Sensitivity of k_∞ to Homogenization, and Dimension and Composition Uncertainties for Plate Type Research Reactor Fuel

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Abstract

As a part of the Department of Energy's Innovations in Nuclear Infrastructure and Education (INIE) Program a full facility model is being built of the Ohio State University Research Reactor (OSURR) using the discrete ordinates transport code, PENTRAN. Since the thickness of the fuel plate of OSURR is very small, billions of spatial meshes are required in order to represent the whole reactor core. This, however, is not practical even with the PENTRAN code which is capable of partitioning the memory among processors. Hence, it is essential to consider a certain level of homogenization of fuel, clad, and/or moderator/coolant. Further, since fuel and cladding materials contain impurities and dimensions include tolerances, it also is important to estimate their impacts on the core eigenvalue. The impacts of different homogenization cases as well as the uncertainties in composition and dimensions of the fuel plates on k_∞ are examined. To estimate the accuracy of different cases, Monte Carlo reference calculations are performed using the MCNP5 code. The selected combination will be used for full-facility simulation.

KEYWORDS: Research Reactor Model, Discrete Ordinates Modeling, Homogenization

1. Introduction

In support of the nation's nuclear energy industry, the Innovations in Nuclear Infrastructure and Education (INIE) program was established in 2002 by the Department of Energy. Its function is to strengthen university nuclear engineering education programs through improved/original use of university research and training reactors [1].

The Ohio State University (OSU) is part of the INIE consortium consisting of Penn State University, OSU, Purdue University, University of Illinois (Urbana-Champaign), University of Michigan and University of Wisconsin – Madison. For improving research reactor utilization and to meet objectives consistent with the goals of the INIE program, a full facility model of the OSU Research Reactor (OSURR) is being assembled using the PENTRAN 3-D discrete ordinates code (version 9.36b) [2].

Traditionally, diffusion codes were used to model research reactors for parametric

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studies [3, 4, 5]. Such codes, however, cannot accurately model transport effects that are associated with a high-leakage research reactor. The advent of parallel computers and faster computer chips have allowed development of relatively fast parallel transport theory codes [6, 7, 8] that are capable of accurately simulating high-leakage cores. Further, in order to characterize the facility completely, it is essential to model components such as beam tubes and thermal columns. For these "deep penetration" problems, deterministic transport methods are usually more computationally effective.

Storing the full phase-space information for an exact geometry model of the OSURR would require a few thousand gigabytes. This large memory requirement is a result of the fine spatial meshing essential for modeling the very thin layers of cladding (0.038 cm thick by 6.66 cm long on each side of the fuel) and the fuel meat (0.051 cm thick and 6.10 cm long) over the whole core. Such a large model (about 2×10^9 spatial meshes) is unrealistically cumbersome even considering the parallel memory and phase-space decomposition capability of PENTRAN. Hence, it is essential to consider some level of homogenization of different material regions including fuel, clad, and/or moderator/coolant.

In order to optimize the reduction in model size, evaluate the possible bias introduced in the calculation by the homogenization, and understand the impact of systematic uncertainties in the models, this paper investigates the effects of the homogenization and the uncertainties due material impurities based on eigenvalue calculations for a unit cell in an infinite lattice of OSURR.

2. The OSURR Fuel Description and Homogenization Schemes

The OSURR is fueled with MTR plate-type elements. The height of the fueled portion (often referred to as the meat) of the fuel plate is 57.14 cm and composed of U_3Si_2 powder dispersed (40% of the meat volume) in an aluminum matrix. The cladding composed of aluminum alloy T-6061 was modeled in the homogenization studies as pure aluminum. To examine the effect of homogenization, we developed a reference fuel cell (Case 1) and three homogenization cases (Cases 2-4). Figure 1 shows the schematic of an OSURR fuel cell (i.e. Case 1), which includes a fuel plate, and its surrounding coolant/moderator and two aluminum T-6061 end plates.

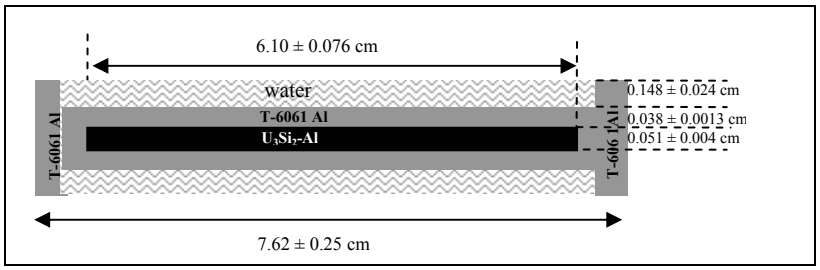

Figure 1: Schematic of the Exact Fuel Plate Geometry

Figures 2a-2b show the three homogenization cases considered in this study.

