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Received by OSTI

February 8, 1974

FEB 08 1991

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TO: R. J. PRYOR

FROM: D. R. FINCH *DRF*

IMPROVED RESONANCE REACTION RATE CALCULATION FOR
LATTICE PHYSICS SUBSYSTEM

DISTRIBUTION:

J. W. Croach - A. A. Johnson, Wilm.
C. H. Ice - L. H. Meyer, SRL
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H. K. Clark
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A. N. Mallen

E. J. Hennelly, SRL
J. A. Smith
J. D. Spencer
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N. H. Kuehn III
G. M. Morris
F. J. McCrosson
R. W. Benjamin
R. L. Reed
D. A. Sharp
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Contents

1. Introduction
2. Summary
3. Discussion
 - 3.1 Review of Previous Computational Methods
 - 3.1.1 Reaction Rate Equation
 - 3.1.2 Lattice Cell Geometry
 - 3.1.3 Solution for Resonance Integral in HAMMER
 - 3.1.3.1 HAMMER Solution for Resolved Resonances
 - 3.1.3.2 HAMMER Solution for Unresolved Resonances
 - 3.1.3.3 Resonance Cross Sections in HAMMER
 - 3.1.3.4 Deficiencies in HAMMER Resonance Calculation
 - 3.1.4 Solution for Resonance Integrals in HAMBUR
 - 3.1.4.1 HAMBUR Solution for Resolved Resonances
 - 3.1.4.2 HAMBUR Solution for Unresolved Resonances
 - 3.1.4.3 Resonance Cross Sections in HAMBUR
 - 3.1.4.4 Deficiencies in HAMBUR Resonance Calculation
 - 3.2 Improved Resonance Calculations
 - 3.2.1 Resonance Flux Equation
 - 3.2.2 Lattice Cell Geometry and Composition
 - 3.2.3 Solution of Slowing Down Integrals
 - 3.2.4 Selection of Energy Grid
 - 3.2.5 Cross Sections
 - 3.2.5.1 Resonance Cross Sections
 - 3.2.5.1.1 Breit-Wigner Resolved Resonance Formulae
 - 3.2.5.1.2 Adler-Adler Resolved Resonance Formulae
 - 3.2.5.1.3 Single Level Breit-Wigner Unresolved Resonance Formulae

Contents

- 3.2.5.2 Smooth Multigroup Cross Section
- 3.2.6 Resonance Flux Calculation
- 3.2.7 Generation of Output Reaction Rates

4. References

Appendices

- A. New LIDS Data Set Blocks and Temporary Storage Blocks.
- B. New RILIB and NUCPARAM Data Set Records.
- C. Mathematical Details of Flux and Collision Probability Calculation.
- D. Calculation of $\psi(\theta, X)$ and $\chi(\theta, X)$ Resonance Line Shape Functions.
- E. Calculation of Fluctuation Integrals for Unresolved Resonant Cross Sections.

1. Introduction

The calculation of resonance reaction rates in the present SRL Lattice Physics codes and modules is based upon methods developed more than ten years ago. Virtually all of the current calculations are based directly on the methods of Lothar Nordheim¹ published in 1961.

The first widely used resonance calculation at Savannah River Laboratory was developed by J. E. Suich in 1964 in the HAMMER System². The HAMMER treatment incorporated versions of the Nordheim codes ZUT³ and TUZ for resolved and unresolved resonance integral calculations, respectively. The HAMMER treatment was extended by the author in 1967 to enable spatial resonance effects to be resolved in Lattice Physics cell calculations. This extension was incorporated into the HAMBUR System⁴. The currently used resonance capture treatment is the CREEP module⁵ used by the RAHAB⁶ lattice physics module. CREEP contains the same physics as the HAMBUR System resonance treatment with some improvements, made by D. A. Sharp, in numerical techniques that reduce execution times.

There have been significant changes since the last improvements to the theoretical methods employed in SRL resonance codes were made. Of prime importance is the considerable improvement in CPU speed of the SRL digital computers which allows a more complete mathematical description of the resonance physics to be employed at reasonable cost to the user. Also of prime importance are the several new resonance formalisms that take multi-level effects into account. Prominent among these formalisms are the Reich-Moore⁷ and Adler-Adler⁸ formulations as well as modification of the classic Breit-Wigner⁹ formalism to take multi-level scattering effects into account. All of these new formalisms are of importance as they are acceptable forms for resonance data in the ENDF/B data file from which SRL will derive much of its present and future cross sections.

It is appropriate at this time to review on a common basis the calculational methods used in existing resonance capture codes, and to propose improvements seen necessary and useful to enable present and future resonance calculation needs to be implemented. This is the purpose of this memorandum.

2. Summary

The resonance capture calculations of the HAMMER System and HAMBUR (also CREEP) System are derived from a consistent statement of the integral slowing down equation and definitions of the resonance integral. The assumptions made in these treatments are explicitly stated, and an attempt is made to estimate the possible error in the resonance integral arising from these assumptions. This analysis is made to pin-point those parts of the calculation that can be improved and updated.

Based on the analysis of existing calculations a method of calculation is derived which avoids most of the problems encountered in HAMMER and HAMBUR. The chief improvements that result are as follows:

- Careful attention is paid to calculation of the resonance flux as most errors in existing calculations result from consistently overpredicting fluxes in all regions of a lattice cell.
- The calculation can be modified to produce as crude or detailed a resonance calculation, at the expense of computer time, as required by the user.
- Resonances that overlap group boundaries contribute the correct contribution to each group's reaction rates.
- Overlap between resonances of different isotopes is correctly accounted for.
- Up-to-date resonance formalisms are used including the Adler-Adler multi-level formulations. Provision is made to easily add new formalisms when required.
- Streaming effects from neutrons leaking into a cell may optionally be included in the calculation of resonance reaction rates.

A complete description of the physics contained in this new computational module is provided along with additional information on the numerical techniques employed in the module. The module is currently in a check-out status and much of the numerical methodology described in this respect is subject to change without notice. Persons interested in using this module should check with the author for up-to-date information.

3. Discussion

3.1 Review of Previous Computational Methods

3.1.1 Reaction Rate Equation

The equations solved by existing and previous resonance treatments at SRL have utilized the integral slowing down equation in a multi-region lattice cell. This equation is an expression of neutron balance in which the total collision rate at an energy E in a region n is equated to the sum over all regions n'

$$\sum_{n'}^+ P_{n'n}(E) V_n \varphi_n(E) = \sum_{n'=1}^M P_{n'n}(E) V_n \sum_{i \in n'}^J \frac{N_{n'i}}{1 - \alpha_i} \int_E^{E/\alpha_i} \frac{\sigma_i^s(E')}{E'} H(E - \alpha_i E') \varphi_{n'}(E') dE' \quad (1)$$

where:

$\Sigma_n^+(E)$ = total macroscopic cross section in region n at energy E

V_n = volume of region n

$\phi_n(E)$ = flux in region n at energy E

N_{ni} = concentration (atm/bn-cm) of isotope i in region n

$\sigma_i^s(E)$ = microscopic scattering cross section (bns) of isotope i at energy E

α_1 = $[(A_1 - 1)/(A_1 + 1)]^2$

A_1 = mass ratio of isotope 1 to neutron mass

$P_{n'n}(E)$ = probability that a neutron born in region n' at energy E will first collide in region n

$H(E - \alpha_1 E')$ = Heviside Function = $H(X) = 1 \quad X \geq 0$
 $H(X) = 0 \quad X < 0$

Equation 1 is applicable under the assumptions that the only scattering process is elastic scattering and that all scattering is isotropic in the CM system. Flux $\phi_n(E)$ is the average flux in region n at energy E. This is a good approximation, although the spatial flux detail is ignored in the region, if the sources are taken in the flat flux approximation as is done in most cases. This has been shown to be perfectly adequate for practical lattice calculations¹⁰. Improvements in cell detailed fluxes can be made by subdividing the lattice geometry into smaller regions.

In HAMMER, HAMBUR, and CREEP the approach has been to evaluate the resonance integral

$$I^a = \int_{R_{res}} \sigma^a(E) \phi(E) dE, \quad (2)$$

In the resolved regions the integrals over each resonance are evaluated, and in the unresolved regions the integrals over the statistically averaged cross sections are performed. The result is expressed in the form of an effective resonance integral defined as that microscopic cross section which, when multiplied by the asymptotic flux, region volume, and isotopic concentration in the appropriate region, yields the reaction rate due to

one resonance of an isotope, i.e.

$$N_n V_n \phi_n^{\text{asy}} I_{n_i}^X = \int_{R_{es}} dE \int_{V_n} d\vec{r} \phi(\vec{r}, E) \sum_{n_i}^X (\vec{r}, E) \quad (2a)$$

where X is either fission or capture. The asymptotic flux is defined as that flux that would exist in the region n at energy E in the absence of the resonance.

3.1.2 Lattice Cell Geometry

The lattice geometry for resonance calculations has always been a one-dimensional annular geometry. Square and hexagonal lattice cells are reduced to the annular geometry as Wigner-Seitz equivalent cells. In HAMMER and HAMBUR this same geometry is used for the transport theory solution for the neutron flux, while in CREEP this geometry is derived from the CARD Block in the LIDS data for a lattice case.

In this geometry a flux solution is performed for each region using flat flux sources. These fluxes are then utilized in Equations 1 and 2.

HAMMER and HAMBUR proceed differently in solving Equation 2, hence they will be described separately below. The solution of Equation 2 in CREEP is basically the same as for HAMBUR with a few numerical differences that will be noted.

3.1.3 Solution for Resonance Integrals in HAMMER

The basic method of solution of Equation 2 in HAMMER was adopted from the ZUT and TUZ codes³ by J. E. Suich in 1964. It provides a method of performing the integration in Equation 2 utilizing fluxes derived from Equation 1.

The following assumptions are made:

- The separated absorber regions in the annular geometry are represented by a single equivalent absorber region having volume equal to the total absorber region volume and isotopic concentrations equal to the volume average concentration over all absorber regions.
- Regions not containing the resonance absorber are assumed to be moderator regions.
- Fluxes are assumed to have reached their asymptotic $1/E$ values both above and below each resolved resonance.
- Resolved resonances of different isotopes do not overlap in energy.
- Slowing down sources in the moderator region are computed in the Narrow Resonance (NR) approximation.

- o In an absorber region only a few isotopes contribute to the slowing down source. Specifically the lightest and most abundant isotopes in addition to the absorber isotope, selected mutually exclusive.

The effect of each assumption on the solution will be examined in a later section.

3.1.3.1 Solution by HAMMER for Resolved Resonances

Equation 1 is summed over all fuel regions and written

$$\sum_f^+ (\bar{\epsilon}) V_f \bar{\phi}_f(\bar{\epsilon}) = \sum_{n \in f} \sum_{n'=1}^M P_{n'n}(\bar{\epsilon}) V_{n'} \sum_{l \in n'}^J \frac{N_{n'l}}{1 - \alpha_l} \int_{\bar{\epsilon}}^{\bar{\epsilon}/\alpha_l} \frac{\sigma_l^s(\bar{\epsilon}')}{\bar{\epsilon}'} H(\bar{\epsilon} - \alpha_l \bar{\epsilon}') \phi_{n'}(\bar{\epsilon}') d\bar{\epsilon}' \quad (3)$$

where we define

$$\sum_f^+ (\bar{\epsilon}) = \frac{\sum_{n \in f} \sum_{l \in n} N_{nl} \sigma_l^+(\bar{\epsilon}) V_n}{\sum_{n \in f} V_n} = \sum_{l \in f} \sigma_l^+(\bar{\epsilon}) \frac{\sum_{n \in f} N_{nl} V_n}{\sum_{n \in f} V_n} = \sum_{l \in f} N_{0l} \sigma_l^+(\bar{\epsilon}) \quad (4)$$

$$\text{and } N_{01} = \sum_{n \in f} N_{n1} V_n / \sum_{n \in f} V_n$$

is the volume average concentration of isotope 1 in the equivalent absorber region. Subscript f is used to indicate the absorber region.

With the definitions of Equation 4, Equation 3 can be taken as defining the average flux in the absorber region as

$$\bar{\phi}_f(\bar{\epsilon}) = \frac{1}{\sum_{l \in f} N_{0l} \sigma_l^+(\bar{\epsilon})} \sum_{n \in f} \sum_{n'=1}^M P_{n'n}(\bar{\epsilon}) V_{n'} \sum_{l \in n'}^J \frac{N_{n'l}}{1 - \alpha_l} \int_{\bar{\epsilon}}^{\bar{\epsilon}/\alpha_l} \frac{\sigma_l^s(\bar{\epsilon}')}{\bar{\epsilon}'} H(\bar{\epsilon} - \alpha_l \bar{\epsilon}') \phi_{n'}(\bar{\epsilon}') d\bar{\epsilon}' \quad (5)$$

The sum over n' in Equation 5 is now broken into two sums over the absorber regions and moderator regions respectively to yield

$$\bar{\varphi}_f(E) = \frac{1}{\sum_{i \in f} N_{0i} \sigma_i^r(E)} \sum_{n \in f} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{i \in n'} \frac{J}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_i^s(E')}{E'} H(E - \alpha_i E') \varphi_{n'}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \sum_{i \in n'} \frac{J}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_i^s(E')}{E'} H(E - \alpha_i E') \varphi_{n'}(E') dE' \right\} \quad (5a)$$

The second term of the right side of Equation 5a is evaluated by the stated assumption of the Narrow Resonance Approximation in the moderator. These assumptions require that

$$\varphi_{n'}(E') = \frac{\varphi_{n'}^{asr}}{E'} \quad \text{and} \quad \sigma_i^r(E') = \sigma_i^s(E') = \text{constant}$$

so that the integral in the second sum on the right side of 5a becomes

$$\frac{1}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_i^s(E')}{E'} H(E - \alpha_i E') \varphi_{n'}(E') dE' = \frac{\sigma_i^s(E) \varphi_{n'}^{asr}}{E} \quad (6)$$

and equation 5a becomes

$$\bar{\varphi}_f(E) = \frac{1}{\sum_{i \in f} N_{0i} \sigma_i^r(E)} \sum_{n \in f} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{i \in n'} \frac{J'}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_i^s(E')}{E'} H(E - \alpha_i E') \varphi_{n'}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\sum_{i \in n'} \sigma_i^s(E) \varphi_{n'}^{asr}}{E} \right\} \quad (7)$$

where $\Sigma_n^s(E) = \sum_{i \in n} N_{n,i} \sigma_i^s(E)$ and the J' in the isotope

sum in the absorber regions indicates only the selected isotopes are included in the sum.

Inserting Equation 7 into Equation 2 for isotope j gives

$$I_j^a = \int_{res} dE \frac{\sigma_j^a}{\sum_{n \in f} N_{o,n} \sigma_{c,n}^+(E)} \sum_{n \in f} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{n'' \in n'} \frac{N_{n''}}{1 - \alpha_{n''}} \int_E^{E/\alpha_{n''}} \frac{\sigma_{c,n''}^s(E')}{E'} H(E - \alpha_{n''} E') \phi_{n''}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\sum_{n'' \in n'}^s \phi_{n''}^{asy}}{E} \right\} \quad (8)$$

where only the absorption integral is computed. The fission integral is derived from capture to fission ratios, or ratios of fission width to capture width.

We have assumed that there is no overlap between resonances in evaluating Equation 8. Therefore the sum over isotopes in the denominator of Equation 8 is written

$$\sum_{n \in f} N_{o,n} \sigma_{c,n}^+(E) = N_{o,j} \left\{ \sigma_j^+(E) + \frac{\sigma_{m_1}^s N_{o,m_1}}{N_{o,j}} + \frac{\sigma_{m_2}^s N_{o,m_2}}{N_{o,j}} \right\} = N_{o,j} \bar{\sigma}_j^+(E) \quad (9)$$

where m_1 and m_2 are subscripts indicating the two admixed moderator materials. Equation 8 is now written

$$I_j^a = \int_{res} dE \frac{\sigma_j^a}{\bar{\sigma}_j^+(E)} \sum_{n \in f} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \left[\frac{1}{1 - \alpha_j} \int_E^{E/\alpha_j} \frac{\sigma_j^s(E')}{E'} H(E - \alpha_j E') \phi_{n'}(E') dE' \right. \right. \\ \left. \left. + \sum_{m=1}^2 \frac{N_{o,m}}{N_{o,j}(1 - \alpha_{j,m})} \int_E^{E/\alpha_{j,m}} \frac{\sigma_m^s(E')}{E'} H(E - \alpha_{j,m} E') \phi_{n'}(E') dE' \right] \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\sum_{n'' \in n'}^s \phi_{n''}^{asy}}{N_{o,j} E} \right\} \quad (10)$$

where the source integrals for the absorber isotope and admixed moderator isotopes have been separated.

