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Diffusion coefficients for LMFBR cells calculated with MOC and Monte Carlo methods

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ABSTRACT

The present work discusses the calculation of the diffusion coefficient of a lattice of hexagonal cells, with both "sodium present" and "sodium absent" conditions. Calculations are performed in the framework of lattice theory (also known as fundamental mode approximation). Unlike the classical approaches, our heterogeneous leakage model allows the calculation of diffusion coefficients under all conditions, even if planar voids are present in the lattice. Equations resulting from this model are solved using the method of characteristics (MOC). Independent confirmation of the MOC result comes from Monte Carlo calculations, in which the diffusion coefficient is obtained without any of the assumptions of lattice theory. It is shown by comparison to the Monte Carlo results that the MOC solution yields correct values of the diffusion coefficient under all conditions, even in cases where the classic calculation of the diffusion coefficient fails. This work is a first step in the development of a robust method to calculate the diffusion coefficient of lattice cells. Adoption into production codes will require more development and validation of the method.

1. Introduction

Since the sodium void reactivity worth (SVRW) is one of the most important neutronic parameters of fast reactors with respect to safety, the accurate prediction of SVRW is required to carry out core design studies efficiently. Sodium voiding changes the core reactivity (criticality) through an increase of neutron leakage and a shift of the neutron energy spectrum. Both these phenomena should be taken into account properly for the accurate prediction of SVRW.

A fast reactor fuel subassembly consists of a cluster of fuel pins with cladding, which is surrounded by a hexagonal wrapper tube. Since the exact representation of such a complicated system is unrealistic in numerical calculations for a whole core, homogenization procedures have been widely and effectively used. This homogenization is usually performed on the basis of a unit lattice cell using reflective or periodic boundary conditions, while neutron leakage from the lattice is taken into account by the buckling concept. The lattice-averaged diffusion coefficient is an important parameter since it is used in core design calculations based on diffusion theory. Furthermore, the directional diffusion coefficient is beneficial to estimate the magnitude of anisotropic neutron streaming effects due to the heterogeneous configuration of the unit lattice.

In order to define the diffusion coefficient, many important studies have been carried out in the past and several definitions of diffusion coefficients have been proposed (Deniz, 1986). Among these, Benoist's classical diffusion coefficients are utilized in lattice codes for fast reactors, and can be calculated by codes such as ECCO (Rimpault, 1997) and SLAROM-UF (Hazama et al., 2009), because they are relatively simple to implement into numerical calculation tools. However, Benoist's definition has a drawback, which is well-known, namely the "divergence" of the diffusion coefficient in the case of a lattice containing planar voids (a planar void is a void region of such a shape that a slab of infinite lateral dimensions and a finite thickness can be contained in it (Gelbard, 1983)). Hence, approximations are used in the application of Benoist's classical theory to such a system, such as the introduction of a fictitious cross section into the void regions corresponding to the buckling or smearing surrounding structural materials into the void regions.

Remedies for the divergence problem have been also proposed in earlier work. The work done by Grimstone (1980), which uses the theory originally proposed by Brissenden and Green (1973), is straightforward and is founded on the same theoretical basis as Benoist's theory. In the work of Grimstone, the lattice flux functions are calculated using one-dimensional S_n theory rather than collision probabilities. The method was not applied to a hexagonal fast reactor pin cell directly. Rather, Grimstone applied it to a cylindrical cell model which can be treated by a one-dimensional discrete ordinates method.

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In the present study, we apply a similar procedure as Grimstone to a rigorous fast reactor pin cell model of hexagonal geometry with the help of the method of characteristics (MOC). MOC is chosen as a solution strategy because the calculation of the diffusion coefficient under void conditions requires a solution with angular resolution of the transport equation, as will be illustrated later. Furthermore, MOC has the potential to handle highly complex geometries. We will obtain diffusion coefficients defined by Grimstone's procedure and Benoist's classical theory, and quantify the accuracy of Benoist's classical procedures in a realistic fast reactor lattice model. Through this numerical study, we will quantify errors induced by the divergence problem, and also determine the dependence of the diffusion coefficient on the buckling value which is ignored in Benoist's classical theory. In addition, in order to assess our numerical procedure for diffusion coefficient calculations with MOC, an independent calculation with a Monte Carlo method is employed to obtain diffusion coefficients. A comparison between deterministic-based and Monte Carlo-based diffusion coefficients will be carried out as well. This work is a first step in the development of a robust method to calculate the diffusion coefficient of lattice cells without or with voided regions.