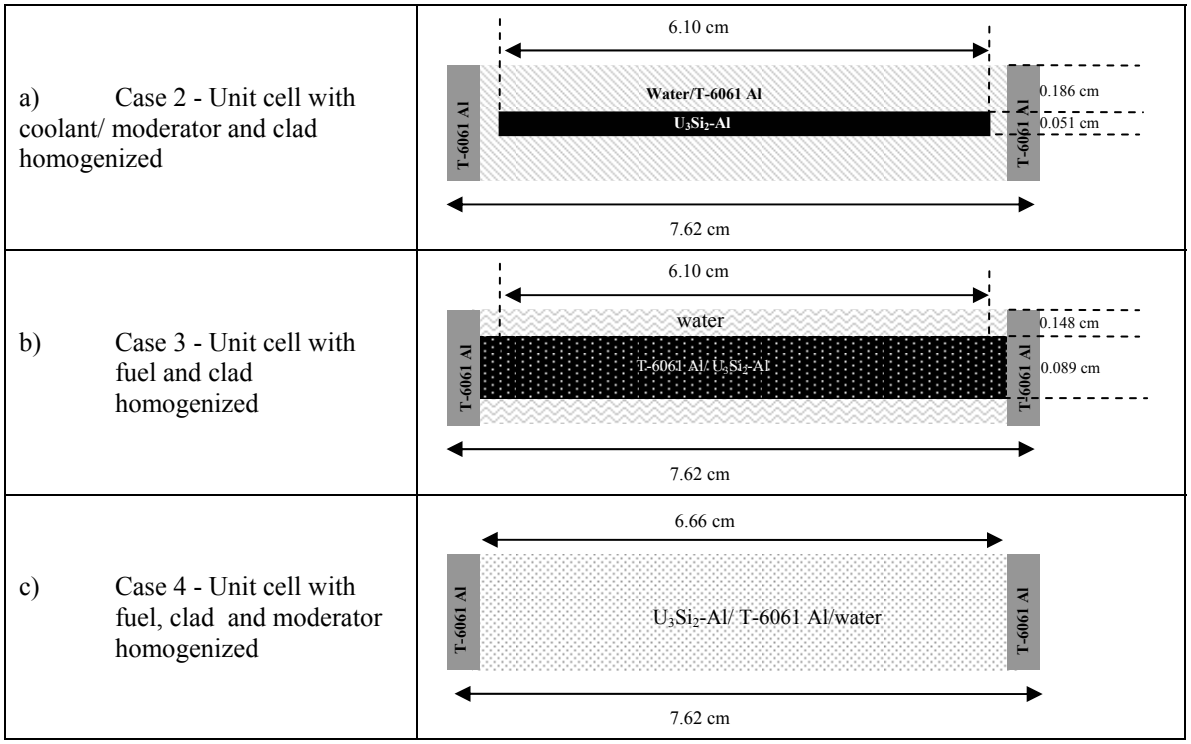

Figure 2: Schematics of the Homogenized Cases

3. Methodology

To study the impact of the homogenization and the material/geometry uncertainties, an OSURR unit cell in an infinite lattice is modeled in PENTRAN and MCNP5 [9]. The multigroup cross section data necessary for PENTRAN are obtained from the SCALE5 (Standardized Computer Analyses for Licensing Evaluation) [10] package.

3.1 Description of Modeling Software

PENTRAN (Parallel Environment Neutral-particle TRANsport) performs 3-D SN transport calculation with the capability of performing full domain decomposition (space, angle and energy) and memory partitioning in parallel environments. PENTRAN also possesses adaptive differencing schemes and different special quadrature sets.

MCNP (Monte Carlo N-Particle) is the well known general purpose Monte Carlo code developed by Los Alamos that can be used for particle transport through an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. It uses point-wise (continuous) or multigroup cross section data and contains many flexible tallies and variance reduction techniques.

SCALE is a modular code system developed and maintained by Oak Ridge National Laboratory. The development of SCALE has been focused on problem dependent cross-

section processing and analysis of criticality safety, shielding, depletion/decay, and heat transfer problems.

