Evaluation of PBMR-400 Core Design Steady State Condition with Serpent and AGREE

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Abstract. The significant recent advances in computer speed and memory have made possible an increasing fidelity and accuracy in reactor core simulation with minimal increase in the computational burden. This has been important for modeling some of the smaller advanced reactor designs for which simplified approximations such as few groups homogenized diffusion theory are not as accurate as they were for large light water reactor cores. For narrow cylindrical cores with large surface to volume ratios such the Ped Bed Modular Reactor (PBMR), neutron leakage from the core can be significant, particularly with the harder neutron spectrum and longer mean free path than a light water reactor. In this paper the core from the OECD PBMR-400 benchmark was analyzed using multigroup Monte Carlo cross sections in the HTR reactor core simulation code AGREE. Homogenized cross sections were generated for each of the discrete regions of the AGREE model using a full core SERPENT Monte Carlo model. The cross sections were generated for a variety of group structures in AGREE to assess the importance of finer group discretization on the accuracy of the core eigenvalue and flux predictions compared to the SERPENT full core Monte Carlo solution. A significant increase in the accuracy was observed by increasing the number of energy groups, with as much as a 530 pcm improvement in the eigenvalue calculation when increasing the number of energy groups from 2 to 14. Significant improvements were also observed in the AGREE neutron flux distributions compared to the SERPENT full core calculation.

1. Introduction

The "two-step" few group, homogenized method for solving the neutron transport equation has been used successfully for the analysis of most all large Light Water Reactors [1]–[4]. However, the methods have not been as accurate for reactor cores that are not as optically thick and are not scattering-dominant system which is the case for some of the smaller advanced reactor concepts. The research here focused on the High Temperature Reactor (HTR) which is one of the six type reactor designs that were proposed in the Generation IV Forum (GIF) in 2002 [5]. The neutronic modeling of the HTR using the few group homogenized diffusion approximations has several limitations, particularly for the PBMR-400 core analyzed here which introduces the additional complexity of the double heterogeneity in modeling Pebbles with TRISO fuel [5].

The analysis here was performed using the OECD PBMR-400 Benchmark. The Monte Carlo Code SERPENT and the deterministic core simulator AGREE were used to analyze the PBMR-400. PBMR-400 is the reactor of choice in this analysis due to the data availability of PBMR-400 benchmark results. Some works related to PBMR-400 steady-state and transient analysis has been done in the past [6][7]. This work is meant to be a part to verify the use of two-step method using Monte Carlo generated cross sections and diffusion theory to obtain k-eigenvalue, power, and flux distribution. Using this analysis, similar analysis can be done in the future for any advanced reactor, especially HTR, which has similar system to PBMR-400.

This work was performed as part of a collaboration between ORNL and Department of Nuclear Engineering and Radiological Sciences, University of Michigan to assess and verify the SCALE/PARCS/AGREE code system for advanced reactor analysis. One particular task in this project is to perform full core analyses of PBMR-400 benchmark by generating nodal data from Monte Carlo method to model the full core with the cylindrical diffusion kernel in the AGREE code.

2. OECD PBMR-400 Benchmark

The Pebble-Bed Modular Reactor (PBMR) is a pebble-type High Temperature Gas Cooled Reactor (HTGR) that incorporates a closed cycle primary coolant system utilizing helium as coolant to transfer heat energy from modular core to a recuperative Brayton Cycle power conversion unit with a single-shaft turbine/compressor/generator. This type of reactor provides simplification and a substantial increase in overall system and efficiency and inherent safety with lower capital and operational cost.

The core contains approximately 451,527 fuel pebbles with a packing fraction of 0.61. The packing fraction of 0.61 was achieved by randomizing the pebble positions using Serpent's capability to model pebble position explicitly. The uranium loading is 9 g per fuel-sphere with the ^{235}U enrichment at 9.6%. The inner 5 cm of the fuel sphere contains about 15,000 UO_2 TRISO-coated micro-spheres within a graphite matrix and surrounded by an outer graphite fuel free zone. Each coated particle acts as a fission product barrier [6].

