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Homogenised group constants generation using Monte Carlo codes for diffusion calculation of pebble bed reactor

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Abstract. This study is focused on the development of homogenization technique for the ASTRA pebble bed critical facility. The methods of generating homogenized few-group cross sections using continuous energy Monte Carlo codes MCU-PTR and Serpent 2.1.29 for full core diffusion calculation of pebble bed reactor were studied. 13-group cross sections were used in the SHIPR diffusion code to calculate the simplified cores of the ASTRA critical facility with HTGR-type fuel and a graphite reflector. Cross-verification of Serpent and MCU-PTR applied to HTGR system was carried out. Different homogenization schemes were tested for the SHIPR model and compared against Monte Carlo solutions. Diffusion coefficients for the fuel calculated using out-scatter approximation and cumulative migration method (CMM) were compared. It was shown that diffusion coefficients for fuel of pebble bed reactor calculated by CMM may reduce the difference between the diffusion and Monte Carlo simulation. The abilities of Serpent and MCU-PTR for modelling pebble bed reactors were compared.

1. Introduction

Analysis of the ASTRA facility critical experiments is an important part of international HTGR verification and validation activities for the pebble bed design. A set of critical pebble bed configurations of the ASTRA-HTGR facility [1] was previously analyzed using SHIPR [2,3] diffusion code with 13-group cross sections (XS) generated with WIMS-D code [3,4]. Full 3-D model for the ASTRA-HTGR facility was developed using MCU-PTR code. Neutron multiplication factor, control rod worth, and fission reaction rate distribution over the core obtained in the diffusion and Monte Carlo simulations were compared with the measured results [5,6]. The diffusion and Monte Carlo results showed a good agreement with the measured data. However, in some cases the diffusion model gives larger error than Monte Carlo simulation. In this study, the attempt was made to improve the diffusion model by generating XS with Monte Carlo code.

The experience of testing of homogenization techniques for small-size light water research reactors showed that using of several Monte Carlo codes for generating few-group XS is useful [7]. MCU-PTR [7] and Serpent [8] were used for XS generation of the fuel and water reflector. Comparison of different homogenization options used in MCU and Serpent enables to reveal the main issues of few group XS generation. We extend this approach to the development of diffusion model for the pebble bed reactor.



2. Models and codes

Model problems calculations were performed using continuous-energy Monte Carlo codes Serpent 2.1.29 and MCU-PTR. The ENDF/B-VII.0 nuclear data library was used in Serpent simulations. The MCU-PTR calculations were performed using the ACE/MCU library for the energy region of $100 \text{ keV} < E < 20 \text{ MeV}$ and the BNAB/MCU library for the energy region of $2.15 \text{ eV} < E < 100 \text{ keV}$. ACE/MCU is the library of cross sections of neutron interaction with nuclei in the epithermal energy region in a pointwise representation obtained from the ENDF/B-VII.0 files for the most part. BNAB/MCU is an expanded and modified version of the BNAB-93 26-group system of constants. In the thermalization region, the simulations were performed using continuous-energy neutron interaction data. Graphite cross sections used in MCU-PTR calculations were obtained from the ENDF/B-VII.0 files.

The fuel pebbles were modeled in Serpent and MCU simulations as shown in figure 1. The unit cell of fuel lattice is presented. The distance between the pebbles centers was selected so that packing factor is equal to 0.609. Explicit particle fuel model was used in Serpent simulations. MCU uses the implicit particle fuel model that works by sampling new particles on the neutron flight path (CORN option).

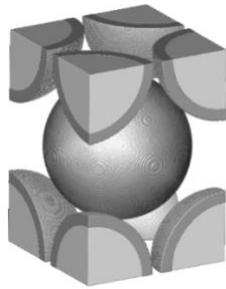


Figure 1. The ASTRA fuel cell.

A simplified model of the ASTRA facility was considered. Model #1 consists of the main structural components of the critical facility: the core, top, bottom, side, and inner reflector (figure 2). The geometry and the materials compositions used in Serpent and MCU simulations are the same.

Homogenized 13-group constants for the core and graphite reflectors were generated using MCU-PTR and Serpent in full-core and cell simulations. Energy group boundaries (in MeV) used in this study are as follows: $5.80\text{E-}08$; $1.00\text{E-}07$; $3.00\text{E-}07$; $4.00\text{E-}07$; $6.25\text{E-}07$; $7.80\text{E-}07$; $1.30\text{E-}06$; $2.10\text{E-}06$; $4.00\text{E-}06$; $1.60\text{E-}05$; $9.07\text{E-}04$; 0.183 . These group constants were then used in the SHIPR diffusion code. The spatial nodalization in SHIPR is the same as in the calculations presented in [5,6].