3.2 Group structure and Cross Section Generation

The group structure for the discrete ordinates calculation was chosen from the analysis of the flux spectrum generated in MCNP5 for a single fuel plate model as described in Section 2. The MCNP5 modeling scheme is described in Section 3.3. This flux spectrum, and the selected group structure which is indicated by vertical divisions, is illustrated below in Figure 3.

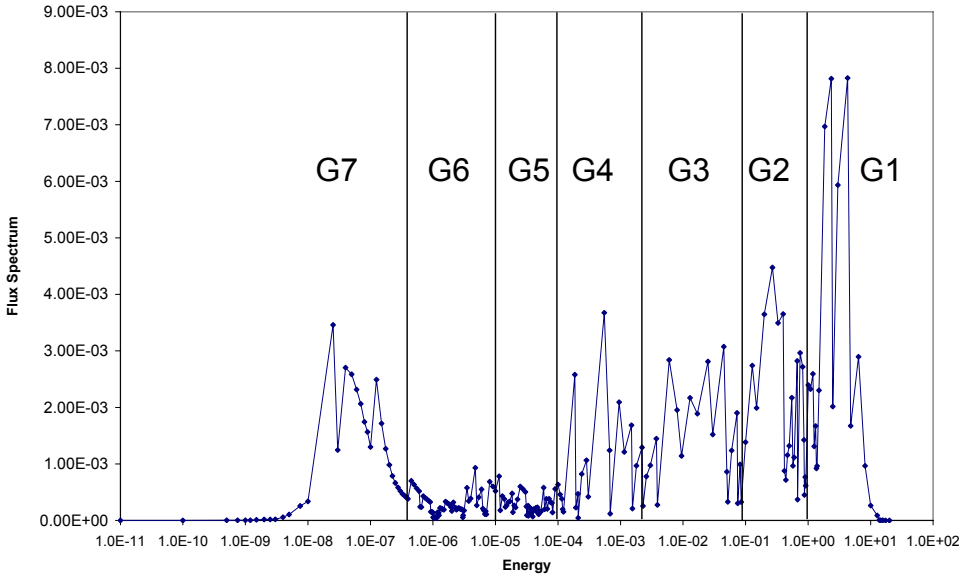

Figure 3: The flux spectrum for the fuel plate unit cell with the selected group structure indicated by the vertical divisions on the plot.

The seven groups were chosen for proper grouping of the resonance peaks with upper limits 4.0E-7 MeV, 1.0E-05 MeV, 1.0E-04 MeV, 2.0E-03 MeV, 1.0E-01 MeV, 1.1 MeV, and 20 MeV. .

In order to generate the cross-sections used in PENTRAN, the SCALE5 [10] code package was used in conjunction with SCALFORM [11] and GMIX [11]. The SCALE5 modules used included TRITON, CENTRM, NEWT, and ALPO in order to extract the seven group cross-sections from a 238-group general purpose library derived from the ENDF/B-V libraries. These microscopic cross-sections were then reformatted using the code SCALEFORM and used in GMIX to calculate the macroscopic cross sections of the mixture for all the cases. The anisotropic scattering cross-sections used in the analyses were evaluated for up to a third order Legendre polynomial expansion.

3.3 Description of the Reference Models

Fig. 4 shows the spatial mesh distribution used in PENTRAN calculations.

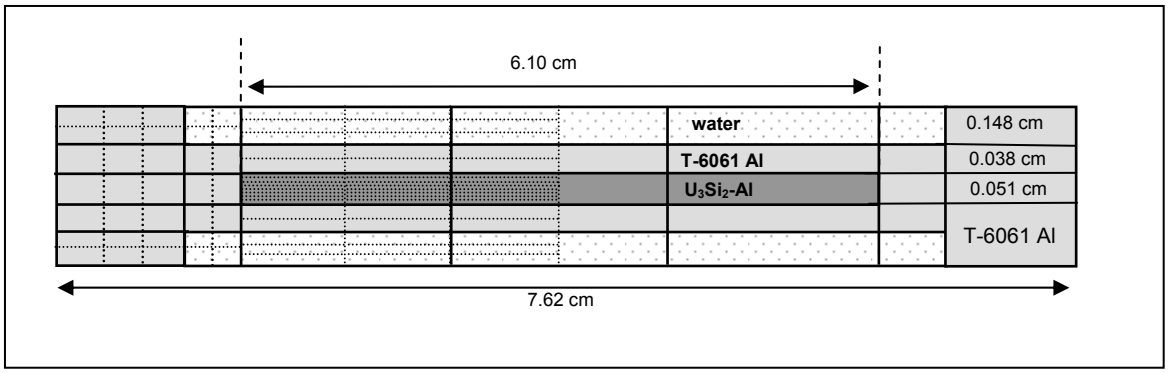

Figure 4: Illustration of the fine spatial meshing (on the left half of the figure) coarse spatial meshing (on the right half of the figure) and the as used in PENTRAN

