Annals of Nuclear Energy 90 (2016) 353–363

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

A comparative study of leakage and diffusion coefficient models for few-group cross section generation with the Monte Carlo method

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ARTICLE INFO

Article history:
Received 23 October 2015
Received in revised form 16 December 2015
Accepted 20 December 2015
Available online 31 December 2015

Keywords:
Serpent
Monte Carlo
Neutron leakage
CANDU
Directional diffusion coefficient

ABSTRACT

The quality of few-group cross section data generated for core diffusion solvers depends on the treatment of the neutron leakage at lattice level. In this work, we propose a study about the relative performance of three assembly leakage models in the Monte Carlo code Serpent. Additionally, the extension of a novel method for the generation of directional diffusion coefficients to different reactor types is studied. Using Monte Carlo full core results as reference values, leakage and diffusion coefficient models are contrasted in terms of system eigenvalue and power distributions in a simplified heavy-water-moderated reactor system. Heterogeneous leakage models yielded the best results. Standard diffusion coefficients showed the best performance, due to difficulties arising from the volume-averaging of directional diffusion coefficients in cluster geometry. The results of this work suggest that the generation of directional diffusion coefficients could be extended to graphite-moderated gas-cooled reactors.

1. Introduction

Monte Carlo (MC) neutron transport codes are increasingly used in nuclear engineering studies. The Monte Carlo method makes use of the best available interaction models with very few approximations. The treatment of arbitrary geometries confers a great versatility which, combined with the use of continuous energy cross section (XS) data and parallelization techniques, allows the calculation of reference solutions for various applications.

In the field of reactor physics, large heterogeneous systems need to be calculated with sufficient accuracy in a reasonable time. In order to attain this target, a two-step calculation procedure is often adopted. The first step involves a solution of the neutron transport problem in a sub-domain of the original system, generally limited to periodic or reflective boundary conditions (BCs). As a result, homogenized XS data is obtained. This data is then used in the second step, i.e., the core level solver, generally based on few-group diffusion theory.

The Monte Carlo method has been gaining more relevance in the calculation of homogenized XS constants, a field typically dominated by deterministic methods. Examples of the application of the 2-step approach with Monte Carlo techniques at cell level may be found in Park et al. (2012), Ilas and Rahnema (2003), Rachamin et al. (2013), and Leppänen et al. (2014).

The adoption of the 2-step approach is not free from drawbacks. At cell level, zero-net-leakage boundary conditions are approximate and imply that volume-averaged scalar fluxes calculated at cell and core level will, in the general case, not match. Smith (1986) highlights that the definition of a homogenized diffusion coefficient constitutes the most inaccurate approximation frequently made. He introduces additional degrees of freedom in the homogenized diffusion equation by relaxing the continuity of scalar flux at assembly interfaces. To that end, Smith introduces the concept of *discontinuity factors* (DFs).

Previous work (Fridman et al., 2013; Leppänen et al., 2014) has been conducted in connection with the computation of discontinuity factors with the Monte Carlo code Serpent (Leppänen, 2007). Additionally, a recent work compared the performance of a new directional diffusion coefficient model with that of discontinuity factors (Dorval, 2016).

Pertaining the use of zero-net-leakage boundary conditions at cell level, there are different models (Park et al., 2012; Martin and Hébert, 2011; Fridman and Leppänen, 2011; Yun and Cho, 2010) to account for neutron leakage in the framework of Monte Carlo XS generation. In particular, we would like to test the performance of a recently proposed method (Dorval, 2016).

The aim of this work is twofold: to compare different leakage models on a simplified reactor problem following a MC plus diffusion 2-step scheme, as well as to study the relative performance of standard (isotropic) and directional diffusion coefficients. Prior to

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http://dx.doi.org/10.1016/j.anucene.2015.12.021
0306-4549/

this, it is necessary to extend the directional diffusion coefficient model to other reactor types.

The rest of this article is structured as follows: Section 2 provides preliminary concepts and references to the methods studied in this work, whilst Section 3 presents the main results and discusses their significance. Finally, the conclusions are collected in Section 4. Appendix A provides support for some of the findings of Section 3.

2. Methods

2.1. Diffusion coefficients in the Serpent code

The detailed derivation of the anisotropic diffusion coefficient calculation method to be studied in this work may be found in Dorval and Leppänen (2015). This Monte Carlo-specific methodology is based on the computation of a special score upon surface crossings. When a neutron crosses a specific plane, denoted by $\mathcal{S}$, a neutron-current-weighted estimate of the transport cross section is tallied. This estimate is expressed as follows:

$$\langle \Sigma_{tr} \rangle|_{\mathbb{J}} = (1-m)\frac{\alpha}{\langle D_n \rangle} + m\langle \Sigma_t \rangle|_{\mathbb{J}} - \overline{\mu}_0 \langle \Sigma_s \rangle|_{\mathbb{J}}, \quad 0 \leqslant m \leqslant 1, \tag{1}$$

where the subscript $\mathbb{J}$ stands for neutron-current-weighted quantities. $\langle \Sigma_{tr} \rangle$ is the transport XS estimate; $\overline{\mu}_0$ is the average scattering cosine in the laboratory system, extended over the cell; m is an interpolation constant; and $\langle \Sigma_t \rangle|_{\mathbb{J}}$ and $\langle \Sigma_s \rangle|_{\mathbb{J}}$ are the total and scattering macroscopic cross sections, respectively. The latter quantities are weighted with the total neutron current.

