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Predicting spatially dependent reaction rate for problem with nonuniform temperature distribution by subgroup method

Qingming He [a,b], Liangzhi Cao [a,*], Hongchun Wu [a], Benoit Forget [b], Kord Smith [b]

[a] Xi'an Jiaotong University, 28 Xianning West Road, Xi'an, Shaanxi 710049, China
[b] Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, United States

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ABSTRACT

The subgroup methods based on partial cross section fit scheme (PXSFS) and simplified partial cross section fit scheme (SPXSFS) are proposed in this paper to treat problems with non-uniform temperature distribution. These methods fit the cross sections at different temperatures as partial cross sections and share a same set of subgroup probabilities. The new methods are compared to the pre-existing methods: conventional subgroup method (CSM), the correlation model (CM), the subgroup level adjustment scheme (SLAS) and the number density adjustment scheme (NDAS). The numerical results show that the new methods can better predict the spatially dependent reaction rates than pre-existing methods. Within the new methods, the simplified scheme consumes less computation time and is more numerically stable. Additionally, the superhomogenization (SPH) correction method is studied, which is used to treat the multi-group (MG) equivalence effect. It is found that the subgroup-one-group (subgroup-1G) calculation can fully capture the MG equivalence effect.

1. Introduction

The subgroup method has long been used for self-shielding calculation in lattice codes for its geometrical adaptability and balance between precision and computational time (Nikolaev et al., 1970; Chiba and Unesaki, 2006; Hébert, 2009a; Li et al., 2015). Recently, the direct whole-core high-fidelity neutronics calculation codes, such as DeCART (Joo et al., 2004), nTRACER (Jung et al., 2013) and MPACT (Liu et al., 2013), were developed taking advantage of advancements in high performance computing. These codes all select the subgroup method to perform the self-shielding calculation step. One of the challenges newly encountered in the direct whole-core high-fidelity self-shielding calculation is how to obtain precise spatially dependent reaction rates within a pin cell. Many effects impact the spatially dependent reaction rate, such as the spatial self-shielding effect (Stoker and Weiss, 1996), the resonance interference effect (Williams, 1983; He et al., 2016), the non-uniform temperature distribution effect (Jung et al., 2016) and the multi-group (MG) equivalence effect (Hébert, 2009b). This paper focuses on the non-uniform temperature distribution effect and the MG equivalence effect.

Generally, the subgroup method divides an energy group into several subgroups according to the magnitude of the cross section (XS) rather than the energy. The ratio of the energy range of a subgroup to the energy range of an energy group is the subgroup probability and the average XS in a subgroup is the subgroup level, which are called the probability table in combination. There are two kinds of probability tables. The first one is the physical probability table which preserves the resonance integral (RI) (Halsall, 1995; Casal et al., 1991). Another is the mathematical probability table which preserves the XS moments (Cullen, 1974; Grimstone et al., 1990). Neither of these method is guaranteed to share the same set of subgroup probabilities for a resonant nuclide at different temperatures. This means that the subgroup fixed-source equation cannot be formulated based on the energy range of a subgroup as energy ranges for different temperatures are different. In this paper, the conventional subgroup method (CSM) refers to the subgroup method based on physical probability table.

Many schemes have been developed to overcome this defect: the correlation model (CM) (Nikolaev et al., 1970; Hébert, 2009a; Takeda and Kanayama, 1999), the subgroup level adjustment scheme (SLAS) (Joo et al., 2005) and the number density adjustment scheme (NDAS) (Jung et al., 2016; Wemple et al., 2007). The CM finds the overlap energy range of subgroups of one resonant nuclide at different temperatures. Then the probability table is redefined by the shared subgroup probabilities. The

* Corresponding author.
E-mail address: caolz@mail.xjtu.edu.cn (L. Cao).

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disadvantage is an increase in the number of subgroups with the increase in the number of temperatures. Therefore the computational time will increase accordingly. The SLAS forces subgroup probabilities at different temperatures to be same and then adjusts the subgroup levels by preserving the RI at infinite dilution. However, the RIs at other dilutions will not be preserved. The NDAS uses the probability table at average temperature for all temperatures and adjusts the number density accordingly. However, the assumption that the number density adjustment factor is the same for different subgroups is adopted, which will introduce errors in computation.