This mesh distribution includes 35 coarse meshes, which are divided into block adaptive fine meshes used by PENTRAN. The reflective boundary condition is prescribed on all boundaries for both PENTRAN and MCNP5 calculations. All the deterministic calculations performed in this paper used 80 directions (S8) and a third-order Legendre expansion (P3) for the scattering cross-section. The convergence criteria for the inner and outer iterations were set to 1E-5 and 1E-04, respectively.

For the MCNP5 calculation, the continuous-energy ENDF/B-VI cross section library is used. A reference simulation for the Monte Carlo calculations used the values of 5000 particle histories per cycle and 30 skipped cycles with a total of 300 cycles. These parameters were tested against the reference values. The number of cycles skipped was tested at 30, 50, 100, and 150. The reference value of 30 cycles skipped was chosen because it demonstrated source convergence. The total number of cycles and the number of particle histories per cycle were also examined to determine the optimum calculation time versus calculation accuracy. The number of particle histories per cycle was tested using 1,000, 5,000, 10,000 histories per cycle for 500 cycles, 400 of them being active cycles. The number of total cycles was tested at 100, 300, and 500. The results for these calculations indicated that the reference values of 5000 particle histories with 300 total cycles gave a maximum uncertainty of 0.050%.

4. Results

4.1 Impact of Homogenization

The k_∞ results for the MCNP calculations for Cases 1-4 are presented in Table 1.

Table 1: MCNP5 Unit Cell Homogenization Results

Case	*Materials Homogenized*	k_∞	*Uncertainty*[*]	*$\|\Delta k\|/k$ with respect to Case 1(%)*
Case 1	----------	1.67337	±0.00041	----------
Case 2	clad and water	1.67161	±0.00043	0.105±0.0037
Case 3	fuel and clad	1.67408	±0.00042	0.0424±0.0015
Case 4	fuel, water, and clad	1.65694	±0.00046	0.9820±0.0364
[*] one standard deviation				

Table 1 results show that the differences between exact geometry (Case 1), water/clad homogenization (Case 2) and fuel/clad homogenization (Case 3) are less than 0.11%. In fact, the difference between Cases 1 and 3 is within the statistical uncertainty of the results. Case 4 and Case 1 results differ by about 1% $|\Delta k|/k$.

The results from the homogenization studies performed in PENTRAN are shown in Table 2.

Table 2: PENTRAN Unit Cell Homogenization Results

Case	k_∞	$\|\Delta k\|/k$ *with respect to Case 1(%)*	$\|\Delta k\|/k$ *with respect to MCNP Case 1 (%)*
Case 1	1.67291	0.0	0.0275
Case 2	1.67717	0.25465±2.15E-4	0.2271
Case 3	1.67752	0.27557±2.33E-4	0.2480
Case 4	1.67809	0.30964±2.61E-4	0.2821

The changes as a result of homogenization in Cases 2 and 3 are both within 0.25% $|\Delta k|/k$. Case 4 also shows good agreement with the reference Case 1. Also shown in Table 2 are the results between MCNP5 and PENTRAN for each respective case studied. The most notably different results occur in Case 4 when all of the materials are homogenized together. PENTRAN shows only a 0.3% $|\Delta k|/k$ between the full homogenization case and the reference case. When Case 4 in PENTRAN is compared to MCNP5, $|\Delta k|/k$ is 1.4%. This difference arises from the differences in the treatment of the cross sections. In SCALE5 the cross sections are modified to account for the space and energy shielding effects so that these effects are preserved in homogenized geometries when used in PENTRAN. In MCNP5 these effects are not taken into account when using the volume weighted homogenization. A more accurate MCNP5 homogenization scheme would involve preserving the reaction rates.

