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A CORRELATION TECHNIQUE FOR RESONANCE CALCULATIONS

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ABSTRACT

A correlation technique has been developed to make the accuracy of complex and long running resonance treatments available in fast, routine calculations. The technique is based on the subgroup method and is used to generate group-averaged resonance reaction rates. By fitting the correlation to several detailed auxiliary resonance calculations, a set of weights (the Lebesgue measure) is obtained. The weights may then be applied to a wider range of new cases. Use of the correlation technique results in one-tenth the computational burden of the detailed resonance treatment; yet, the results duplicate the detailed calculations to within 1/100% in k_{eff} .

INTRODUCTION

The Generalized Lattice Analysis Subsystem

In a typical lattice physics calculation at the Savannah River Laboratory, approximately 25 to 50% of the computational time is expended in the resonance calculation. The Generalized

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Lattice Analysis Subsystem (GLASS)¹ modules performing this calculation use the Nordheim integral treatment, with the Breit-Wigner single level model providing the cross sections. Recent work^{2,3} has demonstrated some deficiencies in the present calculation. These deficiencies lead to a consistent overprediction of the resonance integral and resonance reaction rates. The most important of these deficiencies are 1) the assumption of nonoverlap of resonances between isotopes, 2) the assumption of 1/E flux dependence both above and below the resonance, 3) the treatment of all nonabsorber regions as moderator regions with the Narrow Resonance Approximation, and 4) the calculation of the resonance integrals in a manner which overlaps the multigroup boundaries.

An improved resonance calculation³ has been developed which overcomes these deficiencies, but the more-detailed modeling increases the running time by at least an order of magnitude. These realities have stimulated the present effort to develop a simple and rapid correlation technique which will make the accuracy of the improved resonance calculation available with a minimal expenditure of computer time.

These resonance calculations are performed by the modular computational system GLASS (see Figure 1). Each box in the Figure represents one or more modules performing a basic function. The significant output of the modules calculating the resonances is represented by a single block of data: a table of resonance

reaction rate per unit slowing down density by isotope, energy group, and cell subregion. These normalized resonance reaction rates are then input to the modules performing the neutron flux calculation and are used to calculate the volume source terms in the multigroup integral transport equations. Whether the flux solution is obtained by the collision probability method, the transmission probability method, or the Monte Carlo method (all available for the user's selection), the data interface between the resonance calculation and the flux calculation modules remains identical in form.

In this paper, the correlation to be described simply replaces the modules labeled "Calculate Resonances" in Figure 1. Due to the interface requirements of GLASS, the basic quantity to be calculated by the correlation is constrained to be the resonance reaction rate per unit slowing down density. If the GLASS interface were structured differently, the correlation could conceivably be in terms of average microscopic cross sections instead of normalized resonance reaction rates; however, the present work will be in terms of reaction rates.

The Subgroup Method

The correlation presented will be cast in terms of the subgroup method. That term should not be confused with the more familiar terms multigroup or group, which refer to a collection of neutrons, all approximately similar in energy. A subgroup refers to a collection of neutrons all "seeing" approximately

the same total cross section. Thus, a group of neutrons consists of those neutrons whose energy lies in the interval ΔE about E ; a subgroup of neutrons consists of those neutrons which experience a total cross section in the interval $\Delta \Sigma^t$ about Σ^t . The subgroup method was originally formulated by Nikolaev⁴ and has been applied in a collision probability, integral transport framework by Roth.⁵ This method has similarities with the histogram approach of MacDougall and Rowlands⁶ and the probability table method of Levitt.⁷

The current method represents a specialization of Roth's subgroup method.⁵ In this earlier work, Roth used the subgroup method to calculate group-averaged resonance cross sections and relied upon the availability of a data base of homogeneous resonance integrals. In the current work, the subgroup method is used to suggest the form for a correlation which can be employed as an interpolation tool to calculate group-averaged resonance reaction rates. A library of homogenized cell data is not required.