Table 1. PBMR-400 design characteristics

Installed thermal capacity (MW)	400
Core height (m)	11
Core configuration	Vertical with fixed center graphite reflector
Inner core diameter (m)	2
Outer core diameter (m)	3.7
Primary coolant	Helium
Primary coolant pressure (MPa)	9
Moderator	Graphite
Core outlet temperature (°C)	900
Core inlet temperature (°C)	500

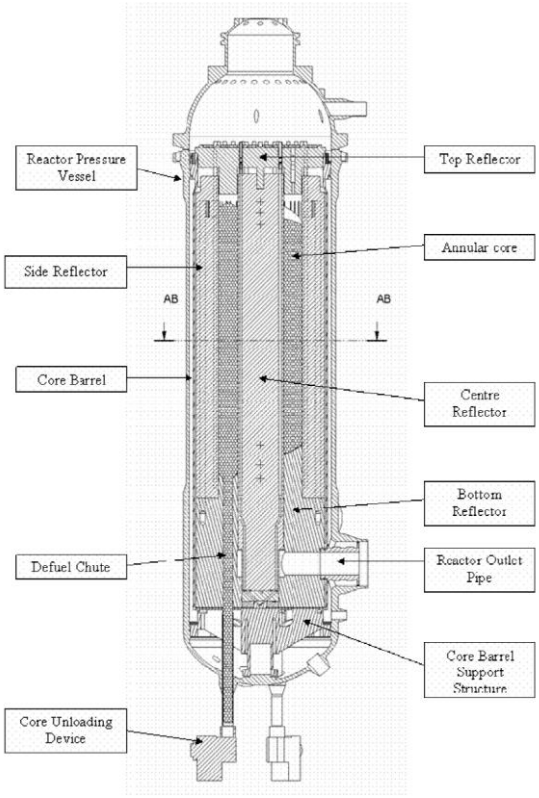

Figure 1. PBMR schematics

Table 2. PBMR-400 core characteristics

Fuel pebble diameter	6 cm
Outer graphite shell thickness	0.5 cm
Heavy metal content per pebble	9 g
Fuel enrichment	9.6%
Number of fuel kernels	15000
UO_2 kernel radius	0.0025 cm
UO_2 density	10.4 g/cm^3
Coating layer material	PyC/PyC/SiC/PyC
Coating layer thickness	0.0095/0.004/0.0035/0.004 cm
Coating layer densities	1.05/1.9/3.18/1.9 g/cm^3
Density of graphite matrix	1.77 g/cm^3
Reflector material	Graphite
Reflector density	1.78 g/cm^3
Control rod material	B_4C
B-10 content of B_4C	6 ppm
Total number of pebbles	451,527

In the benchmark design, core analysis was performed using the Very Superior Old Program (VSOP) which utilized a set of two-group macroscopic cross-section data for each distinct core region which included fuel regions with different mixtures of burned pebbles, as well as reflector and control rod regions [8]. The cross sections were prepared stored in multi-dimensional tables as a function of five state-parameters, to include fuel temperature, moderator temperature, xenon concentration, as well as fast and thermal buckling to represent the leakage spectral effects. All cross terms dependencies were included which were determined by linear interpolation on a 5-dimensional space [6].

3. Core Simulation

3.1. Monte Carlo Neutronics

The Serpent Monte Carlo code, developed at VTT Technical Research Centre of Finland, is a continuous-energy Monte Carlo particle code. It has been enabled to perform lattice physics calculations to obtain homogenized cross sections for use in nodal diffusion calculations. Although a large number of particle histories can be required to minimize the statistical uncertainty and provide accurate multi-group data, Monte Carlo methods are attractive for lattice physics calculations since they are able to solve any arbitrary and complicated three-dimensional problems with minimal physics approximations [9], [10]. This is particularly attractive for modeling the HTR with complex physics such as the double heterogeneity introduced by the TRISO fuel form.

Serpent has unique capabilities with regards to the modeling of pebble bed reactors. Serpent can not only model the random pebble distribution, but it can also model the random TRISO distribution inside the pebbles. This modeling is done explicitly in which the location of each pebble is generated using an automated disperser routine. Serpent only requires a file with the position of each pebble's center point. Serpent uses this information to explicitly represent the location of pebbles in the core without applying any homogenization.

For the analysis of the PBMR-400 in this work, Serpent was used for preparation of the multi-group homogenized cross sections as well as to provide a detailed reference calculation without energy, angular, or spatial discretization error. The version of Serpent used in this work is 2.1.31.

