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A new procedure to generate resonance integral table with an explicit resonance interference for transport lattice codes

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ABSTRACT

Resonance interference could not be considered explicitly in the conventional resonance treatment employing subgroup and direct resonance integral methods when using coarse energy group structure. This problem comes from the lack of information for the resonance shapes of resonant nuclides in the resonance interference formulas. As energy group boundaries get coarser, inaccuracy in estimating self-shielded cross sections with resonance interference gets bigger. A new method has been proposed to conserve the self-shielded cross sections for each group through an explicit consideration of resonance interference effect, which results in a good accuracy in predicting the multiplication factor. This method can be applicable to various mixing combinations of constituent resonant nuclides with resonance interference and can cover wide dilution range. The MERIT code has been used to generate resonance integral tables and to estimate resonance interference effects. And the 2-D transport lattice code KARMA has been used to perform sample calculations to see the effectiveness of the newly developed method. Sample calculations have been performed for single pins with various temperatures, ^{235}U enrichments and dilution levels with the 47 and 190 energy group structures. The computational results show that this method is able to estimate self-shielded cross sections in each coarse energy group accurately for various temperatures and various geometry and composition configurations.

1. Introduction

Typical neutron energy group structure for the thermal reactor fuels includes thermal, resonance and fast energy groups in which the energy group boundaries are about 1–2 eV for thermal and resonance groups, and about 10 keV for resonance and fast energy groups, respectively. Since 40–200 energy groups are used for the thermal reactor physics analysis because of the limitation on the computing capacity, it is almost impossible to consider the complicated resonance behavior precisely. Therefore, some special resonance treatment for the resonance energy groups is indispensable in the deterministic neutron transport lattice and whole-core calculations upon which the accuracy of transport codes are mainly dependent.

The conventional resonance treatment requires resonance integral (RI) tables in which resonance integrals are tabulated as a function of the background cross sections to be a measure of dilution. RI tables can be generated by performing slowing down calculations with point-wise cross sections defined on an ultra fine energy grid and then by obtaining the corresponding background cross sections. Slowing down calculation is performed to obtain the self-shielded cross section for coarse energy group by flux weighting for which the homogeneous or the heterogeneous pin configurations can be utilized. The corresponding background cross section can be obtained from the Dancoff factor (Leslie et al., 1965) calculation or the transport fixed source calculation with the intermediate resonance approximation (Goldstein and Cohen, 1962) and the equivalence theory (Stamm'ler and Abbate, 1983) between the homogeneous and the heterogeneous geometries. Various background cross sections can be achieved by using various compositional and geometrical configurations. In order to generate RI tables, slowing down equation is solved by assuming only one resonant nuclide with scattering and absorption cross sections for this nuclide and background nuclides with only potential cross sections. Resonance interference between resonance nuclides is not considered at this stage but at the transport calculation through the resonance interference formula. In the transport lattice calculation, the RI tables will be used in estimating the self-shielded cross sections for coarse energy groups in which the background cross sections are calculated from the Dancoff factor or the fixed source transport calculations. Sometimes RI tables are converted into subgroup data to be used in the physical subgroup method (Nikolaev, 1976). Subgroup data from RI table are also called physical probability table. Another method to generate probability table (subgroup data) is the mathematical probability table method (Coste and Mengelle, 1996) which is to employ the

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cross section moment conservation principle in the direct processing of point-wise cross sections. In this study only the physical probability table method is considered. In the subgroup method, resonances are divided by the subgroup levels and the corresponding probability for each subgroup level defined as a subgroup weight. Subgroup data can be generated from RI table through the least square fitting. In the HELIOS code (Stamm'ler et al., 1998) subgroup data were generated by assuming constant background cross sections regardless of subgroup levels. Recently a new method was proposed to generate subgroup data with conserving self-shielded cross sections. (Joo et al., 2009) In this study, Joo's method has been modified to generate subgroup data for more convenient and simple application.

In the subgroup method, resonance interference is considered not at the stage of generating RI table and subgroup data but at the use of subgroup data through the resonance interference iterations in which the formula for the self-shielded scalar flux is replaced with the formula for the interfered self-shielded scalar flux. Unfortunately the formula for resonance interference is not enough to consider resonance interference explicitly which results in some errors in estimating effective self-shielded cross sections. As energy group width for each resonance group becomes larger, error gets larger. In reality resonant nuclides include their own resonance shapes in a coarse energy group, in which resonance interference occurs complicatedly. The only way to resolve this problem is to increase the number of resonance energy groups sufficiently and to decide the group boundaries appropriately to consider resonance interference properly. However, due to the limited computing capacity even about 70 resonance energy group structure may be too much burden to the transport lattice and whole-core calculations. Therefore, some adjustments for RI table have been required. Adjustment for resonance integrals has been performed to have same fraction of epithermal-to-thermal reaction rates with the experimental results such as TRX-1 and TRX-2. (Askew, 1975; Decher, 1994) This adjustment has been applied to all the resonance integrals by the same amount. The authors applied this method to conserve total reaction rates for the whole resonance energy range to be close to those from the MCNP calculation. (Kim et al., 2009a) Joo proposed a new method to obtain relatively better self-shielded cross sections by adjusting the geometrical configuration and including resonance nuclides in advance. (Joo et al., 2009) However, his method could not give the self-shielded cross sections conserved for each energy group. And since adjustment was performed only for the specified mixture of ^{235}U and ^{238}U, error might be increased for other mixtures of two resonant nuclides. This problem comes from the imperfect resonance interference treatment in the subgroup method.