The subgroup method allows the difficult Riemann integrals required in the integration over resonances to be replaced by the simpler Lebesgue-Stieltjes integrals.⁵ Integrals of the form $\int \sigma(E) \phi(E) dE$ must be calculated where $\sigma(E)$ varies rapidly with energy. In the multigroup method, the integral is solved laboriously over a fine energy mesh. In the subgroup method, the key is to note that $\phi(E)$ is a function of $\sigma(E)$; thus a more convenient form of the integral is $\int f[\sigma(E)] dE$, where $f[\sigma(E)]$ is $\sigma(E) \phi[\sigma(E)]$. By dividing the range of σ into intervals (i.e., the subgroups), the Lebesgue-Stieltjes integral may then be defined:

$$\int f[\sigma(E)] dE = \lim_{N \rightarrow \infty} \sum_{i=1}^N f(\sigma_i) w_i \quad (1)$$

where σ_i is a point in the subgroup $[\sigma_{i-1}^*, \sigma_i^*]$. In the numerical calculation, N is limited to a finite value; σ_i values are chosen and $f(\sigma_i)$ is evaluated. The integral is obtained by multiplying by the appropriate Lebesgue measure w_i (the weight) and carrying out the summation. For the present correlation, the means of obtaining $f(\sigma_i)$ and w_i for the purpose of calculating resonance reaction rates will be described in succeeding sections.

SUBGROUP FORMULATION OF RESONANCE REACTION RATES

Due to the requirements of the GLASS interface, the result needed at the conclusion of the resonance calculation is the resonance reaction rate in energy group j , per unit slowing down density into group j , in spatial region k , and for isotope ℓ

$$R_{jk}^{\ell} = \int_{\Delta V_k} \int_{\Delta E_j} N_k^{\ell} \sigma^{\ell}(E) \phi(\underline{r}, E) dE d\underline{r} \quad (2)$$

where

ΔV_k = the volume of region k

N_k^{ℓ} = the uniform number density of isotope ℓ in region k

σ^{ℓ} = the resonance cross section (fission or absorption)

ϕ = the flux normalized to the unit slowing down density

ΔE_j = the width of energy group j .

The subgroup method suggests that this integral may be written as

$$R_{jk}^{\ell} = V_k N_k^{\ell} \sum_{i=1}^I \sigma_i \phi_{ikj} w_{ij}^{\ell} \quad (3)$$

where

V_k = the volume of region k

σ_i = the microscopic cross section of subgroup i

w_{ij}^{ℓ} = the appropriate weight

ϕ_{ikj} = the subgroup flux.

The ϕ_{ikj} may be thought of as the flux of neutrons in subgroup i and in region k. The product of ϕ_{ikj} and the "cross section" $\sigma_i w_{ij}^{\ell}$ is that subgroup's contribution to the normalized resonance reaction rate in group j. Alternatively, σ_i may be thought of as the i-th "contribution" to the resonance cross section, ϕ_{ikj} as the resonance flux in group j due to that i-th contribution; and w_{ij}^{ℓ} as the weight of that contribution such that the summation totals the correct resonance reaction rate. If these heuristic arguments attempting to transform cross section space into energy space are to no avail, Equation 3 may be considered simply the definition of a correlation in which the σ_i are given constants, the w_{ij}^{ℓ} are fitting parameters, and the ϕ_{ikj} are functions given by the model described in the next section.

CALCULATION OF SUBGROUP FLUXES

The concept of the subgroup as the collection of all neutrons "seeing" a similar total cross section suggests that the subgroup fluxes ϕ_{ikj} in Equation 3 may be obtained by solving the one-group integral transport equation. By definition, all neutrons in a single region in the same energy group "see" the same cross section. The collision probability form of the transport equation is:

$$V_k \Sigma_{ikj}^t \phi_{ikj} = \sum_m V_m P_{mk} (\Sigma_{mj}^s \phi_{imj} + S_{mj}) \quad (4)$$

where

P_{mk} = the probability that a neutron born in region m has its first collision in region k

Σ_{mj}^s = the self-scattering cross section in region m and group j

S_{mj} = the source into the group j in region m.