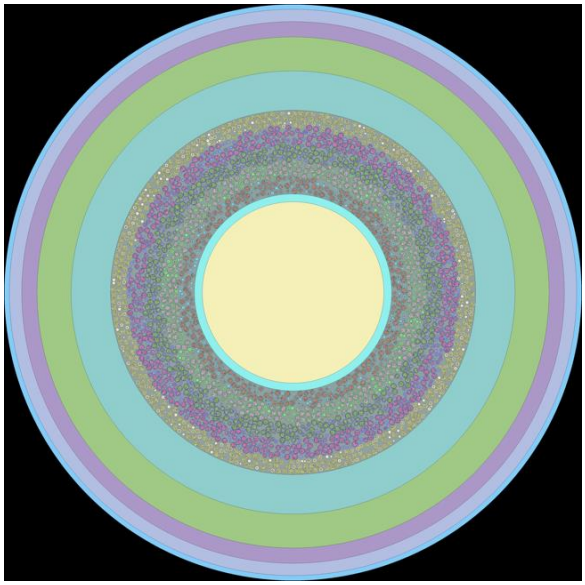

Figure 2. Radial configuration of Serpent PBMR-400

3.2. AGREE HTR Simulator

Cross sections that were calculated in Serpent were processed by the cross-section data converter GenPMAXS to generate a PMAXS cross section file that would be read by AGREE. Cross section was prepared for each of the distinct core regions of the PBMR-400. These cross sections contain 110 cross section data for 110 fuel regions and 470 reflector region that has been defined in the benchmark document. region division is shown in Figures 2 and 3.

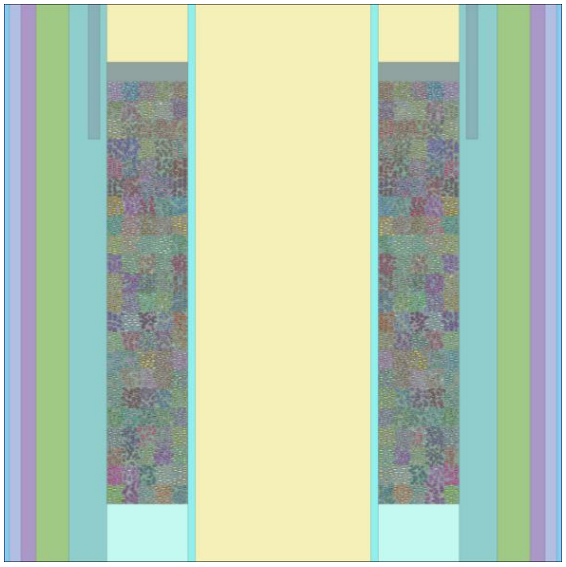

Figure 3. Axial configuration of Serpent PBMR-400

The AGREE (Advance Gas Reactor Evaluator) was developed for the U.S. NRC as a thermo-fluids code to solve the steady state and time dependent mass, momentum, and energy equations in three-dimensions for High Temperature Gas Cooled reactor analyses. AGREE has two separate versions, one for Pebble Bed type reactor applications and another for Prismatic type reactors. The pebble bed version of AGREE was recently updated to provide functionality for the Fluoride salt-cooled High temperature Reactor (FHR) designed by Kairos Power [11].

3.3. Core Calculation

The procedure used here to perform core simulation is depicted in Fig. 5. Serpent was used to generate nodal cross sections for the AGREE code, as well as full core reference calculations. The Serpent k-eff eigenvalue and power distribution results will be used as reference for AGREE results.

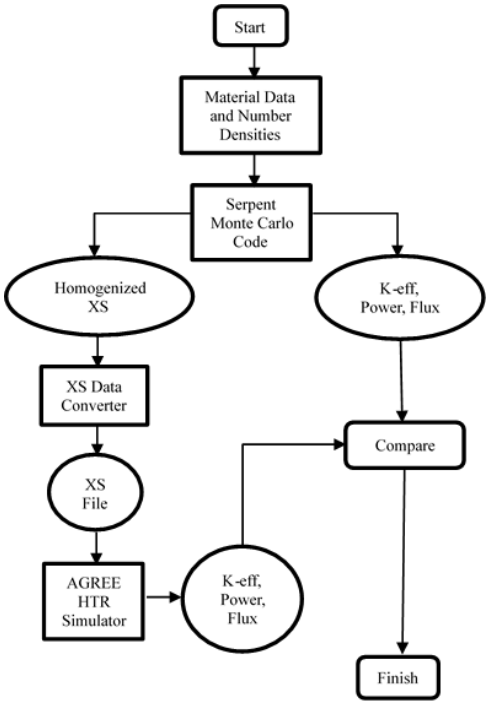

Figure 4. Research method employed in this work

The type of two-step code system method has been used in previous modeling of High-Temperature Gas Reactor, as for example by Argonne National Laboratory (ANL) using DRAGON as lattice transport code and DIF3D as nodal diffusion code. In this study, significant errors were reported using the two-step method compared to the result of Monte-Carlo code [12].

