

Argonne National Laboratory

**EFFECT OF RESONANCE SCATTERING
ON CRITICALITY CALCULATIONS
OF FAST ASSEMBLIES**

by

D. Meneghetti

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EFFECT OF RESONANCE SCATTERING ON CRITICALITY
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ABSTRACT

Critical masses of representative ZPR-III fast assemblies containing resonance scatterers are calculated using the SNG transport code. THE IBM-704 ELMOE code of Hummel and Rago, however, was used to evaluate group transport and group elastic transfer cross sections in the cores in conjunction with the 16-group cross section set of Yiftah, Okrent, and Moldauer. (By using hundreds of neutron energy groups and the detailed elastic scattering matrices for the resonance scatterers, ELMOE carries out a fundamental mode analysis. It thereby obtains material buckling and the detailed fine structure flux dependence upon energy. It then re-evaluates the gross group cross sections for transport and elastic transfer.)

Consideration of the resonance scattering effects due to aluminum and stainless steel increase the calculated critical masses of ZPR-III assemblies 23, 31, and 32 by about 15 kg, 21 kg, and 21 kg, respectively. Corresponding reactivity decreases are about -1%, -0.7%, and -2% keffective, respectively.

I. INTRODUCTION

Numerous fast neutron multigroup cross-section parameters have been used for the analyses of the fast critical assemblies^(1,2,3) constructed on the Argonne Fast Critical Facility ZPR-III. These have generally ranged from about 10 to 16 energy groups. As the successive assemblies have been studied, comparison with experimental results have shown that a seemingly adequate set of cross sections for a large range of previous assemblies does not necessarily enable subsequent assemblies to be adequately predicted. For example, an 11-group cross-section set^(2,3) used for much of the analyses provided a good fit to the moderately dilute assemblies. It has been found, however, to overpredict the critical mass of the more highly dilute assemblies, Nos. 24 and 25, by about 30%. (Assemblies 24

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ABSTRACT

Critical masses of representative ZPR-III fast assemblies containing resonance scatterers are calculated using the SNO transport code. THE IBM-704 ELMOE code of Hansen and Rago, however, was used to evaluate group and group elastic transfer cross sections in the cores in conjunction with the 16-group cross section set of Yllescu, Oxtun, and Moldauer. (By using hundreds of neutron energy groups and the detailed elastic scattering matrices for the resonance scatterers, ELMOE carries out a fundamental mode analysis. It thereby obtains material buckling and the detailed fine structure flux dependence upon energy. It then re-evaluates the group cross sections for transport and elastic transfer.)

Consideration of the resonance scattering effects due to aluminum and stainless steel increase the calculated critical masses of ZPR-III assemblies 2.5, 3.1, and 3.5 percent, respectively. Corresponding reactivity decreases are about -1.5, -0.75, and -1.5 percent, respectively.

1. INTRODUCTION

Numerous fast neutron multigroup cross-section parameters have been used for the analyses of the fast critical assemblies (1,2,3) constructed on the Argonne Fast Critical Facility ZPR-III. These have generally ranged from about 10 to 16 energy groups. As the successive assemblies have been studied, comparison with experimental results have shown that a reasonably adequate set of cross sections for a large range of previous assemblies does not necessarily enable subsequent assemblies to be adequately predicted. For example, an 11-group cross-section set (2,3) used for much of the analyses provided a good fit to the moderately dense assemblies. It has been found, however, to overpredict the critical mass of the more highly dense assemblies. Nos. 54 and 55 by about 10%. (Assemblies 54

and 25 contain nominal U^{238}/U^{235} atomic ratios of about 9.5 and 10.4, respectively. They have corrected experimental critical masses of about 490 kg and 620 kg, respectively.)

Yiftah et al.⁽⁴⁾ have recently prepared a 16-group fast reactor cross-section set. An effort was made to explain and document all choices and assumptions made in the set of cross sections. This enables an analyst to assess the present reliability of the constants and readily make suitably assessed modifications as new microscopic data and/or improved calculational procedures are employed.