2. Definition of the diffusion coefficient in lattice theory

The work presented in this paper is based on classic lattice theory, also known as the *fundamental mode approximation*. The system under investigation is assumed to be a finite lattice, made up of repeating unit cells. In the present work, the unit cells are assumed to be symmetric, and the unit cells could themselves be comprised of a cluster of smaller cells. A three-dimensional system is considered, described by variables for spatial position $\boldsymbol{r}$, neutron energy E and direction of propagation $\boldsymbol{\Omega}$. The problem is treated for the critical eigenvalue of the lattice.

In the finite lattice, the flux has a gross asymptotic curvature which is the same for all neutron energies and directions of propagation. The curvature is represented by the buckling vector $\boldsymbol{B}$, the square of whose length is the geometric buckling B^2. To analyze the finite lattice, it is assumed to extend to infinity (so-called image piles approximation). This removes any transient effects due to boundaries, and the solution becomes the deep-interior asymptotic solution. Thus, the flux is assumed to be described by the real part of a complex lattice flux:

$$\begin{aligned}\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) &= \mathrm{Re}\{f_B(\boldsymbol{r},E,\boldsymbol{\Omega})\exp(i\boldsymbol{B}\cdot\boldsymbol{r})\}\\ f_B(\boldsymbol{r},E,\boldsymbol{\Omega}) &= g_B(\boldsymbol{r},E,\boldsymbol{\Omega}) + ih_B(\boldsymbol{r},E,\boldsymbol{\Omega})\end{aligned} \tag{1}$$

The function f_B describes the intra-cell variation of the flux, with g_B and h_B periodic with the cell. The exponential term, whose real part is $\cos(\boldsymbol{B}\cdot\boldsymbol{r})$, describes the gross curvature of the flux in the lattice. This flux shape corresponds to a slab reactor with its boundaries oriented perpendicular to the direction of $\boldsymbol{B}$, and the width of which is given by $a^2 = \pi^2/B^2$, where $B^2 = \|\boldsymbol{B}\|^2$. The philosophical considerations which lead to this factorization of the lattice flux will not be discussed here. Deniz gives some indications for the validity of the factorization in Deniz (1986). By contrast, Gelbard (1983) seems to state that the choice is more based on physical intuition and expendiency of analysis. Furthermore, Deniz (1986) states that the unit cells can be asymmetric. Again, Gelbard and Lell (1977) claims the opposite, and provides a simple example of a finite lattice of asymetric cells and shows that the resulting macroscopic flux shape is not a cosine. In the present work, which focuses on fast reactors, the assumption of a symmetric unit cell seems to be justified, and the flux factorization of Eq. (1) is assumed valid. Taking the real part of Eq. (1), the lattice flux is given as:

$$\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) = g_B(\boldsymbol{r},E,\boldsymbol{\Omega})\cos(\boldsymbol{B}\cdot\boldsymbol{r}) - h_B(\boldsymbol{r},E,\boldsymbol{\Omega})\sin(\boldsymbol{B}\cdot\boldsymbol{r}) \tag{2}$$

2.1. Properties of the lattice flux functions

Assume that the point $\boldsymbol{r} = 0$ corresponds to a symmetry point of the lattice. Any position $\boldsymbol{r}$ can be written as $\boldsymbol{r} = n^{*}\boldsymbol{r_c} + \boldsymbol{r}'$, with n an integer, $\boldsymbol{r}_c$ the lattice offset vector, and $\boldsymbol{r}'$ measured in the coordinate frame of a unit cell. The lattice functions g_B and h_B are periodic with the lattice. They are the same for each unit cell, and therefore they can be defined uniquely in the coordinate system of the unit cell $\boldsymbol{r}'$. In other words:

$$\begin{aligned}g_B &= g_B(\boldsymbol{r}',E,\boldsymbol{\Omega})\\ h_B &= h_B(\boldsymbol{r}',E,\boldsymbol{\Omega})\end{aligned} \tag{3}$$