Σ_{ikj}^t is the subgroup-modified total cross section and defined to be

$$\Sigma_{ikj}^t = \Sigma_{kj}^o + \Sigma_{ki}^r \quad (5)$$

where Σ_{kj}^o is the smooth (nonresonance) total cross section in group j and region k; Σ_{ki}^r is the "resonance" cross section in subgroup i. Σ_{ki}^r is calculated by taking σ_i as the microscopic "resonance" cross section.

To calculate the subgroup fluxes ϕ_{ikj} , Σ_{ikj}^t from Equation 5 takes on $i=1,2,\dots,I$ values (for each σ_i) which are used successively in Equation 4. The collision probabilities P_{mk} would similarly be

calculated for the Σ_{ikj}^t appropriate to each region of the cell. In the end, Equation 4 will have been solved I times for each energy group, once for each value of σ_i . The desired normalized resonance reaction rate is calculated by multiplying the resulting ϕ_{ikj} by the appropriate w_{ij}^l and σ_i and carrying out the summation of Equation 3. Such a formulation is consistent with the alternative argument for Equation 3: σ_i is the i-th contribution to the resonance cross section, and ϕ_{ikj} is the resonance flux in group j due to that contribution.

The definition of the source term S_{mj} in the one-group form of Equation 4 is ambiguous. The magnitude of the source is unimportant due to the normalization to a unit slowing down density which is implicit in the method. However, the shape of the source is important. Initially, the assumption of a source proportional to the inverse of the volume of each region was tested. This formulation resulted in a correlation which worked well within the range spanned by the calculations used to generate the fitting coefficients. But the correlation could not be used to extrapolate outside that range. A more-detailed source model was then adopted: the source was assumed to be that calculated for the case with all smooth cross sections. Namely, the coupled set of multigroup transport equations is solved:

$$V_k \Sigma_{kj}^0 \phi_{kj} = \sum_m V_m P_{mk} (\Sigma_{mj}^S \phi_{mj} + S_{mj}) \quad (6)$$

where ϕ_{kj} is the usual multigroup flux in group j and region k .

The source was separated into a fission source and a slowing down source:

$$S_{mj} = S_{mj}^f + S_{mj}^{sd} \quad (7)$$

where

$$S_{mj}^f = \frac{1}{k_{eff}} \sum_g \left(\sum_n \chi_{g \rightarrow j} v \Sigma_{fg}^{nm} \right) \phi_{mg} \quad (7a)$$

$$k_{eff} = \frac{\sum_k \sum_n \sum_g (v \Sigma_{fg}^{nk} \phi_{kg})}{\sum_k \sum_n \sum_g (\Sigma_{ag}^{nk} \phi_{kg})} \quad (7b)$$

$$S_{mj}^{sd} = \sum_g \Sigma_{s,g \rightarrow j}^m \phi_{mg} \quad (7c)$$

where

Σ_{fg}^{nm} = the fission cross section in group g for isotope n in region m

Σ_{ag}^{nm} = the similar absorption cross section

$\Sigma_{s,g \rightarrow j}^m$ = the scattering cross section from group g to group j

$\chi_{g \rightarrow j}$ = the fission spectrum.

To solve Equation 6, a standard fission source iteration procedure is used for the outer iterations, and a successive over-relaxation matrix inversion is used for the inner iterations. The P_{mk} are calculated by using Kennedy's method.⁸

The S_{mj} matrix resulting from this procedure is then considered to be a fixed source term in Equation 4. The equation may then be solved directly (through a simple matrix inversion) to calculate the ϕ_{ikj} . Use of this more-detailed representation of the source results in a correlation which demonstrates more reasonable behavior, both as an extrapolation and an interpolation tool (see "Testing the Correlation" in this paper). Equation 4 could be solved iteratively, but then the computational burden would increase by a factor of I . Experience to date has shown this ultimate source treatment to be unnecessary and has shown that the source matrix obtained from Equation 6 works satisfactorily (i.e., the deficiencies in the model are corrected through the w_{ij}^ℓ fitting coefficients).