Perusal of the calculated and corrected experimental masses listed by Yiftah et al. indicates that the listed calculated critical masses are underpredicted by about -6% to -17%. (By use of "conservative" U^{235} values for ν , the predicted critical deviations from observed values range from about +2% to -11%.) Those calculated assemblies listed which contain appreciable resonance scattering materials such as aluminum and/or stainless steel tend to be most in error on the side of overreactivity.

Recent ZPR-III assemblies 23, 29, 30, 31, and 32, which contain large volume fractions of aluminum and/or stainless steel, have emphasized this aspect. They are underpredicted by about -19% to -26% in the critical masses. The large overpredictions of reactivity in such systems are observed also with previous sets.^(3,5) This suggested that these excessive deviations might in part be due to not having considered the detailed fluctuations of the energy dependence of the flux within groups due to scattering resonances of, for example, aluminum and the components of stainless steel in the evaluation of the group cross-section parameters.

In the present study, the contribution of these resonance effects toward improving the critical mass predictions is determined. The group transport and group elastic transfer cross sections were re-evaluated using the recent ELMOE code.^(6,7) ELMOE is an IBM-704 code. It uses hundreds of neutron energy groups to describe the detailed elastic scattering matrix for the resonance scatterers. It carries out a fundamental mode analysis to obtain material buckling and the detailed fine structure flux dependence upon energy. The program then re-evaluates the gross group cross sections for transport and elastic transfer for an energy group structure such as in the 16-group set. The present study employs ELMOE calculations in the P-1 approximation.

II. CRITICAL MASSES AND CORE MATERIAL BUCKLINGS

Assemblies 23, 29, 30, 31, and 32 contained appreciable volume fractions of aluminum and/or stainless steel. These cylindrical assemblies had approximately the core composition given in Table I, which are the

values used in the calculations. The reflector in all cases was about 30 cm of depleted uranium. The critical mass calculations were carried out in spherical geometry using the SNG transport code^(8,9) in S_4 approximation. The 16-group set without and with the ELMOE-evaluated group cross sections for transport and elastic transfer was used. The modified aluminum cross sections for transport and elastic transfer employed are those based upon an ELMOE calculation for a core composition as in the aluminum assembly 23 but without stainless steel. The modified stainless steel cross sections are those obtained by an ELMOE calculation of the steel assembly 32. The error incurred in simple volume fraction weighting of modified aluminum and steel cross sections for cores containing both materials is evaluated for assembly 31. The core of assembly 31 consisted approximately of equal volumes of aluminum and stainless steel resonance scattering materials. The cylindrical critical masses were obtained by use of estimated shape factors.^(2,3) The reported experimental critical masses were corrected for the effects of slab geometry plate heterogeneities, either by auxiliary calculations or by estimates based on results⁽¹⁰⁾ of heterogeneity experiments, so as to represent homogeneous cores.

Table I

CORE AND REFLECTOR COMPOSITIONS (Volume Fractions)

Assembly No.	U^{235} (0.048) ^a	U^{238} (0.048)	Al (0.0603)	Stainless Steel ^b	O (0.096)
23	0.0942	0.0071	0.4473	0.0916	0
29	0.0497	0.0997	0.2438	0.2475	0.1446
30	0.0592	0.0906	0.2341	0.2460	0.0728
31	0.0581	0.0914	0.2349	0.2449	0
32	0.0942	0.0071	0	0.801	0
Reflector	0.0019	0.833	0	0.0731	0

a. N - values in units of 10^{24} per cm^3 .

b. Stainless steel (assuming ~71.3 at-% iron, 8.5 at-% nickel, and 20.2 at-% chromium having N-values for pure elements of 0.0847, 0.0913, and 0.0801, respectively).