In this paper, the subgroup methods based on partial cross section fit scheme (PXSFS) and the simplified partial cross section fit scheme (SPXSFS) are proposed. These methods define partial XS at different temperatures with shared continuous-energy (CE) flux spectrum. The newly defined partial XS is an extension of the definition of partial XSs in the CSM (including total XS, absorption XS, scattering XS and neutron production XS). In the CSM, the subgroup probabilities are shared among different partial subgroup levels in the fitting procedure as the CE flux spectrum for MG condensation is shared among these partial XSs. In light of this, the subgroup probabilities can also be shared among partial XSs at different temperatures. The differences between PXSFS and SPXSFS will be discussed in Section 2. The new schemes are compared to the pre-existing schemes: CSM, CM, SLAS and NDAS. A simple pin cell problem is analyzed and the numerical results show that the new schemes can predict the spatially dependent reaction rates better than the pre-existing schemes.

Another important effect that impacts the spatially dependent reaction rates is the MG equivalence effect (Hébert, 2009b). The essence of the self-shielding calculation is to condense the CE XSs to MG XSs with problem-dependent flux spectrum. However, the reaction rates obtained by the MG calculation are not consistent with those obtained by the CE calculation even when the flux spectrum is correct, which is the MG equivalence effect. The super-homogenization (SPH) correction method (Hébert, 2005; Peng et al., 2013; Yamamoto et al., 2011; Sugimura and Yamamoto, 2007; Park and Joo, 2017) and discontinuity factor (DF) method (Smith, 1986; Sanchez, 2009), which is originally employed to capture the spatial homogenization effect can be used to treat the MG equivalence effect. The SPH correction method is adopted in this paper.

The rest of the paper is organized as follows. The theory of the pre-existing schemes, the new schemes and the SPH correction method will be given in Section 2. The numerical results will be given and analyzed in detail in Section 3. The conclusions will be given in the last Section.

2. Theory

2.1. Conventional subgroup method

There are different implementations of the subgroup method. The subgroup method can be classified according to how the probability tables are obtained. The physical probability table tries to preserve the RI table or XS table and the mathematical probability table tries to preserve the XS moments (Hébert, 2005). The physical probability table is preferred in this paper for that the mathematical probability table needs more energy groups to capture the slowing-down effect (Joo et al., 2009). The physical probability table can be classified into homogeneous table and heterogeneous table (Joo et al., 2009; Liu and Martin, 2016). The difference is that the homogeneous table tabulates XSs by solving homogeneous slowing-down equations with varying dilution XSs while the heterogeneous table tabulates XSs by solving heterogeneous slowing-down equations with varying pin cell properties (typically 1D cylindrical geometry). The homogeneous table is preferred for its simplicity. There are also several scattering models in the subgroup fixed-source equation. The scattering model based on the intermediate resonance (IR) approximation is adopted (Ishiguro and Takano, 1969).

In the resonance energy range (4.0 eV ~ 9118.0 eV in this paper), the neutron slowing-down is dominated by the elastic scattering and the CE neutron slowing-down equation can be written as:

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega},u)+\Sigma_{\mathrm{t}}(\mathbf{r},u)\psi(\mathbf{r},\mathbf{\Omega},u)=\frac{1}{4\pi}\int_0^{\infty}\Sigma_{\mathrm{s}}(\mathbf{r},u'\rightarrow u)\phi(\mathbf{r},u')\,\mathrm{d}u' \tag{1}$$

where $\mathbf{\Omega}$ is the angular variable; $\mathbf{r}$ is the coordinate in space; u is the lethargy; $\psi(\mathbf{r},\mathbf{\Omega},u)$ is the angular flux; $\phi(\mathbf{r},u)$ is the scalar flux; $\Sigma_{\mathrm{t}}(\mathbf{r},u)$ is the total XS; $\Sigma_{\mathrm{s}}(\mathbf{r},u'\rightarrow u)$ is the scattering kernel.