Since the absorber and admixed moderator isotope concentrations have been homogenized over all regions and the average values used in Equation 10 (all absorber regions have the same concentration) the slowing-down density will be very nearly the same for all regions. In addition, the solution will generate the values of $\phi_f(E)$ rather than $\phi_f(E')$ as required for Equation 10, hence the average source value, S_0 , is used in all regions. This uniform absorber region slowing-down density is defined by

$$S_0(E) = \frac{1}{1-\alpha_j} \int_E^{E/d_j} \frac{\sigma_j(E')}{E'} H(E-\alpha_j E') \bar{\phi}_f(E') dE' + \sum_{m=1}^2 \frac{N_{0m}}{N_{0j}(1-\alpha_m)} \int_E^{E/d_m} \frac{\sigma_m^s(E')}{E'} H(E-\alpha_m E') \bar{\phi}_f(E') dE' \quad (11)$$

Equation 10 can be written with this approximation as

$$I_j^a = \int_{E \in S} dE \frac{\sigma_j^a(E)}{\sigma_j^t(E)} \left\{ \sum_{n \in f} \sum_{n' \in f} P_{n'n}(E) V_{n'} S_0(E) + \sum_{n \in f} \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\bar{\Sigma}_{n'}^s(E) \phi_{n'}^{asy}}{N_{0j} E} \right\} \quad (12)$$

Define now

$$P_0(E) = \sum_{n \in f} \sum_{n' \in f} P_{n'n}(E) V_{n'}$$

$$P_1(E) = \sum_{n \in f} \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\bar{\Sigma}_{n'}^s(E) \phi_{n'}^{asy}}{N_{0j} E}$$

so that Equation 12 becomes

$$I_j^a = \int_{k_{0.5}} dE \frac{\sigma_j^a(E)}{\sigma_j^T(E)} \left\{ P_0(E) S_0(E) + \frac{P_1(E)}{E} \right\}. \quad (14)$$

Equation 14 is used in HAMMER to compute the resolved absorption resonance integrals for each isotope j . A fine interval Simpson's rule integration (actually performed in lethargy space) is performed over a range of ± 5 times the practical width of the resonance about the central energy of the resonance. In each interval the absorber region slowing-down source is obtained from Equation 11 and collision sums defined by Equation 13 are obtained from a cosine current collision probability calculation (details of this calculation are described in Appendix C). Cross sections for the absorber material are obtained from Single Level Breit Wigner resonance parameters (S wave only) with Doppler broadening effects included (See Section 3.1.3.3). Equation 11 is evaluated by separate Simpson rule integrations for the absorber and each admixed moderator from stored flux tables.

Corrections are made to the result of integrating Equation 14 to account for very small contributions in the wings of the resonances. These corrections are analytic expressions based on assumed $1/E$ fluxes in the wings and will not be discussed in detail here.

It will be noted that the asymptotic fluxes enter the calculation via Equations 13. These fluxes are derived from a P_0 Legendre order cosine currents calculation using the smooth multigroup cross sections and the slowing-down densities from the next higher energy group. This procedure allows some spatial detail to enter the calculation of the moderator slowing-down source.

3.1.3.2 Solution for Unresolved Resonances in HAMMER

The HAMMER calculation of unresolved resonance integrals is that of Adler, Hinman, and Nordheim as described in Ref. 11. Basically it treats resonance integrals of homogeneous regions in the Narrow Resonance Approximation with a statistical average over the Porter-Thomas distribution (∞ degrees of freedom) of neutron width. Only S wave resonances are treated in this method.

The unresolved resonance integral is defined by

$$I_j^{\text{unres}} = \frac{(\sigma_p + \sigma_m)}{D} \int_{E_r}^{\infty} \bar{J}(E) dE \quad (15)$$

where

$$\bar{J}(E) = \frac{1}{12\pi G} \int_0^{\infty} \frac{d\tau}{\sqrt{\tau}} J(\tau, B) e^{-(\tau+B)/2G} \quad (16)$$

and

$$G = \langle \Gamma_n^0 \rangle \sqrt{\frac{A}{4kT}} = \langle \Gamma_n^0 \rangle \sqrt{E} / \beta$$

$$\tau = \frac{\Gamma}{\beta} = G + B + \frac{\Gamma_f}{\beta} \quad (17)$$

$$B = \Gamma \sqrt{\frac{A}{4kT}} = \frac{\Gamma}{\beta}$$

$$C = 3.842 \times 10^{-7} (\sigma_p + \sigma_m) E$$

$$\beta = \frac{C \tau}{\tau - B}$$

$$J(\tau, B) = \int_0^{\infty} \frac{\psi}{\psi + \beta} dx$$

$\langle \Gamma_n^0 \rangle$ = average neutron width at 1 ev

D = mean level spacing

E_c = cut-off energy above which the resonances are considered unresolved.

The integrations in Equations 15 and 16 are carried out numerically using stored tables of the J function. The upper limits of the integration are $J = 1$ in Equation 16 and $E = E_c$ in Equation 15.

3.1.3.3 Resonance Cross Sections in HAMMER

The cross sections for resolved resonances are calculated from Single Level Breit-Wigner resonance parameters. These parameters define the Maxwell average for the Doppler-broadened cross section as

$$\bar{\sigma}(E) = \frac{1}{\sqrt{\pi} \Gamma_D} \int_0^\infty dE_r \sqrt{E_r} \sigma(E_r) e^{-(E-E_r)^2/\Gamma_D^2} \quad (18)$$

where

$$\Gamma_D = \text{Doppler width} = \sqrt{\frac{4E kT}{A}}$$

E = neutron energy (ev) lab system

E_r = relative energy between neutron and target nucleus.

The Breit-Wigner Single Level Cross Sections for absorption (or fission) and scattering are

$$\sigma_a = \sigma_0 \frac{\Gamma_r}{\Gamma} \sqrt{\frac{E_0}{E}} \frac{1}{1 + 4 \frac{(E-E_0)^2}{\Gamma^2}} \quad (19)$$

$$\sigma_s = \sigma_0 \frac{\Gamma_n^0}{\Gamma} \frac{1}{1 + 4 \frac{(E-E_0)^2}{\Gamma^2}} + \left(\sigma_0 \sigma_p \frac{\Gamma_n^0}{\Gamma} \right)^{1/2} \frac{2(E-E_0)/\Gamma}{1 + 4 \frac{(E-E_0)^2}{\Gamma^2}} + \sigma_p$$

where:

Γ_n^0 is the neutron width at resonance

$$\sigma_0 = 4\pi g \lambda_0^2 \frac{\Gamma_n^0}{\Gamma} = \text{peak cross section at resonance}$$

$$g = \frac{2J+1}{2(2I+1)}$$

I = nuclear spin

J = channel spin

Substituting Equation 19 into Equation 18 and changing variables to

$$\chi = 2(\epsilon - \epsilon_0)/\Gamma \quad \eta = 2(\epsilon_r - \epsilon)/\Gamma$$

yields the normal Doppler-broadened formulas

$$\bar{\sigma}_2(\epsilon) = \frac{\Gamma}{\Gamma} \sqrt{\frac{\epsilon_0}{\epsilon}} \sigma_0 \psi(\tau, \chi) \quad (20)$$

$$\bar{\sigma}_3(\epsilon) = \frac{\Gamma_n^0}{\Gamma} \sigma_0 \psi(\tau, \chi) + \left(\sigma_0 \sigma_r g \frac{\Gamma_n^0}{\Gamma} \right)^{1/2} \chi(\tau, \chi) + \sigma_p$$

where:

$$\tau = \frac{\Gamma}{\Gamma_D} = \sqrt{\frac{A \Gamma^2}{4 \epsilon^2 \lambda^2}} = \text{ratio of material to Doppler width.}$$

The $\psi(\tau, \chi)$ and $\chi(\tau, \chi)$ are the standard line shape integrals defined by

$$\psi(\tau, \chi) = \frac{\tau}{\sqrt{4\pi}} \int_{-\infty}^{\infty} d\eta \frac{e^{-\tau^2(\chi - \eta)^2/4}}{1 + \eta^2} \quad (21)$$

$$\chi(\tau, \chi) = \frac{\tau}{\sqrt{4\pi}} \int_{-\infty}^{\infty} \frac{2\eta d\eta e^{-\tau^2(\chi - \eta)^2/4}}{1 + \eta^2} = 2\chi\psi(\tau, \chi) - 4 \frac{d\psi(\tau, \chi)}{d\chi}$$

In HAMMER the Ψ and χ functions of Equation 21 are evaluated by asymptotic and convergent series expansions of the Incomplete Gamma Function. This procedure is credited to Y. D. Naliboff¹⁹ and inserted in a 1963 version of the ZUT program designated the NIT program.

The unresolved cross sections are evaluated by the equations given in Section 3.1.3.2. The resonance parameters here modify the integrations over the tabular tables of the $J(\epsilon, \beta)$ functions.

3.1.3.4 Deficiencies in the HAMMER Resonance Calculation

The major deficiencies in the HAMMER calculation of resonance integrals arise from the original six assumptions stated in Section 3.1.3.0. One must remember that this calculation represents the state-of-the-art in 1964 and represents assumptions that could be economically handled on the 7090 speed computers.

The assumption of a single equivalent absorber region of uniform composition produces the most serious errors in the resonance integral calculation. Large differences in isotopic concentration in different absorber regions can produce significant changes in the calculated resonance integral. In HAMMER, as long as the sum $\sum_{i=1}^N N_i V_i$ remains constant the material may be distributed in any fashion among the absorber regions and will produce the same resonance integral. The major influence of this effect is in accounting for concentration change effects in depletion-production calculations, particularly for isotopes such as ^{240}Pu which start at zero concentration and build in at a different rate in each absorber region. The actual error in the calculation of the resonance integral is estimated to be as high as 10% with a strong dependence on the lattice cell geometry and composition.

The assumption of non-overlap of resonances between isotopes will lead to an overprediction of the flux in energy regions where overlap truly occurs. This effect could amount to an estimated 3% overprediction in the calculated resonance integral.

The assumption of a $1/E$ flux dependence both above and below the resonance will lead to overprediction of the absorber region fluxes. The magnitude of this error is composition dependent. However, it is well known that resonances are fairly closely spaced in the higher energy resolved resonance range and that recovery of a $1/E$ flux dependence is not achieved. The superposition of all resonances of all isotopes in an absorber region enhances this effect to a considerable extent. This effect could amount to an estimated 3% overprediction of the calculated resonance integral.

The treatment of all non-absorber regions as moderator regions, hence by the NR approximation, can lead to significant over-estimation of absorber region fluxes, particularly for assemblies containing target tubes. The treatment of a target tube by the NR approximation (in which $\sigma_t \sim \sigma_s \sim \sigma_f \sim \text{constant}$) cannot account for the depressed flux in the region. This will result in too high a slowing-down source in the target region, and the collision probabilities for the region will be too low. The absorber region collision probabilities will be too high, leading to overprediction of the resonance integral. A partial account is taken for this effect in the calculation of the asymptotic fluxes since the correct total cross section is used in the calculation. The error in the computed resonance integral could be as much as 3% higher from this effect.

The resonance integrals are performed over a range of energies symmetrical about the central energy of the resonance. This range can and often does overlap the multigroup boundaries over which the transport calculation of net flux is carried out. In HAMMER the total effect of a resonance integral is inserted into the multigroup containing the central energy. This can lead to an underprediction of the net flux in the multigroup containing the central energy and an overprediction of the net flux in the next lower multigroup. Over all the reaction rates for isotopes computed from these fluxes will be in error. The net effect can be in either overprediction or underprediction of the reaction rates and can amount to an estimated 2% error.

The effect of ignoring the contributions to the slowing-down density in an absorber region from all but three isotopes is certainly a very small effect and should lead to a slight underprediction of flux and resonance integral. However, the use of the NR approximation in coolant channels directly adjacent to fuel assemblies can clearly lead to overprediction of the slowing-down source in these regions, hence to overprediction of the absorber region flux and resonance integral. This effect could lead to an estimated 2% overprediction of the resonance integral.

All of the above effects can occur to varying degrees in each cell calculated. Some effects will tend to cancel others. It is, however, clear that most of the potential error lies in the calculation of the fluxes, and tends to give high values of the flux everywhere. This leads to consistent overprediction of the resonance integral and resonance reaction rates, a trend that has been observed in virtually all comparisons between HAMMER (HAMBUR and CREEP also) and experiments.

3.1.4 Solution for Resonance Integrals in HAMBUR

The resonance integral calculation in the HAMBUR System was developed as an extension of the HAMMER method by the author in 1967. It eliminates the assumption of a single homogeneous absorber region and computes the resonance integrals at the specified concentrations for each isotope in each region. The physics of this treatment was first presented in a seminar in August, 1967 and is essentially the same as for the CREEP module documented in Volume IV of DPSTM-500.

The basic assumptions in the HAMBUR calculation are the same as set down in Section 3.1.3 for HAMMER with the exception of the first assumption of the equivalent single absorber region

3.1.4.1 Solution by HAMBUR for Resolved Resonances

Equation 1 is written for each absorber region as

$$\sum_n^T(E) V_n \phi_n(E) = \sum_{n'=1}^M P_{n'n}(E) V_{n'} \sum_{l \in n'} \frac{N_{n'l}}{1-\alpha_l} \int_E^{E/d_l} \frac{\sigma_l^s(E')}{E'} H(E-\alpha_l E') \phi_{n'}(E') dE' \quad (22)$$

The sum over n' is broken into a sum over absorber region and a sum over moderator regions, and Equation 22 written

$$\begin{aligned} \phi_n(E) = \frac{1}{\sum_n^T(E) V_n} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{l \in n'} \frac{N_{n'l}}{1-\alpha_l} \int_E^{E/d_l} \frac{\sigma_l^s(E')}{E'} H(E-\alpha_l E') \phi_{n'}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \sum_{l \in n'} \frac{N_{n'l}}{1-\alpha_l} \int_E^{E/d_l} \frac{\sigma_l^s(E')}{E'} H(E-\alpha_l E') \phi_{n'}(E') dE' \right\} \quad (23) \end{aligned}$$

For the second sum in Equation 23 we use the Narrow Resonance Approximation and evaluate the integral as in Equation 6. In the first sum in Equation 23 the isotopes are limited to the selected isotopes so that Equation 23 becomes

$$\begin{aligned} \phi_n(E) = \frac{1}{\sum_n^T(E) V_n} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{l \in n'} \frac{N_{n'l}}{1-\alpha_l} \int_E^{E/d_l} \frac{\sigma_l^s(E')}{E'} H(E-\alpha_l E') \phi_{n'}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\sum_{n'}^s(E) \phi_{n'}^{ASY}}{E} \right\} \quad (24) \end{aligned}$$

Equation 24 is inserted into Equation 2 for isotope j in region n as

$$I_{jn}^a = \int_{res} dE \frac{\sigma_j^a(E)}{\sum_n^T(E) V_n} \left\{ \sum_{n' \in f} P_{n'n}(E) V_{n'} \sum_{l \in n'} \frac{\sigma_{nl}^S}{1 - \alpha_l} \int_E^{E/\alpha_l} \frac{\sigma_l^S(E')}{E'} H(E - \alpha_l E') \phi_{n'}(E') dE' \right. \\ \left. + \sum_{n' \in m} P_{n'n}(E) V_{n'} \frac{\sum_{n'}^S(E) \phi_{n'}^{asy}}{E} \right\} \quad (25)$$

We can now expand the total cross section for region n as

$$\sum_n^T(E) = N_{nj} \left\{ \sigma_j^T(E) + \frac{\sigma_m^S(E) N_{nm1}}{N_{nj}} + \frac{\sigma_m^S(E) N_{nm2}}{N_{mj}} \right\} = N_{nj} \sigma_n^T(E) \quad (26)$$

where again the non-overlap of resonances has been used.