Material buckling calculations for the cores have also been calculated using both the 16-group cross-section set unmodified and modified by the re-evaluated transport and elastic transfer cross sections. This was done largely to determine to what extent the reactivity effect of a decrease in transport cross section is in these high-density reflector systems compensated for by an increase in reflector savings.

values used in the calculations. The reflector is assumed to have a value of 0.01. The critical mass of the system was calculated for a spherical geometry using the SNO calculation code. The 10-group set without and with the 2.1-MeV cross-section group were used for transport and elastic scattering calculations. The modified assembly cross-sections for transport and elastic scattering were used for the SNO calculation for system composition as in the assembly. It was found that the critical mass of the assembly is 1.15 kg without elastic scattering. The modified elastic scattering cross-sections are those obtained by an SNO calculation of the elastic scattering. The error incurred in elastic scattering weighting of modified elastic cross-sections for cases consisting both of elastic scattering and steel cross-sections for cases consisting of elastic scattering only. The case of assembly II consisted approximately of equal volumes of aluminum and stainless steel resonance scattering materials. The critical and critical masses were obtained by use of estimated elastic scattering cross-sections. The reported experimental critical masses were compared for the effect of elastic scattering cross-sections, either by multiplying calculations by the correction based on results (10) of heterogeneity experiments, or as in previous homogeneous cases.

Table 1

CORE AND REFLECTOR COMPOSITIONS (Volume Fractions)

Assembly	U_{235} (0.048) ^a	U_{238} (0.048)	Al (0.040)	Stainless Steel ^b	C (0.005)
1	0.042	0.007	0.447	0.046	0
2	0.047	0.007	0.248	0.247	0.144
3	0.022	0.000	0.247	0.246	0.073
4	0.041	0.014	0.248	0.249	0
5	0.042	0.007	0	0.001	0
Reflector	0.001	0.011	0	0.011	0

^a U_{235} in units of 10⁴ per cm³.

^b Stainless steel (assembly - 71.7 at-% iron, 2.4 at-% nickel, 2.9 at-% chromium having Ni-alloy for pure elements 0.0027, 0.0013, and 0.0001, respectively).

Material banking calculations for the core have also been calculated using both the 10-group cross-section set mentioned and modified by the re-evaluated transport and elastic scattering cross-sections. It was found largely to determine to what extent the reactivity effect of a decrease in transport cross-sections is in their high-density reflector systems compared for the decrease in reflector savings.

The factors by which the unmodified 16-group cross sections for aluminum for transport and elastic transfer must be modified if the flux depletion due to resonance scattering is to be accounted for in the predominantly aluminum diluent assembly 23 are listed in Table II. Also listed are the factors for the corresponding stainless steel cross sections for the steel diluent assembly 32.

Table II

RATIO OF MODIFIED TO UNMODIFIED CROSS SECTIONS
FOR ALUMINUM AND FOR STAINLESS STEEL

Energy Group	Group Lower Energy (Mev)	Ratio			
		Aluminum		Stainless Steel	
		Transport	Elastic Transfer	Transport	Elastic Transfer
1	3.668	(1) ^a	(1)	(1)	(1)
2	2.225	0.83	1.11	0.86	0.81
3	1.35	0.95	1.25	0.97	1.14
4	0.825	0.85	1.02	0.91	1.03
5	0.5	0.945	1.11	0.95	1.11
6	0.3	0.94	1.02	0.86	0.78
7	0.18	0.76	0.93	0.94	1.03
8	0.11	0.61	0.84	0.84	0.99
9	0.67	0.475	0.61	0.64	0.80
10	0.0407	0.67	0.68	0.95	0.95
11	0.025	0.24	0.36	0.49	0.75
12	0.015	0.71	~0	0.67	0.73
13	0.0091	0.97	1.00	0.98	0.98
14	0.0055	(1)	(1)	(1)	(1)
15	0.0021	(1)	(1)	(1)	(1)
16	0.0005	(1)	(1)	(1)	(1)

^aIndicates no ELMOE calculation for these groups.

