ON THE USE OF SERPENT MONTE CARLO CODE TO GENERATE FEW GROUP DIFFUSION CONSTANTS

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ABSTRACT

The accuracy of diffusion reactor codes strongly depends on the quality of the group constants processing. For many years, the generation of such constants was based on 1-D infinity cell transport calculations. Some developments using collision probability or the method of characteristics allow, nowadays, 2-D assembly group constants calculations. However, these 1-D and 2-D codes show some limitations as, for example, on complex geometries and in the neighborhood of heavy absorbers. On the other hand, since Monte Carlo (MC) codes provide accurate neutron flux distributions, the possibility of using these solutions to provide group constants to full-core reactor diffusion simulators has been recently investigated, especially for the cases in which the geometry and reactor types are beyond the capability of the conventional deterministic lattice codes. The two greatest difficulties on the use of MC codes to group constant generation and deterministic transport methods based in several approximations. The SERPENT code is a 3-D continuous energy MC transport code with built-in burnup capability that was specially optimized to generate these group constants. In this work, we present the preliminary results of using the SERPENT MC code to generate 3-D two-group diffusion constants for a PWR like assembly. These constants were used in the CITATION diffusion estimate.

1. INTRODUCTION

The evaluation of the neutron flux distribution inside all regions in a reactor core still demands considerable computational resources and direct transport solutions for the entire core is not affordable for day-to-day exploitation. In order to obtain reliable data at the core level, a common procedure is to use various stages of calculations interconnected together.

A reactor core is made of several materials. The relative geometric arrangement of fissile, absorbent, and coolant materials usually follows regular patterns (referred to as lattices)

inside the core. Such lattices are composed of sub elements called unit cells that are repeated throughout the core. The general approach to account for heterogeneous lattice effects is to perform a detailed calculation of the flux distribution in a given unit cell (usually assuming there is zero net current across the boundary of the cell by considering periodic or reflexive boundary conditions) and then calculate the effective group constants characterizing one such cell [1]: after being condensed in few energy groups the various multigroup cross sections characterizing materials in the cell are spatially averaged over the cell using the flux distribution as a weighting function. This procedure results in cell-averaged or so-called self-shielded group constants that can then be used in the analysis of reactor assemblies or of entire cores.

In the 1970s, the calculation flow chart involving reactor core simulations was generally the following [2]:

1. Perform pin-cell calculations using a fine group (few thousands) cross-section library, and condense into fewer (few hundreds) groups and homogenize over the pin-cell's geometry.

2. Perform assembly calculations using homogenized pin-cell cross-section data from step 1, condense into few-group reactor data, and homogenize over assembly's geometry.

3. Perform core calculations using the homogenized assemblies' few-group data from step 2.

Some codes available nowadays are able to perform the first two steps together to calculate 2-D assembly group constants by solving the transport equation in two dimensions using collision probability or the method of characteristics.

For daily core analysis the third step is usually done with few energy groups under the Diffusion approximation. The basic assumption of the Diffusion theory is that the angular neutron flux is weakly dependent on angle in such a way that it can be adequately represented by only a linearly anisotropic angular dependence (i.e., the P1 approximation) [1].

Although not always accurate, diffusion solvers are invaluable in obtaining inexpensive reactor core data since it takes few CPU time to perform full reactor core simulations. However, the key for the success of Diffusion codes lies in the few group constants libraries. Many approximations are done to condense in energy and homogenize in space the unit cells and lattice results [1]. Furthermore, the 1-D pin-cell and 2-D assembly codes show some limitations as, for example, on complex geometries and in the neighborhood of heavy absorbers [2, 3].

On the other hand, since Monte Carlo codes provide accurate neutron flux distributions, the possibility of using these solutions to provide group constants to full reactor core diffusion simulators has been recently investigated [3-10], especially for the cases in which the geometry and reactor types are beyond the capability of the conventional deterministic lattice codes. With Monte Carlo codes the simulation is not limited to simple 2D geometries and the transport process is handled at the level of neutron interactions without major approximations. Also, the same methods can be applied to any fuel or reactor type, without losing the reliability of the calculation scheme and the best available knowledge on neutron interactions is always directly available for the calculation [4].

The two greatest difficulties on the use of Monte Carlo codes to group constant generation are the computational costs and the methodological incompatibility between analog Monte Carlo particle transport simulation and deterministic transport methods based in several approximations. These challenges inspired the development of the SERPENT code which is a 3-D continuous energy Monte Carlo transport code with built-in burnup capability that was specially optimized to generate these group constants [4, 5].