For the slowing-down source in the fuel regions we make use of the average slowing-down value as given in Equation 11, but apply a correction to account for differences in absorber concentration. This is a good assumption since for heterogeneous assemblies over 80% of the slowing-down source comes from the second term of Equation 25. The HAMBUR treatment is valid, therefore, only for heterogeneous assemblies and should not be utilized for homogeneous calculations. Equation 11 represents a source based on the Infinite Mass Approximation of magnitude.

$$S_0(E) = \left\{ \overline{\sum_j^S(E)} + \overline{\sum_m^S(E)} \right\} \phi^{asy}(E) \quad (27)$$

where

$$\overline{\sum_m^S(E)} = \frac{\sum_m \sum_{n \in f} \sigma_m^S(E) N_{nm} V_m}{\sum_{n \in f} V_n} = \text{average admixed moderator scattering cross section} \quad (28)$$

$$\overline{\sum_j^S(E)} = \frac{\sum_{j \in f} \sigma_j^S(E) N_{nj} V_n}{\sum_{n \in f} V_n} = \text{average absorber scattering cross section}$$

The true slowing-down source in Equation 25, based on the Infinite Mass Approximation, is

$$S_{n'}(E) = \lim_{d_i \rightarrow 1} \sum_{i \in n'} \frac{N_{n'i}}{1-d_i} \int_E^{E/d_i} \frac{\sigma_i(E')}{E'} H(E-d_i E') \phi_{n'}(E') dE' = \left\{ \sum_{n'm}^S + \sum_{n'j}^S \right\} \phi_{n'}^{asy} \quad (29)$$

Taking the ratio of Equation 29 and 27 yields

$$S_{n'}(E) = \frac{\sum_{n'm}^S + \sum_{n'j}^S}{\sum_{n'm}^S + \sum_{n'j}^S} S_0 \approx \frac{\sum_{n'm}^S + \sum_{n'j}^S}{\sum_{n'm}^S + \sum_{n'j}^S} S_0 = \left\{ 1 - \frac{\sum_{n'j}^S - \sum_{n'm}^S}{\sum_{n'm}^S + \sum_{n'j}^S} \right\} S_0 \quad (30)$$

Inserting Equation 26 and 30 into Equation 25 then yields

$$I_{jn}^w = \int_{res} dE \frac{\sigma_j^w(E)}{\sigma_n^T(E)} \left\{ \sum_{n' \in f} \frac{P_{n'n}(E) V_{n'}}{N_{nj} V_n} \left[1 - \frac{\sum_{n'j}^S - \sum_{n'm}^S}{\sum_{n'm}^S + \sum_{n'j}^S} \right] S_0 + \sum_{n' \in m} \frac{P_{n'n}(E) V_{n'}}{N_{nj} V_n} \frac{\sum_{n'}^S(E) \phi_{n'}^{asy}}{E} \right\} \quad (31)$$

Define now

$$P_{dn}^w(E) = \sum_{n' \in f} \frac{P_{n'n}(E) V_{n'}}{N_{nj} V_n} \left[1 - \frac{\sum_{n'j}^S - \sum_{n'm}^S}{\sum_{n'm}^S + \sum_{n'j}^S} \right] \quad (32)$$

$$P_{in}^w(E) = \sum_{n' \in m} \frac{P_{n'n}(E) V_{n'}}{N_{nj} V_n} \sum_{n'}^S(E) \phi_{n'}^{asy}$$

so that the final form of the integration is written

$$I_{jn}^e = \int_{res} dE \frac{\sigma_j^a(E)}{\sigma_n^r(E)} \left\{ P_{0n} S_0 + \frac{P_{1n}}{E} \right\} \quad (33)$$

Equation 33 is of the same basic structure as Equation 14 and the integrations are performed in exactly the same manner as for HAMMER. A fine-interval Simpson's rule integration (performed in lethargy space) is carried out over a range of ± 5 times the practical width of the resonance. In each interval the absorber average slowing-down source S_0 is calculated from Equation 11 and the P_{0n} and P_{1n} collision

sums of Equation 32 are evaluated from a cosine current collision probability calculation for each absorber region. Equation 11 is evaluated by a separate Simpson's rule integration and cross sections are evaluated from the Single Level Breit-Wigner parameters (see Section 3.1.3.3). Corrections are made in the wings of the resonances in the same manner as for HAMMER except the correction is applied to each absorber region separately.

This calculational procedure requires considerably more computer time than for HAMMER primarily due to the evaluation of the $P_{0n}(E)$ and $P_{1n}(E)$ terms of Equation 32. In HAMMER the use of the reciprocity theorem allows Equation 13 to be evaluated by a single collision probability calculation. Equations 32 require two collision probability calculations for their evaluation. The CREEP module utilizes work by D. A. Sharp to reduce the time required for these calculations. In CREEP the $P_{0n}(E)$ and $P_{1n}(E)$ are fitted over a selected range of total cross sections to a cubic equation form. These fitted parameters are then used to derive the $P_{0n}(E)$ and $P_{1n}(E)$ values at intermediate values of $\sum_n^r$ for each absorber region.

The asymptotic fluxes that occur in Equation 32 for $P_{1n}(E)$ are evaluated in HAMBUR for each energy group based on smooth cross sections in the multigroup libraries. A slightly different procedure is used in CREEP as the multigroup cross sections are not available. In CREEP a flat flux approximation is used that sets $\phi_{asy} = 1$ wherever it occurs in any equations.

3.1.4.2 Solution for Unresolved Resonances in HAMBUR

In HAMBUR the unresolved resonance integral is computed as an equivalent single absorber region as computed by HAMMER, and a correction factor is applied to relate this average integral

to the correct regionwise value. The calculation of the integral for the equivalent single region absorber is described in Section 3.1.3.2; the description of how it is resolved into the regionwise components will be treated here.

The regionwise resonance integrals are computed so as to maintain the total reaction rate for the assembly the same as computed by Equation 15 for the single equivalent absorber region. This requires that

$$\sum_f \bar{V}_f \bar{\phi}_f = \sum_{n \in f} \bar{Z}_n \bar{V}_n \bar{\phi}_n \quad (34)$$

We desire a set of coefficients f_n such that

$$\bar{\phi}_n \bar{V}_n \bar{Z}_n = f_n \bar{\phi}_f \bar{V}_f \bar{Z}_f \quad (35)$$

or

$$f_n = \frac{\bar{\phi}_n \bar{V}_n \bar{Z}_n}{\bar{\phi}_f \bar{V}_f \bar{Z}_f} = \frac{\bar{\phi}_n \bar{V}_n \bar{Z}_n}{\sum_{n \in f} \bar{\phi}_n \bar{V}_n \bar{Z}_n}$$

The fluxes can be evaluated approximately from Equation 1 by writing it in simplified form

$$\sum_n^T \bar{V}_n \bar{\phi}_n(E) = \sum_{n' \in f} P_{n'n}(E) \bar{V}_n \bar{S}_{n'}(E) + \sum_{n' \in m} P_{n'n}(E) \bar{V}_{n'} \frac{\sum_n^S \bar{V}_n \bar{\phi}_n(E)}{\bar{V}_{n'}} \bar{\phi}_{n'}^{as}$$

where the NR Approximation is used as the moderator source. As a first approximation we ignore the absorber region slowing-down source as contributing since it has only a small effect on the reaction rate. This gives

$$\bar{\phi}_n(E) = \frac{1}{\sum_n^T \bar{V}_n} \sum_{n' \in m} P_{n'n}(E) \bar{V}_{n'} \frac{\sum_n^S \bar{V}_n \bar{\phi}_n(E)}{\bar{V}_{n'}} \quad (36)$$

Inserting Equation 36 into the expression for f_n yields

$$f_n = \frac{\sum_{n' \in m} P_{n'n}(\epsilon) V_{n'} \sum_{n'}^S(\epsilon) \phi_{n'}^{asy}}{\sum_{n \notin f} \sum_{n' \in m} P_{n'n}(\epsilon) V_{n'} \sum_{n'}^S(\epsilon) \phi_{n'}^{asy}} \quad (37)$$

Equation 37 is evaluated in HAMBUR to obtain the regionwise unresolved resonance integrals from the equivalent single region integral calculated in the same manner as in HAMMER. A separate set of f_n are generated for each multigroup within which the integral makes a contribution. Equation 37 uses a cosine currents collision probability routine to generate its solution.

In CREEP a slightly different approach is used to obtain these coefficients. CREEP does not have the multigroup structure available to it hence divides the energy range of the resonance integral into 0.25 lethargy intervals. Within each interval a set of f_n 's are generated and the contribution to the resonance integral (Equation 15) over this lethargy interval computed with these f_n 's. CREEP also uses a flat flux approximation for the ϕ_n^{asy} in Equation 37.

3.1.4.3 Resonance Cross Sections in HAMBUR

The HAMBUR System and CREEP module generate resonance cross sections using exactly the same equations as HAMMER as described in Section 3.1.3.3. The CREEP module has facilities to evaluate the $\psi(\rho, x)$ and $\chi(\rho, x)$ functions by expansion of the complex error function as well as by expansions of the incomplete gamma functions.

3.1.4.4 Deficiencies in the HAMBUR Resonance Calculation

The HAMBUR resonance calculation was developed to enable resonance integrals to be calculated correctly on a regionwise basis. Its basic design did not eliminate errors arising from any other assumptions made in the basic HAMMER calculations. Hence the same basic deficiencies exist for HAMBUR as for HAMMER except for the correct regionwise treatment of integrals. All comments made in Section 3.1.3.4 for HAMMER are also valid for HAMBUR.

The CREEP module has the same discrepancies as HAMBUR. It has, in addition, a possible increased overprediction of the resonance integral due to the use of the flat flux approximation in calculating Equation 32.

3.2 Improved Resonance Calculation

The major discrepancies itemized in Section 3.1.3.4 and 3.1.4.4 for HAMMER, HAMBUR, and CREEP have all been related to the methods used in calculation of the fluxes in each region of a lattice cell. Clearly any new approach to calculation of resonance capture should pay careful attention to this and to the effects arising from the overlap of resonances in different isotopes. There are, however, new effects that arise in the RAHAB calculation in treating multicelled lattices that were not present in the HAMMER and HAMBUR treatments. One effect is that of neutrons streaming into a cell from adjacent cells. Clearly for lattices with voided cells this will have a measurable effect on resonance capture in the adjacent cells.

The resonance reaction rate calculation described below will attempt to enable a good flux calculation to be made, and to account for streaming effects from adjacent cells.

The output from resonance calculation module CREEP is in the form of normalized reaction rates. The resonance reaction rate for isotope j in region n in group g is expressed as

$$S_{nj}^g = R_{nj}^g Q^g \quad (38)$$

where Q^g is the cell average slowing-down density for multigroup g . The coefficients R_{nj}^g are generated by the resonance calculation modules to arbitrary flux normalization and then expressed as a reaction rate/unit slowing-down density. To account for current streaming effects¹² Equation 38 is modified to read

$$S_{nj}^g = R_{nj}^g Q^g + T_{nj}^g J_{in}^g \quad (39)$$

where J_{in}^g is the average boundary current into the cell in group g and T_{nj}^g is the reaction rate/unit current for isotope j in region n in n_j group g .

Equation 39 implies that the boundary current on a cell is not known and all current effects are accounted for in the T_{nj}^g coefficients. The coefficients R_{nj}^g account for all effects generated by neutrons that slow down in the cell itself. In Equation 38 all effects are due to neutrons slowing down in the cell with zero net current on the cell boundary.

In the description that follows, Equation 1 will be rewritten into a slightly different form that allows the boundary currents to be included. The method of solution of this new equation will then be developed in a manner so as to allow full resolution of the resonance fluxes. Finally the method of generating the coefficients in Equation 39 will be described.

3.2.1 Resonance Flux Equation

Assume a cell is broken into N regions (for now, arbitrary in shape). Take a region n of the cell which is surrounded by regions n' (adjacent or otherwise) and we write the total collision rate for this region at energy E as

$$\begin{aligned}
 V_n \sum_n^T(E) \phi_n(E) = & \sum_{\substack{n'=1 \\ n' \neq n}}^N (1 - \tilde{P}_{nn'}(E)) V_n \sum_{i=1}^{M_n} \frac{N_{ni}}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_c^S(E')}{E'} \phi_n(E') dE' \\
 & + \sum_{\substack{n'=1 \\ n' \neq n}}^N \tilde{P}_{n'n}(E) V_{n'} \sum_{i=1}^{M_{n'}} \frac{N_{n'i}}{1 - \alpha_i} \int_E^{E/d_i} \frac{\sigma_c^S(E')}{E'} \phi_n(E') dE' \\
 & + \sum_{\substack{n'=1 \\ n' \neq n}}^N V_{n'} \tilde{P}_{n'n}(E) Q_{n'}(E) + \sum_{\substack{n'=1 \\ n' \neq n}}^N (1 - \tilde{P}_{nn'}(E)) V_n Q_n(E) \\
 & + \sum_{\substack{n'=1 \\ n' \neq n}}^N \tilde{P}_{n'n}^S(E) S_{n'}(E) + \sum_{\substack{n'=1 \\ n' \neq n}}^N (1 - \tilde{P}_{nn'}^S(E)) V_n S_n(E)
 \end{aligned}$$

$$n = 1, 2, 3, \dots, N \quad (40)$$

where:

V_n = volume of region n

$\sum_n^T(E)$ = total macroscopic cross section in region n at energy E

$\phi_n(E)$ = total flux in region n at energy E

$\tilde{P}_{nn'}(E)$ = first flight escape probability from region n to region n' due to unit volume source in region n at energy E

N_{ni} = concentration of isotope i in region n

$\sigma_i^s(E) =$ microscopic scattering cross section of isotope 1 at energy E

$d_i = [(A_i - 1)/(A_i + 1)]^2$ where A_i is the atomic mass ratio of isotope 1 to the neutron mass

$Q_n(E) =$ slowing-down source in region n at energy E from neutrons above energy E_n (top of the resonance region)

$S_n(E) =$ surface source of neutrons in region n at energy E
 $= \vec{J}_n^s(E) \cdot \vec{n}$

$\tilde{p}_{nn'}^s(E) =$ first flight escape probability from region n to region n' from a uniform unit source of neutrons at energy E on the external boundary of region n.
 $= 0$ if region has no cell boundary surface.

Define now

$$\begin{aligned} P_{nn'}(E) &= \tilde{p}_{nn'}(E) \quad \text{if } n \neq n' \\ &= \sum_{\substack{n'=1 \\ n' \neq n}}^N (1 - \tilde{p}_{nn'}(E)) \quad \text{if } n = n' \end{aligned} \quad (4.1)$$

$$\begin{aligned} P_{nn'}^s(E) &= \tilde{p}_{nn'}^s(E) \quad \text{if } n \neq n' \\ &= \sum_{\substack{n'=1 \\ n' \neq n}}^N (1 - \tilde{p}_{nn'}^s(E)) \quad \text{if } n = n' \end{aligned}$$

Also define the Heviside function as

$$H(x) = 1 \quad x \geq 0$$

$$H(x) = 0 \quad x < 0$$

so that Equation 40 can be written

$$\begin{aligned} \sum_n^T(E) V_n \phi_n(E) &= \sum_{n'=1}^N P_{n'n}(E) V_{n'} \sum_{i=1}^{m_{n'}} \frac{A_{n'i}}{1-d_i} \int_E^{E/d_i} \frac{\sigma_i^s(E')}{E'} H(E-d_i E') \phi_n(E') dE' \\ &+ \sum_{n'=1}^N P_{n'n}^s(E) V_{n'} Q_{n'}(E) + \sum_{n'=1}^N P_{n'n}^s(E) S_{n'}(E) \end{aligned} \quad (4.2)$$

$n=1, 2, 3, \dots, N$

We choose the resonance region to fall between two energies, E_L and E_H , the lower and upper limits, respectively. Limit E_L must be lower in energy than the fission production energy, and also low enough in energy that inelastic scattering is negligible since Equations 40 and 42 are based on elastic scattering only. Limit E_H must be high enough in energy so that molecular binding and thermal upscatter are unimportant, i.e., the scattering kernel is obtained from the mechanics of free atom collisions.

Two external neutron sources appear in Equation 2. The $Q_n(E)$ represents the neutron slowing-down density to energy E from neutrons born higher in energy than E_H . The integral in the first term of Equation 42 represents slowing down from neutrons originating at energies between E and E_H . The term $S_n(E)$ is the $\frac{1}{V_n} \cdot \frac{dN}{dt}$ term corresponding to neutrons streaming into the cell from adjacent cells.

The solution of Equation 42 must be separated into two parts corresponding to the two parts of Equation 39. This is done by writing the flux as

$$\phi_n(E) = \phi_n(E) + \psi_n(E) \quad (43)$$

where:

$\phi_n(E)$ = component of flux arising from neutrons born in the cell and slowing down from higher energies

$\psi_n(E)$ = component of flux arising from neutrons born outside the cell plus neutrons slowed down after streaming into the cell

Substituting Equation 43 into Equation 42 yields

$$\begin{aligned} \sum_n^T V_n \phi_n(E) - \sum_{n=1}^N P_{n'n}(E) V_n \sum_{l=1}^{M_{n'l}} \frac{\lambda_{n'l}}{1-\alpha_{n'l}} \int_E^{E_H} \frac{\sigma_{n'l}^s(E')}{E'} H(E-\alpha_{n'l}E') \phi_n(E') dE' - \sum_{n=1}^N P_{n'n}(E) V_n Q_n(E) \\ = \sum_{n=1}^N P_{n'n}(E) V_n \sum_{l=1}^{M_{n'l}} \frac{\lambda_{n'l}}{1-\alpha_{n'l}} \int_E^{E_H} \frac{\sigma_{n'l}^s(E')}{E'} H(E-\alpha_{n'l}E') \psi_n(E') dE' + \sum_{n=1}^N P_{n'n}(E) S_n(E) \\ - V_n \sum_n^T \psi_n(E) \end{aligned}$$

$n=1, 2, 3, \dots, N$

Setting both sides of this equation equal to $\xi_n(E)$ yields the two equations

$$\begin{aligned}
 V_n \sum_{n'=1}^N P_{n'n}(E) \phi_n(E) - \xi_n(E) &= \sum_{n'=1}^N P_{n'n}(E) V_{n'} \sum_{l=1}^{M_{n'l}} \frac{\lambda_{n'l}}{1-\alpha_l} \int_E^{E_{Hl}} \frac{\sigma_l^S(E')}{E'} H(E-\alpha_l E') \phi_{n'}(E') dE' \\
 V_n \sum_{n'=1}^N P_{n'n}(E) \psi_n(E) + \xi_n(E) &= \sum_{n'=1}^N P_{n'n}(E) V_{n'} \sum_{l=1}^{M_{n'l}} \frac{\lambda_{n'l}}{1-\alpha_l} \int_E^{E_{Hl}} \frac{\sigma_l^S(E')}{E'} H(E-\alpha_l E') \psi_{n'}(E') dE' \\
 &+ \sum_{n'=1}^N P_{n'n}^S(E) S_{n'}(E) \quad (44)
 \end{aligned}$$

$n=1, 2, 3, \dots, N$

These Equations 44 have a family of solutions for any choice of the $\xi_n(E)$. We choose the solution $\xi_n(E) = 0.0$ for all n and E , since this choice makes the $\phi_n(E)$ dependent only on neutron sources that slow down from energies above E_H and $\psi_n(E)$ dependent on neutrons streaming in from the boundaries. Choosing this solution has additional advantages. If one desires a solution with no dependence on the boundary currents ($T_{nH} = 0.0$ in Equation 39), then the first of Equations 44 can be solved with the $P_{n'n}(E)$ based on zero currents at the cell boundaries. This is the same type of solution that is performed in HAMMER and HAMBUR. When the boundary current term is included in Equation 39 then Equations 44 are both solved with vacuum boundaries used in generating the $P_{n'n}(E)$.