Homogenized group transport cross sections of the core and group elastic transfer contributions of aluminum and stainless steel were also determined by an ELMOE calculation explicitly for the assembly 31 core, which contained approximately equal parts of aluminum and stainless steel as diluent. Corresponding homogenized group cross sections were constructed by use of volume averaging of the ELMOE-evaluated aluminum cross sections and of the ELMOE-evaluated steel cross sections. The ratios of the homogenized cross sections are listed in Table III.

The factors by which the normalized group transfer cross sections for aluminum, for transport and elastic transfer, were calculated are listed in Table II. The factors for stainless steel were calculated in the same manner as for aluminum. The factors for the transport and elastic transfer cross sections for stainless steel were calculated in the same manner as for aluminum.

Table II
RATIO OF NORMALIZED TO UNNORMALIZED CROSS SECTIONS
FOR ALUMINUM AND FOR STAINLESS STEEL

Group	Group	Ratio			
		Aluminum		Stainless Steel	
		Transport	Elastic Transfer	Transport	Elastic Transfer
1	1	(1) ^a	(1)	(1)	(1)
2	2	0.83	1.1	0.88	0.91
3	3	1.25	1.27	0.97	1.14
4	4	0.85	0.85	0.81	1.03
5	5	0.7	0.75	0.92	1.11
6	6	0.7	1.05	0.86	0.98
7	7	0.18	0.93	0.94	1.03
8	8	0.11	0.94	0.84	0.99
9	9	0.87	0.475	0.84	0.80
10	10	0.007	0.67	0.92	0.98
11	11	0.052	0.51	0.94	0.75
12	12	0.012	0.71	0.67	0.73
13	13	0.007	0.97	0.88	0.88
14	14	0.0024	(1)	(1)	(1)
15	15	0.0031	(1)	(1)	(1)
16	16	0.008	(1)	(1)	(1)

^a Calculated as ELMOE calculation for these groups.

The normalized group transfer cross sections of the core and group elastic transfer contributions of aluminum and stainless steel were also determined by an ELMOE calculation. The results for the assembly 11 core, which contained approximately equal parts of aluminum and stainless steel as shown in Figure 1, are listed in Table III. The results for the assembly 11 core, which contained approximately equal parts of aluminum and stainless steel as shown in Figure 1, are listed in Table III. The results for the assembly 11 core, which contained approximately equal parts of aluminum and stainless steel as shown in Figure 1, are listed in Table III.

Table III

RATIO OF ELMOE CROSS SECTIONS EXPLICITLY EVALUATED FOR
ASSEMBLY 31 TO VOLUME AVERAGE OF ELMOE-EVALUATED
ALUMINUM CROSS SECTIONS AND ELMOE-EVALUATED
STEEL CROSS SECTIONS

Energy Group	Group Lower Energy (Mev)	Ratio	
		Transport ^a	Elastic ^b Transfer
1	3.668	(1) ^c	(1)
2	2.225	1.00	0.97
3	1.35	1.00	0.97
4	0.825	1.01	1.01
5	0.5	1.01	1.02
6	0.3	1.04	1.035
7	0.18	1.06	1.04
8	0.11	1.11	1.09
9	0.67	1.08	1.06
10	0.0407	1.035	1.11
11	0.025	1.13	1.38
12	0.015	1.02	1.07
13	0.0091	1.00	0.92
14	0.0055	(1)	(1)
15	0.0021	(1)	(1)
16	0.0005	(1)	(1)

- a. Includes U^{235} and U^{238} transport contributions.
- b. Does not include U^{235} and U^{238} elastic transfer contributions.
- c. Indicates no ELMOE calculation for these groups.

Results of the calculations of critical mass for the reflected assemblies are given in Table IV. Listed are also experimental^(10,11) and heterogeneity-corrected experimental values. The calculated masses assuming the "conservative" ν^{25} values⁽⁴⁾ were obtained by estimating the fractional increase in critical mass from comparative material buckling calculations. In those assemblies containing oxygen, the intra-group resonance scattering effects of oxygen were not accounted for.