4.2 Impact of Material Composition and Dimension Uncertainties

Sensitivity studies were performed to understand better the influence on the value of k_∞ caused by uncertainties in material composition and dimensions. Such understanding is necessary for future comparison of computational predictions to experimental data. Using MCNP5, a maximum and minimum case (see tolerance values on Case 1 in Figure 1) were modeled and compared to the average value for each dimension. The dimensional tolerances used in the geometry sensitivity study were taken directly from an engineering diagram of a single fuel plate [12].

Uncertainties due to the materials composition were taken into account by examining the changes in materials resulting from the tolerances on the alloy specifications and the presence of various impurities. The aluminum alloy T-6061 contains 9 elements besides the aluminum that were specified by a given range of weight percents. The percent weight of aluminum ranged from 96.0% to 98.6% [13]. The effect of the additional elements in the cladding was modeled using the maximum percentage of each element, the minimum percentage of each element (which in some cases was zero), and their average value. The fuel itself contains 29 impurities which make up 0.654% of the fuel's

overall weight [13]. The only data available for the fuel provided the average percent by weight for each one of these impurities. In the case of the fuel material, there was not enough information available to determine a range on the k_∞ value. Table 3 lists the cases considered in the sensitivity study.

Table 3: List of Cases used in Sensitivity Analyses

Case	Description
5	Maximum dimensional tolerance value modeled
6	Minimum dimensional tolerance value modeled
7	Maximum percent of additional elements in the clad (96.0% Al)
8	Minimum percent of additional elements in clad (98.6% Al)
9	Average value of additional element modeling in cladding
10	Average value of impurities modeled in the fuel

Table 4 compares Case 5 through 10 results to the reference Case 1.

Table 4: MCNP5 Unit Cell Sensitivity Results

Case	k_∞	*Uncertainty*	$\|\Delta k\|/k$ *with respect to Case 1*
Case 1	1.67337	±0.00041	0.0
Case 5	1.67197	±0.00044	0.0837±0.0030%
Case 6	1.67617	±0.00042	0.1141±0.0040%
Case 7	1.66612	±0.00042	0.4680±0.0165%
Case 8	1.67371	±0.00046	0.0330±0.0012%
Case 9	1.66889	±0.00042	0.3210±0.0113%
Case 10	1.66684	±0.00041	0.3902±0.0135%

Above table indicates that composition uncertainties may influence the results by a maximum absolute difference of ~0.5% $|\Delta k|/k$, while the dimensional tolerance may impact the results by a maximum absolute difference of ~0.1% $|\Delta k|/k$.

Hence the uncertainties in material composition have non-negligible effect on the system eigenvalue.

5. Conclusion

This paper investigates the effects of the homogenization and material/geometry uncertainties on the k_∞ of an infinite lattice composed of unit cells based on the OSURR MTR fuel plate design in order to: a) optimize the reduction in PENTRAN model size, b) evaluate the possible bias introduced in the calculation by the homogenization, and c) understand the impact of systematic uncertainties in the models. The k_∞ results from different homogenization schemes using the different code packages indicate that the best homogenization scheme for the discrete ordinates model is the homogenization of the fuel, cladding, and water (Case 4). This homogenization scheme introduces a small, but acceptable bias in unit cell k_∞ (0.30964±2.61E-4 %$|\Delta k|/k$) and is not expected to have significant effect in the modeling of the full research reactor facility. The results from the

comparison between the SCALE5/PENTRAN homogenizations and the MCNP5 homogenizations indicate that volume weighted homogenization of the fuel, clad and the moderator introduces approximately 1% $|\Delta k|/k$ error in MCNP5 unit cell calculations. This error is attributed to space and energy shielding effects which are not taken into account in homogenized MCNP5 calculations. However, shielding effects were not found to be appreciable (less than 0.1% $|\Delta k|/k$) for homogenized coolant/moderator-clad and fuel-clad MCNP5 runs.

Homogenization of the fuel and the cladding is expected to reduce the number of mesh points required for the PENTRAN calculations by approximately three orders of magnitude. The k_∞ was found to be insensitive (0.10%) to the tolerances in the physical dimensions of the fuel plate's geometry as taken from the engineering diagrams. The sensitivity studies performed on the material composition included the modeling of the impurities in the fuel and the alloy components in the cladding. The changes in the materials showed that an appreciable effect on the k_∞ (up to 0.6%) could be observed when the two sources of uncertainties are combined. Such changes need to be considered when considering the full facility model comparison to physical data.

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