To solve Equation 44 an arbitrary normalization must be provided. We choose to normalize the first of Equations 44 to one neutron slowing down into the Resonance Region at energy E_H . Further we assume that the flux above energy E_H is everywhere $1/E$, is spatially flat and the scattering is isotropic with constant cross section $\sigma_l^S(E) = \text{constant}$. With these assumptions we write

$$V_n \sum_{n'=1}^N P_{n'n}(E_H) \phi_{n'}(E_H) = \sum_{n'=1}^N P_{n'n}(E_H) V_{n'} Q_{n'}(E_H)$$

and

$$Q_{n'}(E_H) = \sum_{l=1}^{M_{n'l}} \frac{\lambda_{n'l}}{1-\alpha_l} \int_{E_H}^{E_{Hl}} \frac{\sigma_l^S(E')}{E'} H(E_H - \alpha_l E') \phi_{n'}(E') dE'$$

now

$$\phi_n(\epsilon') = \frac{A}{\epsilon'} \quad \text{and} \quad \sigma_c^s(\epsilon') = \text{constant}$$

hence,

$$Q_n(\epsilon_H) = \sum_{c=1}^{m_n'} \frac{N_{n,c}}{1-\alpha_c} A \sigma_c^s \int_{\epsilon_H}^{\epsilon_H/\alpha_c} H(\epsilon_H - \alpha_c \epsilon') \frac{d\epsilon'}{\epsilon'^2}$$

$$Q_n(\epsilon_H) = \sum_{c=1}^{m_n'} \frac{N_{n,c}}{1-\alpha_c} A \sigma_c^s \left(\frac{1}{\epsilon_H} - \frac{\alpha_c}{\epsilon_H} \right) = \frac{A}{\epsilon_H} \sum_{c=1}^{m_n'} N_{n,c} \sigma_c^s$$

The normalizing condition then becomes

$$\sum_{n=1}^N V_n Q_n(\epsilon_H) = \frac{A}{\epsilon_H} \sum_{n=1}^N V_n \sum_{c=1}^{m_n'} N_{n,c} \sigma_c^s = 1 \quad (45)$$

$$\text{or,} \quad A = \frac{\epsilon_H}{\sum_{n=1}^N V_n \sum_{c=1}^{m_n'} N_{n,c} \sigma_c^s}$$

At an energy $E < E_H$ the contribution from sources above E_H in energy may be written as

$$Q_n(E) = \frac{E_H \sum_{c=1}^{m_n'} \frac{N_{n,c}}{1-\alpha_c} \sigma_c^s \left(\frac{1}{E_H} - \frac{\alpha_c}{E} \right) H(E - \alpha_c E_H)}{\sum_{n=1}^N V_n \sum_{c=1}^{m_n'} N_{n,c} \sigma_c^s} \quad (46)$$

Normalization of the second of Equations 44 is performed as follows

$$\begin{aligned}
 S_{n'}(E) &= 0 & E > E_H \\
 \sum_{n'=1}^N S_{n'}(E) &= 1.0 & E = E_H \\
 S_{n'}(E) &= B/E & E_L \leq E \leq E_H
 \end{aligned} \tag{47}$$

hence

$$B = E_H \text{ and } S_{n'}(E) = E_H/E \quad E_L \leq E \leq E_H$$

With Equations 45 and 47 the fluxes at energy E_H may be written as

$$\phi_n(E_H) = \frac{1}{V_n \sum_{n'} P_{n'n}(E_H)} \sum_{n'=1}^N P_{n'n}(E_H) Q_{n'}(E_H) V_{n'}$$

$$\phi_n(E_H) = \frac{1}{V_n \sum_{n'} P_{n'n}(E_H)} \sum_{n'=1}^N P_{n'n}(E_H) V_{n'} \frac{\sum_{l=1}^{m_{n'}} N_{n'l} \sigma_l^S}{\sum_{n'=1}^N V_{n'} \sum_{l=1}^{m_{n'}} N_{n'l} \sigma_l^S}$$

and

$$\phi_n(E_H) = \frac{\sum_{n'=1}^N P_{n'n}^S(E_H)}{V_n \sum_{n'} P_{n'n}(E_H)} \tag{48}$$

To achieve accuracy in the solution of the resonance fluxes, Equation 44 will be solved directly throughout the resonance region. The procedure will be to select a grid of energy points adequate for accuracy of the flux solution and to enable accurate interpolation of the fluxes between energy points. The techniques of selecting energy points will be described below. Cross sections at energy E will represent the total contribution from all isotopes in each region of the lattice cell, both smooth and resonance contributions.

The reaction rates for each isotope in each region can be generated from the flux solution by a finely detailed integration over each resonance with fluxes interpolated from the solution of

Equation 44 at all energies.

Several approximations can be made to accelerate the solution of Equation 44. The sections below will discuss those that are available to the user in obtaining the slowing-down integrals in Equation 44.

The sections that follow will describe the numerical methods used to evaluate the slowing-down integrals, the grid selection, the cross section representation, the generation of the output coefficients $R_{n,j}$ and $\tau_{n,j}$ in Equation 39, and the numerical methods used in the solution. Please be aware that these methods are experimental and are subject to change without notice.

The module that performs this calculation is called RRRID. Because of its inclusion of the current source term in Equation 39 and its use of newly defined NUCPARAM, RILIB, and LIDS data set records it can only be used with a special version of the RAHAB module.

3.2.2 Cell Geometry and Composition

The cell geometry used in RRRID is similar to that used in HAMMER, HAMBUR, and CREEP. Each region in this geometry is numbered from the center out and is an annular ring of uniform composition over which the flat source approximation may be used in the flux solution. This geometry allows a one-dimensional solution for the collision probabilities $P_{n,n'}(E)$ and $P_{n,n'}^S(E)$ in Equation 44 by the method described in Appendix C.

There is only one region having a cell boundary, that being the highest numbered region in the geometry. The current source applied to this boundary is arbitrarily chosen as $1/E$ in shape in Equation 47. The proper current to utilize in Equation 39 for the reaction rates should be the inward current averaged over the entire cell boundary. The linearity of the transport equation makes it unimportant where a current of neutrons enters a cell in calculating cell average resonance effects.

The geometrical description of all cells in the lattice is contained in the GEOR block in the LIDS data set. The composition of all cells in the lattice are contained in the COMR block in the LIDS data set. A description of these blocks appears in Appendix A. These blocks are prepared as a first step in executing RRRID from the GEOM and COMP blocks in LIDS. These blocks may be saved and reused as ordered by the user.

3.2.3 Solution of Slowing Down Integrals

In a region n' the slowing-down density $Q_{n'}(E)$ is written as

$$Q_n(E) = \sum_{l=1}^{M_n'} \frac{N_n l}{1-\alpha_l} \int_E^{E/\alpha_l} \frac{\sigma_l^s(E')}{E'} H(E-\alpha_l E') \bar{\Phi}_n(E') dE' \quad (49)$$

where $\bar{\Phi}_n(E')$ can be $\phi_n(E')$ or $\psi_n(E')$. The regions in a lattice cell can be placed into one of three categories for computation of the slowing-down density.

1. Absorber regions where $\bar{\Phi}_n(E')$ varies rapidly.
2. Moderator regions where $\bar{\Phi}_n(E')$ varies rapidly.
3. Moderator regions where $\bar{\Phi}_n(E')$ can be taken as $1/E$.

The first of these categories consists of those regions where we desire the flux solution to be very accurate, hence we wish to obtain the slowing-down source from accurate numerical integrations over points higher in energy than E . The second of these categories are those regions where flux depression is evident due to proximity of a fuel tube or a target tube, and an accurate slowing-down source is necessary to predict the effects in the absorber regions that arise from these flux variations. For this second category we wish to obtain the slowing-down source from numerical integration of flux points higher in energy than E . The third category are those moderator regions whose fluxes are not materially affected by the presence of a resonance absorber hence can be treated as having relatively constant scattering properties and $1/E$ fluxes.

The regions in category 3 will be treated first. Here the flux is $1/E$ and we treat the scattering cross section as a constant $\sigma_l^s(E') = \sigma_l^p(E')$ where $\sigma_l^p(E')$ is the potential scattering cross section for the isotope l . We use Equation 45 as the normalizing equation for the $1/E$ flux, hence Equation 49 is written

$$Q_n(E) = \frac{M_n'}{\sum_{l=1}^{M_n'} \frac{N_n l}{1-\alpha_l} \frac{\sigma_l^p}{\sum_{n=1}^N V_n \sum_{l=1}^{M_n} N_n \sigma_l^s}} \int_E^{E/\alpha_l} H(E-\alpha_l E') \frac{dE'}{E^2}$$

or

$$Q_n(E) = \frac{1}{E \sum_{n=1}^N V_n \sum_{l=1}^{M_n} N_n \sigma_l^p} \sum_{l=1}^{M_n'} N_n l \sigma_l^p \quad (50)$$

Note that the energy range between E_H and E/α_1 , if present, is included in the integration of Equation 50. This makes it easier to evaluate each region source.

To evaluate the slowing-down density integrals for regions in categories 1 and 2 we wish to numerically integrate for each isotope i in region n' at energy point E_j the integral

$$K_{n'i}(E_j) = \int_{E_j}^{E_j/\alpha_1} \frac{\sigma_i^s(E')}{E'} H(E_j - \alpha_i E') \Phi_{n'}(E') dE'. \quad (51)$$

To perform this integration we first put a restriction on the energy grid chosen for the flux solution that $\sigma_i^s(E') \Phi_{n'}(E')$ vary linearly with E' between discrete energy points E_m at which the flux solution is made. The details of the grid selection is contained in Section 3.2.4 and this will be pursued further there. With this assumption we write the $\sigma_i^s \Phi_{n'}$ product between points at energies E_m and E_{m-1} as

$$\sigma_i^s(E') \Phi_{n'}(E') = \frac{1}{E_{m-1} - E_m} \{ (E' - E_m) \sigma_{n-1}^s \Phi_{m-1} + (E_{m-1} - E') \sigma_m^s \Phi_m \} \quad (52)$$

where the points are numbered starting at higher energies and going to lower energies. Hence $E_1 = E_H$ and $E_{LAST} = E_L$. Rewriting Equation 51 yields

$$K_{n'i}(E_j) = \int_{E_j}^{E_j/\alpha_1} \frac{\sigma_i^s(E')}{E'} H(E_j - \alpha_i E') \Phi_{n'}(E') dE' = \sum_{m=j}^{P+1} \int_{E_m}^{E_{m-1}} \sigma_i^s(E') \Phi_{n'}(E') dE'/E' + \int_{E_p}^{E_j/\alpha_1} \frac{\sigma_i^s(E')}{E'} H(E_j - \alpha_i E') \Phi_{n'}(E') dE'$$

where energy E_j/α_1 is assumed to fall between energy points at E_p and E_{p-1} . If $E_j/\alpha_1 > E_H$ the integration is terminated at E_H and the contribution from Equation 46 is added. Putting Equation 52 into Equation 51 then yields

$$K_{n'i}(E_j) = \sum_{m=j}^{P+1} \int_{E_m}^{E_{m-1}} \frac{1}{E_{m-1} - E_m} \{ (E' - E_m) \sigma_{n-1}^s \Phi_{m-1} + (E_{m-1} - E') \sigma_m^s \Phi_m \} \frac{dE'}{E'} + \int_{E_p}^{E_j/\alpha_1} \frac{1}{E_{p-1} - E_p} \{ (E' - E_p) \sigma_p^s \Phi_{p-1} + (E_{p-1} - E') \sigma_p^s \Phi_p \} \frac{dE'}{E'}$$

where:

$$E^* = \min(E_H, E_j/d_i)$$

Integrating and collecting terms yields

$$K_{ni}(\epsilon_j) = \sum_{m=j}^{j+1} \left\{ \left(\frac{E_{m-1} \ln \frac{E_{m-1}}{E_m}}{E_{m-1} - E_m} - 1 \right) \sigma_m^S \Phi_m + \left(1 - \frac{E_m \ln \frac{E_{m+1}}{E_m}}{E_{m+1} - E_m} \right) \sigma_{m+1}^S \Phi_{m+1} \right\} \\ + \frac{1}{E_{p-1} - E_p} \left\{ (E_{p-1} \ln \frac{E_i^*}{E_p} - E_i^* + E_p) \sigma_p^S \Phi_p + (E_i^* - E_p - E_p \ln \frac{E_i^*}{E_p}) \sigma_{p+1}^S \Phi_{p+1} \right\}$$

Changing indices and rewriting this last expression yields

$$K_{ni}(\epsilon_j) = \left(1 - \frac{E_{p+1}}{E_p - E_{p+1}} \ln \frac{E_p}{E_{p+1}} \right) \sigma_{i,p}^S \Phi_{i,p} + \left(\frac{E_{j-1}}{E_{j-1} - E_j} \ln \frac{E_{j-1}}{E_j} - 1 \right) \sigma_{i,j}^S \Phi_{i,j} \\ + \sum_{m=p+1}^{j-1} \left\{ \left(\frac{E_{m-1}}{E_{m-1} - E_m} \ln \frac{E_{m-1}}{E_m} - 1 \right) + \left(1 - \frac{E_{m+1}}{E_m - E_{m+1}} \ln \frac{E_m}{E_{m+1}} \right) \right\} \sigma_{i,m}^S \Phi_{i,m} \\ + \frac{1}{E_{p-1} - E_p} \left\{ (E_{p-1} \ln \frac{E_i^*}{E_p} - E_i^* + E_p) \sigma_{i,p}^S \Phi_{i,p} + (E_i^* - E_p - E_p \ln \frac{E_i^*}{E_p}) \sigma_{i,p+1}^S \Phi_{i,p+1} \right\} \quad (53)$$

Define now

$$\gamma_m = 1 - \frac{E_{m+1}}{E_m - E_{m+1}} \ln \frac{E_m}{E_{m+1}} \quad (a)$$

$$\rho_m = \frac{E_{m-1}}{E_{m-1} - E_m} \ln \frac{E_{m-1}}{E_m} - 1 \quad (b)$$

$$\delta_m = \gamma_m + \rho_m \quad (c)$$

$$C_p^{(in)} = \frac{1}{E_{p-1} - E_p} \left\{ (E_{p-1} \ln \frac{E_i^*}{E_p} - E_i^* + E_p) \sigma_{i,p}^S \Phi_{i,p} + (E_i^* - E_p - E_p \ln \frac{E_i^*}{E_p}) \sigma_{i,p+1}^S \Phi_{i,p+1} \right\} \quad (54)$$

so that Equation 53 becomes

$$K_{n,i}(E_j) = \sigma_{ip}^s \Phi_{n,p} \gamma_p + \sigma_{ij}^s \Phi_{n,j} \gamma_j + \sum_{m=p+1}^{j-1} \sigma_{im}^s \Phi_{n,m} \gamma_m + C_p^{in'} \quad (55)$$

If $E_j/\alpha_i < E_{j-1}$, Equation 55 reduces to $C_p^{in'}$ corresponding to widely spaced points for isotope 1. This would be a typical case for energy points lying between resonances where the gridding routine would select widely spaced points. Note also that the flux term $\Phi_{n,j}$ at energy point E_j appears in Equation 55. Since this flux has not yet been solved for a linear extrapolation of the fluxes at points E_{j-1} and E_{j-2} is used of the form

$$\Phi_j = \Phi_{j-2} + \frac{\Phi_{j-1} - \Phi_{j-2}}{E_{j-1} - E_{j-2}} (E_j - E_{j-2}) \quad (56)$$

this approximation should introduce little error due to 1) the assumptions contained in Equation 52, 2) the flux will be solved for from Equations 44 - a small error in the slowing-down source for one region will have little influence on the flux, and 3) the gridding routine checks to assure the flux solution obtained is consistent within a specified ϵ , ϵ .

There are five possible cases that arise in the evaluation of Equation 55, and are shown in Figure 1.

Figure 1

The X's indicate the high energy limit for each case for scattering to energy E_j . Case I contains all terms of Equation 55 except the ϕ_j and has an additional component computed from Equation 46 for neutrons scattering from energies between E_j and E_j/α_1 to energy E . Case II contains all terms of Equation 55. Cases III, IV, and V are special cases arising for heavy mass isotopes and at the beginning of a calculation.