Results of corresponding material buckling calculations (16 groups) are given in Table V. These were carried out by means of asymptotic transport leakage.⁽¹²⁾

Table IV
RESONANCE-CORRECTED AND -UNCORRECTED CALCULATED CRITICAL MASSES
(kg U^{235} in Core)

Assembly No.	Experimental		Calculated Critical Masses ^a				Calculated Value of $\frac{(\Delta M/M)}{\text{core edge } (\Delta k/k)}$
			Regular ν^{25} Values		Conservative ν^{25} Values ^b		
	Measured (Refs. 7, 9)	Corrected ^c	Without Resonance Corrections	With Resonance Corrections	Without Resonance Corrections	With Resonance Corrections	
23	258	271	219	233	241	257	5.1
29	422	449	352	386	369	404	4.3
30	395	422	326	353	345	374	4.5
31	463	494	387	417 (407) ^d	414	447 (436) ^d	5.5
32	227.5	239	176	197	188	210	4.5

a. Assumes shape factors of 0.94 for sphere to cylinder.

b. Extrapolated from the listed results, of the regular ν^{25} , by comparative bare core calculations using "regular" and "conservative" ν^{25} values.

c. Assumes 1% k heterogeneity effects in assemblies 23 and 32, and 1.5% k heterogeneity effects in assemblies 29, 30, and 31.

d. Using cross sections obtained by ELMOE program explicitly for assembly 31.

Table V
RESONANCE-CORRECTED AND -UNCORRECTED CALCULATED B VALUES
(B^2 = MATERIAL BUCKLING) AND PER CENT CHANGES IN
BARE CORE REACTIVITIES

Assembly No.	Regular ν^{25} Values			Conservative ν^{25} Values	
	B, cm^{-1}		% $\Delta k/k^a$	B, cm^{-1}	% $\Delta k/k^b$
	Without Resonance Correction	With Resonance Correction		With Resonance Correction	
23	0.0590	0.0558	-5.8	0.0548	-2.0
29	0.0526	0.0502	-3.8	0.0496	-1.1
30	0.0536	0.0512	-4.0	0.0505	-1.3
31	0.0486	0.0464 (0.0472) ^c	-4.2	0.0457	-1.3
32	0.0746	0.0712	-4.7	0.0702	-1.5

a. Relative to bare core calculated without resonance corrections and with regular ν^{25} values.

b. Relative to bare core calculated with resonance corrections and with regular ν^{25} values.

c. Using cross sections obtained by ELMOE program expressly for assembly 31.

The increases in calculated critical masses for the reflected assemblies 23, 31, and 32 due to consideration of the resonance scattering effects correspond to reactivity decreases of about -1%, -0.7%, and -2% k, respectively. Corresponding decrease for assembly 31 using the composite cross sections is about -1%. Thus the results obtained for assembly 31 by means of the separately re-evaluated aluminum and stainless steel cross sections shows that the composite of the steel and aluminum resonance structures are such that they lessen the overall resonance effect on calculations of critical mass.

Reactivity decreases obtained for the bare cores by use of the ELMOE-corrected cross sections are greater by factors of two to three than the reactivity decreases which may be deduced from the increases in the reflected critical masses. That this is due largely to the compensating effect of the reflector saving, of the high-density reflector, increasing as the core leakage increases due to the changes of cross sections for transport and elastic transfer is seen in Table VI. (The values of reflector savings listed are the differences between the bare core radii obtained by the 16-group fundamental mode analysis using asymptotic transport leakage and by the critical core radii as obtained by the 16-group S_4 solutions.)

