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Effect and treatment of angular dependency of multi-group total cross section and anisotropic scattering in fine-mesh transport calculation

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ABSTRACT

The whole core heterogeneous high-fidelity transport calculation is widely researched recently, where the spatial meshes reach sub-pin level to provide accurate results. In this context, two issues, namely angular dependency of total cross section and anisotropic scattering, which greatly affect the precision of multi-group transport calculation are assessed in this paper. Two pin cell problems respectively fueled with UO_2 and MOX are calculated. The numerical results show that neglecting angular dependency of total cross section leads to over-estimation of flux in resonance groups in fuel pellet and under-estimation of eigenvalue. Using angular-flux-weighted total cross sections can effectively reduce the error of flux in resonance groups. For UO_2 fuel pin cell, angular dependency of total cross section is more important than anisotropic scattering. While for MOX fuel pin cell, anisotropic scattering is more important. And then SPH method and a newly developed method called auxiliary term method are introduced and tested on UO_2 and MOX pin cell and 3×3 super cell with control rod. The numerical results show that both of these two methods are capable of capturing the effect of the angular dependency of total cross section. The accuracies of the methods are comparable.

1. Introduction

High accuracy and multi-physics coupling simulation are required for reactors design and analysis for higher safety and economy. In this context, the high-fidelity direct whole core neutronics calculation is being studied worldwide. In order to provide accurate results for the following thermal-hydraulics and fuel performance simulations, the meshes used in the neutronics calculation reach sub-pin level. Due to its high calculation efficiency, the deterministic method is widely used for high-fidelity calculation.

To reduce the computational burden, some important approximations are adopted in the deterministic method. The continuous variables i.e. space, angle and energy are treated by orthogonal polynomials or discretization methods. For the energy variable, the multi-group approximation divides the energy domain into a series of energy intervals which are called energy groups. Therefore, before performing the transport calculation, the continuous energy cross sections are condensed into multi-group format using flux-volume weight. Theoretically, the angular flux should be used as the weighting function to collapse the cross sections to preserve the reaction rate, as a result, the multi-group total cross sections become angular dependent (Bell and Glasstone, 1970). The angular flux is always replaced by the scalar flux in the process of condensation to avoid the angular dependent total cross sections, because it is not convenient to use the angular dependent total cross sections in the following transport calculation or diffusion calculation. This approximation will introduce significant impact on the accuracy of the transport calculation which greatly depends on accuracy of the multi-group cross sections. This limitation has been recognized for a long time (Bell and Glasstone, 1970). It is conventionally solved by consistent-P or transport correction method. The work by Won and Cho (2011) proved that the results of effective multiplication factor are significantly improved when the angular dependent total cross sections are directly applied in local/global iteration. In recent work by Gibson (2016), the issues caused by multi-group resonance cross sections condensed using scalar flux were noted, and two correction methods were analyzed to capture angular dependency, i.e. the SPH factor and transport correction methods. RecentlyPark and Joo (2017) analyzed the impact of neglecting the angular dependency of multi-group resonance cross sections, and proposed to use the parametrized region-wise spectral SPH factors to correct the scalar-flux-weighted total cross sections. The present work is carried out independently, and some comparable results are obtained. Besides, a new method adding

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an auxiliary term to the transport equation will be introduced to take account of the angular dependency of the total cross section in this paper. Numerical tests show that the latter can get more precise results than SPH method in some cases.

Moreover, multi-group scattering cross sections are dependent on angle because of the effect of anisotropic scattering. The effect of anisotropic scattering is very important, especially for the problems containing control rods or MOX fuel. In the deterministic method, scattering cross sections are usually expanded in Legendre polynomials. It's very time-consuming to perform high order calculation, so the transport equation is always solved by assuming the isotropic scattering. This approximation is mitigated by performing transport correction which was firstly derived by Bell et al. (1967), and simultaneously applied to take account of the angular dependency of total cross section. By using transport correction which assumes that the order of anisotropic scattering is L and makes $L+1$ order as zero, total and scattering cross sections are replaced by transport corrected ones. Now, the widely used transport correction methods include the consistent P_N, the outflow transport correction and the inflow transport correction. Choi et al. (2015) found that the inflow transport correction shows more accurate results than other methods from most of the verification problems.

The multi-group cross sections are fundamental issue for the transport calculation. In the conventional neutronics models such as assembly or pin homogenization technique, the above mentioned approximation can provide satisfied accuracy. However, it's more complex to generate accurate multi-group cross sections for the heterogeneous high-fidelity transport calculation. In this paper, we firstly revisit the multi-group theory, and discuss the treatment for the angular dependency of total cross section and effect of anisotropic scattering. And then the errors introduced by these two phenomena are quantified based on numerical analysis. Finally, the SPH method and a new correction method are proposed to capture the angular dependency of multi-group total cross section.

This paper is organized as follows. Section 2 describes the multi-group theory, SPH method and the new correction method. In Section 3, some problems are analyzed to show the effect of angular dependency of the total cross section and anisotropic scattering, and then SPH method and the new proposed method are tested. Some conclusions are given in the last section.