3.2.4 Selection of the Energy Grid

The selection of the energy points at which the flux solution is performed is based upon a number of criteria. One approach would be to select a uniformly fine energy mesh adequate to ensure all flux variations from all resonances are accounted for. This procedure would be time consuming and expensive in terms of computer cost and would surely generate many more flux solutions than are necessary to ensure the validity of Equation 52.

The grid selection method used in RRR1D selects the energy points based on the position and widths of all resonances in an absorber region. At energies that lie between resonances (all cross sections represented by smooth cross sections) the grid is selected as very widely spaced energy points due to the slow variation of flux at these energies. At energies that lie at or near a resonance of some isotopes the grid is selected more closely spaced.

The criteria used to select energy point E_j having already obtained flux solutions at energy points E_{j-1} , E_{j-2} , and E_{j-3} are the following:

1. The energy E_j is selected so that $\left| \frac{\phi_j - \phi_{j-1}}{\phi_{j-1}} \right| < \epsilon$ where ϵ is user specified.
2. The maximum $\Delta E = E_{j-1} - E_j \leq \delta_{\max} E_{j-1}$ where $\delta_{\max}$ is user specified.
3. The minimum $\Delta E = E_{j-1} - E_j \geq \delta_{\min} E_{j-1}$ where $\delta_{\min}$ is user specified.
4. If energy E_{j-1} is within the energy range W associated with resonance R the maximum $\Delta E = W/M \log E_h/E_l$ where E_h and E_l are the upper and lower energies of W_R , respectively, and M is based on the strength of the resonance.
5. If energy E_{j-1} lies between all resonances the maximum $\Delta E = E_{j-1} - E_{\text{next}}$ where E_{next} is the upper energy of the next resonance to be encountered.

Of these criteria 1 and 3 are absolute. The maximum ΔE is selected as the smallest of criteria 2, 4, and 5 but not less than the minimum ΔE selected by criterion 3.

Only absorber regions are considered in selecting an energy point since the fluxes are subject to more variation in these regions. The final energy point is selected by the smallest ΔE for any absorber region.

The steps involved in selecting energy point E_j are the following

1. $\Delta E_{\max}$ is selected from criteria 2, 4, and 5.
2. $\Delta E_{\min}$ is selected from criterion 3.
3. A quadratic fit is made of the fluxes at energy points E_{j-1} , E_{j-2} , and E_{j-3} and the derivative of the flux at E_{j-1} is evaluated, i.e.,

$$\begin{aligned}\phi(E) &= a + bE + cE^2 \\ \left. \frac{d\phi}{dE} \right|_{j-1} &= b + 2cE_{j-1}\end{aligned}\tag{57}$$

4. The flux at E_j is written as

$$\phi_j = \phi_{j-1} + \left. \frac{d\phi}{dE} \right|_{j-1} (E_{j-1} - E_j)$$

or

$$\Delta E = \frac{\phi_j - \phi_{j-1}}{\left. \frac{d\phi}{dE} \right|_{j-1}} = \frac{\Delta \phi}{\left. \frac{d\phi}{dE} \right|_{j-1}}$$

5. Criterion 1 states $\Delta \phi \leq \epsilon \phi_{j-1}$ so that

$$\Delta E \left. \frac{d\phi}{dE} \right|_{j-1} \leq \epsilon \phi_{j-1}$$

$$\text{and } \Delta E \leq \frac{\epsilon \phi_{j-1}}{\left. \frac{d\phi}{dE} \right|_{j-1}}\tag{58}$$

Equations 57 and 58 are used to obtain the ΔE under equality conditions in Equation 58. This value is then modified to conform to the $\Delta E_{\min}$ and $\Delta E_{\max}$ conditions in steps 1 and 2.

Following the flux solution the gridding routine is re-entered and the condition imposed by criterion 1 is checked. If this test fails the energy E_j is set to

$$E_j^{\text{new}} = \frac{E_j^{\text{old}} + E_{j-1}}{2} \leq E_{j-1} - \Delta E_{\min}\tag{59}$$

In the event $\Delta E = E_{j-1} - E_j^{old} = \Delta E_{min}$ the flux solution is accepted and a new energy point E_j is selected.

3.2.5 Cross Sections

Two types of cross sections are needed to obtain the flux solution at each energy point. The values $\sigma_i^f(E)$ are needed to evaluate Equation 49 for the slowing-down sources for each isotope in each region, and the values of $\Sigma_n^T(E)$ are needed to solve for the fluxes via Equation 44. We shall also need at a later time, the values of $\sigma_i^c(E)$ and $\sigma_i^f(E)$ to evaluate the reaction rates in each absorber region once the flux solution is obtained.

The values of $\sigma_i^f(E)$ are relatively easy to obtain and are usually set to the isotopic potential scattering cross section in the resonance region. Some isotopes, however, do have significant resonance scattering components and should properly be taken into account. The procedure used in RRR1D is to evaluate $\sigma_i^f(E)$ as the potential scattering cross section unless the user specifies the scattering to be calculated from resonance formulae which will be written down later.

The values of $\Sigma_n^T(E)$ are dependent upon all isotopes in region n and require both the smooth multigroup cross sections and the resonance cross sections as well as isotopic concentrations for computation. The smooth cross sections are stored in the XREC block of the LIDS data set along with the potential scattering cross section. Resonance parameters are stored in the RESP block of the LIDS data set for immediate access. Isotopic concentrations are stored in the COMR block in the LIDS data set. These LIDS blocks are described in Appendix A. The values of $\Sigma_n^T(E)$ are evaluated using the isotopic concentrations from the COMR block, smooth cross sections from the XREC block, and resonance parameters from the RESP block.

In the output phase the values of $\sigma_i^c(E)$ and $\sigma_i^f(E)$ will be required. Only the resonance component of these cross sections are required since the smooth components are already included in the epithermal transport computation.

3.2.5.1 Resonance Cross Sections

Many new resonance formalisms have come into usage since the ZUT and TUZ codes³ were written in 1961. The HAMMER, HAMBUR, and CREEP calculations utilize the same formalisms as ZUT and TUZ in their resonance cross section calculations which are computed from Single Level Breit-Wigner resonance parameters. The use of multi-level equations in the Reich-Moore⁷ or Adler-Adler⁸ formalisms are in common usage as well as a so-called multi-level Breit-Wigner formalism⁹. An attempt has been made in the RRR1D module to make the more useful of these formalisms available for cross section representation, and to make the module easily modifiable to add other formalisms as required.

Module RRRID can handle the following resonance formulae in the evaluation of isotopic cross sections:

Resolved Resonance Region:

- Single Level Breit-Wigner
- Multi-Level Breit-Wigner
- Adler-Adler Multi-Level

Unresolved Resonance Region:

- Single Level Breit-Wigner with competition reaction effects included.

The cross sections produced from these formalisms are Doppler-broadened values. The paragraphs below will give the formulae used in the evaluation of cross sections by each formalism. The details of how each set of resonance parameters for an isotope are stored in the RESP block are given in Appendix A.

3.2.5.1.1 Breit-Wigner Resolved Resonance Formulae

The Breit-Wigner resolved resonance formulae used in RRRID are those of Gregson, et.al⁹. They are consistent with the recommended formulae of the Resonance Region Subcommittee of the Cross Section Evaluation Working Group¹³ and can be considered proper formulae for use with ENDF/B parameters. Since a considerable fraction of present and future resonance parameters will be derived from ENDF/B it is desirable to implement consistent formulae.

These formulae are written in the Laboratory system for all ℓ values without Doppler broadening as follows:

◦ Elastic Scattering Cross Section

$$\sigma^j(\epsilon) = \sum_{\ell=0}^{\infty} \left\{ (2\ell+1) \frac{4\pi}{k^2} \sin^2 \phi_{\ell} + \frac{\pi}{k^2} \sum_{\substack{r=1 \\ r \neq j}}^{\infty} g_r \left(\Gamma_r^2 \cos^2 \phi_{\ell} - 2\Gamma_r(\Gamma_r + \Gamma_r') \sin^2 \phi_{\ell} + 2(\epsilon - \epsilon_r') \Gamma_r \sin^2 \phi_{\ell} \right) / ((\epsilon - \epsilon_r')^2 + \frac{\Gamma_r^2}{4}) \right\}$$

(60)

o. Capture Cross Section

$$\sigma^c(E) = \sum_{l=0}^{ULS} \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr} \Gamma_r}{(E-E_r)^2 + \Gamma_r^2/4}$$

o. Fission Cross Section

(60)

$$\sigma^f(E) = \sum_{l=0}^{ULS} \frac{\pi}{k^2} \sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr} \Gamma_r}{(E-E_r)^2 + \Gamma_r^2/4}$$

where

$$g_J = \frac{2J+1}{2(2I+1)}$$

I = spin of target nucleus

J = spin of compound nucleus

$\Gamma_{nr}(E_r)$ = neutron width (ev) for the r^{th} resonance evaluated at resonance energy E_r . For bound levels the absolute value $|\Gamma_r|$ is used.

$$\Gamma_{nr}(E) = P_L(E) \Gamma_{nr}(E_r) / P_L(E_r)$$

$$\Gamma_r(E) = \text{total width (ev)} = \Gamma_{nr}(E) + \Gamma_r + \Gamma_{fr}$$

$$E_r' = E_r + \frac{S_L(E_r) - S_L(E)}{2 P_L(E_r)} \Gamma_{nr}(E_r)$$

$$k = 2.196771 \times 10^{-3} \left(\frac{A}{A+1} \right) \sqrt{E} \quad = \text{neutron wave number}$$

E = neutron energy (ev) in the Laboratory system

S_L = shift factor

$$S_0 = 0$$

$$S_1 = 1/(1+\rho^2)$$

$$S_2 = -(18+3\rho^2)/(9+3\rho^2+\rho^4)$$

P_e = penetration factor

$$P_0 = P$$

$$P_1 = P^3 / (1 + P^2)$$

$$P_2 = P^5 / (9 + 3P^2 + P^4)$$

ρ = ka

$$a = (1.23A^{1/3} + 0.8) / 10$$

ψ_e = phase shift

$$\psi_0 = \hat{\rho}$$

$$\psi_1 = \hat{\rho} - \tan^{-1} \hat{\rho}$$

$$\psi_2 = \hat{\rho} - \tan^{-1} (3\hat{\rho} / (3 - \hat{\rho}^2))$$

$$\hat{\rho} = k\hat{a}$$

$\hat{a}$ = effective scattering radius (fermis)

The RESP block contains the following data for each resonance from which Equation 60 may be evaluated.

E_r = resonance energy (ev)

g_r = g factor for each resonance

l = angular momentum for each resonance

$\Gamma_{nr}(E_r)$ = neutron width (ev) at resonance energy E_r

Γ_r = radiation width (ev)

Γ_{fr} = fission width

The directory blocks for each isotope contained in the RESP block contain the following data:

A = atomic mass ratio to neutron mass

ABN = abundance of an isotope in a material

$\hat{a}$ = effective scattering radius

The cross sections given by Equation 60 are unbroadened. The broadened cross sections may be written as

$$E^{1/2} \sigma_0(E) = \frac{1}{\Delta \sqrt{\pi}} \int_0^{\infty} E'^{1/2} \sigma(E') e^{-\left(\frac{E-E'}{\Delta}\right)^2} dE' \quad (61)$$

where:

$$\Delta = \text{Doppler width} = \sqrt{\frac{4kT}{A}}$$

$$k = \text{Boltzmann's constant } (8.6167 \times 10^{-5} \text{ eV/}^\circ\text{K})$$

$$T = \text{Temperature } (^\circ\text{K})$$

Applying Equation 61 to Equation 60 yields the Doppler broadened cross sections as

o. Elastic Scattering

$$\sigma_a^S(E) = \frac{4\pi}{k^2} \sum_{L=0}^{NLS} \left\{ (2L+1) \sin^2 \varphi_L + \sum_J g_J \sum_{r=1}^{NR_J} \left[\frac{(\Gamma_{nr}^2 \cos^2 \varphi_L - 2\Gamma_{nr}(\Gamma_{rr} + \Gamma_{rr}) \sin^2 \varphi_L) \psi(\theta, x)}{\Gamma_r^2} + \frac{\Gamma_{nr} \sin^2 \varphi_L \chi(\theta, x)}{2\Gamma_r} \right] \right\}$$

o. Capture

$$\sigma_a^C(E) = \frac{4\pi}{k^2} \sum_{L=0}^{NLS} \sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr} \Gamma_{rr}}{\Gamma_r^2} \psi(\theta, x) \quad (62)$$

o. Fission

$$\sigma_a^f(E) = \frac{4\pi}{k^2} \sum_{L=0}^{NLS} \sum_J g_J \sum_{r=1}^{NR_J} \frac{\Gamma_{nr} \Gamma_{rr}}{\Gamma_r^2} \psi(\theta, x)$$

where: $\theta = \Gamma/\Delta$

$$x = 2(E - E_r)/\Gamma_r$$

$$\psi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2} dy \quad (63)$$

$$\chi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2} 2y dy$$

The $\psi(\theta, \chi)$ and $\chi(\theta, \chi)$ are evaluated by the method of Matta and Reichel¹⁴ which provides a rapid evaluation of Equation 63 by contour integration.

Equations 62 are used to evaluate resolved resonance cross sections in the Single Level Breit-Wigner formalism at an energy E.

For the Breit-Wigner multi-level formalism an additional term is added to the first of Equations 60. This equation then becomes

$$\sigma_{\Delta}^S(E) = \sigma_{\Delta SW}^S(E) + \sum_{\ell=0}^{\infty} \frac{\pi}{k^2} \sum_J g_J \sum_{r=2}^{\infty} \sum_{s=1}^{r-1} \frac{2\Gamma_r \Gamma_s [(\bar{E}-E_r)(\bar{E}-E_s) + \Gamma_r \Gamma_s / 4]}{[(\bar{E}-E_r)^2 + \Gamma_r^2 / 4][(\bar{E}-E_s)^2 + \Gamma_s^2 / 4]} \quad (64)$$

where $\sigma_{\Delta SW}^S(E)$ is given by Equation 60.

The resonances in Equation 64 are assumed to be ordered by increasing energy for each ℓ -J combination. This equation contains the interference terms between resonances in these sequences. Applying Equation 61 to Equation 64 yields the Doppler broadened cross section as

$$\sigma_{\Delta}^S(E) = \sigma_{\Delta SW}^S(E) + \sum_{\ell=0}^{\infty} \frac{4\pi}{k^2} \sum_J g_J \sum_{r=2}^{\infty} \sum_{s=1}^{r-1} \frac{32\Gamma_r \Gamma_s}{\Gamma_r^3 \Gamma_s^3} \left\{ 4\psi(\theta_r, \chi)\psi(\theta_s, \chi) + \chi(\theta_r, \chi)\chi(\theta_s, \chi) \right\} \quad (65)$$

where:

$$\sigma_{\Delta SW}^S(E)$$

is the contribution from Equation 62.

3.2.5.1.2 Adler-Adler Resolved Resonance Formulas

The formulas given here are based on the parameters contained in the ENDF/B representation of the Adler-Adler formalism described in Appendix D of Reference 13. The physical basis of this formalism is described in Reference 6.

The unbroadened cross sections are obtained from the formula

$$\begin{aligned} \sigma_x^X(E) = & \frac{2C}{E} (1 - \cos \omega) + \\ & + \frac{C}{\sqrt{E}} \sum_k \frac{J_k^X (G_k^X \cos \omega + H_k^X \sin \omega) + (\mu_k^X - E)(H_k^X \cos \omega - G_k^X \sin \omega)}{(\mu_k^X - E)^2 + J_k^{X2}} \\ & + \frac{C}{\sqrt{E}} \left\{ A_1^X + \frac{A_2^X}{E} + \frac{A_3^X}{E^2} + \frac{A_4^X}{E^3} + B_1^X E + B_2^X E^2 \right\} \quad (66) \end{aligned}$$

where:

$\sigma_x^X(E)$ = cross section from reaction type X at energy E.

$C = \pi E / k$

$k = 2.196771 \times 10^{-3} \left(\frac{A}{A+1} \right) \sqrt{E}$ = neutron wave number

A = atomic mass ratio of isotope to neutron mass

$\frac{2C}{E} (1 - \cos \omega)$ = potential scattering cross section. Term is non-zero only for scattering and total cross section.

$\omega = 2k\hat{a} = 4.393542 \times 10^{-3} \left(\frac{A}{A+1} \right) \hat{a} \sqrt{E}$

$\hat{a}$ = effective scattering radius (fermis)

$A_1^X, A_2^X, A_3^X, A_4^X, B_1^X, B_2^X$ = background parameters giving the contribution of "tails" of resonances lying outside the resonance region. Each reaction X has a different set of parameters.

G_k^X = symmetrical term resonance parameter (ev)

H_k^X = asymmetrical term resonance parameter (ev)

J_k^X = total width parameter (ev)

μ_k^x = energy parameter (ev)

E = neutron incident energy in Laboratory system (ev)

X = reaction designator. X can be total, capture, or fission in ENDF/B data. Any one, all, or any two reactions can be specified. See Appendix A for details of storage of parameters in the RESP block.