Table VI

CALCULATED SPHERICAL REFLECTOR SAVINGS WITHOUT
AND WITH RESONANCE-CORRECTED CORES

Assembly No.	Reflector Saving, ^a cm	
	Without Resonance Corrections	With Resonance Corrections
23	22.9	24.4
29	15.8	17.3
30	18.3	19.8
31	21.6	23.6
	21.6	(22.7) ^b
32	13.4	14.8

- a. Difference of bare core fundamental mode calculation using asymptotic transport leakage and of reflected S_4 calculation.
- b. Using cross sections obtained by ELMOE program explicitly for assembly 31.

III. CONCLUSIONS

For the aluminum diluent assembly 23 the consideration of the resonance scattering effects can be said to reduce the overprediction of reactivity to about the same range of overprediction as for assemblies⁽⁴⁾ not containing appreciable aluminum and/or stainless steel. The overreactivity of the calculated assembly 23 is reduced to +2.7% k and +1.0% k, respectively, when the standard values of νU^{235} and conservative νU^{235} are used, respectively. For comparison, the uncorrected 16-group set gives +3.8% k and +2.2% k, respectively.

The calculation for the stainless steel assembly 32 has been improved by reduction of the reactivity error to +3.8% k and +2.7% k, respectively, by means of the two sets of values of νU^{235} . The predicted overreactivity is still, however, overly excessive in comparison with the calculated critical masses of assemblies not containing appreciable stainless steel. Similarly, the calculated overreactivity of assembly 31, containing about equal parts aluminum and stainless steel, though reduced to +3.2% k and +2.1% k, respectively, is still overly excessive, as are also assemblies 29 and 30 which, in addition, contain oxygen. It thus appears that the stainless steel 16-group cross sections are still too reactive (by about 1% k or 2% k in assembly 32). An increase in the average stainless steel capture cross section by about 40% in the energy groups between 9 kev and 1.35 Mev would reduce the assembly 32 reactivity by about 1% k.

The problem of the general underprediction of critical mass, aside from the stainless steel overreactivity, appears to be due largely to the overreactivity of the U^{235} group cross sections. Thus use of the "conservative νU^{235} " values⁽⁴⁾ improves agreement with experiment. These correspond to a value for $(d\bar{\nu}/dE)U^{235}$ of about 0.1, with a normalization of 2.42 at thermal, over most of the energy range, except above about 3.7 Mev for which the value of $\bar{\nu}U^{235}$ is taken to be 2.71. Recent measurements^(13,14) of νU^{235} suggest that a lowering of $(d\bar{\nu}/dE)U^{235}$ is indeed indicated.

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The calculation for the stainless steel assembly 32 has been improved by reduction of the reactivity error to $\pm 0.5\%$ and $\pm 0.1\%$ respectively, by means of the two sets of values of W^{235} . The provided overreactivity is still, however, overly excessive in comparison with the calculated critical masses of assemblies not containing appreciable stainless steel. Similarly, the calculated overreactivity of assembly 31, containing about equal parts of stainless and stainless steel, though reduced to $\pm 0.1\%$ and $\pm 0.1\%$ respectively, is still overly excessive, as are also assemblies 19 and 20 which, in addition, contain oxygen. It thus appears that the stainless steel 19-group cross sections are still too reactive (by about 1% or 1% in assembly 32). An increase in the average stainless steel capture cross section by about 40% in the energy groups between 9 keV and 1.35 MeV would reduce the assembly 32 reactivity by about 1% .

The problem of the general underprediction of critical mass, aside from the stainless steel overreactivity, appears to be due largely to the overreactivity of the U^{235} group cross sections. The use of the "corrected" values of W^{235} improves agreement with experiment. These corrections to a value for $(\sigma/\epsilon)U^{235}$ of about 0.1, with a normalization of 1.45 at thermal, over most of the energy range, except above about 3.7 MeV for which the value of W^{235} is taken to be 5.71. Recent measurements (1,3,14) of W^{235} suggest that a lowering of $(\sigma/\epsilon)U^{235}$ is indeed indicated.

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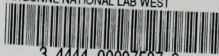
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