## MERIT Code Development for the Generation of Intermediate Resonance Parameters and Resonance Integral Tables

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#### 1. Introduction

Resonance treatment is the most important part in the deterministic transport lattice calculation. The conventional resonance treatment requires resonance integrals tabulated as a function of the background cross section ( $\sigma_h$ ) in advance. In the transport lattice calculation, a background cross section is estimated at first, and then the self-shielded resonance cross section can be obtained by looking up a resonance integral (RI) table. This RI table can be prepared by various methods, which include the Bondarenko method<sup>[1]</sup>, the homogeneous method and the heterogeneous method<sup>[2,3]</sup>. These methods are categorized by how to calculate the ultra fine group selfshielded fluxes. The third one is the best because it solves the slowing down equation in a heterogeneous geometry. P. H. Kier<sup>[2]</sup> at Argonne national laboratory developed the RABBLE code and F. Leszczynski<sup>[3]</sup> at CNEA in Argentina developed RMET21 for this purpose. One of the drawbacks in these codes is that they do not include a module to generate the corresponding  $\sigma_b$ 's.

A new transport lattice code LIBERTE has been developed which adopts a subgroup method for a resonance treatment. This subgroup method requires RI tables and intermediate resonance parameters<sup>[4]</sup> ( $\lambda$ ) generated by the heterogeneous method. Therefore, we have developed a new code MERIT (program for <u>Multiregional Effective Resonance Integral Table</u>) to generate RI tables and  $\lambda$ 's. This code includes a module to edit ultra fine group (> millions) cross sections with an equal lethargy width, a module to solve the slowing down equation in the homogeneous and 1-D cylindrical geometries by integral transport, a module to calculate the corresponding  $\sigma_b$ 's by the method of characteristics, and a module to calculate  $\lambda$ 's.

#### 2. Methods and Results

# 2.1 Slowing down calculation<sup>[2]</sup>

In order to obtain the effective resonance cross sections the self-shielded neutron spectra should be obtained by solving a slowing down equation. The MERIT code solves a slowing down equation in the homogeneous and heterogeneous 1-D cylindrical geometries by an integral transport. In the integral transport theory the integrated flux is

$$\phi_{ig} = \frac{C_{ig}}{\Sigma_{ig}},\tag{1}$$

where  $C_{ig}$  is the collision rate in region *i* for group *g* and  $\Sigma_{ig}$  the macroscopic total cross section. In this formulation, the collision rate is obtained from the expressions involving the slow-down sources, the first-flight escape and transmission probabilities, and the interface currents. The calculation of a regional slowing down is based on the assumption that neutrons are scattered elastically and isotropically.

The source for a region is

$$S_{g} = \sum_{j=1}^{J} \sum_{n=1}^{L_{j}} P_{nj} \Sigma_{s,g-n}^{j} \phi_{g-n} \Delta u_{f} , \qquad (2)$$

where  $P_{nj}$  is the probability per unit lethargy that a neutron is scattered down *n* groups in a scattering collision with material *j*,  $L_j$  is the maximum number of group through which a neutron can be down-scattered in a scattering collision with material *j*,  $\sum_{s,g-n}\phi_{g-n}$  is the reaction rate at which neutrons are scattered by material *j* in group *g*-*n*, and  $\Delta u_f$  is the lethargy width of a fine group.  $P_n$  is as follows:

$$P_n \Delta u_f = \frac{1}{1-\alpha} (1 - e^{-\Delta u_f})^2 e^{-(n-1)\Delta u_f}, \qquad (3)$$
$$\alpha = \left(\frac{A-1}{A+1}\right)^2,$$

where A is the atomic mass.

The next step is to calculate the collision rates. The collision rate in the homogeneous case is

$$C_i = S_i \,. \tag{4}$$

The collision rate in the 1-D cylindrical geometry is

$$C_{i} = \begin{cases} (1 - T_{i}^{OO})J_{i}^{-} + (1 - P_{i}^{+})S_{i}, & i = 1\\ (1 - T_{i}^{OI})J_{i-1}^{+} + (1 - T_{i}^{OO} - T_{i}^{IO})J_{i}^{-} + , & (5)\\ (1 - P_{i}^{+} - P_{i}^{-})S_{i}, & i = 2, I \end{cases}$$

where  $J_i$  is the cosine current,  $P_i$  is the escape probability, and  $T_i$  is the transmission probability. The effective microscopic resonance cross sections can be obtained by a flux volume weighting.

### 2.2 Hydrogen-equivalent parameter

Intermediate resonance parameter  $(\lambda)$  is also called a hydrogen-equivalent parameter which was introduced in the intermediate resonance approximation proposed by

Goldstein and Cohen<sup>[4]</sup>. This parameter is a probability that a neutron passes through a resonance.  $\lambda=1$  means a narrow resonance and  $\lambda=0$  the wide resonance. Resonance integrals are tabulated as a function of  $\sigma_b (\equiv \lambda \sigma_p)$  where  $\lambda$ is defined as 1 for hydrogen. For other nuclides,  $\lambda$  can be obtained by comparing solutions in U<sup>238</sup>/H mixtures with mixtures where the hydrogen was partly replaced by the other nuclides.

## 2.3 Background cross section

Resonance integrals are expressed as a function of  $\sigma_b$ . After an effective resonance cross section is obtained through the ultra fine group slowing down calculation, the corresponding  $\sigma_b$  should be obtained in the same geometry and composition by solving a broad group slowing down equation:

$$\hat{\Omega}_{m} \cdot \nabla \varphi_{mg}(\vec{r}) + \Sigma_{tg}(\vec{r}) \varphi_{mg}(\vec{r}) = \frac{1}{4\pi} \lambda_{g} \Sigma_{pg}, \qquad (6)$$

where  $\Sigma_{tg}$  and  $\Sigma_{pg}$  are total and potential cross section and  $\varphi_{mg}$  is a self-shielded angular flux. The corresponding  $\sigma_b$  is obtained as follows:

$$\Sigma_{bg}(\sigma_{ag}) = \frac{\Sigma_{ag}\phi_g}{1 - \phi_g}, \quad \sigma_{bg} = \Sigma_{bg} / N_R, \quad (7)$$

where  $\Sigma_{ag}$  is the absorption cross section,  $\phi_g$  is the selfshielded scalar flux and  $N_R$  is the particle number density of the representative resonant nuclide.

## 2.4 Calculation and results

Figures 1 and 2 show the comparisons of RI's from the MERIT calculations with RI's from the HELIOS<sup>[5]</sup> library for the 59<sup>th</sup> resonance group and  $\sigma_b$ =57.9 barn of U<sup>238</sup>. The overall trend is very similar, and the differences came from using different ENDF/B versions, which shows that the MERI code is working reasonably well. Hydrogen-equivalent parameters calculated from the RI tables are very consistent with the HELIOS ones for the resonant energy groups.

#### 3. Conclusion

We developed a new code MERIT to generate the hydrogen-equivalent parameters and the resonance integral tables. Results of the sample calculations showed that this MERIT code is working reasonably well. RI table and the hydrogen-equivalent parameters generated by the MERIT code will be used in the new library for LIBERTE<sup>[6]</sup>.



Figure 1.  $U^{238}$  resonance integral vs.  $\sigma_b$  in the 59<sup>th</sup> group



Figure 2. Group-wise  $U^{238}$  resonance integrals at  $\sigma_b$  =57.9 barn

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