PBMR-400 cross sections were calculated using Serpent with various few-group configurations using ENDF 7.1 Library. Energy cut-offs for each group is tabulated in Table 3. In each calculation, 500,000 neutron histories were used in order to minimize statistical standard deviation to approximately 10pcm. For full core calculations, a vacuum boundary condition was used.

Table 3. Energy cut-off boundaries (Unit: eV) [13]

23	14	7	4	2
3.679E+06				
1.353E+06				
5.000E+05	5.000E+05	5.000E+05		
1.110E+05	1.110E+05			
6.738E+04	6.738E+04			
9.118E+03	9.118E+03	9.118E+03	9.118E+03	
3.673E+02	3.673E+02			
4.000E+00	4.000E+00	4.000E+00		
				3.059E+00
1.500E+00				
1.097E+00	1.097E+00	1.097E+00		
1.045E+00				
9.720E-01	9.720E-01			
8.500E-01	8.500E-01		8.500E-01	
5.000E-01	5.000E-01	5.000E-01		
4.000E-01				
3.500E-01	3.500E-01			
3.000E-01				
2.500E-01				
1.800E-01				
1.400E-01	1.400E-01			
1.000E-01		1.000E-01	1.000E-01	
5.000E-02	5.000E-02			

4. Results and discussions

4.1. k-eff Eigenvalue Comparison

Homogenized multi-group cross section data was generated for 580 regions of the full core model of the PBMR-400, including 110 regions of fuel assemblies and 470 region of non-fuel assemblies. In this section, comparison of k-eff eigenvalue results between Serpent and AGREE is provided with the standard deviation for Monte Carlo calculation and also the overall absolute difference between Serpent and AGREE. These results are tabulated in Table 4.

As indicated in Table 4 the k-eff eigenvalue difference between Serpent and AGREE decreases as the number of energy groups used in the calculation increases. However, from 14-groups to 23-groups, the difference is not as significant as the previous few-groups. In Serpent, the number of neutrons used per cycle is 500,000. To assess the statistical uncertainty of the results, 1,000,000 neutrons per cycle is also calculated and the results are tabulated in Table 5 and as indicated 500,000 histories appear to be sufficient.

Table 4. k-eff eigenvalue results of AGREE and Serpent with 500,000 neutrons per cycle, 600 cycles

Groups	Serpent		AGREE	Δk-eff (pcm)
	k-eff	σ (pcm)	k-eff	
2	0.995002	4.6	1.002107	710.5
4	0.995039	4.6	0.999852	481.3
7	0.994955	4.6	0.997337	238.2
14	0.994805	4.7	0.996580	177.5
23	0.994795	4.6	0.995914	111.9

Table 5. k-eff eigenvalue results of AGREE and Serpent with 1,000,000 neutrons per cycle, 1200 cycles

Groups	Serpent		AGREE	Δk-eff (pcm)
	k-eff	σ (pcm)	k-eff	
2	0.995028	2.3	1.002132	710.4
4	0.995034	2.4	0.999804	477.0
7	0.995005	2.1	0.997323	231.8
14	0.994788	2.2	0.996559	177.1
23	0.994763	2.3	0.995913	115.0

The general conclusion from the eigenvalue results is that more than 2 or 4 energy groups are necessary to accurately describe the core leakage and achieve a reasonable prediction of the core eigenvalue for modeling the PBMR-400.

4.2. Flux Distribution Comparison

The group-wise neutron fluxes from the full core Serpent calculation are compared to the AGREE calculation in this section. Because of space limitations, the results shown focus on the radially and integrated distributions of the thermal fluxes for each of the multi-group calculations shown in Table 5. The radial flux distributions are obtained by volume averaging the axial fluxes in each ring. The results are displayed in Fig. 5 to Fig. 9.