CALCULATION OF THE WEIGHTS

Since the σ_i are predefined, and the ϕ_{ikj} are calculated by using Equation 4, the remaining unknowns in the equation for the resonance reaction rates are the weights w_{ij}^ℓ . At this point, the current method becomes a correlation technique: the weights are obtained by fitting to the results of auxiliary calculations. The quantity to be preserved by the fitting is the cell-total resonance reaction rate:

$$R_j^\ell \equiv \sum_i R_{rj}^\ell = \sum_i \sigma_i w_{ij}^\ell \sum_k V_k N_k^\ell \phi_{ikj} \quad (8)$$

The auxiliary calculations are detailed resonance calculations: they provide the truth (the left-hand side of Equation 8) which the correlation is to duplicate. Solution of Equation 4 for the lattices analyzed in the auxiliary calculations provides the ϕ_{ikj} for the right-hand side of Equation 8. Thus, the only unknown remaining in Equation 8 is w_{ij}^{λ} , the set of weights. If the number of auxiliary calculations exceeds the number of subgroups, the w_{ij}^{λ} may be obtained from least squares fitting. For the purpose of this work, the number of auxiliary calculations was assumed to be equal to the number of subgroups, in which case Equation 8 becomes I equations in I unknowns for each isotope and energy group.

To summarize the correlation procedure: I states of the lattice are analyzed by using the detailed (expensive) resonance treatment. These states are chosen so that they span the range of cases which future analyses will cover (e.g., at I different ^{235}U enrichments, if the correlation is to calculate burnup dependent resonance data). The weights are then obtained through fitting to the detailed calculations by using Equation 8 and Equation 4. The resulting set of weights may then be used to calculate new lattice states with the subgroup fluxes resulting from Equation 4 and the resonance reaction rates resulting from Equation 3. The new state calculations with the correlation are fast, yet preserve the accuracy of the detailed auxiliary calculations.

TESTING THE CORRELATION

The unit cell illustrated in Figure 2 was set up as a test case for the method discussed here. The set of subgroups (i.e., the σ_i) was defined to be 3, 10, 30, 270, 2000, and 7000 barns. In order to generate the weights, auxiliary calculations with GLASS were performed for six ^{235}U enrichments: 1%, 3%, 5%, 7%, 9%, and 11%. With the weights catalogued, the first 16 new lattices (none of which were used to generate the weights) described in Table 1 were calculated with the correlation. In cases 1 through 5, the ^{235}U enrichment was varied over a somewhat wider range (0.75% to 20%) than that used to generate the weights (1% to 11%). Cases 2 through 4 are new lattices within the range spanned by the auxiliary calculations. Reference calculations with GLASS and the calculations with the correlation were compared and agreed well (to at least the fourth significant figure in k_{eff}). This result illustrates the usefulness of the method as an interpolation tool. In addition, the good agreement for Cases 1 and 5, which are outside the fitted range, suggests a limited extrapolation capability for the method.

In Cases 6 through 10, the correlation was applied to new lattices in which the ^{235}U enrichment always remained in the range spanned by the fittings, but the moderator and fuel densities were varied. The intent was to investigate the effect of spectral changes which were not tied to ^{235}U concentration (e.g., the moderator density variation). Again, the results yielded by use of the correlation agreed well with those of the confirming GLASS

calculations (k_{eff} was duplicated to at least the third significant figure). Recall that the weights were calculated by fitting to cases in which fuel and moderator densities did not vary from their 100% nominal values. Thus, the reasonably accurate predictions with the correlation suggest a wider applicability than that implied by the process of fitting the auxiliary calculations. This result suggests the usefulness of the method as a tool for extrapolation.