Based on the IR approximation, the neutron slowing-down equation can be simplified to:

$$\begin{aligned}&\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega},u)+\Sigma_{\mathrm{t}}(\mathbf{r},u)\psi(\mathbf{r},\mathbf{\Omega},u)\\&=\frac{1}{4\pi}\sum_k\left\{\lambda_k(u)\Sigma_{\mathrm{p},k}(\mathbf{r})+[1-\lambda_k(u)]\Sigma_{\mathrm{s},k}(\mathbf{r},u)\phi(\mathbf{r},u)\right\}\end{aligned} \tag{2}$$

where k is the nuclide index; $\lambda_k(u)$ is the Goldstein-Cohen (GC) factor (MacFarlane, 1999); $\Sigma_{\mathrm{p},k}(\mathbf{r})$ is the potential elastic scattering XS; $\Sigma_{\mathrm{s},k}(\mathbf{r},u)$ is the scattering XS;

As the treatment of the resonance interference effect is outside the scope of this paper, the following derivation is based on the assumption that there is only one resonant nuclide in the problem to be solved.

For an homogeneous system consisting of a resonant nuclide and the corresponding background nuclide of ^{1}H (the scattering XS is assumed to be 20 barns, the absorption XS is 0 barn and atomic weight ratio is identical to that of ^{1}H), the solution of Eq. (2) is:

$$\phi(u)=\frac{\sigma_{\mathrm{b}}(u)}{\sigma_{\mathrm{inter,res}}(u)+\sigma_{\mathrm{b}}(u)} \tag{3}$$

where $\sigma_{\mathrm{b}}(u)=\sigma_0+\lambda_{\mathrm{res}}(u)\sigma_{\mathrm{p,res}}$ is the background XS; $\sigma_0=N_{\mathrm{back}}\sigma_{\mathrm{p,back}}/N_{\mathrm{res}}$ is the dilution XS; $\sigma_{\mathrm{inter,res}}(u)=\sigma_{\mathrm{a,res}}(u)+\lambda_{\mathrm{res}}(u)\left[\sigma_{\mathrm{s,res}}(u)-\sigma_{\mathrm{p,res}}\right]$ is the intermediate XS.

The definition of the MG XS is:

$$\sigma_{x,\mathrm{res},g}(\mathbf{r})=\frac{\int_{\Delta u_g}\sigma_{x,\mathrm{res}}(u)\phi(\mathbf{r},u)\,\mathrm{d}u}{\int_{\Delta u_g}\phi(\mathbf{r},u)\,\mathrm{d}u} \tag{4}$$

where g is the energy group index; Δu_g is the lethargy range of energy group g.

For an homogeneous system, Eq. (3) is replaced in Eq. (4) to yield the following subgroup form:

$$\begin{aligned}\sigma_{x,\mathrm{res},g}(\sigma_{\mathrm{b},g})&=\frac{\sum_i\int_{\Delta u_{g,i}}\sigma_{x,\mathrm{res}}(u)\phi(u)\,\mathrm{d}u}{\sum_i\int_{\Delta u_{g,i}}\phi(u)\,\mathrm{d}u}\\&=\frac{\sum_i\sigma_{x,\mathrm{res},g,i}\phi_{g,i}}{\sum_i\phi_{g,i}}\\&=\frac{\sum_i\sigma_{x,\mathrm{res},g,i}\frac{p_{\mathrm{res},g,i}\sigma_{\mathrm{b},g}}{\sigma_{\mathrm{inter,res},g,i}+\sigma_{\mathrm{b},g}}}{\sum_i\frac{p_{\mathrm{res},g,i}\sigma_{\mathrm{b},g}}{\sigma_{\mathrm{inter,res},g,i}+\sigma_{\mathrm{b},g}}}\end{aligned} \tag{5}$$

where i is the subgroup index; x is the reaction type; $\sigma_{x,\mathrm{res},g}(\sigma_{\mathrm{b},g})$ is the MG XS as a function of background XS; $\Delta u_{g,i}$ is the lethargy range of subgroup; $\sigma_{x,\mathrm{res},g,i}$ is the subgroup level; $\phi_{g,i}$ is the subgroup flux; $p_{\mathrm{res},g,i}$ is the subgroup probability. The resonance XS table consists of MG XS over a range of background XSs. In this paper,