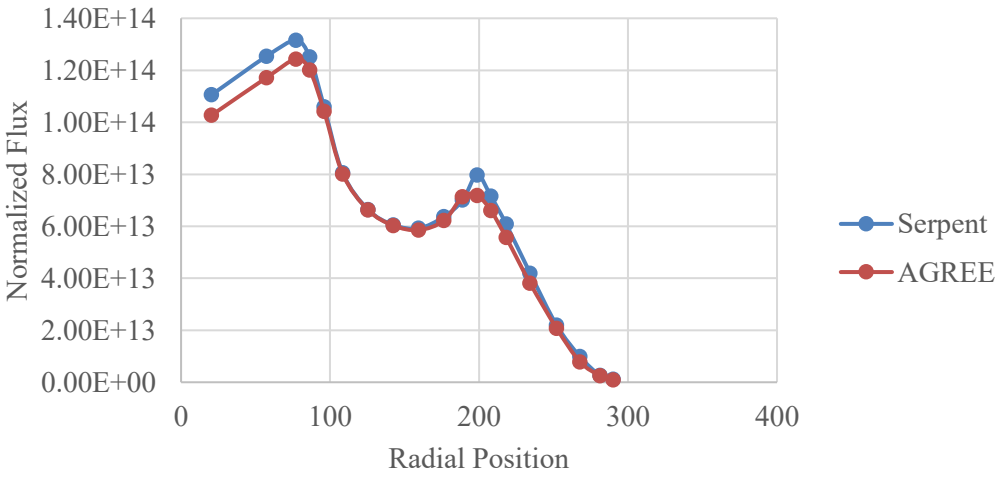

Figure 5. Radial thermal flux of 2-groups core

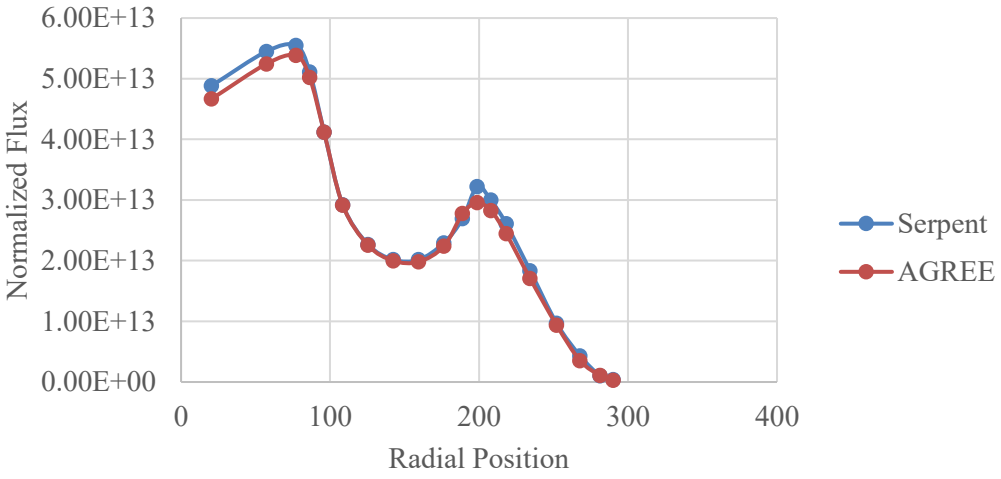

Figure 6. Radial thermal flux of 4-groups core

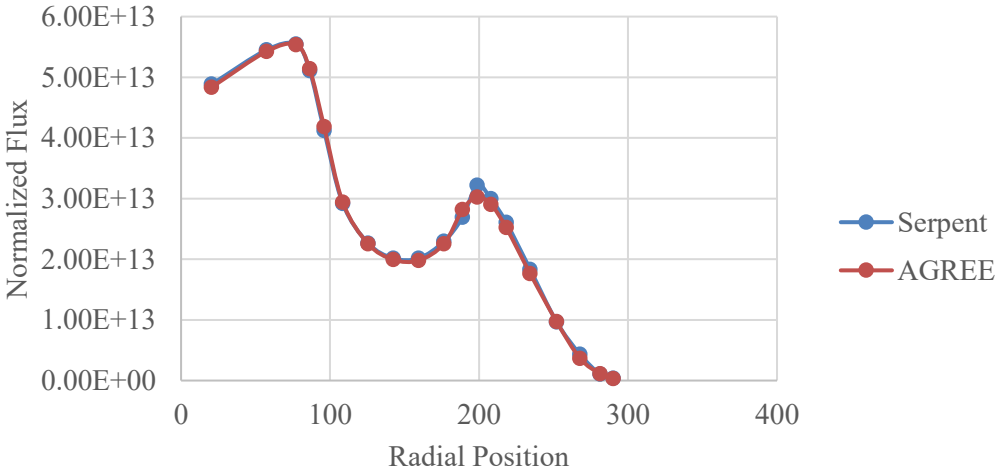

Figure 7. Radial thermal flux of 7-groups core

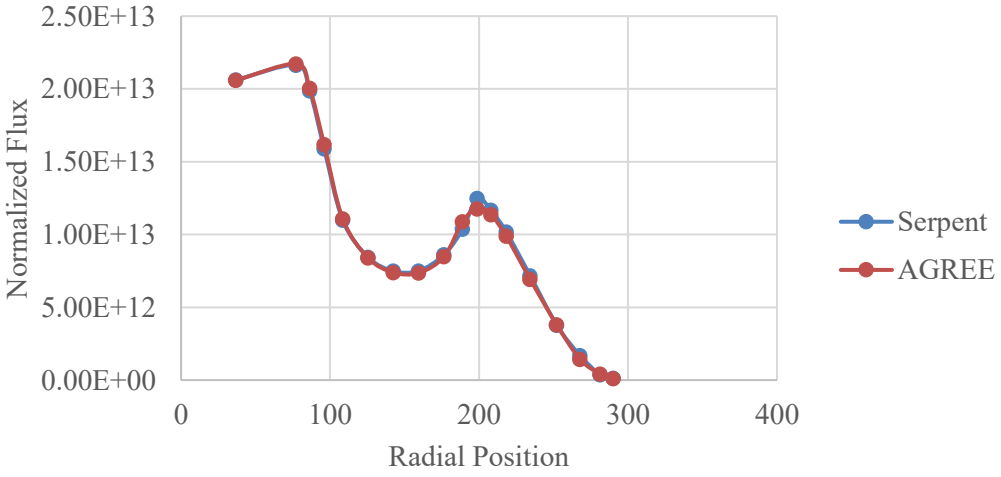

Figure 8. Radial thermal flux of 14-groups core

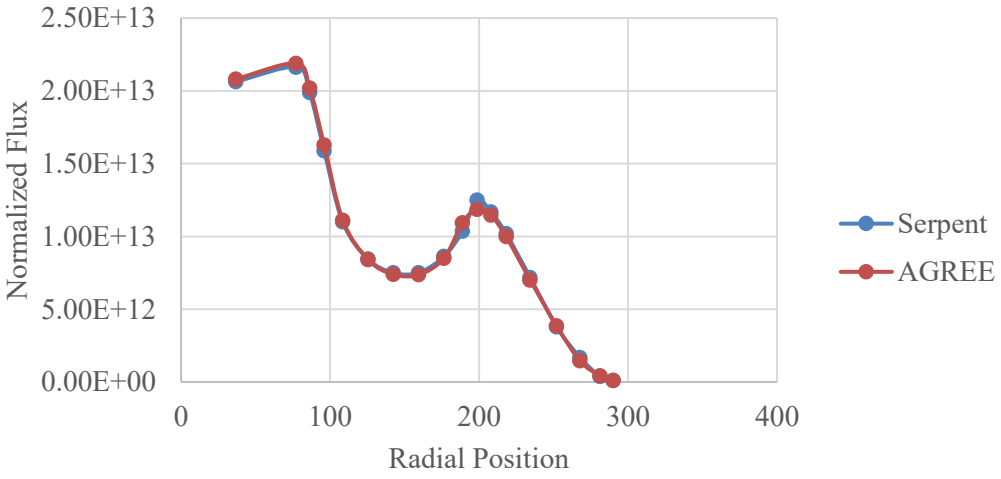

Figure 9. Radial thermal flux of 23-groups core

Similar to the results for the eigenvalue calculation shown in Tables 4 and 5, the results for the radial thermal flux distributions indicate better agreement of the Serpent and AGREE results as the number of groups increases. For the 23-group core, the maximum relative error is 14.5% at the outermost position of the core. Noticeable relative errors are observed at position 96.025 cm and 188.975 cm, which is the interface between the reflector and fuel regions. In general, there is good agreement between the radial flux distributions of AGREE and Serpent.

4.3. Power Distribution Comparison

The radially integrated axial power distributions were also edited and are shown in this section for each of the few group calculations in Fig. 10 to Fig. 14.