Cases 11 through 14 were calculated to demonstrate that this correlation, like all others, can get into difficulties outside its range of applicability. By applying the correlation to a ^{235}U enrichment far outside the fitted range (i.e. a very subcritical lattice) or by making drastic changes in the fuel and moderator densities, results which are in error by several percent in k_{eff} can be obtained.

In Cases 15 and 16, the effect of changing lattice geometry was investigated by increasing the outside diameter of the fuel rod and thus displacing moderator. As expected, the correlation gave a reasonable result (1/2% error in k_{eff}) for a small perturbation in rod diameter (5% increase) and a significant error (4% error in k_{eff}) for a major change in rod diameter (40% increase).

The point to be emphasized is that these first 16 cases in Table 1 were all calculated with the single set of weights obtained by fitting the six auxiliary calculations in which only the ^{235}U enrichment was varied. Thus, the correlation could be used for resonance calculations during a reactor depletion analysis with a single set of weights.

A second set of weights was generated by performing GLASS calculations for six different moderator densities: 40%, 50%, 70%, 80%, 100%, and 200%. In this series, the ^{235}U enrichment was fixed at 5.2% and the fuel density at 100%. The resulting weights were used in the correlation to calculate the two new lattices in Cases 17 and 18 in Table 1. Again, the results with the correlation agree well with the results of the confirming GLASS calculations (to at least the fourth significant figure in k_{eff}). These results support the use of the correlation as an interpolation tool, in this case for resonance calculations during a voiding accident analysis.

Overall, the comparisons suggest that the correlation yields excellent results within the range spanned by the fitting and still yields reasonable results outside that range. The single most important benefit of the correlation technique was that it required approximately 2 seconds of CPU time on an IBM 360/195 for the resonance calculation in each of the cases in Table 1, while each confirming GLASS calculation required approximately 20 seconds.

CONCLUSIONS

The correlation technique for group-averaged resonance reaction rates developed in the current work duplicates the results of detailed resonance treatments for approximately one-tenth the computational cost. The set of subgroup weights obtained by

fitting detailed auxiliary calculations has a range of validity which exceeds that spanned by the original fitting calculations. Thus, the method may be used both as an interpolation tool with high accuracy (with an error of approximately 1/100% in k_{eff}) and an extrapolation tool with reasonable accuracy (with an error of approximately 1/10% in k_{eff}).

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TABLE 1

Test Results

Case	^{235}U Enrichment, %	Fuel Density, %	Moderator Density, %	k_{eff}		Error, Δk_{eff}
				Correlation	GLASS	
1	0.75	100	100	0.99080	0.98585	+0.00495
2	2	100	100	1.24172	1.24143	+0.00029
3	6	100	100	1.40913	1.40936	-0.00023
4	10	100	100	1.46865	1.45864	+0.00001
5	20	100	100	1.55692	1.55575	+0.00117
6	2	100	90	1.25687	1.25627	+0.00060
7	5.2	100	95	1.37584	1.37666	-0.00082
8	5.2	100	80	1.32265	1.32675	-0.00410
9	5.2	100	70	1.28104	1.23854	-0.00750
10	4	105	95	1.33564	1.33758	-0.00194
11	0.2	100	100	0.62255	0.56057	+0.06198
12	5.2	100	200	1.57390	1.57154	+0.00236
13	4	120	95	1.32844	1.31560	+0.01284
14	3.7	194	80	1.25955	1.18083	+0.07872
15	5.2	100	100	1.35770	1.36571	-0.00801
16	5.2	100	100	1.21533	1.26767	-0.05234
17	5.2	100	90	1.36125	1.36094	+0.00031
18	5.2	100	150	1.50383	1.50386	-0.00003

Note: Case 15 — fuel OD = 2.10 in.

Case 16 — fuel OD = 2.50 in.

fuel: ^{235}U and ^{238}U in 2" OD rod

clad: ^{56}Fe 0.01" thick

moderator: D_2O

hexagonal pitch: 5"

FIGURE 2. Unit Cell for Test Problems

FIGURE 1. Generalized Lattice Analysis Subsystem (GLASS)