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Cumulative migration method for computing rigorous diffusion coefficients and transport cross sections from Monte Carlo

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ABSTRACT

The cumulative migration method (CMM) for computing lattice-homogenized multi-group neutron diffusion coefficients and transport cross sections from Monte Carlo is proposed in this paper. CMM is demonstrated to be both rigorous and computationally efficient, while eliminating inaccuracies inherent in commonly-applied transport approximations. In the limit of a homogeneous hydrogen slab, the new method is shown to be equivalent to the long-used, and only-recently-published CASMO transport correction method employed for production LWR analysis. Results demonstrate that CMM can produce rigorous few-group assembly-homogenized diffusion coefficients directly from heterogeneous Monte Carlo lattice tallies—without requiring the intermediate step of tallying of fine-group cross section data commonly required for P_1 or B_1 calculations of diffusion coefficients. Comparisons with several common diffusion coefficient approximations are made for both simple homogeneous media and fully heterogeneous lattices. CMM is demonstrated to produce 2-group diffusion data for the BEAVRS PWR lattices, as well as 11-group directional-dependent diffusion coefficients for the TREAT graphite/fuel lattices. Core flux distributions and eigenvalues computed using CMM diffusion coefficients are demonstrated to be more accurate than those obtained with traditional methods for approximating diffusion coefficients.

1. Introduction

Many deterministic nuclear reactor calculations utilize transport-corrected-P_0 transport or diffusion theory to model neutron transport within fuel assemblies and adjoining reflecting regions. The accuracy of such core models is inherently tied to approximations made in obtaining multi-group transport cross sections or diffusion coefficients. While classic reactor physics textbooks (George et al., 1979; Lamarsh, 1966) offer insights and plausible arguments for computing transport cross sections and diffusion coefficients, there appears to be no rigorous theory for, nor quantification of errors introduced by, these approximations. Consequently, the computational accuracy of both heterogeneous (e.g. explicit fuel pin) and nodal (e.g. homogenized fuel assemblies) core calculations is often seriously compromised by inaccurate transport approximations, and little guidance is available in the literature to assist code developers and analysts in choosing the appropriate transport approximation.

1.1. Background

The generation of multi-group cross section data for LWR analysis usually starts by identifying some characteristic "lattice"—be it a pin-cell, a fuel assembly, or a collection of fuel assemblies. For each such lattice, a very-fine-group transport calculation (e.g., 50–10,000 groups) is performed to obtain the neutron flux and reaction rate distributions within the lattice. Unless this transport calculation explicitly models anisotropic scattering, an approximation for transport-corrected-P_0 cross sections for each nuclide must be introduced before the multi-group lattice transport calculation can be performed.

In addition, lattice reaction rates and fluxes are used to compute energy-condensed and/or spatially-homogenized transport cross sections (or diffusion coefficients) for use in downstream multi-group (e.g., 2–100 groups) core calculations. Here, additional approximations are required to compute the appropriate transport cross section that preserves some selected characteristic of the lattice calculation.

All production lattice physics codes (Newton and Hutton, 2002; Huria et al., 1994; Marleau et al., 1994; Villarino, 1992) make such approximations, often without substantial justification. Moreover, the most useful of these approximations are often considered to

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be proprietary, and the literature remains largely silent on useful methods. One example might be that of the transport-corrected-P_0 methods that have been employed in CASMO for more than 40 years. Only recently has Herman (Herman et al., 6052) published details of the method used in CASMO to generate transport-corrected-P_0 cross sections for ^{H} in LWR lattices. Herman was able to compute CASMO's "exact" transport cross section that matched continuous-energy Monte Carlo (MC) neutron leakages (integrated into 70 fine energy groups) for a slab of pure hydrogen. This transport correction is markedly different from that computed using the "micro-balance" argument (Stamm'ler and Abbate, 1983) which produces the classic "out-scatter" approximation—with its transport-to-total ratio of 1/3 for purely isotropic center-of-mass neutron scattering with ^{1}H in a free gas model. CASMO developers recognized long ago that this definition of transport cross section produced excellent eigenvalues for small LWR critical assemblies with large neutron leakages, while the classic out-scatter approximation produced errors in eigenvalue as large as 1000 pcm. In addition, SIMULATE-3 nodal code developers observed (more than 30 years ago) that the CASMO transport cross section also produced two-group diffusion coefficients that eliminated radial power tilts observed in large 4-loop PWR cores when using the out-scatter approximation.

1.2. Various deterministic approximation methods for transport cross sections

Many approximation methods for computing diffusion coefficients have been investigated in the past 40 years, among which the "out-scatter" approximation based on the "micro-balance" argument is probably the most often used one, assuming that the in-scatter rate of neutrons from energies E' to E will approximately balance the out-scatter rate of neutrons from E to all other energies (Stamm'ler and Abbate, 1983). The approximation can be represented as.

$$\int_0^\infty \Sigma_{s1}(\vec{r}, E' \to E)\vec{J}(\vec{r}, E')dE' \approx \int_0^\infty \Sigma_{s1}(\vec{r}, E \to E')\vec{J}(\vec{r}, E)dE' \tag{1}$$

in which $\Sigma_{s1}(\vec{r}, E' \to E)$ is P_1 scattering cross section from E' to E at $\vec{r}$, and $\vec{J}(\vec{r}, E')$ is the neutron current of energy E' at $\vec{r}$. Based on this approximation, the multi-group transport cross section can be derived to be the expression in Eq. (2).

$$\Sigma_{tr,g}^{os} = \Sigma_{t,g} - \overline{\mu}_g \Sigma_{s0,g} \tag{2}$$

In this equation, $\Sigma_{tr,g}^{os}$ is the transport cross section from the out-scatter approximation, $\Sigma_{t,g}$ is the total cross section, $\Sigma_{s0,g}$ is the P_0 scattering cross section, $\overline{\mu}_g$ is the average scattering cosine of the neutrons, and subscript g denotes the group index. The spatial dependence on $\vec{r}$ is omitted in most equations in this paper for clarity and generally all the terms refer to the same spatial position.