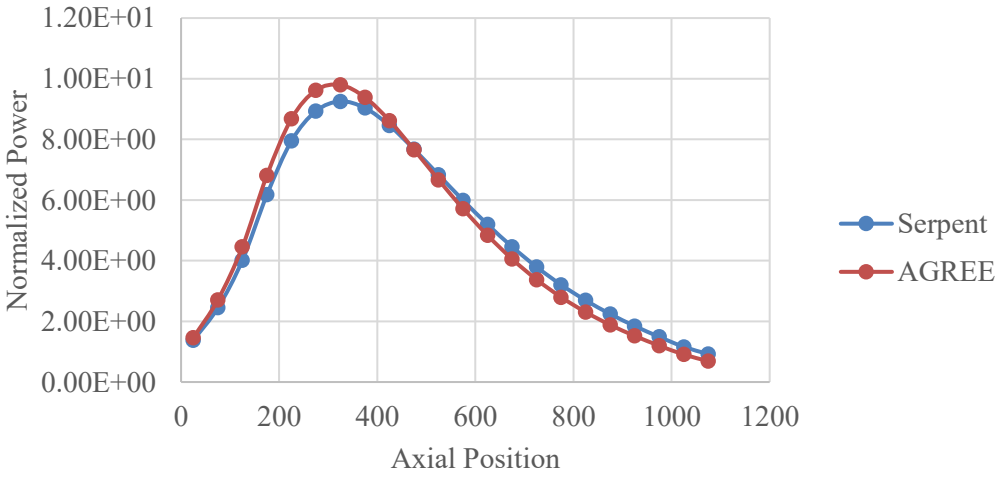

Figure 10. Axial power distribution of 2-groups core

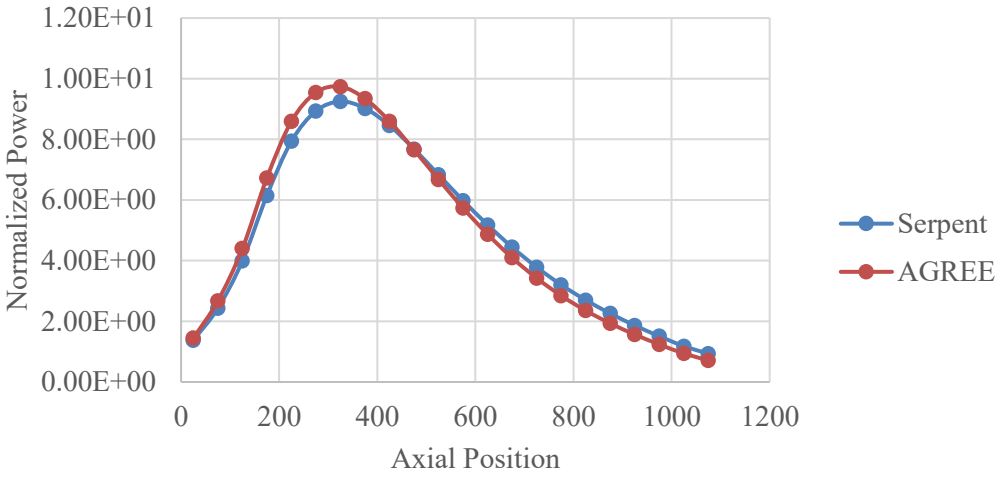

Figure 11. Axial power distribution of 4-groups core

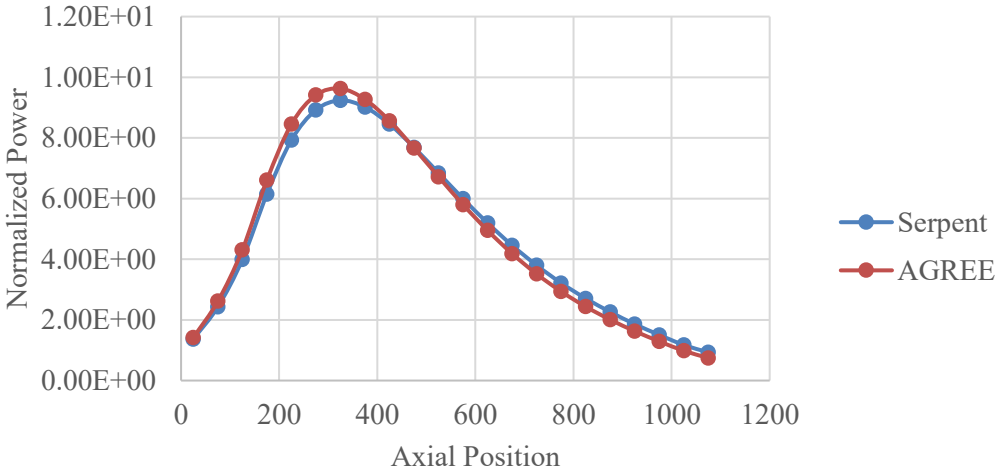

Figure 12 . Axial power distribution of 7-groups core

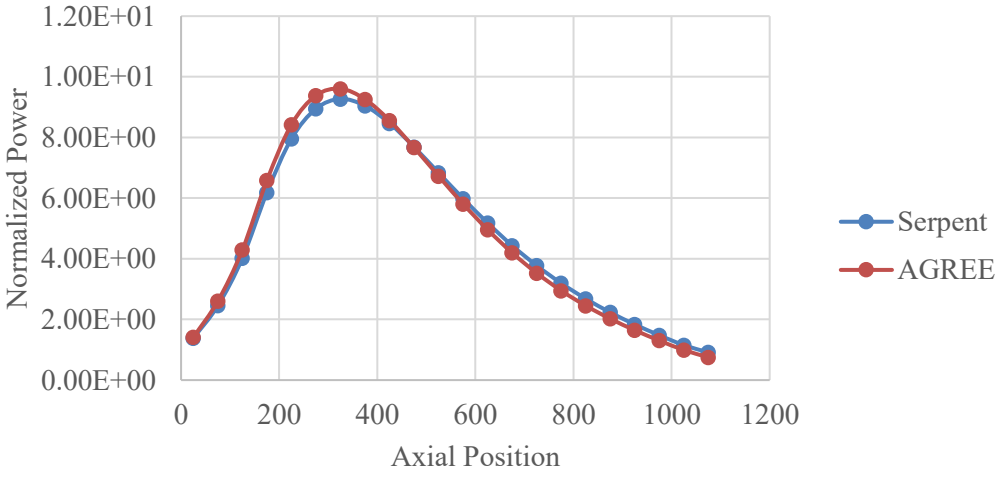

Figure 13. Axial power distribution of 14-groups core

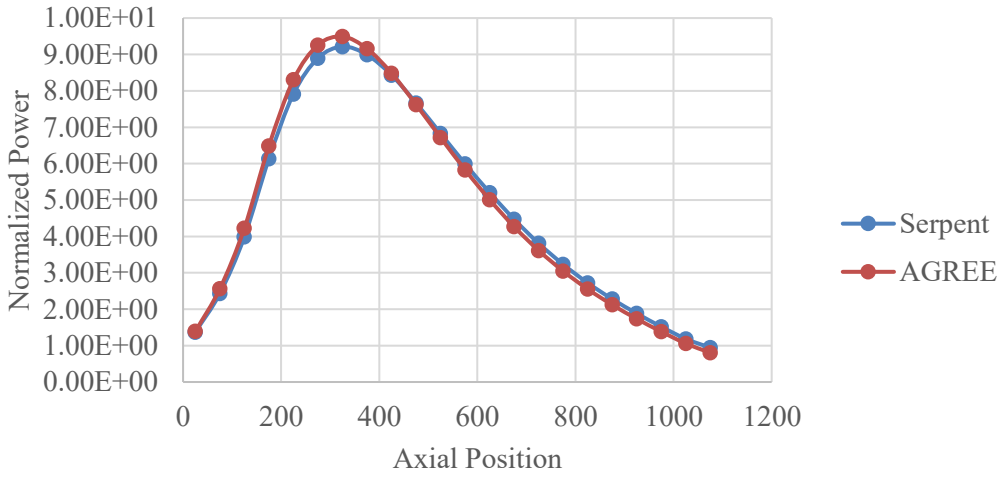

Figure 14. Axial power distribution of 23-groups core

As indicated in the figures, the agreement between AGREE and Serpent again improves with increasing number of groups. It is also apparent that the highest relative error from each few-group core is at the bottom of the core at the fuel and reflector interface.

5. Conclusions

The neutronics simulation of the PBMR-400 using the deterministic core simulator AGREE with multi-group cross sections generated using the Monte Carlo code Serpent showed considerable improvement in the agreement with the full core Serpent result as the number of energy groups was increased. An eigenvalue improvement of approximately 530 pcm was observed when the number of energy groups was increased from 2 to 23. However, even with 7 energy groups sufficiently accurate results were obtained with could be considered acceptable for core analysis. Similar improvements were observed in the flux and power distributions as the number of energy groups were increased.

Work is continuing on the incorporation of assembly discontinuity factors into the deterministic core calculation, as well as the analysis of calculations at the full range of core power and temperature conditions. This work will involve the assessment of using color set or supercell models at the various temperature conditions instead of relying on full core Monte Carlo for every branch calculation necessary for practical reactor simulation.

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