A MONTE CARLO ESTIMATE OF THE DIFFUSION COEFFICIENT FOR A CANDU CELL

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Abstract

In this paper, the radial diffusion coefficient for a CANDU cell is calculated by using the Monte Carlo code MCNP [1]. The calculation uses the conventional definition of the diffusion coefficient which is based on the transport cross section. The latter is estimated from an MCNP simulation of the CANDU cell with a reflective boundary condition. These MCNP-based two-group diffusion coefficients are compared to the corresponding result obtained with the transport and depletion code HELIOS [2]. The calculations are performed for two burnup states: 0 and 4 GWd/TU.

Introduction

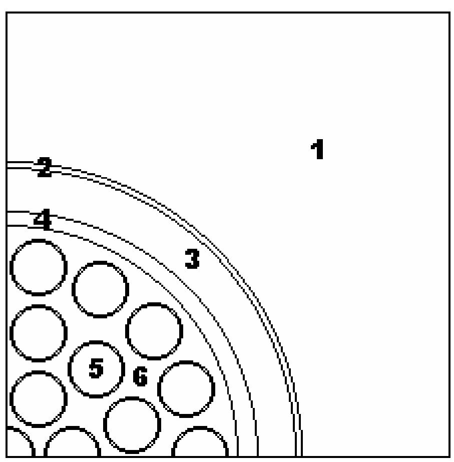
The calculation of the homogenized diffusion coefficient constitutes one of the main issues to be addressed when using nodal diffusion theory to describe the neutron balance in a reactor core. The diffusion coefficient can be defined in different ways, in order to preserve parameters of interest such as reaction rates, eigenvalue, surface leakage and node-averaged leakage [3,4,5]. Both deterministic and Monte Carlo techniques have been used to calculate the node-averaged diffusion coefficient. For a CANDU cell, no Monte Carlo estimate of the radial diffusion coefficient has been reported so far in the literature. A computational method to calculate the axial diffusion coefficient of a heterogeneous reactor lattice based on MCNP was developed and applied to a CANDU fuel channel by Milgram [6].

In this paper an estimate of the radial diffusion coefficient is calculated using MCNP. The calculation uses the conventional definition of the diffusion coefficient which is based on the transport cross section. The latter is estimated from an MCNP simulation of the CANDU cell with a reflective boundary condition. This method to calculate the homogenized diffusion coefficient has been shown to assure a good accuracy of the nodal calculation of spent fuel lattice configurations [7].

Method

The analyzed CANDU cell is a typical square lattice cell with a single CANDU cluster of 37 fuel rods, as given in reference 8. Only one quarter of the cell is considered due to the symmetry (see Figure 1). The fuel rods are made of natural uranium dioxide and have a Zircaloy cladding. Heavy water is used both as the coolant inside the pressure tube and as the moderator surrounding the calandria tube. The gap is filled with helium. The geometry is fully modeled in 2-D with MCNP, with a specular reflective boundary condition.

Two burnup states are considered: 0 GWd/TU and 4 GWd/TU, respectively. Both states are analyzed at operating temperatures (687^{o}C in the fuel, 288.5^{o}C in the coolant, 68^{o}C in the moderator) and a nominal coolant density of 0.80623 g/cc. The continuous energy cross section libraries used in the MCNP calculations are based on the ENDF/B-VI data files. An additional case is analyzed for the fresh fuel state, with all cross sections at 300K (the standard MCNP continuous energy libraries based on the ENDF/B-VI data files are used) and the coolant density of 1.1020 g/cc. In all cases the coolant is assumed to be uniformly distributed inside the pressure tube.



1 Moderator
2 Calandria Tube
3 Gap
4 Pressure Tube
5 Fuel Rod
6 Coolant

Figure 1. Geometry Model

The calculation with MCNP of the cell-averaged diffusion coefficient for group g, $\overline{D}_g$, is based on the conventional definition:

$$\overline{D}_g = 1/\left(3\overline{\Sigma}_{tr,g}\right) \tag{1}$$

The cell-averaged transport cross section in group g, $\overline{\Sigma}_{tr,g}$, is given by:

$$\overline{\Sigma}_{tr,g} = \frac{\int_g dE \int_{\vec{r}} d\vec{r}\, \Sigma_{tr}(\vec{r},E)\Phi(\vec{r},E)}{\int_g dE \int_{\vec{r}} d\vec{r}\, \Phi(\vec{r},E)} \tag{2}$$

where $\vec{r}$ represents the spatial variable, E the neutron energy, $\Phi(\vec{r},E)$ the scalar flux, and $\Sigma_{tr}(\vec{r},E)$ is given by:

$$\Sigma_{tr}(\vec{r},E) = \Sigma_t(\vec{r},E) - \mu(E)\Sigma_s(\vec{r},E) \tag{3}$$

$\mu(E)$ is the average cosine of the scattering angle in the laboratory system. $\Sigma_t(\vec{r},E)$ and $\Sigma_s(\vec{r},E)$ are the total and the scattering cross sections, respectively.