A new method to consider resonance interference explicitly has been proposed in this study. A perturbation term for resonance interference between two resonant nuclides is added to the conventional resonance integral which is dependent upon a fraction of one nuclide to the total.

The MERIT code (Kim et al., 2009a) was used to generate RI tables by solving the slowing down and the fixed source transport equations, and to estimate the resonance interference effects explicitly which are added to the conventional RI table. The SUBDATA code (Kim et al., 2009a) was used to generate subgroup data from RI table. In order to see the effectiveness for the proposed method the 2-D transport lattice code KARMA (Kim et al., 2009b) adopting the subgroup and the direct RI methods was used for sample calculations by incorporating the proposed method for an explicit resonance interference. The conventional method to generate RI table is introduced in Section 2. The subgroup method and the procedure to generate subgroup data are introduced in Section 3, and the conventional and new methods to consider resonance interference are also introduced in Section 3. In Section 4, the detailed description for sample calculations is included to show the effectiveness of the newly proposed method. Characteristics of resonance interference are shown, and the estimated self-shielded cross sections and the multiplication factors by KARMA are compared with the reference solutions.

2. Generation of resonance integral table

Typical energy range for the resolved resonance is 1.0 eV–10 keV. Since fission neutron energy is mostly higher than 10 keV, no fission source can be assumed. There is almost no inelstic scattering in the neutron energy range less than 10 keV. The scattering source in the transport equation can be simplified by assuming isotropic scattering, only elastic scattering (s-wave) and no up-scattering. (Duderstadt and Hamilton, 1976) The slowing down equation can be written as follows:

$$\hat{\Omega}\cdot\nabla\psi(\vec{r},u,\hat{\Omega})+\Sigma_t(\vec{r},u)\psi(\vec{r},u,\hat{\Omega}) = \int_{u-\ln(1/\alpha)}^{u}\frac{\Sigma_s(\vec{r},u')\phi(\vec{r},u')}{(1-\alpha)}e^{u'-u}du', \tag{1}$$

where $\alpha=[(A-1)/(A+1)]^2$, A denotes atomic mass, and u lethargy ($u=ln(E_0/E)$, $E_0=10$ MeV). When region k includes several nuclides, Eq. (1) can be rewritten for this region as follows:

$$\hat{\Omega}\cdot\nabla\psi_k(u,\hat{\Omega})+\sum_i\Sigma_{i,t}^k(u)\psi_k(u,\hat{\Omega}) = \sum_i\int_{u-\Delta_i}^{u}\Sigma_{i,s}^k(u')\phi_k(u')\frac{e^{u'-u}}{1-\alpha_i}du', \tag{2}$$

where

$$\begin{aligned}&\Sigma_{i,x}=N_i\sigma_{i,x},\\ &\Sigma_{i,s}^k(u)=\Sigma_{i,p}^k+\Sigma_{i,rs}^k(u),\\ &\Sigma_{i,t}^k(u)=\Sigma_{i,s}^k(u)+\Sigma_{i,ra}^k(u),\\ &\alpha_i=(A_i-1)^2/(A_i+1)^2,\\ &\Delta_i=-\ln(\alpha_i).\end{aligned} \tag{3}$$

In Eqs. (2) and (3), N_i is atomic number density of nuclide i, $\sigma_{i,x}$ and $\Sigma_{i,x}$ microscopic and macroscopic cross sections of reaction type x, respectively, $\Sigma_{i,p}(u)$ potential, $\Sigma_{i,rs}(u)$ resonance scattering, $\Sigma_{i,ra}(u)$ resonance absorption, $\Sigma_{i,t}(u)$ total cross sections. Δ_i is the maximum lethargy gain and $1-\alpha_i$ is the maximum fractional energy loss per collision with isotope i, respectively. The continuous scalar flux can be obtained by solving Eq. (2) using the point-wise cross sections. The effective self-shielded cross section of the resonance isotope for each coarse group can be obtained by using the following equation.

$$\sigma_{x,g}=\frac{\int_{\Delta u_g}\sigma_x(u)\phi(u)du}{\int_{\Delta u_g}\phi(u)du}. \tag{4}$$

Conventionally resonance integrals for the transport lattice codes are obtained with the following two assumptions for Eq. (2). (Leszczynski et al., 2007)

a. Only one resonant nuclide is assumed in the mixture with a constant potential scattering cross section (σ_p), a resonance scattering cross section ($\sigma_{rs}(u)$) and a resonance absorption cross section ($\sigma_{ra}(u)$).
b. Non-resonant nuclides are considered to have negligible absorption and constant potential scattering cross sections.

With the intermediate resonance approximation, Eq. (2) can be rewritten for the coarse energy groups.