For neutron energies relevant to nuclear reactor physics, elastic scattering with ^{H} can be seen as approximately isotropic in the center-of-mass system, and $\overline{\mu}_g$ can be calculated to be 2/3 when thermal upscattering is not taken into account. This leads to a simple prescription for computing diffusion coefficients by taking $\overline{\mu}_g$ to be 2/3 for all groups, which produces

$$\Sigma_{tr,g}^{as} = \Sigma_{t,g} - \frac{2}{3}\Sigma_{s0,g} \tag{3}$$

in which $\Sigma_{tr,g}^{as}$ is the transport cross section from the "asymptotic" out-scatter approximation.

Another approximation makes the hypothesis that the neutron current cannot exceed the scalar flux and it uses the scalar flux spectrum instead of neutron current spectrum for weighting P_1 scattering cross sections (Pomraning, 1984). The transport cross section computed by this method as shown in Eq. (4) can be called "flux-limited" transport cross section.

$$\Sigma_{tr,g}^{fl} = \Sigma_{t,g} - \sum_{g'=1}^{G} \frac{\Sigma_{s1,g' \to g}\phi_{g'}}{\phi_g} \tag{4}$$

In Eq. (4) ϕ_g is scalar flux in group g and $\Sigma_{s1,g' \to g}$ is the P_1 cross section of scattering from group g' to group g.

Actually according to P_1 theory, the in-scatter can be treated exactly with given multi-group cross sections. In recent research on the transport correction for hydrogen (Herman, 2014), a 70-group library for ^{H} bound in water molecules was generated using NJOY (Macfarlane et al., 2000), including a 70-group P_0 and P_1 scattering matrix with the thermal scattering effect (using $s(\alpha, \beta)$ tables for light water molecules). Using the group data, the multi-group P_1 equations can be solved numerically to get the flux and current spectrum. Then the transport cross section can be computed directly following the definition as

$$\Sigma_{tr,g}^{in} = \Sigma_{t,g} - \sum_{g'=1}^{G} \frac{\Sigma_{s1,g' \to g}\vec{J}_{g'}}{\vec{J}_g} \tag{5}$$

in which $\Sigma_{tr,g}^{in}$ is the transport cross section with in-scatter calculated directly and the result of this method will be used as reference for comparison with other approximation methods.

2. Analytical derivation and numerical comparison of transport cross section ratio

2.1. Analytical derivation of transport cross section ratio

The analytical transport correction ratio for an isotope with atomic mass A can be derived in an infinite homogeneous medium with the assumption of only down scatter. In this case the diffusion coefficient can be derived from the second P_1 equation (Hebert, 2009), as shown in Eq. (6).

$$D(E) = \frac{1}{3\Sigma_t(E)}\left[1 + \frac{3}{\phi(E)}\int_E^{\frac{E}{\alpha}} \Sigma_{s1}(E' \to E)D(E')\phi(E')dE'\right] \tag{6}$$

In Eq. (6) $\alpha = (A-1)^2/(A+1)^2$. The differential P_1 scattering cross sections can be expressed as

$$\Sigma_{s1}(E' \to E) = \bar{\mu}\frac{\Sigma_t(E')}{(1-\alpha)E'} = \frac{2}{3A}\frac{\Sigma_t(E')}{(1-\alpha)E'}. \tag{7}$$

Through the relationship between diffusion coefficient and transport cross section $D = 1/(3\Sigma_{tr})$, Eq. (6) can be re-written as

$$\frac{1}{3\Sigma_{tr}(E)} = \frac{1}{3\Sigma_t(E)}\left[1 + \frac{3}{\phi(E)}\int_E^{\frac{E}{\alpha}} \frac{2}{3A}\frac{\Sigma_t(E')}{(1-\alpha)E'}\frac{1}{3\Sigma_{tr}(E')}\phi(E')dE'\right] \tag{8}$$

The transport correction ratio is defined as $f(E) = \frac{\Sigma_{tr}(E)}{\Sigma_t(E)}$. The ratio can be derived by rearranging Eq. (8).

$$f(E) = \left[1 + \frac{2}{3A(1-\alpha)\phi(E)}\int_E^{\frac{E}{\alpha}} \frac{\phi(E')}{f(E')E'}dE'\right]^{-1} \tag{9}$$

According to slowing down theory, flux density at energy E can be approximated as

$$\phi(E) = \int_E^\infty \frac{\chi(E')}{\xi\Sigma_s(E)E}dE' \tag{10}$$

in which $\chi(E')$ is the source density at energy E' from Watt fission spectrum, and $\xi = 1 + \frac{\alpha}{(1-\alpha)\ln(\alpha)}$. Under the approximation, Eq. (10) holds for $A = 1$, but for $A > 1$ it doesn't take the Placzek transient