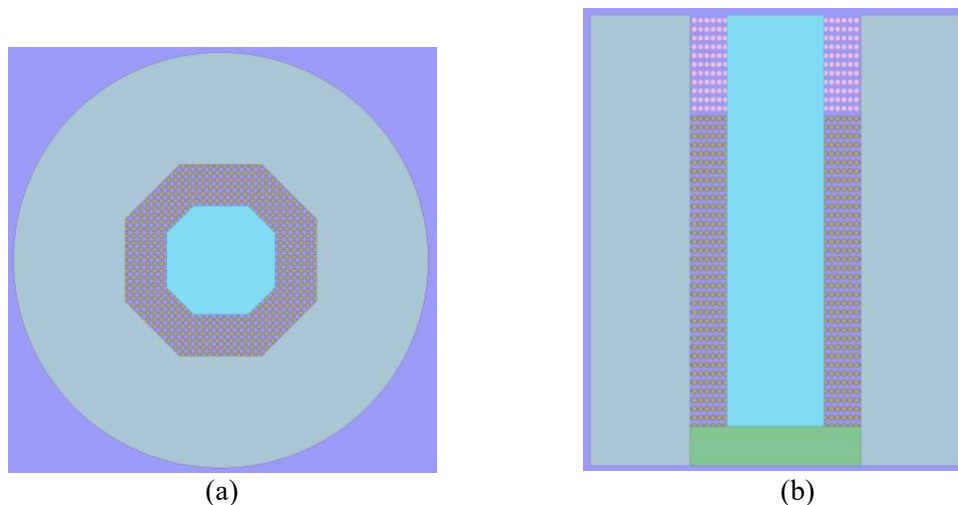


Figure 2. Horizontal (a) and vertical (b) cross section of the ASTRA simplified model #1.

3. Calculated results

Table 1 presents infinite multiplication factors and multiplication factors for model #1 calculated using Serpent and MCU.

Table 1. Comparison of multiplication factors calculated using Serpent and MCU.

Configuration	MCU	Serpent	Difference, % $\Delta k/k$
Unit cell	1.7718 ± 0.00008	1.7748 ± 0.00008	0.10
Model #1	1.1855 ± 0.00015	1.1963 ± 0.00015	0.76

A good agreement in infinite multiplication factor between Serpent and MCU is observed. Serpent overestimates the multiplication factor by 0.76% $\Delta k/k$ in comparison with MCU. Similar difference between MCU and Serpent with JEFF-3.1.1, JEFF-3.1, and ENDF/B-VII.0 data libraries was reported in [10]. Large difference in multiplication factor can be caused by differences in the graphite absorption cross section in different libraries [10]. But in our case the difference cannot be explained by the difference in graphite cross sections because the same graphite cross section libraries (ENDF/B-VII.0) were used in Serpent and MCU simulations. Comparison of the reaction balance of Serpent and MCU calculations showed that the difference in fission reaction is the major source of discrepancy.

The results of the described simulations performed by Serpent and MCU-PTR were further used as reference solutions.

13-group constants for the fuel zone and for the reflectors were generated in full-core 3D calculation using Serpent and MCU-PTR. 13-group constants for fuel were also generated in the unit cell model (with reflective boundary condition) using Serpent and MCU-PTR. Three options of diffusion coefficient calculation available in Serpent were tested: out-scatter approximation (D_INF), B1 approximation, and cumulative migration method (CMM) based on the calculation of the average square of the length of a neutron displacement before it is absorbed or removed from the energy group. CMM in Serpent can be used only for the cell with reflective boundary conditions. The method of diffusion coefficient calculation used in MCU is similar to the cumulative migration method, but it can be applied in full-core simulation in some cases.

Figure 3 shows the 13-group diffusion coefficients of the fuel zone, consisting of spherical fuel elements and air between them. Diffusion coefficients were obtained as a result of cell and full-scale calculations using MCU, Serpent, and WIMS.

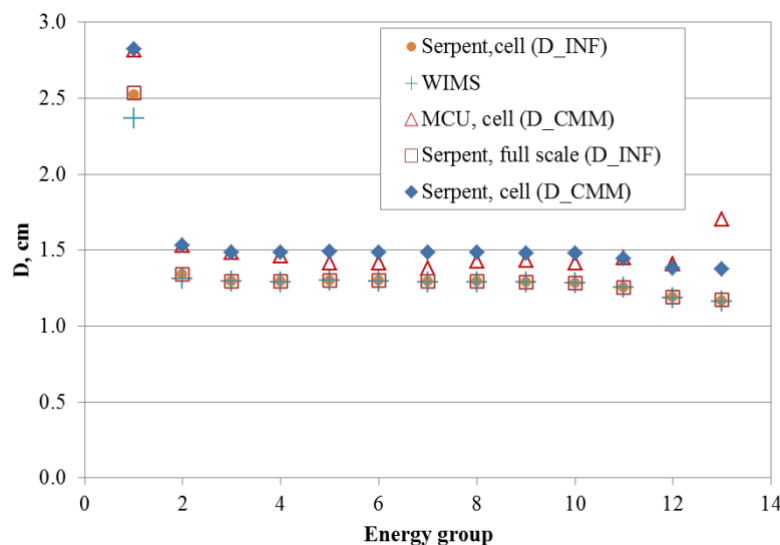


Figure 3. Fuel diffusion coefficients calculated using Serpent and MCU.