2. Theory and methodology

2.1. Multi-group approximation

The neutron interaction cross sections are very complicated functions of energy, so that enormous number of data points are required to represent energy dependent cross sections. In deterministic method, too many energy points heavily increase the computational burden. To reduce the burden, multi-group approximation is applied, where the energy domain is divided into a series of energy intervals which are called energy groups, and in each group flux and cross sections are all average values. The continuous energy eigenvalue problem of the neutron transport equation can be written as:

$$\begin{aligned}&\Omega\cdot\nabla\psi(r,\Omega,E)+\Sigma_t(r,E)\psi(r,\Omega,E)\\&=\frac{\chi(r,E)}{4\pi k}\int_0^\infty\int_{4\pi}\nu\Sigma_f(r,E')\psi(r,\Omega',E')\mathrm{d}\Omega'\mathrm{d}E'\\&\quad+\int_0^\infty\int_{4\pi}\Sigma_s(r,\Omega'\to\Omega,E'\to E)\psi(r,\Omega',E')\mathrm{d}\Omega'\mathrm{d}E'\end{aligned}\tag{1}$$

where $\psi(r,\Omega,E)$ is the neutron angular flux. $\chi(r,E)$ is the fission energy spectrum. k represents the eigenvalue. The total, fission production and scattering cross sections are represented by $\Sigma_t(r,E)$, $\nu\Sigma_f(r,E)$ and $\Sigma_s(r,\Omega'\to\Omega,E'\to E)$, respectively.

The multi-group form of the transport equation is attained by integrating Eq. (1) over the energies defining a group $[E_{g-1},E_g]$:

$$\begin{aligned}&\Omega\cdot\nabla\psi_g(r,\Omega)+\Sigma_{t,g}(r,\Omega)\psi_g(r,\Omega)\\&=\frac{\chi_g(r)}{4\pi k}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(r)\phi_{g'}(r)+\sum_{g'=1}^{G}\int_{4\pi}\Sigma_{s,g'\to g}(r,\Omega'\to\Omega)\psi_{g'}(r,\Omega')\end{aligned}\tag{2}$$

The multi-group angular flux $\psi_g(r,\Omega)$ and scalar flux $\phi_g(r)$ are defined as:

$$\psi_g(r,\Omega)=\int_{E_g}^{E_{g-1}}\psi(r,\Omega,E)\mathrm{d}E\tag{3}$$

$$\phi_g(r)=\int_{4\pi}\int_{E_g}^{E_{g-1}}\psi(r,\Omega,E)\mathrm{d}E\mathrm{d}\Omega\tag{4}$$

To get multi-group form, cross sections are condensed by flux-volume weight to preserve the reaction rates. The multi-group total, fission production and scattering cross sections and fission spectrum can be written as:

$$\Sigma_{t,g}(r,\Omega)=\frac{\int_{E_g}^{E_{g-1}}\Sigma_t(r,E)\psi(r,\Omega,E)\mathrm{d}E}{\int_{E_g}^{E_{g-1}}\psi(r,\Omega,E)\mathrm{d}E}\tag{5}$$

$$\begin{aligned}\nu\Sigma_{f,g'}(r)&=\frac{\int_{E_g}^{E_{g-1}}\int_{4\pi}\nu\Sigma_f(r,E')\psi(r,\Omega',E')\mathrm{d}\Omega'\mathrm{d}E'}{\int_{E_g}^{E_{g-1}}\int_{4\pi}\psi(r,\Omega',E')\mathrm{d}\Omega'\mathrm{d}E'}\\&=\frac{\int_{E_g}^{E_{g-1}}\nu\Sigma_f(r,E')\phi(r,E')\mathrm{d}E'}{\int_{E_g}^{E_{g-1}}\phi(r,E')\mathrm{d}E'}\end{aligned}\tag{6}$$

$$\begin{aligned}&\Sigma_{s,g'\to g}(r,\Omega'\to\Omega)\\&\quad=\frac{\int_{E_g}^{E_{g-1}}\int_{E_{g'}}^{E_{g'-1}}\Sigma_s(r,\Omega'\to\Omega,E'\to E)\psi(r,\Omega',E')\mathrm{d}E'\mathrm{d}E}{\int_{E_{g'}}^{E_{g'-1}}\psi(r,\Omega',E')\mathrm{d}E'}\end{aligned}\tag{7}$$

$$\chi_g(r)=\int_{E_g}^{E_{g-1}}\chi(r,E)\mathrm{d}E\tag{8}$$

It can be observed that the continuous energy total cross sections only rely on space and energy in Eq. (1), while after energy condensation, the multi-group form is also dependent on angle shown in Eq. (5). Because of the inconvenience to use angular dependent total cross sections in transport calculation or diffusion calculation, scalar flux instead of angular flux is used to collapse multi-group total cross sections. See as follows:

$$\begin{aligned}\Sigma_{t,g}(r,\Omega)\approx\Sigma_{t,g}(r)&=\frac{\int_{4\pi}\int_{E_g}^{E_{g-1}}\Sigma_t(r,E)\psi(r,\Omega,E)\mathrm{d}E\mathrm{d}\Omega}{\int_{4\pi}\int_{E_g}^{E_{g-1}}\psi(r,\Omega,E)\mathrm{d}E\mathrm{d}\Omega}\\&=\frac{\int_{E_g}^{E_{g-1}}\Sigma_t(r,E)\phi(r,E)\mathrm{d}E}{\int_{E_g}^{E_{g-1}}\phi(r,E)\mathrm{d}E}\end{aligned}\tag{9}$$

This treatment causes discrepancy between continuous energy and multi-group equation which will be discussed below.

To treat anisotropic scattering the multi-group scattering cross sections are usually expanded using Legendre polynomials:

$$\Sigma_{s,g'\to g}(r,\Omega'\to\Omega)=\sum_{n=0}^{N}\frac{2n+1}{4\pi}\Sigma_{s,n,g'\to g}(r)P_n(\Omega'\cdot\Omega)\tag{10}$$

As mentioned above, it's time-consuming to perform high order calculation, therefore, the transport correction method which is an isotropic approximation is widely used to treat anisotropic scatter-