Applying Equation 61 to Equation 66 yields the Doppler broadened cross section as

$$\begin{aligned} \sigma_D^x(E) = & \frac{2c}{E}(1 - \cos \omega) + \frac{c}{\sqrt{E}} \sum_k \frac{\psi(\mu_k^x)}{v_k^x} \{ G_k^x \cos \omega + H_k^x \sin \omega \} \\ & + \frac{c}{2\sqrt{E}} \sum_k \frac{\chi(\mu_k^x)}{v_k^x} \{ H_k^x \cos \omega + G_k^x \sin \omega \} \quad (67) \\ & + \frac{c}{\sqrt{E}} \left\{ A_1^x + \frac{A_2^x}{E} + \frac{A_3^x}{E^2} + \frac{A_4^x}{E^3} + B_1^x E + B_2^x E^2 \right\} \end{aligned}$$

where:

$$\beta = \frac{\omega}{2} = \frac{\gamma}{2\Delta}$$

$$x = (\mu - E)/\gamma$$

and the $\psi(\mu, x)$ and $\chi(\mu, x)$ are defined in Equation 63.

Equations 67 and 63 are used to evaluate the cross sections based on the Adler-Adler multi-level formalism.

3.2.5.1.3 Single Level Breit-Wigner Unresolved Resonance Formulas

The only unresolved formalism employed in RRR1D is the Single Level Breit-Wigner. The formulas used are based on the recommendations of the Resonance Region Subcommittee of the CSEWG and follow the derivation of J. E. Lynn in Reference 16.

The Doppler broadened cross sections are written as

o. Elastic Scattering

$$\sigma^S(E) = \frac{4\pi}{k^2} \sum_{l=0}^{ULS} \sum_J g_J \left\{ (2l+1) \sin^2 \phi_l + \frac{\pi}{2 D_{lJ}} \left[\left\langle \frac{\bar{n}_n \bar{n}_n}{\bar{n}} \right\rangle_{lJ} - 2 \bar{n}_{lJ} \sin^2 \phi_l \right] \right\}$$

o. Capture

$$\sigma^C(E) = \frac{2\pi^2}{k^2} \sum_{l=0}^{ULS} \sum_J \frac{g_J}{D_{lJ}} \left\langle \frac{\bar{n}_n \bar{n}_f}{\bar{n}} \right\rangle_{lJ} \quad (68)$$

o. Fission

$$\sigma^f(E) = \frac{2\pi^2}{k^2} \sum_{l=0}^{ULS} \sum_J \frac{g_J}{D_{lJ}} \left\langle \frac{\bar{n}_n \bar{n}_f}{\bar{n}} \right\rangle_{lJ}$$

where:

$$\left\langle \frac{\bar{n}_n \bar{n}_n}{\bar{n}} \right\rangle_{lJ} = \left\{ \frac{\bar{n}_{n,lJ} \bar{n}_{n,lJ}}{\bar{n}_{lJ}} \right\} R_{n,lJ}$$

$$\left\langle \frac{\bar{n}_n \bar{n}_r}{\bar{n}} \right\rangle_{lJ} = \left\{ \frac{\bar{n}_{n,lJ} \bar{n}_{r,lJ}}{\bar{n}_{lJ}} \right\} R_{r,lJ}$$

$$\left\langle \frac{\bar{n}_n \bar{n}_f}{\bar{n}} \right\rangle_{lJ} = \left\{ \frac{\bar{n}_{n,lJ} \bar{n}_{f,lJ}}{\bar{n}_{lJ}} \right\} R_{f,lJ}$$

$$\begin{aligned} \bar{n}_{n,lJ} &= \text{average neutron width} = \bar{n}_{n,lJ}^0 \sqrt{E} \sqrt{V_0} \mu_{n,lJ} \\ V_0 &= \text{penetrability} \end{aligned}$$

$$V_0 = 1$$

$$V_1 = \rho^2 / (1 + \rho^2)$$

$$V_2 = \rho^4 / (1 + 3\rho^2 + \rho^4)$$

- $\mu_{n\ell J}$ = number of degrees of freedom for neutron widths
 $\mu_{f\ell J}$ = number of degrees of freedom for fission widths
 $\mu_{r\ell J}$ = number of degrees of freedom for radiation widths
 $\mu_{c\ell J}$ = number of degrees of freedom for competition widths

$\bar{\Gamma}_{n\ell J}^0$ = average reduced neutron width (ev)

$\bar{\Gamma}_{r\ell J}$ = average radiation width (ev)

$\bar{\Gamma}_{f\ell J}$ = average fission width (ev)

$\bar{\Gamma}_{c\ell J}$ = average competition width (ev)

$\bar{D}_{\ell J}$ = average level spacing (ev)

$g_J = \frac{2J+1}{2(2I+1)}$ = statistical spin factor

I = nuclear spin

J = compound nucleus spin

$\bar{\Gamma}_{\ell J} = \text{average total widths (ev)} = \bar{\Gamma}_{n\ell J} + \bar{\Gamma}_{r\ell J} + \bar{\Gamma}_{f\ell J} + \bar{\Gamma}_{c\ell J}$

$\rho = k a$

$k = 2.196771 \times 10^{-3} \left(\frac{A}{A+1} \right) \sqrt{E}$ = neutron wave number

a = channel radius (fermis) = $[1.23 A^{1/3} + 0.8] / 10$

A = atomic mass ratio to neutron mass

ϕ_ℓ = phase shift

$$\phi_0 = \hat{\rho}$$

$$\phi_1 = \hat{\rho} - \tan^{-1} \hat{\rho}$$

$$\phi_2 = \hat{\rho} - \tan^{-1} \left(\frac{3\hat{\rho}}{3-\hat{\rho}^2} \right)$$

$$\hat{r} = k \hat{a}$$

$$\hat{a} = \text{effective scattering radius (fermis)}$$

$$R_{n\epsilon\sigma} = \text{fluctuation integral for elastic scattering widths}$$

$$R_{r\epsilon\sigma} = \text{fluctuation integral for radiative capture widths}$$

$$R_{f\epsilon\sigma} = \text{fluctuation integral for fission widths}$$

The fluctuation integrals contain the statistical distribution of resonance widths based on the levels being very narrow (NR Approximation). They are defined as

$$R_{n\epsilon\sigma} = \int_0^\infty P(t|\mu_n) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{t^2}{(t\bar{\mu}_n + r\bar{\mu}_r + s\bar{\mu}_s + z\bar{\mu}_z)} \quad (69)$$

where $P(x|\mu_x)$ is the Porter-Thomas (Chi Square) distribution of neutron widths with μ_x degrees of freedom. This expression allows all widths to have different degrees of freedom. The integration variables t, s, r, z are defined by

$$t = \frac{\Gamma_n}{\bar{\mu}_n}, \quad r = \frac{\Gamma_r}{\bar{\mu}_r}, \quad s = \frac{\Gamma_s}{\bar{\mu}_s}, \quad z = \frac{\Gamma_z}{\bar{\mu}_z}$$

Similarly, for $R_{r\epsilon\sigma}$ and $R_{f\epsilon\sigma}$ we write

$$R_{r\epsilon\sigma} = \int_0^\infty P(t|\mu_t) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{t r}{(t\bar{\mu}_n + r\bar{\mu}_r + s\bar{\mu}_s + z\bar{\mu}_z)}$$

(70)

$$R_{f\epsilon\sigma} = \int_0^\infty P(t|\mu_t) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{s t}{(t\bar{\mu}_n + r\bar{\mu}_r + s\bar{\mu}_s + z\bar{\mu}_z)}$$

Equations 69 and 70 are evaluated by a sample averaging procedure originated by Greebler and Hutchings¹⁷ and modified by Bhat¹⁸. This procedure will evaluate the integrals for $\mu = 1, 2, 3, 4$, and ∞ . A complete description of the numerical techniques used in evaluating Equations 69 and 70 is given in Appendix E.

3.2.5.2 Smooth Multigroup Cross Sections

Smooth cross sections for all isotopes whether they have resonance parameters or not are stored in the XREC block in the LIDS data set as multigroup cross sections. Provision has been made to store the total, capture, and fission cross sections and the potential scattering cross sections. With these cross sections available their effects can be properly accounted for in the resonance flux calculation.

3.2.6 Calculation of Resonance Flux

Returning now to Equation 44 we now describe the over-all method of computing the fluxes $\phi(E)$ and $\psi(E)$ from Equation 44. At an energy E the slowing-down sources are computed by the methods of Section 3.2.4 and the total cross sections evaluated by the methods of Section 3.2.5. Write Equations 44 now as

$$\phi_n(E) = \frac{1}{V_n \Sigma_n^T(E)} \sum_{n'=1}^N P_{n'n}(E) V_{n'} Q_{n'}(E) \quad (71)$$

$$\psi_n(E) = \frac{1}{V_n \Sigma_n^T(E)} \left\{ \sum_{n'=1}^N P_{n'n}(E) V_{n'} \bar{Q}_{n'}(E) + \sum_{n'=1}^N P_{n'n}^S(E) S_{n'}(E) \right\}$$

Equations 71 are solved by a cosine currents P_0 Legendre order flux calculation of the same type as used by HAMMER, HAMBUR and CREEP to evaluate the collision probabilities at energy E . This calculation is described in detail in Appendix C. A choice of boundary conditions is allowed in the calculation so that the second term of Equation 39 may be made optimal. If the boundary conditions on the first of Equation 71 are made reflecting and all $S_{n'}(E) = 0$ in the second of Equation 71 then the calculation will not include streaming effects from adjacent cells and the T_{nj} coefficients in Equation 39 are zero. If the boundary conditions are made vacuum conditions and the $S_{n'}(E) = \beta/E$ then both of Equations 71 are solved, and the $T_{nj} \neq 0$.

This procedure is very efficient in that it requires only one calculation for all $\phi_n(E)$ and one calculation for all $\psi_n(E)$ at any energy E after the sources and cross sections are evaluated at energy E .

The fluxes calculated from Equations 71 are stored in the RFLX block in core. This block is described in Appendix A although it is never written as a LIDS block. This block is used for the flux storage necessary for calculation of the slowing-down sources by Equation 55, and for interpolating the correct fluxes to evaluate the reaction rates for each isotope (See Section 3.2.7 below.).

The RFLX block in core is of finite size and can store only a fixed number of flux solutions (approximately 500) for a given lattice cell. This finite size means that limitations must be imposed on the numerical integrations of the slowing-down density in Equation 55, for it is not possible to store all flux solutions up to energy E_H as described for evaluating Equation 55. The procedure used in the solution is as follows.

1. Starting at energy E_H flux solutions are generated until the RFLX block is full (say 500 points).
2. Reaction rates are generated for each isotope based on the resonance fluxes in the calculation and placed in the RILIB records over the range of energies in the RFLX block.
3. The highest energy 100 points are deleted from the RFLX block.
4. Flux solutions are generated until the RFLX block is again full. The slowing-down calculation will now not have flux solutions up to energy E_H over which to integrate; instead, if a component of slowing down exists for some isotope from energies higher than the highest energy in the RFLX block it is computed from Equation 46 with E_H replaced by the highest energy in the RFLX block. This procedure is probably very good but is at present still being investigated.
5. Steps 2, 3, and 4 are repeated until energy E_L is reached, then Step 2 is executed for a last time.
6. The final step is to convert the reaction rates by energy group stored in the RILIB records into the proper coefficients $\rho_{n_i}^g$ and $\tau_{n_i}^g$ of Equation 39.

3.2.7 Output of Reaction Rates

Periodically during the flux calculation the RFLX block is filled, and the output reaction rates must be generated so that the higher energy flux solutions can be discarded. Only fission and capture reaction rate coefficients are output and are generated from the intermediate integrals.

$$C_{nj}^g = V_n \int_g dE \, N_{nj} \sigma_j^c(E) \Phi_n(E)$$

$$F_{nj}^g = V_n \int_g dE \, N_{nj} \sigma_j^f(E) \Phi_n(E)$$

$$Q^g = \sum_{n=1}^N V_n \int_g dE \, Q_n(E) \quad (72)$$

$$S^g = \sum_{n=1}^N \int_g dE \, S_n(E)$$

where:

C_{nj}^g is the resonance capture reaction rate for isotope j in region n and group g.

F_{nj}^g is the fission reaction rate for isotope j in region n and group g.

Q^g is the total number of neutrons slowing down into group g

S^g is the total number of neutrons leaking into the cell in group g

$\Phi_n(E)$ is either $\phi_n(E)$ or $\psi_n(E)$

The cross sections in Equation 72 contain only the resonance contribution. The integrals in Equation 72 are computed based on a sliding criterion depending on the relative change in the flux across each resonance. Examine only the first of Equations 72 and write it

$$C_{nj}^g = \sum_{r=1}^{R^g} V_n N_{nj} \int_g dE \, \sigma_{jr}^c(E) \Phi_n(E)$$

where the sum over r implies a sum over all resonances r for isotope j in group g.

The contribution from an individual resonance is obtained by integrating over a range $\pm M$ practical widths above and below the resonance or

$$C_{nj}^{gr} = V_n N_{nj} \int_{E_0 - m\Delta}^{E_0 + m\Delta} dE \sigma_{jr}^c(E) \bar{\Phi}_n(E) dE$$

here $\Delta = \sqrt{\sigma_0/\sigma_p}$

where σ_0 = peak cross section at E_0

σ_p = potential scattering cross section

The integration is performed in lethargy space with the lethargy interval selected by the relative change in $\bar{\Phi}_n(E)$ over the range of integration as shown in Table I.

Max. $\frac{\Delta \bar{\Phi}(E)}{\bar{\Phi}(E_0 + m\Delta)}$ in Range	Lethargy Interval
< 10%	1/100
10% to 50%	1/200
> 50%	1/400

Table I

Lethargy Interval Used as a Function of Relative Flux Change Over the Resonance

Hence over resonance r the contribution is

$$C_{nj}^{gr} = V_n N_{nj} \sum_{i=1}^I \int_{u_i}^{u_{i+1}} \sigma_{jr}^c(u) \bar{\Phi}_n(u) du$$

$$u_{i+1} = u_i + \Delta u$$

For simplicity we fit the fluxes $\bar{\Phi}_n(u)$ to a polynomial in the energy region over the resonance. Assume the lethargy range over which the above integral is performed lies between energy points E_k and E_{k+1} (or at lethargies u_k and u_{k+1}) then define

$$\bar{\Phi}_n^k(u) = P(u_k, u_k, u_{k+1}) = a_k + b_k u + c_k u^2$$

and evaluate the integral as

$$C_{nj}^{gr} = V_n N_{nj} \sum_{i=1}^I \sigma_{jr}^c \left(\frac{u_{i+1} + u_i}{2} \right) \left\{ a_k (u_{i+1} - u_i) + b_k \left(\frac{u_{i+1}^2 - u_i^2}{2} \right) + c_k \left(\frac{u_{i+1}^3 - u_i^3}{3} \right) \right\} \quad (73)$$

Fitting the fluxes at a few points avoids the necessity of performing many interpolations at each value of $\frac{u_{i+1} + u_i}{2}$.

The contributions from Equations 72 are stored in core or in the RILIB records described in Appendix B (isotopic and regionwise quantities are stored in RILIB records; cell average values in core). After all contributions have been calculated from Equations 72 from all flux solutions in the energy range E_L to E_H a last pass is made to produce the R_{nj}^2 and T_{nj}^2 coefficients of Equation 39. These are calculated from the equations

$$\begin{aligned} R_{nj}^2 (\text{capture}) &= C_{nj}^2 / Q^2 & \{ \Phi_n(E) = \phi_n(E) \} \\ R_{nj}^2 (\text{fission}) &= F_{nj}^2 / Q^2 & \{ \Phi_n(E) = \phi_n(E) \} \\ T_{nj}^2 (\text{capture}) &= C_{nj}^2 / S^2 & \{ \Phi_n(E) = \psi_n(E) \} \\ T_{nj}^2 (\text{fission}) &= F_{nj}^2 / S^2 & \{ \Phi_n(E) = \psi_n(E) \} \end{aligned} \quad (74)$$

where all terms are defined in Equations 72 and 39. These quantities defined by Equation 74 are the final output of the resonance calculation.

4. References

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APPENDIX ANEW LIDS DATA SET BLOCKS AND TEMPORARY STORAGE BLOCKS

This Appendix contains a description of four new LIDS data set records generated by RRRID for storage of data pertinent to the resonance calculation. These blocks may be saved and reused as desired by the user.

A temporary storage block is defined that is used throughout the resonance calculation and is shown here for information only. This block (the RFLX block) cannot be read or written to or from any data set.

The LIDS data set blocks defined are the following:

- GEOR Block - Resonance geometry block - contains the detailed description of the one-dimensional annular geometry of each cell in the lattice.
- COMR Block - Resonance composition block - contains the isotopic concentrations of each material and pointers to the smooth and resonance cross sections in the XREC and RESP blocks, respectively.
- XREC Block - Smooth cross section block - contains the multigroup cross sections in the resonance energy range for all isotopes, and the potential scattering cross section for each isotope.
- RESP Block - Resonance parameter block - contains the resonance parameters for each absorber isotope in all cells in the lattice.