In this work, we present the preliminary results of using the SERPENT code to generate 3-D two-group diffusion constants for a PWR like reactor. These constants were used in the CITATION diffusion code to investigate the effects of this group constants determination on the neutron multiplication factor diffusion estimate.

2. METHODOLOGY

In order to analyze the differences between two methodologies of group constants generation (i.e. the 1-D unit cell homogenization using HAMMER code and the 3-D region homogenization using SERPENT code) it was considered a 28x26 IPEN/MB-01 reactor core configuration. The main assumptions adopted in this preliminary analysis are presented below.

2.1. The IPEN/MB-01 Reactor Core Configuration

The IPEN/MB-01 research reactor facility is located in the city of São Paulo, Brazil and reached its first criticality on 1988. Since then it has been used for basic reactor-physics research and as an instructional laboratory system [11].

The reactor core is located inside a cylindrical open-top moderator tank which has 1830-mm outside diameter, is 2750 mm high, 8.5 mm thick, and is made of Stainless Steel SS-304. Demineralized light water is used as moderator. Several configurations of cylindrical fuel rods can be arranged in square uniform lattices of 15.0 mm pitch as three grid plates assure the rods' positions. All grids have a square shape (side length is 588 ± 0.5 mm) and are made of SS-304. The bottom grid plate is 22 mm thick and consists of a 30 x 30 square array out of which 852 are 10.4-mm-diameter cavities (not holes), whose purpose is to support the fuel rods. The remaining 48 positions are holes used to fix the guide tubes for the control and safety rods. The intermediate and upper grid plates are located well above the active region and were not considered in this analysis.

Each fuel rod consists of a cladding (SS-304), low enriched (4.3486 wt.% 235U) UO₂ pellets, alumina (Al₂O₃) pellets, a spring (Inconel-600), spacer tube (SS-304) and top and bottom plugs (SS-304). Their dimensions are shown in Figure 1. For this study, we considered fuel rods containing UO₂ arranged in a 28x26 configuration, as shown in Figure 3.

Two banks of control rods control the IPEN/MB-01 reactor. They are located diagonally opposite each other in the core (the grey color in Figure 3 refers to the two control-bank locations, while the black color refers to the locations of the two safety-rod banks). Each of the four control and safety banks is composed of 12 rods held together and supported by a control mechanism above the tank. The absorber rods are clad by SS-304 and the end plugs are made of SS-304. The control rods are filled with an alloy of Ag-In-Cd while the safety rods are filled with B_4C powder. The dimensions of the control rods are shown in Figure 1.

The control and safety banks move through the core inside guide tubes made of SS-304. Their outer diameters are 12.00 mm and the inner diameters are 11.30 mm. Additional information can be obtained in [11].



Figure 1. IPEN/MB-01 fuel and control rods dimensions. Adapted from [11].

As a first analysis, we considered both the safety and control rods completely withdrawn. In fact, during normal operation, the safety banks are always completely withdrawn from the active core. These banks are kept at a removal position of 135% (the absorber is 35% of the active core length above the active core). Therefore when the safety banks are in the totally withdrawn position, they have very little impact on the criticality of the system. For the control rods fully withdrawn (removal position of 100%), on the other hand, the bottom surface of the absorber of the control bank coincides with the top of the active core in such a way that the bottom plug remains inside the active core and the control bank must be considered in the axial reflector for criticality calculations.

2.2. Numerical Codes

This subsection describes the codes used in this analysis and the main assumptions adopted.

2.2.1. The CITATION code for reactor core model

The CITATION code was developed at Oak Ridge National Laboratory in 1971. It is a generic code that solves various kinds of up to 3D multigroup diffusion problems using a finite-difference method in space and time. The neutron-flux-eigenvalue problems are solved by direct iteration to determine the multiplication factor or the nuclide densities required for a critical system [12]. This code was chosen because it is still used a lot in Brazilian organizations such as IPEN.

To model the IPEN/MB-01 reactor core in 3-D using the CITATION code some simplifications had to be made. In the z direction, seven plans were considered from top to bottom: the spacer tube plus control rod plan (24.0 cm high), the top alumina plus control rod plan (5.4 cm high), the active region plus control rod plug plan (2.5 cm high), the active region plus guide tube plan (52.1), the bottom alumina plus guide tube plan (9.0 cm high), the bottom grid plate plan (2.2 cm high), and the bottom reflector plan (30.0 cm high). In the xy direction, we considered a pin-to-pin model (1.5 cm pitch) surrounded by a 30.0 cm water reflector on each side. To account for border effects in the 2-group simulation, this reflector was divided in three parts: the first one next to the core is 1.5 cm width (light blue), the second one is 3.0 cm width and the last one is 25.5 cm width.