The numerator in Eq. (2) is estimated by tallying the following quantity in MCNP:

$$\left\{\Sigma_t(\vec{r},E) - \left[\Sigma_t(\vec{r},E) - \Sigma_c(\vec{r},E) - \Sigma_f(\vec{r},E)\right]\left(uu' + vv' + ww'\right)\right\}\Phi(\vec{r},E) \tag{4}$$

where $\Sigma_c(\vec{r},E)$ and $\Sigma_f(\vec{r},E)$ are the capture cross section and fission cross section, (*u, v, w*) and (*u', v', w'*) define the direction cosines before and after the collision. A patch file is added to MCNP to define user bins through the TALLYX subroutine for tallying the quantity in Eq. (4). The denominator in Eq. (2) is obtained from a standard MCNP F4 (flux) tally.

This estimation of the cell-averaged multigroup transport cross sections is similar to that used by Gast [9] in the Monte Carlo transport code RCP01 [10]. However, for the diffusion coefficients in the fast groups Gast used an empirical correction factor to account for the fact that the flux, and not the current, is used as a weighting function in the Monte Carlo estimate of the transport cross section. This correction is not used in this paper.

Results

The two-group cell-averaged radial diffusion coefficients estimated with MCNP are shown in Table 1. They are compared to the corresponding results obtained with HELIOS when using the same definition (Eq. 1) of the diffusion coefficient (that is, the collapsed and homogenized transport cross section is directly used). The value of the infinite-medium multiplication constant is also shown in the table.

In the HELIOS calculation, the cell configuration shown in Fig. 1 is modeled in 2-D with small approximations of the geometry of the pressure tube, gap, and calandria tube, as described in reference 8. Specular reflection is used as the boundary condition for the cell. The HELIOS calculations used the 45-group cross section library, which does not contain any adjustments to the resonance capture in ^{238}U [11].

The MCNP calculation in each of the three analyzed cases is performed for five million histories. The relative standard deviations for the tallies corresponding to the numerator and denominator in Eq. 2 are 0.0004 for the fast group and 0.0001 for the thermal group. The error shown in Table 1 for the MCNP-based estimate of the diffusion coefficient is calculated by using the error propagation in Eqs. 1 and 2. It is considered that there is no correlation between the two quantities at the numerator and denominator in Eq. 2.

It is observed in Table 1 that the MCNP estimate of the radial diffusion coefficient is systematically smaller than that calculated with HELIOS, for both groups and in all analyzed cases, by about 3-4%.

Table 1. The Radial Diffusion Coefficient

#	$\overline{D}_{1,MCNP}$ (σ)	$\overline{D}_{1,HELIOS}$	Δ (%)	$\overline{D}_{2,MCNP}$ (σ)	$\overline{D}_{2,HELIOS}$	Δ (%)	$K_{\text{inf},MCNP}$ (σ)	$K_{\text{inf},HELIOS}$	Δ (%)
1[a]	1.2344 (0.0002)	1.2823	3.9	0.8167 (0.0005)	0.8465	3.7	1.11877 (0.00018)	1.11411	-0.4
2[b]	1.2344 (0.0002)	1.2828	3.9	0.8150 (0.0005)	0.8442	3.6	1.04533 (0.00018)	1.04703	0.2
3[c]	1.1949 (0.0002)	1.2403	3.8	0.7938 (0.0004)	0.8105	2.1	1.12687 (0.00018)	1.12612	-0.1

[a] 0 GWd, operating temperatures
[b] 4 GWd, operating temperatures
[c] 0 GWd, all temperatures 300K

Conclusion

The radial diffusion coefficient for a CANDU cell is calculated by using the conventional definition of the diffusion coefficient by means of the transport cross section, which is estimated from a 2-D Monte Carlo simulation of the cell with the MCNP code. The MCNP-based estimate of the radial diffusion coefficient is compared to the corresponding result obtained with the collision-probability transport code HELIOS. A further analysis needs to be performed to determine the source of the difference in the results obtained with the two codes. It would also be interesting: 1) to investigate the level of accuracy that can be obtained when using these estimates of the diffusion coefficients in a nodal calculation of the core and 2) to estimate radial, axial and 3-D homogenized diffusion coefficients for each bundle in typical CANDU channels.

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