GEOR BlockResonance Geometry Description in LIDS

KGORG+1	NCLX	KCL1	Number of cells in block; pointer to cell 1.
KCL+0	NCL	KNXTCL	Cell number; pointer to next cell.
+1	NRX	KRO	No. of regions in cell; pointer to region outer radii
+2	KVOL	KTMP	Pointer to region volumes; pointer to region temp.
+3	KNMT	KTYP	Pointer to region material Nos.; pointer to region type flags.
+4	KREG	KNAME	Pointer to region identifiers; pointer to cell name.
KRO+0	Region 1 Outer Radii (cm).	Region Outer Radii (cm).	
	.		
	.		
	Reg.NRX Outer Radii.		
KVOL+0	Region 1 Vol. (cm ²).	Region Volumes (cm ²).	
	.		
	.		
	Region NRX Volume (cm ²).		
KTMP+0	Reg.1 Temp. (°K)	Region Temperatures (°K).	
	.		
	.		
	Reg.NRX Temp. (°K).		
KNMT+0	Reg.1 NMT	Reg.1 KNMT	Region material No.; Pointer to mat. in COMR block.
	.	.	
	.	.	
	Reg.NRX NMT	Reg.NRX KNMT	
KREG+0	Reg.1 Reg.No. in cell.	Pointer to Reg. Name.	Region No. in cell; Pointer to Region Name.
	.	.	
	.	.	
	Reg.NRX Reg.No. in cell.		
KTYP+0	Reg.1 Type.	Reg.2 Type	Region type flag
	.	.	
	.	.	
	Reg.NRX TYP2.		

= 1, absorber region

= 2, non-absorber region, integ.slowing-down source

= 3, non-absorber region, 1/E slowing-down source

COMR BlockResonance Composition Description in LIDS

KCORG+1	NMTX	KMT1	No. of materials in block; Pointer to first material.	
+2	NISX	KIS1	Number of isotopes in block; Point to first isotope.	
KMT+0	NMT	KNXTMT	Material number; Pointer to next material.	
+1	JISX	KMTNAM	No. isotopes in material; Pointer to material name.	
+2	Blank		Always blank.	
+3	NIS ₁	KIS ₁	Isotope number; Pointer to isotope description.	
+4	CONC ₁		Concentration of isotope (atm/bn-cm).	
+5	NIS ₂	KIS ₂		
+6	CONC ₂			
	.			
	.			
	NIS _{JISX}	KIS _{JISX}		
	CONC _{JISX}			
KIS+0	NIS	KNXTIS	Isotope number; Pointer to next isotope.	
+1	ITDC	KISNAM	Temperature (°C); Pointer to isotope name.	
+2	AWR		Atomic mass ratio of isotope to neutron mass.	
+3	ZAS		ZAS designation.	
+4	KRES	KSM	Pointer to resonance parameters in RESP block. If negative isotope is treated as a resonance scatterer.	Pointer to smooth cross sections in XREC block.

XREC BlockSmooth Cross Section Storage in LIDS

KSM+0	NIS	KNXTIS
+1	KTOT	KCAP
+2	KFIS	
+3	σ_P	
KTOT+0	IAT	IBT
+1	$\sigma^T(IAT)$ $\cdot$ $\cdot$ $\cdot$ $\sigma^T(IBT)$	
KCAP+0	IAC	IBC
+1	$\sigma^C(IAC)$ $\cdot$ $\cdot$ $\cdot$ $\sigma^C(IBC)$	
KFIS+0	IAF	IBF
+1	$\sigma^f(IAF)$ $\cdot$ $\cdot$ $\cdot$ $\sigma^f(IBF)$	

Isotope number; Pointer to next isotope.

Pointer to total cross section; Pointer to capture cross section.

Potential scattering cross section (bns).

Lowest group No. for total cross section;
Highest group number for total cross section.

Total cross section (bns).

Lowest group number for capture cross section;
Highest group number for capture cross section.

Capture cross section (bns).

Lowest group number for fission cross section;
Highest group number for fission cross section.

Fission cross section (bns).

Note: If any of the pointers KTOT, KCAP, or KFIS are 0 the corresponding section is omitted from the block.

RESP BlockResonance Parameter Storage Block in LIDS

KRORG+1	NISX	KIS1	Number of isotopes in block; Pointer to 1st isotope
+2	ELOWR		Low energy limit of resonance parameters in block.
+3	EHIGHR		High energy limit of resonance parameters in block.

KIS+0	NIS	KNXTIS	Isotope number; Pointer to next isotope.
+1	NSIX	KSI1	Number sub-isotopes in this isotope; Pointer to first sub-isotope.

KSI+0	NSI	KNXTSI	Sub-isotope number; Pointer to next sub-isotope.
+1	AWRI		Atomic mass ratio of this sub-isotope to neutron mass.
+2	ABN		Fractional abundance of this sub-isotope.
+3	AP		Spin dependent scattering length of this sub-isotope (fermis).
+4	NRPX	KRP1	Number of resonance parameters sets; Pointer to first parameter set.
+5	KSTRT		Starting resonance parameter set in calculation.

Breit-Wigner Resolved Resonance Parameters

KRP+0	NRP	KNXTRP	Resonance number; Pointer to next resonance
+1	IRF	IRU	Resonance formula flag; Resolved/Unresolved flag = 1.
+2	ELR		Low energy of effective range of these parameters (ev).
+3	EHR		High energy of effective range of these parameters (ev).
+4	SP		ℓ value for these parameters
+5	ER		E_0 (ev) central energy of resonance.
+6	G		$g = \frac{2I+1}{2(2J+1)}$
+7	Γ_T		Total width (ev)
+8	Γ_n		Neutron width (ev)
+9	Γ_γ		Radiation width (ev)
+10	Γ_f		Fission width (ev)

IRU = Resolved/unresolved flag
 = 1, Resolved Resonance
 = 2, Unresolved Resonance

IRF = Resonance Formula Flag
 = 1, Single level Breit-Wigner
 = 2, Multi-level Breit-Wigner
 = 3, Adler-Adler

RESP Block (Continued)Adler-Adler Resolved Resonance Parameters

KRP1+0

0	KRP2
IRF	IRU
NSX	LDAT
0.0	
0.0	
A1(1)	
A2(1)	
A3(1)	
A4(1)	
B1(1)	
B2(1)	
.	
.	
A1(NSX)	
A2(NSX)	
A3(NSX)	
A4(NSX)	
B1(NSX)	
B2(NSX)	

0 indicating background block; Pointer to first set of resonance parameters.

+1

Resonance formula flag = 3; Resolved/unresolved flag = 1.

+2

Number of sets of data given; Data flag (see below)

+3

Always zero.

+4

Always zero.

+5

Background coefficients for each set 1,2,...,NSX

LDAT = Data Flag

= 1, Total X-section parm. only given.

= 2, Fission X-section " " " "

= 3, Total & Fission X-sect. parm. give

= 4, Capture parm. only given.

= 5, Total and capture parm. given.

= 6, Fission and capture parm. given.

= 7, Total, Fission, and Capture parm. given.

KRP1+

6*(NSX-1)+5

KRP+0

NRP	KNXTRP
IRF	IRU
NSX	KRP1
ELR	
EHR	
DE(1)	
DW(1)	
GR(1)	
GI(1)	
.	
.	
DE(NSX)	
DW(NSX)	
GR(NSX)	
GI(NSX)	

+1

Resonance number; Pointer to next resonance.

+2

Resonance formula flag = 3; Resolved/unresolved flag = 1.

+3

No. parm. sets given; Pointer to background blk

+4

Low energy of effect. range of these parm. (ev)

+5

High energy of effect. range of these parm. (ev)

Resonance energy parameter μ (ev).Width parameter ν (ev).

Symmetrical parameter (ev).

Assymmetrical parameter (ev).

Repeated for NSX sets.

RESP Block (Continued)Breit-Wigner Unresolved Resonance Parameters

KRP+0	NRP	KNXTRP	Resonance number; Pointer to the next resonance.
+1	IRF	IRU	Resonance formula flag = 1; Resolved/unresolved flag = 2.
+2	NFN	NFG	No. degrees of freedom in neutron width; No. degrees of freedom in radiation width.
+3	NFF	NFX	No. degrees of freedom in fission width; No. degrees of freedom in competition width.
+4	ELR		Low energy of effect.range of these parm. (ev).
+5	EHR		High energy of effect.range of these parm. (ev).
+6	SP		4 value for these parameters
+7	D		Mean level spacing (ev).
+8	G		$g = \frac{2I+1}{2(2J+1)}$
+9	Γ_n^0		Reduced neutron width (ev).
+10	Γ_γ		Average radiation width (ev).
+11	Γ_f		Average fission width (ev).
+12	Γ_x		Average competition width (ev).

RFLX BlockTemporary Storage of Resonance Fluxes

KFORG+1

NEPX	KEP1
------	------

Number of energy points in block; Pointer to first energy point.

KEP+0

NEP	KNXTEP
E	
S	
Q	
ϕ_1	
ψ_1	
ϕ_2	
ψ_2	
.	
.	
ϕ_{NRX}	
ψ_{NRX}	

Point number; Pointer to next energy point.

Energy (ev) at this flux solution.

External current source into cell (neut/sec).

Slowing-down source for entire cell (neut/sec).

Flux due to slowing-down sources in region 1.

Flux due to current sources in region 1.

Flux due to slowing-down sources in region 2.

Flux due to current sources in region 2.

APPENDIX BNEW RECORDS DEFINED FOR NUCPARAM AND RILIB DATA SETS

The descriptions in this Appendix itemize the additions and changes to the NUCPARAM and RILIB data sets as a result of implementing the improved resonance capture calculation. Changes in the NUCPARAM data set are made to provide storage for the Adler-Adler multilevel resonance parameters. Changes in the RILIB data set are to provide records to output the reaction rate on a groupwise basis for each isotope in each region and for all isotopes in each region.

NUCPARAM

1/8/74

LIST OF ISOTOPES IN A MATERIAL (?DISC?) WITH RESOLVED RESONANCE
PARAMETERS IN A VERSION OF DATA SET

NAME = 'NUCPARAM'.?VERSN?.?DISC?. 'RESOLVED'. 'CONTENTS'

LIST = NRIX, (IZASRI(NRI), ABUN(NRI), AWR(NRI), IRF(NRI), AP(NRI), AM(NRI),
EL(NRI), NRI=1, NRIX)

SYMBOL	DEFINITION	TYPE
ABUN	FRACTIONAL ABUNDANCE OF SUB-ISOTOPE I IN ISOTOPE	R4
AM	SPIN DOWN SCATTERING LENGTH (FERMIS)	R4
AP	SPIN UP SCATTERING LENGTH (FERMIS)	R4
AWR	ATOMIC MASS RATIO OF SUB-ISOTOPE I TO NEUTRON MASS	R4
DISC	ISOTOPE NAME	C8
EL	LOW ENERGY (EV) BELOW WHICH RESONANCE CONTRIBUTION SHOULD NOT BE COMPUTED	R4
IRF	RESOLVED RESONANCE FORMULA FLAG: ALLOWED VALUES ARE: IRF = 1 - SINGLE LEVEL BREIT-VIGNER FORMULA WITH NO INTERFERENCE TERMS IN SCATTERING. IRF = 2 - SINGLE LEVEL BREIT-VIGNER FORMULA WITH INTERFERENCE SCATTERING TERMS INCLUDED. IRF = 3 - ADLER-ADLER MULTILEVEL FORMULA	I4
IZASRI	INTEGER SUB-ISOTOPE DESIGNATION IN FORM ZZAAS	I4
NRIX	NUMBER OF SUB-ISOTOPES WITH RESONANCE PARAMETERS IN THIS ISOTOPE	I4
VERSN	NUCPARAM DATA SET VERSION NAME	C8

ADLER-ADLER MULTILEVEL RESOLVED RESONANCE PARAMETERS FOR
ISOTOPE (?IZASRI?) IN MATERIAL (?DISO?) IN VERSION
(?VERSN?) OF DATA SET

NAME - 'NUCPARAM'.?VERSN?.?DISO?.?ADLER?.?IZASRI?

LIST - NSX,NRX,LDAT,(A1(NS),A2(NS),A3(NS),A4(NS),P1(NS),P2(NS),
NS=1,NSX),(SP(NS,NR),G(NS,NR),DE(NS,NR),DW(NS,NR),
GR(NS,NR),GI(NS,NR),NS=1,NSX),NR=1,NRX)

SYMBOL	DEFINITION	TYPE
A1	A1 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
A2	A2 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
A3	A3 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
A4	A4 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
B1	B1 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
B2	B2 COEFFICIENT IN BACKGROUND SERIES FOR SET NS	R4
DE	ENERGY PARAMETER (EV) FOR RESONANCE NR IN SET NS	R4
DISO	ISOTOPE NAME	C8
DW	WIDTH PARAMETER (EV) FOR RESONANCE NR IN SET NS	R4
G	STATISTICAL SPIN FACTOR = $(2*I+1)/(2*J+1)/2$ FOR RESONANCE NR IN SET NS	R4
GI	ASSYMETRICAL PARAMETER (EV) FOR RESONANCE NR IN SET NS	R4
GR	SYMMETRICAL PARAMETER (EV) FOR RESONANCE NR IN SET NS	R4
IZASRI	INTEGER ISOTOPE DESIGNATOR IN FORM ZZAAAS	I4
LDAT	DATA INDICATOR FLAG =1, TOTAL CROSS SECTION PARAMETERS ONLY GIVEN =2, FISSION CROSS SECTION PARAMETERS ONLY GIVEN =3, TOTAL AND FISSION CROSS SECTION PARAMETERS GIVEN	I4

SYMBOL	DEFINITION	TYPE
	=4, CAPTURE CROSS SECTION PARAMETERS ONLY GIVEN	
	=5, TOTAL AND CAPTURE CROSS SECTION PARAMETERS GIVEN	
	=6, FISSION AND CAPTURE PARAMETERS GIVEN	
	=7, TOTAL, FISSION, AND CAPTURE PARAMETERS GIVEN	
NR	INDEX OF RESONANCES	I4
NRX	NUMBER OF RESONANCES GIVEN	I4
NS	INDEX OF PARAMETER SETS	I4
NSX	NUMBER OF PARAMETER SETS GIVEN =1 FOR LDAT = 1,2, OR 4 =2 FOR LDAT = 3,5, OR 6 =3 FOR LDAT = 7	I4
SP	L VALUE FOR RESONANCE NR IN SET NS	R4
VERSN	VERSION NAME OF DATA SET	C2

RILIB

1/8/74

 RESONANCE REACTION RATES FOR ISOTOPE (?DISO?), IN REGION (?DREG?)

NAME - 'RILIB'.?DCEL?.?VCEL?.?DISO?.?DREG?.?RATES'

LIST - IA,IB,(RCO(I),RFQ(I),RCJ(I),RFJ(I),I=IA,IB)

SYMBOL	DEFINITION	TYPE
DCEL	CELL NAME	C8
DISO	ISOTOPE NAME IN CELL ?DCEL?	C8
DREG	REGION NAME IN CELL ?DCEL?	C8
IA	LOWEST GROUP INDEX FOR NON-ZERO DATA	I4
IB	HIGHEST GROUP INDEX FOR NON-ZERO DATA	I4
RCJ	CAPTURE REACTION RATE PER NEUTRON STREAMING INTO CELL IN GROUP J	R4
RCO	CAPTURE REACTION RATE PER NEUTRON SLOWING DOWN INTO GROUP I	R4
RFJ	FISSION REACTION RATE PER NEUTRON STREAMING INTO CELL IN GROUP J	R4
RFQ	FISSION REACTION RATE PER NEUTRON SLOWING DOWN INTO GROUP I	R4
VCEL	CELL VERSION NAME	C8

PILIB

1/8/74

RESONANCE REACTION RATES FOR ALL ISOTOPES IN REGION (2DREG?)

NAME - 'PILIB', 2DCEL?, 2VCEL?, 'ALLISO', 2DREG?, 'RATES'

LIST - IA, IB, (RCO(I), RFO(I), RCJ(I), RFJ(I), I=IA, IB)

SYMBOL	DEFINITION	TYPE
DCEL	CELL NAME	CR
DREG	REGION NAME IN CELL 2DCEL?	CR
IA	LOWEST GROUP INDEX FOR NON-ZERO DATA	I4
IB	HIGHEST GROUP INDEX FOR NON-ZERO DATA	I4
RCJ	CAPTURE REACTION RATE PER NEUTRON STREAMING INTO CELL IN GROUP J	R4
RCO	CAPTURE REACTION RATE PER NEUTRON SLOWING DOWN INTO GROUP I	R4
RFJ	FISSION REACTION RATE PER NEUTRON STREAMING INTO CELL IN GROUP J	R4
RFO	FISSION REACTION RATE PER NEUTRON SLOWING DOWN INTO GROUP I	R4
VCEL	CELL VERSION NAME	CR

APPENDIX C

MATHEMATICAL DETAILS OF FLUX AND COLLISION PROBABILITY CALCULATION

The method of solution for collision probabilities in HAMMER, HAMBUR, and CREEP and for total collision rates in RRR1D is based on the method of H. Markl²⁰. The cell is assumed to be a Wigner-Seitz cell consisting of N annular regions. Define the following terms:

V_n = Volume/unit axial length of region n (cm^3)

S_n = Outer surface area/unit axial length of region n (cm^2)

q_n = Average source density of neutrons in region n assumed to be uniform over the entire volume of region n . The total source in region n is then $Q_n = q_n V_n$.