Whenever a neutron crosses the surface $\mathcal{S}$, the total and scattering cross sections at the crossing point are retrieved, as well as the neutron weight. If we denote every such surface crossing event by the index i, then the surface-averaged XSs are computed as:

$$\langle \Sigma_{\{t,s\}} \rangle|_{\mathbb{J}} = \frac{\sum_i (\Sigma_{\{t,s\}} w_i)}{\sum_i w_i} \tag{2}$$

The sense in which neutrons traverse the surface $\mathcal{S}$ is not taken into account in Eq. (2). The directional dependence of the averaged cross sections is implicit in the choice of $\mathcal{S}$.

In Eq. (1), the hard-coded constant α is needed for normalization purposes. Its complete derivation may be found in Dorval (2013). Based on the assumptions of an infinite homogeneous medium and isotropic angular flux, the constant α is expressed in terms of the Exponential Integral function Ei (Harris, 1957), through:

$$\alpha = 2e^2\,\mathrm{Ei}(-2) + 1 \simeq 0.2773427662 \tag{3}$$

In Eq. (1), $\langle D_n \rangle$ is the total-current-weighted average of the score:

$$D_n = \frac{R}{2 + R\Sigma_t|_R}, \tag{4}$$

where R is the distance between the last source or collision point and the crossing position on $\mathcal{S}$. $\Sigma_t|_R$ is the total XS evaluated at that crossing point. Once the transport cross section is determined, the directional diffusion coefficient is calculated through:

$$D_{\mathbb{J}} = \frac{1}{3\langle \Sigma_{tr} \rangle|_{\mathbb{J}}} \tag{5}$$

In Eq. (5), the transport cross section is a scalar quantity which depends on the surface under scrutiny. By setting up surfaces along three orthogonal directions, an equal number of equations arises, and a directional diffusion coefficient component for every direction is determined. In Eqs. (1), (4), and (5), energy group indexes have been omitted in order to ease the syntax. Detailed information on the treatment of the energy variable is reported in Dorval (2016).

In the same article, an extension of the original methodology to the treatment of multiple parallel surfaces per direction is also presented. Such extension is aimed at obtaining volume-averaged anisotropic diffusion coefficients per direction. The situation is sketched in Fig. 1. There, we introduce a superimposed regular Cartesian mesh in order to score surface crossings per direction in different locations.

With regards to standard diffusion coefficients, Fridman et al. (2013) describe how these are calculated in the Serpent code, whereas the work by Fridman and Leppänen (2011) deals with the implementation of the B_1 critical spectrum corrections and associated diffusion coefficients in Serpent.

2.2. Assembly leakage models in Monte Carlo

In this work, only three different methods for the treatment of neutron leakage will be dealt with. These methods are used in order to correct neutron spectra and associated few-group XS data when the calculation domain has reflective or periodic boundary conditions.

The first method is based on the solution of the B_1 equations (Stamm'ler and Abbate, 1983). The second one is based on the albedo search proposed by Yun and Cho (2010). Both methods are implemented in the Serpent code from version 2.1.16 onwards.

The third method is the layer-expansion leakage model, which has been recently proposed (Dorval, 2016) as an alternative to albedo search iterations. In the layer-expansion method, special indexes are updated when a neutron reaches a periodic or reflective boundary. These indexes provide information about the location of the neutron in a fictitious homologous system where the boundary condition is replaced by an identical lattice element.

After some initial iterations, it is possible to modify the neutrons' weight at particular locations in this homologous system until the eigenvalue reaches a pre-defined target value. The main advantages of this method are that leakage is treated in a heterogeneous configuration (as in the albedo method) and that the expanded system does not need to be explicitly represented and stored in the computer memory. For further details and preliminary tests, the reader is referred to Dorval (2016).

The methods described so far are usually applied to single assemblies. In the work by Leppänen et al. (2014), cross sections and leakage-corrected discontinuity factors generation through colorsets was shown to be an accurate approach for the study of a complex heterogeneous reactor involving UO_2 fuel assemblies. We do not intend to incur in such an extent of complexity in this work, given that our aim is to conduct a comparative study.

3. Results and discussion

3.1. Determination of interpolation constants

In our previous work (Dorval and Leppänen, 2015), the interpolation constant m in Eq. (1) was adjusted in a sodium-cooled fast reactor (SFR) environment. Here, we perform scoping one-dimensional (1-D) calculations in order to adjust m in other types of reactor fuel assemblies.

The adjustment of m is carried out by optimizing the eigenvalue agreement between Monte Carlo and diffusion results. MC techniques are applied to 1-D axial problems, from which system eigenvalues are obtained, and homogenized few-group XS constants are generated. These constants are then fed to a diffusion solver, and the eigenvalues are compared. The differences in eigen-