For each one of these zones the macroscopic nuclear properties are assumed constant by the numerical code. The diffusion coefficient, the macroscopic absorption cross section, the macroscopic production cross section ($v\Sigma_F$), the macroscopic reciprocal velocity cross section and the macroscopic cross section for scatter from group *k* (above) to each of the other groups below *k* must be given as input data for CITATION.

In order to provide the energy and space homogenized group constants, two different approaches were considered: one using the HAMMER-TECHNION code and other using the SERPENT Monte Carlo code. The next two subsections describe these approaches. In both cases, the energy groups were divided in two ranges: from 0 to 0.625 eV for the thermal group and from 0.625 eV to 10 MeV for the epithermal-fast group.

2.2.2. The HAMMER-TECHNNION code for cross-section generation

The HAMMER-TECHNNION code (an acronym for Heterogeneous Analysis by Multigroup Methods of Exponentials and Reactors) was jointly developed at Brookhaven National Laboratory and at the Savannah River Laboratory in 1978 [13].

It performs a 1-D unit cell spectrum calculation using 54 fast and 30 thermal groups (obtained from ENDEF/B-IV microscopic cross section library), a detailed resonance treatment, a Fourier transform leakage treatment and integral transport theory for up to 20 spatial mesh points. Once the 54 and 30 neutron spectra are calculated, they are collapsed into two (one fast and one thermal) or more broad energy groups. Group constants are then obtained for the entire cell, each homogeneous region and combination of the homogeneous region.

To model the two-group constants for IPEN/MB-01 reactor core at HAMMER, nine unit cells were considered: three for the fuel rods (UO2, Alumina, and Spacer Tube), two for the control rods (Ag-In-Cd rod and its end fixture), one for the safety rods (guide tube only), one for the grid plate, one for the water below the grid plate, and one for the water around the array. For the fuel, safety and control rods' non-fissile materials, "super cell" models were considered like the one illustrated in Figure 3 for the control rod.



Figure 2. Super cell model for the control rod.

2.2.3. The SERPENT code for cross-section generation

Serpent is a three-dimensional continuous-energy Monte Carlo reactor physics code which has a built-in burnup calculation capability. It has been developed at VTT Technical Research Centre of Finland since 2004 and has been publicly distributed by OECD/NEA Data Bank and RSICC since 2009. Recently, the code is gaining the international community attention being already used by 43 organizations in 20 countries around the world.

From geometrical point of view, Serpent is similar to other Monte Carlo codes (e.g. MCNP and KENO) as it uses a universe-based geometry model that allows the description of complicated three-dimensional reactor geometries (e.g. ATR reactor [9, 10]).

One of the main advantages of Serpent, however, is the option to combine Woodcock deltatracking with ray-tracing for neutron transport. In traditional ray-tracing MC, the collision distance has to be adjusted each time the neutron enters a new region with higher or lower interaction probability so the distance to the nearest boundary surface has to be calculated each time the next collision site is sampled. The calculation of the surface distances demands a major part of the computational time especially if the neutron mean free path is long compared to the characteristic dimensions of the geometry.

The key idea in the delta-tracking method is to add an appropriate virtual collision cross section to each material total cross-section in such a way that the modified total cross section has the same value in all materials. The result is that the total interaction probability, in this case the sum of real and virtual collision probabilities, is the same in all materials. This eliminates the need to calculate the free path length each time the neutron enters a new material, and eventually, the need to calculate the surface distances. The problem of calculating the shortest optical surface distance is reduced to the calculation of in which cell

the collision point is located. Consequently, the neutron flight direction plays no role and the maximum number of free variables is reduced from six to three.

The combination of surface-to-surface ray-tracing and the Woodcock delta-tracking method can speed up the simulation up to 20 times for PWR calculations without losing accuracy [8]. This overcomes the efficiency problems normally encountered with delta-tracking in the presence of localized heavy absorbers [14]. On the other hand, the main drawback of delta-tracking is that the track-length estimate of neutron flux is not available and reaction rates have to be calculated using the potentially less-efficient collision estimator.