Diffusion coefficients calculated using Serpent in out-scatter approximation (D_{INF}) practically coincide with that calculated using WIMS (except for a small difference in the 1st group). The diffusion coefficients calculated in infinite lattice using Serpent and MCU using cumulative migration method (D_{CMM}) are close to each other and are larger than the coefficients in out-scatter approximation by $\sim 15\%$. This can be attributed to the fact that cumulative migration method describes heterogeneity effect in the fuel zone consisting of fuel pebbles in air better than out-scatter approximation. Diffusion coefficients calculated using B1 approximation is similar to that obtained using out-scatter approximation.

Figure 4 shows the 13-group diffusion coefficients of the external graphite reflector. For solid graphite, the diffusion coefficients calculated in out-scatter approximation (Serpent D_{INF} and WIMS) practically coincide with CMM diffusion coefficients (except for the 13th group for MCU). This can be attributed to low anisotropy of scattering in graphite. The diffusion coefficient of the 13th group, calculated by MCU, as in the case of fuel, increases in comparison with the previous groups. This can be explained by the peculiarities of calculating thermalization in the MCU.

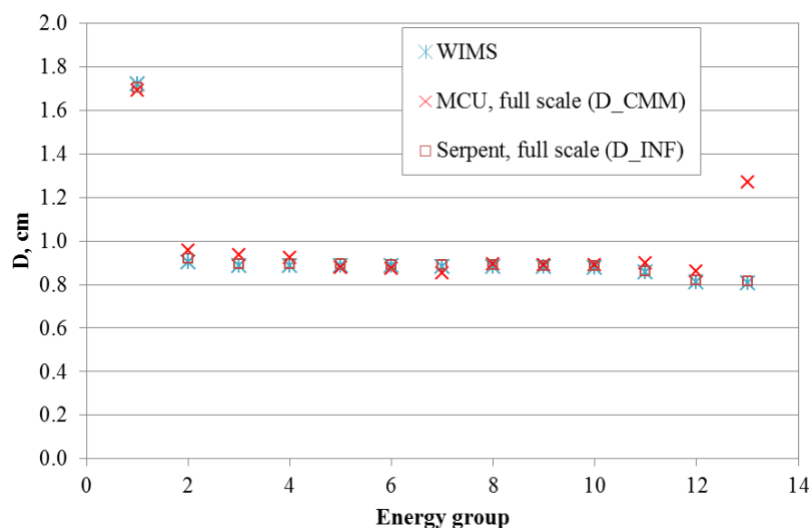


Figure 4. Graphite reflector diffusion coefficients calculated using Serpent and MCU.

The obtained diffusion coefficients and cross sections for fuel and graphite were tested by comparing the corresponding diffusion calculations of model #1 with the results of Monte Carlo calculations. The results of k_{eff} calculations for model #1 are shown in tables 2 and 3. The deviation of the multiplication factor calculated using the diffusion code SHIPR from the result of the Monte Carlo calculation is also presented. For calculations with XS prepared using Serpent (cases #1-#3), the Serpent results were used as the reference solution. For calculations with XS prepared using MCU (cases #4-#5), the MCU results were used as the reference solution. Diffusion coefficients and XS generated in infinite lattice (cell) and in full-core simulation (full-core) were used. In case of full-core simulation by Serpent, diffusion coefficients were generated using out-scatter approximation (D_{INF}). In infinite lattice simulation diffusion coefficients were generated using CMM (D_{CMM}). In case of full-core and infinite lattice simulation by MCU diffusion coefficients were generated using CMM.

It can be seen from table 2, that using of diffusion coefficients for fuel from CMM improves the agreement between the diffusion and Monte Carlo simulation. Using of out-scatter diffusion coefficients for fuel leads to the overestimation of k_{eff} by $0.25\% \Delta k/k$. As for the diffusion calculation with MCU XS, better agreement in case of using of group constants from full-core Monte Carlo simulation is shown.

Table 2. The results of diffusion calculation with various XS generated using Serpent.

Case #	Fuel		Reflector		k_{eff}	Deviation, % $\Delta k/k$
	D	XS	D	XS		
1	cell (D_CMM)	cell	full-core (D_INF)	full-core	1.2016	0.37
2	full-core (D_INF)	full-core	full-core (D_INF)	full-core	1.2041	0.54
3	cell (D_CMM)	full-core	full-core (D_INF)	full-core	1.2004	0.29

Table 3. The results of diffusion calculation with various XS generated using MCU.

Case #	Fuel		Reflector		k_{eff}	Deviation, % $\Delta k/k$
	D	XS	D	XS		
4	cell	cell	full-core	full-core	1.1774	-0.58
5	full-core	full-core	full-core	full-core	1.1821	-0.24

4. Conclusions

13-group diffusion XS generated using MCU-PTR and Serpent 2.1.29 for the simplified core of pebble bed reactor were tested. The difference in k_{eff} between the diffusion and Monte Carlo calculation is less than 0.6% $\Delta k/k$ for all considered variants. It was shown that diffusion coefficients for fuel of pebble bed reactor calculated by CMM may reduce the difference between the diffusion and Monte Carlo simulation. Out-scatter approximation is suitable for the calculation of diffusion coefficients of solid graphite reflector. Further investigations are needed to extend the obtained results to real configuration of ASTRA facility.

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