	1.00278	1.00278
JEZEBEL-Pu (pmf-002)	1.00025(20)	1.00336	1.00336
umf002-1	0.99891 (21)	1.00337/1.00294	1.00337/1.00294
umf002-2	1.00002 (21)	1.00527/1.00469	1.00527/1.00419
umf005-1	0.99396 (21)	1.00136/0.99749	1.00089/0.99748
umf005-2	0.99201 (23)	1.00089/0.99686	1.00089/0.99686
pci-001	1.01150(28)	1.00991	1.00497
hci-004	0.98781(24)	0.99223	0.98942
ORNL-1 (hst-013 Case 1)		0.99890	0.99881
ORNL-2 (hst-013 Case 2)		0.99802	0.99787
ORNL-10 (hst-032)		0.99925	0.99926
L-7 (hst009-3)		1.00577	1.00485
L-8		1.00639	1.00632
L-9		1.00380	1.00367
L-10		1.00298	1.00247
L-11 (hst012)		1.00183	1.00175
PNL-1		1.01074	1.01031
PNL-2		1.00741	1.00687
PNL-3		0.99623	0.99596
PNL-4		1.00202	1.00169
TRX1-r[*]	0.99908(29)	1.00254	0.99890
TRX2-r[**]	0.99908(28)	1.00501	1.00316
BAPL1-r[**]		1.00465	1.00395
BAPL2-r[**]		1.00167	1.00169
BAPL3-r[**]		1.00286	1.00301

Note: /1-D transport correction

Table D.5: Calculated keff eigenvalues against the measured keff =1.000 B3 and Sn Transport Correction

| | k_{eff} | | |
| | | COMBINE7.0 | |
IHECB/CSEWG Benchmarks	mcnp	Bondarenko Self shielding	Bondarenko + Nordheim self shielding
GODIVA (hmf-001)	1.00014(22)	1.00268	1.00266
FLATTOP-25 (hmf-028)	1.00275(24)	1.00653	1.00632
FLATTOP-Pu (pmf-006)	1.00067(25)	1.00491	1.00484
JEZEBEL (pmf-001 bare)	1.0001(20)	1.00268	1.00267
JEZEBEL-23 (umf-001)	1.00032(21)	1.00261	1.00259
JEZEBEL-Pu (pmf-002)	1.00025(20)	1.00334	1.00333
ORNL-1 (hst-013 Case 1)	0.99891 (21)	0.99768	0.99758
umf002-1	1.00002 (21)	1.00325/1.00282	1.00323/1.00288
umf002-2	0.99396 (21)	1.00517/1.00459	1.00514/1.00456
umf005-1	0.99201 (23)	0.99999/0.99574	0.99954/0.99572
umf005-2	1.01150(28)	0.99655/0.99469	0.99654/0.99469
pci-001	0.98781(24)	1.00991	1.00497
hci-004		0.99223	0.98936
ORNL-2 (hst-013 Case 2)		0.99679	0.99666
ORNL-10 (hst-032)		0.99867	0.99868
L-7 (hst009-3)		1.00446	1.00355
L-8		1.00487	1.00480
L-9		1.00260	1.00250
L-10		1.00167	1.00116
L-11 (hst012)		1.00073	1.00064
PNL-1		1.00848	1.00806
PNL-2		1.00428	1.00373
PNL-3		0.99429	0.99401
PNL-4		0.99975	0.99943
TRX1-r[*]	0.99908(29)	1.00162	0.99807
TRX2-r[**]	0.99908(28)	1.00432	1.00245
BAPL1-r[**]		1.00387	1.00318
BAPL2-r[**]		1.00095	1.00096
BAPL3-r[**]		1.00227	1.00243

Note: /1-D transport correction

D. REFERENCE

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