From the physical interaction point of view, Serpent reads continuous-energy cross sections from MCNP ACE format data libraries. The interaction physics is based on classical collision kinematics and ENDF reaction laws and unresolved resonance cross sections can be sampled from probability tables.

Serpent also uses a unionized reconstruct energy grid for all reaction modes. This approach speed-up the calculation at the cost of large memory consumption, that may be a problem in burnup calculations and in parallel processing with Message Passing Information (MPI). In Serpent, parallelization is implemented by dividing the neutron histories to several tasks and combining the results after the transport cycle.

Serpent has been extensively validated in LWR lattice calculations [9, 10]. Effective multiplication factors are within the statistical accuracy from reference MCNP results, when the same ACE libraries are used in the calculations. Differences to other Monte Carlo codes (Keno-VI) are small, but statistically significant discrepancies can be observed in some cases due mainly to differences in SCALE/AMPX cross section processing [15].

Furthermore, the SERPENT code was specially designed for group constants generation, including calculation techniques beyond the standard tally features of general-purpose Monte Carlo codes: in order to account for the non-physical infinite-lattice approximation, B1 methodology, routinely used by deterministic lattice transport codes, is used for generation of leakage-corrected few-group cross sections [4].

To model the two-group constants for IPEN/MB-01 reactor core at SERPENT, 3-D homogenization regions were considered. To account for longitudinal flux variations, the z-direction was divided in seven regions like the z-structure used for CITATION.

To account for radial flux variations, a chess-like structure was adopted, as indicated in Figure 3. The green, yellow and red circles represent the fuel rods while the gray and black circles are the control and safety rods, respectively. This chess-like structure in important for B1 approximation used to determine the diffusion coefficient.

Finally, the water around the array was divided in four regions as indicated in blue colors. It is important to divide the reflector around the array because in the limit of few-energy groups there is a thermal flux peak in the reflector near the core-reflector border. This peak arises from the slowing down in the reflector of fast neutrons which escape from the core. Since the absorption cross section of the reflector is small, the thermalized neutrons accumulate in this region until they eventually diffuse back into the core, escape from the outer surface of the reflector, or are captured [1].



Figure 3. IPEN/MB-01 homogenization regions for SERPENT two-group constants' generation. Green, yellow and red circles are fuel rods. Gray and black circles are control and safety rods. Blue colors represent the water around the array.

3. RESULTS AND DISCUSSION

The division of the cells in different types for homogenization plays an important role in cross section generation since there are noticeable differences in the two-group constants for cells with same materials. This feature can be illustrated by Table 1 which compares the two-group constants obtained for the three regions of water cells adopted. In fact, this effect is more pronounced for the diffusion coefficient values.

One may also notice that HAMMER fast group constants are closer to the values obtained with SERPENT for the water region closest to the fuel rods array while the HAMMER thermal group constants are closer to the values obtained with SERPENT for the water cell represented by the external blue region of the Figure 3.

| Constant | SERPENT constants (cm ⁻¹) | | | |
|-----------------------|---------------------------------------|--|--|-------------------------|
| | first water | second water | third water | constants |
| D ₁ | 1.536±0.001 | 2.085±0.001 | 4.614±0.002 | 1.1873 |
| \sum_{A1} | $(4.609 \pm 0.002) \times 10^{-4}$ | $(5.124 \pm 0.002) \times 10^{-4}$ | $(5.575 \pm 0.002) \times 10^{-4}$ | 4.6913x10 ⁻⁴ |
| $\sum_{1,2}$ | (5.121 ± 0.002) x10 ⁻² | $(5.943 \pm 0.002) \times 10^{-2}$ | $(6.045 \pm 0.001) \times 10^{-2}$ | 4.6196×10^{-2} |
| D ₂ | (7.295 ± 0.008) x10 ⁻² | $(8.567 \pm 0.006) \times 10^{-2}$ | $(1.5877 \pm 0.0001) \times 10^{-1}$ | 1.4818x10 ⁻¹ |
| \sum_{A2} | $(1.8480\pm0.0006)x10^{-2}$ | $(1.88631 \pm 0.00009) \times 10^{-2}$ | $(1.91080 \pm 0.00006) \times 10^{-2}$ | 1.8793x10 ⁻² |

Table 1. Water cell two-group constants

Figure 4 shows the collision density (cold colors) and power density (hot colors) for an azimuthally and a radial plans obtained with the SERPENTcode. Since these quantities are proportional to the neutron flux, Figure 4 reinforces the importance of dividing the water cells in three regions for collapsing the group constants.



Figure 4. Collision density (cold colors) and power density (hot colors) for an azimuthally (zx) and a radial (xy) plans obtained by SERPENT.

Although the chess like configuration is important for the difusion coeficient estimate, the differences in the fuel rods cross sections are less pronounceated than for the water cells values, as shown in Table 2. The fuel rods fast diffusion coefficients obtained with SERPENT are around 55% smaller than the HAMMER ones. These differences must be better investigated. For the thermal diffusion coefficients, relative good agreement is noted for the green and red fuel rods, however, for the yelllow fuel rod, the diffucion coefficient is twice bigger than the HAMMER value. This may be physically explained by the bigger leakage expected for the boundary cells.

| Constant | SERPENT constants (cm ⁻¹) | | | HAMMER |
|-----------------|---------------------------------------|--------------------------------------|--------------------------------------|-------------------------|
| | Yellow fuel rod | Green fuel rod | Red fuel rod | constants |
| D ₁ | (5.140 ± 0.005) x10 ⁻¹ | $(5.065 \pm 0.001) \times 10^{-1}$ | $(5.004 \pm 0.002) \times 10^{-1}$ | 1.1074 |
| \sum_{A1} | (8.735 ± 0.007) x10 ⁻³ | (8.785 ± 0.002) x10 ⁻³ | (8.945 ± 0.003) x10 ⁻³ | 9.1071x10 ⁻³ |
| $\nu \sum_{F1}$ | $(7.437 \pm 0.005) \times 10^{-3}$ | $(7.245 \pm 0.001) \times 10^{-3}$ | $(7.317 \pm 0.002) \times 10^{-3}$ | 7.3829x10 ⁻³ |
| $\sum_{1,2}$ | $(2.679 \pm 0.002) \times 10^{-2}$ | $(2.6874 \pm 0.0004) \times 10^{-2}$ | $(2.7426 \pm 0.0007) \times 10^{-2}$ | 2.6847×10^{-2} |
| D ₂ | $(4.492 \pm 0.006) \times 10^{-1}$ | $(2.793 \pm 0.001) \times 10^{-1}$ | (2.512 ± 0.002) x10 ⁻¹ | 2.2342×10^{-1} |
| \sum_{A2} | $(1.3065 \pm 0.007) \times 10^{-1}$ | $(1.2279 \pm 0.0001) \times 10^{-1}$ | $(1.2349 \pm 0.0002) \times 10^{-1}$ | 1.2002×10^{-1} |
| $\nu \sum_{F2}$ | $(1.9947 \pm 0.008) \times 10^{-1}$ | $(1.8721 \pm 0.0002) \times 10^{-1}$ | $(1.8832 \pm 0.0004) \times 10^{-1}$ | 1.8165×10^{-1} |

| Table 2. U | UO ₂ fuel | rods tw | o-group | constants |
|------------|----------------------|---------|---------|-----------|
|------------|----------------------|---------|---------|-----------|

Table 3 shows the comparison among the multiplication factors obtained with the CITATION code using the two methodogies for constants generation (i.e. CITATION/SERPENT and CITATION/HAMMER) and the SERPENT MC transport one, taken as reference. One may note that the results obtained by the proposed methodology is 7255 pcm bigger than the transport SERPENT MC reference solution while the HAMMER multiplication factor is 1365 pcm smaller. A superestimated k_{eff} value using the proposed methodology was in fact expected since the chosen configuration was supercritical. In a supercritical configuration, there is an overstimative of the fission spectrum contribution. This leads to understimated values of homogenized group constants, which in turn results in larger values for k_{eff} [4].

| SERPENT | CITATION/SERPENT | CITATION/HAMMER |
|---------------------|------------------|-----------------|
| 1.0255 ± 0.0001 | 1.0999 | 1.0115 |

Table 3. Multiplication factors comparison

4. FINAL REMARKS

In this work, the SERPENT MC code was used to generate 3-D two-group diffusion constants for a supercritical configuration of IPEN/MB-01 reactor (i.e. with control rods withdraw). These constants were used in the CITATION diffusion code and compared with constants produced by the classical code HAMMER. Although the proposed methodology showed itself feasible, further investigations must be done. The next step of this study is to perform simulations of critical benchmarks. As demonstrated in [3, 4], the generation of few group constant for 2D infinity lattice has been successfully performed. However, for 3D finite reactors the diffusion coefficient estimate methodology has to be analyzed in detail.

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