$j_n^{+(-)}$ = Neutron current density through S_n in outward (+) and inward (-) direction, respectively. Total current across surface n is

$$J_n^{+(-)} = j_n^{+(-)} S_n$$

These quantities are diagrammed in Figure C-1.

Figure C-1

Markl shows that the total collision rate C in region n may be written as

$$C_n = Q_n W_n^{VV} + J_{n-1}^+ W_n^{iV} + J_n^- W_n^{oV} \quad (1-C)$$

where:

W_n^{VV} = Number of first collisions in region n due to one neutron born in region n .

W_n^{iV} = Number of neutrons having first collisions in region n due to one neutron entering region n through its inner surface.

W_n^{oV} = Number of neutrons having first collisions in region n due to one neutron entering region n through its outer surface.

Equation 1-C is based on the following assumptions:

- Cross sections, sources, and collision rates are spatially constant and isotropic over each region n .
- The distribution of neutrons crossing any surface S follow a cosine angular distribution. (Cosine-currents approximation.)

We define other W^{ij} quantities in analogy with the three defined above. Specifically we will use W_n^{Vi} , W_n^{Vo} , W_n^{iO} , W_n^{oO} , and W_n^{oo} where $i = S$ inner, $O = S$ outer, $V = S$ volume n . These quantities are related by reciprocity relations as follows:

$$\begin{aligned} W_n^{iV} &= \frac{4V_n}{S_{n-1}} \sum_{t_n} W_n^{Vi} & W_n^{oV} &= \frac{4V_n}{S_n} \sum_{t_n} W_n^{Vo} \\ W_n^{iO} &= 1 - W_n^{iV} & W_n^{oO} &= \frac{S_{n-1}}{S_n} W_n^{iO} \\ W_n^{oo} &= 1 - W_n^{oO} - W_n^{oV} & W_n^{VV} &= 1 - W_n^{Vi} - W_n^{Vo} \end{aligned} \quad (2-C)$$

Using these reciprocity relations Equation 1-C may be written

$$C_n = Q_n - Q_n W_n^{Vi} - Q_n W_n^{Vo} + J_{n-1}^+ (1 - W_n^{iO}) + J_n^- (1 - W_n^{oO} - W_n^{oo})$$

or

$$C_n = Q_n - (Q_n W_n^{Vo} + J_{n-1}^+ W_n^{iO} + J_n^- W_n^{oo}) - (Q_n W_n^{Vi} + J_n^- W_n^{oO}) + J_{n-1}^+ + J_n^-$$

We define now the currents J_n^+ and J_n^- as

$$J_n^+ = Q_n W_n^{v_0} + J_{n-1}^+ W_n^{i_0} + J_n^- W_n^{o_0} \quad (3-C)$$

$$J_{n-1}^- = Q_n W_n^{v_i} + J_n^- W_n^{o_i}$$

so that 1-C becomes

$$C_n = Q_n - J_n^+ - J_{n-1}^- + J_{n-1}^+ + J_n^- \quad (4-C)$$

It is these Equations (3-C) and (4-C) that are used to solve for the collision rate in all resonance capture treatments at Savannah River Laboratory. The Q_n are given, then Equations (3-C) are solved for the J_n^+ and J_n^- based on the specified boundary conditions. The method of solution is adapted from the work of A. Muller and E. Linnartz²¹. The W_n^{ij} are evaluated using Equations 2-C from the geometrical specification and cross section. Examination of Equations 3-C and 2-C shows the only W_n^{ij} that must be computed are $W_n^{v_0}$ and $W_n^{v_i}$, and these are computed by the method of J. M. Kennedy²².

The method of solution is altered according to the boundary conditions chosen. HAMMER, HAMBUR, and CREEP use reflecting boundary conditions at surface S_N . RRRID has an optional choice of reflecting boundary conditions or vacuum boundary conditions with J_N^- specified. These two cases will be treated separately.

Vacuum Boundary Conditions

In this case the Q_n ($n=1, 2, \dots, \infty$), and J_N^- are given. All W_n^{ij} are computed from Equations 2-C and the values of $W_n^{v_i}$ and $W_n^{v_0}$ (see below). Equations 3-C are used to evaluate the J_n^+ and J_n^- . This case is very simple as the second of Equations 3-C is solved successively for all values of the J_n^- .

Current J_1^+ is then computed from the boundary condition at the center of the cell

$$J_1^+ = Q_1 W_1^{v_0} + J_1^- W_1^{o_0} \quad (5-C)$$

The remaining J_n^+ are generated successively from the first of Equations (3-C).

Having solved for the J_n^+ and J_n^- ($n=1, 2, \dots, \infty$) Equation 4-C is used to generate the collision rate for each region due to sources Q_n and surface current J_N^- .

Reflecting Boundary Conditions

In this case the Q_n ($n=1,2,\dots,N$) are given, but the required surface current J_N^- is not known and must be evaluated from the outer boundary condition

$$J_N^- = \alpha J_N^+ \quad (6-C)$$

where α is an optional albedo factor. Equations 3-C are solved by generating two solutions $J_{n_0}^+$ and $J_{n_1}^+$ at two known values of J_N^- , specifically $J_{N_0}^- = 0$ and $J_{N_1}^- = 1$. This is done exactly as described for the vacuum boundary condition case. Equations 3-C are linear in the boundary current J_N^- so that we may write J_N^+ as a linear combination of $J_{N_0}^+$ and $J_{N_1}^+$ as

$$J_N^+ = J_{N_0}^+ + \frac{(J_{N_1}^+ - J_{N_0}^+)}{(J_{N_1}^- - J_{N_0}^-)} J_N^- \quad (7-C)$$

substituting 7-C into 6-C and solving for J_N^- yields

$$J_N^- = \frac{\alpha J_{N_0}^+}{1 - \alpha \frac{(J_{N_1}^+ - J_{N_0}^+)}{(J_{N_1}^- - J_{N_0}^-)}} \quad (8-C)$$

which is the correct surface current into the cell to satisfy Equation 6-C. The remaining J_n^+ are generated from

$$J_n^- = J_{n_0}^- + J_N^- \frac{(J_{n_1}^- - J_{n_0}^-)}{(J_{N_1}^- - J_{N_0}^-)} \quad (9-C)$$

$$J_n^+ = J_{n_0}^+ + J_N^- \frac{(J_{n_1}^+ - J_{n_0}^+)}{(J_{N_1}^- - J_{N_0}^-)}$$

Having solved for the J_n^+ ($n=1,2,\dots,N$), Equation 4-C is used to generate the collision rate for each region n from sources Q_n ($n=1,2,\dots,N$) and reflecting boundary conditions.

Generating Coefficients $W_n^{v_0}$ and $W_n^{v_i}$

The method used to generate the $W_n^{v_0}$ and $W_n^{v_i}$ is due to J. M. Kennedy²² and is accurate to 0.6% (relative) over all radii and mean free paths.

Let r_1 and r_2 be the inner and outer radii of an annulus and define

$$k = r_1 / r_2$$

$$x = (r_2 - r_1) \bar{\Sigma}_t$$

(10-C)

where $\bar{\Sigma}_t$ = total macroscopic cross section of region bounded by radii r_1 and r_2 .

Let $P(k, x) =$ inward escape probability $= W_n^{V_i}$

$Q(k, x) =$ outward escape probability $= V_n^{V_o}$.

The method of solving for P and Q is based on approximations to the two auxiliary functions

$$S = P + Q$$

$$G = \frac{1+k}{k} P$$

(11-C)

The method is obtaining accurate values for S and G at $k = 0$ and $k = 1$, then using suitably weighted interpolations to give approximate values at other k values.

The basic formulas at $k = 0$ and $k = 1$ are

$$S(0, x) = \frac{2}{3} \{ (2x^2 + 1) I_1(x) K_1(x) + 2x [(x K_0(x) + K_1(x)) I_2(x) - 1] - 1 \}$$

$$S(1, x) = \frac{1}{x} \left[\frac{1}{2} - E_3(x) \right]$$

$$G(0, x) = \frac{1}{x} \left[\frac{1}{2} - \frac{2}{\pi} K_3(x) \right]$$

$$G(1, x) = S(1, x)$$

(12-C)

The S function is interpolated by the formula

$$S(k, x) = \frac{(\bar{k} - L) S(0, x) + k S(1, x)}{1 - L}$$

(13-C)

where $\bar{k} = 1 - k$ and $L = \frac{k \bar{k} (6x - 3)}{2x + 1}$

Equation 13-C gives 0.3% relative accuracy for all k and x .

Interpolation in G is more complicated and is given by

$$G(k, x) = (1-\alpha)G(0, x) + \alpha G(1, x) \quad (14-C)$$

where:

$$\begin{aligned} \alpha &= k - (k-2)e^{-\lambda x} \\ \lambda &= 1.8 + \frac{0.3}{(1.01-k)(1+x)} \\ \lambda &= \frac{1}{\pi-2} \left\{ \frac{\sqrt{1-k^2} + \frac{\tan^{-1}k}{k} - \frac{\pi}{2}k}{1-k} - 2 \right\} \end{aligned} \quad (15-C)$$

and finally

$$W_n^{V_i} = P = \frac{k}{k+1} G(k, x) \quad \text{and} \quad W_n^{V_o} = Q = S(k, x) - P \quad \text{from Equation (11-C).}$$

APPENDIX D

CALCULATION OF $\psi(\theta, x)$ AND $\chi(\theta, x)$ RESONANCE LINE SHAPE FUNCTIONS

The resonance line shape functions used in computing Doppler broadened resonance cross sections are defined as

$$\psi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2} dy \quad (1-D)$$

$$\chi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2} 2y dy$$

where

$$\theta = \Gamma(4kTE_0/A)^{1/2} \quad \text{and} \quad x = 2(E-E_0)/\Gamma$$

An excellent discussion of the relative speeds and accuracies obtainable for evaluation of Equations 1-C is contained in Reference 15. The method used in module RRRID is a very rapid method based on contour integrals developed by Matta and Reichel¹⁴. This method involves the evaluation of a contour integral of the form $\int_{-\infty}^{\infty} f(t) e^{-t^2} dt$

by numerical integration. The integral is expanded into a series with a parameter h (and corresponding error estimate $E(h)$) which can be varied to achieve any desired accuracy. In addition to this series contribution, there are contributions due to poles (places where $f(t) \rightarrow \infty$) which depend upon whether θ is chosen inside, on, or outside the contour of integration.

The method of Matta and Reichel sets $t = 1/\theta^2$ and writes Equations 1-D in the form

$$\psi(t, x) = \frac{h}{\sqrt{\pi}(1+x^2)} + \frac{2h}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{e^{-n^2 h^2}}{(1+x^2+4tn^2 h^2)} + PP_1 - \frac{E(h)}{t} \quad (2-D)$$

$$\chi(t, h) = \frac{2hx}{\sqrt{\pi}(1+x^2)} + \frac{4hx}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{e^{-n^2 h^2}}{(1+x^2+4tn^2 h^2)^2 + 4x^2} - 2\left\{PQ_1 + \frac{x}{t} E(h)\right\}$$

where:

$$P = 0 \quad \text{for } \theta > \frac{2\pi}{h} \quad \text{or } t < \frac{h^2}{4\pi^2}$$

$$P = 1/2 \quad \text{for } \theta = \frac{2\pi}{h} \quad \text{or } t = \frac{h^2}{4\pi^2}$$

$$P = 1 \quad \text{for } \theta < \frac{2\pi}{h} \quad \text{or } t > \frac{h^2}{4\pi^2}$$

$$P_1 = \alpha \left(\frac{Ac - Bd}{c^2 + d^2} \right) \quad Q_1 = \alpha \left(\frac{Bc + Ad}{c^2 + d^2} \right)$$

$$\alpha = \sqrt{\frac{\pi}{t}} e^{-\left(\frac{x^2}{4t} + \frac{\pi}{h\sqrt{t}} - \frac{1}{4t}\right)}$$

$$A = \cos \frac{x}{2t} \quad B = \sin \frac{x}{2t}$$

$$C = e^{-\frac{\pi}{h\sqrt{t}}} - \cos \frac{\pi x}{h\sqrt{t}}$$

$$D = \sin \frac{\pi x}{h\sqrt{t}}$$

$$|E(h)| \leq \frac{e^{-\pi^2/h^2}}{2(1 - e^{-\pi^2/h^2})}$$

The routine used in RRR1D truncates the series in Equations 2-D at nine terms and uses $h = 0.75$. At the very worst this routine will provide four significant digits in $\psi(\theta, x)$ and one significant digit in $\chi(\theta, x)$. Over a very wide range the routine provides seven significant digits in $\psi(\theta, x)$ and four significant digits in $\chi(\theta, x)$. The error estimate $|E(h)|$ for this choice of parameters is $|E(h)| \leq 1.2 \times 10^{-8}$.

APPENDIX ECALCULATION OF FLUCTUATION INTEGRALS
FOR UNRESOLVED RESONANT CROSS SECTIONS

In Section 3.2.5.1.3 the statistical fluctuation integrals for evaluating the effects of the statistical distribution of resonance widths on the cross sections were introduced as

$$R_{n,t} = \int_0^\infty P(t|\mu_t) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{t^2}{(t\bar{\Gamma}_n + r\bar{\Gamma}_r + s\bar{\Gamma}_s + z\bar{\Gamma}_z)}$$

$$R_{r,t} = \int_0^\infty P(t|\mu_t) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{tr}{(t\bar{\Gamma}_n + r\bar{\Gamma}_r + s\bar{\Gamma}_s + z\bar{\Gamma}_z)} \quad (1-E)$$

$$R_{s,t} = \int_0^\infty P(t|\mu_t) dt \int_0^\infty P(r|\mu_r) dr \int_0^\infty P(s|\mu_s) ds \int_0^\infty P(z|\mu_z) dz \frac{ts}{(t\bar{\Gamma}_n + r\bar{\Gamma}_r + s\bar{\Gamma}_s + z\bar{\Gamma}_z)}$$

where: $t = \frac{\Gamma_n}{\bar{\Gamma}_n}$, $r = \frac{\Gamma_r}{\bar{\Gamma}_r}$, $s = \frac{\Gamma_s}{\bar{\Gamma}_s}$, $z = \frac{\Gamma_z}{\bar{\Gamma}_z}$

and $P(\chi^2/\mu)$ is the Porter-Thomas (chi-square) distribution with μ degrees of freedom defined as

$$P(\chi^2/\mu) = [2^{\mu/2} \Gamma(\frac{\mu}{2})]^{-1} \int_0^{\chi^2} y^{\frac{\mu}{2}-1} e^{-y/2} dy \quad (2-E)$$

The method used to evaluate Equations 1-E is that of Greebler and Hutchins¹⁷. In this method the width distributions are approximated by discrete widths, each representing a given fraction of the total distribution. Ten discrete widths are used to represent the distribution of each set of widths represented by variables t , r , s , and z . The discrete widths chosen are the values $\bar{\chi}^i$ for $i = 1, 2, \dots, 10$ corresponding to

$$\int_0^{\bar{x}^i} P(x|\mu) dx = 0.05, 0.15, 0.25, 0.35, 0.45, 0.55, 0.65, 0.75, 0.85, 0.95 \quad (3-E)$$

but normalized to give

$$\sum_{i=1}^{10} \bar{x}^i = 10 \quad (4-E)$$

Note also that in the limit of $\mu \rightarrow \infty$ (which is typical for Γ)

$$\lim_{\mu \rightarrow \infty} \int_0^{\infty} P(x|\mu) dx = 1 \quad (5-E)$$

hence these terms are easily evaluated.

With these approximations Equations 1-E can be reduced to

$$R_{n25} = \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} \sum_{l=1}^{N_l} \frac{\bar{t}^i \bar{r}^j}{(\bar{t}^i \bar{r}^j + \bar{r}^j \bar{r}^i + \bar{s}^k \bar{r}^j + \bar{z}^l \bar{r}^j)} (N_i N_j N_k N_l)$$

$$R_{r25} = \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} \sum_{l=1}^{N_l} \frac{\bar{t}^i \bar{r}^j}{(\bar{t}^i \bar{r}^j + \bar{r}^j \bar{r}^i + \bar{s}^k \bar{r}^j + \bar{z}^l \bar{r}^j)} (N_i N_j N_k N_l) \quad (6-E)$$

$$R_{f25} = \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \sum_{k=1}^{N_k} \sum_{l=1}^{N_l} \frac{\bar{t}^i \bar{s}^k}{(\bar{t}^i \bar{r}^j + \bar{r}^j \bar{r}^i + \bar{s}^k \bar{r}^j + \bar{z}^l \bar{r}^j)} (N_i N_j N_k N_l)$$

where the $\bar{t}^i, \bar{r}^j, \bar{s}^k$, and $\bar{z}^l$ depend upon the number of degrees of freedom through Equations 3-E, and the sum over i, j, k , or l is normally over 10 terms, but reduces to 1 term if the $\mu \rightarrow \infty$ for that width.

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