Whether the system is finite or infinite in size, symmetry implies that $\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) = \Psi_B(-\boldsymbol{r},E,-\boldsymbol{\Omega})$, as long as $\boldsymbol{r} = 0$ is chosen to be a symmetry point of the lattice. Furthermore, it assumes that the materials are isotropic for neutron movement (see note in Appendix B). Thus, for a lattice of symmetric unit cells, we expect that the flux Ψ_B is even in $\boldsymbol{r}$ and $\boldsymbol{\Omega}$. The symmetry property of the lattice flux thus implies:

$$\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) = g_B(\boldsymbol{r}',E,\boldsymbol{\Omega})\cos(\boldsymbol{B}\cdot\boldsymbol{r}) - h_B(\boldsymbol{r}',E,\boldsymbol{\Omega})\sin(\boldsymbol{B}\cdot\boldsymbol{r}) \tag{4}$$

$$\begin{aligned}\Psi_B(-\boldsymbol{r},E,-\boldsymbol{\Omega}) &= g_B(-\boldsymbol{r}',E,-\boldsymbol{\Omega})\cos(-\boldsymbol{B}\cdot\boldsymbol{r}) - h_B(-\boldsymbol{r}',E,-\boldsymbol{\Omega})\sin(-\boldsymbol{B}\cdot\boldsymbol{r})\\ &= g_B(-\boldsymbol{r}',E,-\boldsymbol{\Omega})\cos(\boldsymbol{B}\cdot\boldsymbol{r}) + h_B(-\boldsymbol{r}',E,-\boldsymbol{\Omega})\sin(\boldsymbol{B}\cdot\boldsymbol{r})\end{aligned} \tag{5}$$

and thus for symmetric unit cells g_B is even in $\boldsymbol{r}$ and $\boldsymbol{\Omega}$, and h_B is odd in $\boldsymbol{r}$ and $\boldsymbol{\Omega}$. As shown in Deniz (1986), the function g_B is also even in $\boldsymbol{B}$, and h_B is odd in $\boldsymbol{B}$.

2.2. Transport equation for the lattice flux functions

We start off by introducing several operators:

$$L\Psi_B \equiv \nabla\cdot\boldsymbol{\Omega}\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) \tag{6}$$

$$\Sigma_t\Psi_B \equiv \Sigma_t(\boldsymbol{r},E)\Psi_B(\boldsymbol{r},E,\boldsymbol{\Omega}) \tag{7}$$

$$S_{in}\Psi_B \equiv \int_0^\infty dE'\int_{4\pi} d\boldsymbol{\Omega}'\Sigma_s(\boldsymbol{r},E'\to E,\boldsymbol{\Omega}'\to\boldsymbol{\Omega})\Psi_B(\boldsymbol{r},E',\boldsymbol{\Omega}') \tag{8}$$

$$S_f\Psi_B \equiv \int_0^\infty dE'\int_{4\pi} d\boldsymbol{\Omega}'\frac{\chi(E)}{4\pi}\nu\Sigma_f(\boldsymbol{r},E')\Psi_B(\boldsymbol{r},E',\boldsymbol{\Omega}') \tag{9}$$

The transport equation for the critical eigenvalue then becomes, upon substitution of the lattice flux:

$$\exp(i\boldsymbol{B}\cdot\boldsymbol{r})\left[\left(L + i\boldsymbol{\Omega}\cdot\boldsymbol{B} + \Sigma_t - S_{in} - \frac{1}{k}S_f\right)f_B\right] = 0 \tag{10}$$

Since this equation is valid for any buckling vector $\boldsymbol{B}$, the term in brackets must be equal to zero. Upon substitution of $f_B = g_B + ih_B$, a coupled transport equation for the lattice flux functions is found by separating the real and imaginary parts:

$$\begin{bmatrix}\nabla\cdot\boldsymbol{\Omega} + \Sigma_t - S_{in} & -\boldsymbol{\Omega}\cdot\boldsymbol{B}\\ +\boldsymbol{\Omega}\cdot\boldsymbol{B} & \nabla\cdot\boldsymbol{\Omega} + \Sigma_t - S_{in}\end{bmatrix}\begin{bmatrix}g_B(\boldsymbol{r},E,\boldsymbol{\Omega})\\ h_B(\boldsymbol{r},E,\boldsymbol{\Omega})\end{bmatrix} = \frac{1}{k}\begin{bmatrix}S_f g_B(\boldsymbol{r},E,\boldsymbol{\Omega})\\ S_f h_B(\boldsymbol{r},E,\boldsymbol{\Omega})\end{bmatrix} \tag{11}$$

In the present work, we have implemented a solver based on the Method of Characteristics (MOC) to find the solutions g_B and h_B. These solutions are rigorous within lattice theory, and may be solved with the accuracy allowed by the MOC solver. In the conventional approach to lattice calculations, one proceeds further, and develops g_B (even in $\boldsymbol{B}$) and h_B (odd in $\boldsymbol{B}$) as a power series of the buckling: