The Monte Carlo Method: Versatility Unbounded In A Dynamic Computing World
Chattanooga, Tennessee, April 17–21, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

Accuracy of MICROX-2 for PBR Analysis Using Monte Carlo Technique

Nathanael Hudson, Germina Ilas[a], Farzad Rahnema[*]
Nuclear and Radiological Engineering/ Medical Physics Program
George W. Woodruff School of Mechanical Engineering
Georgia Institute of Technology, Atlanta, GA 30332-0405
farzad.rahnema@nre.gatech.edu

Abderrafi Ougouag[**], Hans Gougar, and William Terry
Idaho National Laboratory
Idaho Falls, Idaho 83415-3885
oom@inel.gov

Ramatsemela Mphahlele
National Nuclear Regulator
PO Box 7106, Centurion 0046, South Africa

ABSTRACT

One of the important issues in a nodal diffusion analysis of a PBR core is the generation of accurate nodal constants. As compared to a light water reactor (LWR) lattice, in which the variation of the core properties in the axial direction is relatively weak and therefore a 2-D modeling appropriate, the calculation at the core sub-region level for a PBR needs to account for the third spatial dimension because of the complex geometry (double heterogeneity) of packed arrangements of spherical pebbles.

The purpose of the present work was to assess the capability of the MICROX-2 code to generate accurate nodal cross sections for PBR lattices. This preliminary evaluation was based on comparison to a continuous-energy, doubly heterogeneous MCNP reference model. The terms of the comparison were the infinite medium multiplication factor, the few-group cell-homogenized total, capture and fission cross-sections, and the spectral indices. The principal phenomena covered by these choices pertain to resonance treatment and double heterogeneity. The models developed here do not attempt to evaluate the effect of packing randomness at either heterogeneity level. Such a study will be discussed elsewhere.

The double heterogeneity of the lattice cell was fully modeled in the MCNP reference model. The cell-homogenized few-group cross sections and spectral parameters were calculated in MCNP by using the reaction rates and flux tallies. A spherical geometry model was used with MICROX-2. The analysis was completed at cold, room temperature (296 K) and at hot operating conditions (1073 K). For consistency, the same cross section data files were used for generating both the pointwise cross sections for MCNP and the fine-group cross sections for MICROX-2. Results showed significant differences between the MCNP and the MICROX-2 results, especially in the thermal and resonance energy range.

Key Words: nodal cross section(s), MICROX-2, PBR

---

[a] current address: Oak Ridge National Laboratory, Oak Ridge, TN 37831-6172
ilasg@ornl.gov

1 INTRODUCTION

One of the important issues in a nodal diffusion analysis of a pebble-bed reactor (PBR) core is the generation of accurate nodal constants, which strongly influences the accuracy of the diffusion approximation. The calculation at the core sub-region level for a PBR needs to consider or account for the third spatial dimension because of the complex geometry (double heterogeneity) of packed arrangements of spherical pebbles. There are two levels of heterogeneity: a three-dimensional random distribution of fuel grains within the pebble core and a three-dimensional packing of the pebbles within the reactor core.

The purpose of the present work is to assess the capability of the MICROX-2 [1] code to generate accurate nodal cross sections for PBR lattices. Previous evaluations of MICROX-2 for the PBR [2] compared the code to a singly heterogeneous MCNP benchmark and reported as a basis for comparison solely the spectral indices. This current assessment is based on the comparison to a continuous-energy doubly heterogeneous MCNP [3] reference model. The terms of the comparison are the multiplication factor, the few-group cell-homogenized total, capture and fission cross sections, and the spectral indices of a Body-Centered-Cubic (BCC) pebble lattice cell at a 61% packing fraction. The spectral indices calculated are the ratio of epithermal to thermal U^{238} captures (ρ^{28}), the ratio of epithermal to thermal U^{235} fissions (ρ^{25}), the ratio of U^{238} fissions to U^{235} fissions (δ^{28}), and the ratio of U^{238} capture to U^{235} fissions (C*). Two temperature conditions are considered: a cold case at 296 K and a hot case at 1073 K for the pebble and 998 K for the coolant.

2 PROBLEM DESCRIPTION

2.1 Reference Model

The reference geometry model is a BCC arrangement of 3-cm-radius pebbles, as shown in Figure 1, with a packing fraction of 61 %. This packing fraction was chosen as it has been indicated [4] as the closest approximation to the real random distribution of the pebbles in a reactor core. Each pebble has a 2.5-cm-radius inner region containing 15,000 spherical fuel grains in a graphite matrix and a graphite outer shell. Each fuel grain consists of a uranium oxide kernel 0.025 cm in radius at 8% enrichment, coated with four carbon-based layers for an outer radius of 0.045 cm [5].

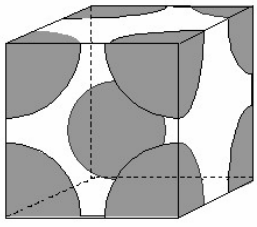

Figure 1: Body-Centered-Cubic Lattice

The side of the cubic cell in Figure 1 is 6.298 cm. The region around the pebbles in the cell contains helium as a coolant. A reflective boundary condition is used on the outer surfaces of the cubic cell.

2.2 MCNP Model

The double heterogeneity of the lattice cell is fully modeled in MCNP. The fuel grains within the pebble core are explicitly modeled using, for convenience, a BCC arrangement as used for the pebble lattice. As noticed by Karriem, et al. [6], the type of the lattice used to model the arrangement of the fuel grains is generally unimportant because of the large inter-grain distance with respect to the grain diameter. The grain packing fraction here is approximately 9%.

In order to be completely consistent when comparing cross sections, a cold/hot MCNP continuous-energy library was generated based on the same ENDF/B-VI data files as used to generate the fine-group library for use with MICROX-2. The NJOY99.90 [7] code was employed, with 0.001 as tolerance value. The cell-homogenized cross sections and spectral indices were calculated by using the reaction rates and flux tallies in MCNP.

2.3 MICROX-2 Model

The MICROX-2 code solves the B-1 slowing-down equations at 10000 lethargy points for a fine-group spectrum. This spectrum is then collapsed to the coarse group structure of interest. The geometry considered is a 1-D two-region cell, the two regions being coupled through collision probabilities. The inner region models the fuel zone of the pebble, and the outer region is a homogenized mixture of the graphite shell and helium coolant. The volume of the outer region is calculated to ensure the same pebble packing fraction as used for the reference MCNP model.

MICROX-2 accounts for the double heterogeneity of the pebble-bed lattice cell through the use of two Dancoff factors, one for the grain structure and the other for the pebble lattice. While the former is calculated internally through the Wälti Method [1], the latter Dancoff factor must be provided by the user, along with the corresponding total macroscopic cross section of the moderator region for which this factor was calculated. Only one pebble lattice Dancoff factor must be input for the geometry of interest, as a table of energy-dependent Dancoff factors is generated internally within MICROX-2.

As MICROX-2 is a one-dimensional code, the three-dimensionality of the lattice and the leakage is taken into account through the user-input Dancoff factor and the buckling. It is recommended in the user manual [1] that the determination of this Dancoff factor be consistent with the boundary condition desired for the analyzed system. In this study, the formulae derived by Westfall [8] and employed by Bende *et. al.* [9] were the basis for the computation of grey pebble lattice Dancoff factors for the geometric arrangement and packing fraction under consideration. The geometry model for which these formulae were developed consists of two concentric spheres (one fuel zone surrounded by a moderator region) with a white boundary condition on the outer surface. For the configuration analyzed in our study, we determined the following values of the pebble lattice Dancoff factor: 0.499288 and 0.498826 for the cold and hot temperature case, respectively. The moderator region macroscopic cross sections at which these Dancoff factors were calculated were both tallied in MCNP in the resonance region

between 7102 eV and 2.28 eV. The values of these cross sections were calculated as 0.408483 cm^{-1} and 0.408716 cm^{-1}, respectively. The fuel zone total cross sections used for the calculation of the pebble-lattice Dancoff factors were also tallied in MCNP as 0.416130 cm^{-1} and 0.417597 cm^{-1} for the cold and hot cases.

MICROX-2 requires a fine-group pointwise and groupwise library, which necessitates the use of the NJOY/MICROR system developed at the Paul Scherrer Institut [10]. The fine groupwise constants are created with NJOY99.90 in the General Atomics 193-group structure. The formatting code MICROR is used to transfer the NJOY point/group data to a binary form suitable for MICROX-2. The MICROX fast library data, which are temperature and dilution dependent, consists of 92 fine groups covering the 14.9 MeV to 2.38 eV energy range. The resonance library was created with 60000 data points between 8 keV and 0.414 eV, equally spaced in lethargy. The thermal library was constructed with temperature-dependent thermal neutron data sets covering 2.37 eV to 0.001 eV, with 101 variably spaced points in the energy structure.

3 RESULTS AND DISCUSSION

The cell-homogenized cross sections were calculated for a six-group structure. The energy boundaries considered, as shown in Table I, were based upon the V.S.O.P. [11,12] energy structure, with the additional boundaries of 7102 eV and 2.38 eV introduced due to limitations in MICROX-2 (all coarse-group boundaries must be a subset of the 193-group General Atomics structure).

Table I. Broad-Group Boundaries (eV)

	Group 6	Group 5	Group 4	Group 3	Group 2	Group 1	
E_6	E_5	E_4	E_3	E_2	E_1	E_0	
0.0	1.86	2.38	29.0	7102	0.111E6	1.49E7	

The results of the few-group cross sections and infinite-medium multiplication factor at room temperature are presented in Table II. As observed, the differences in the total and fission cross sections are less than 2.43 %. However, the comparison shows a large overestimation of the capture in the resonance region: 3.09 % and 11.35 % in groups 3 and 4, respectively. The infinite medium multiplication constant is under estimated by 1.84 %.

The results of the comparison at hot operating conditions are shown in Table III. At operating temperature the over (under)estimation does not change considerably as compared to the cold temperature, except in the case of the lower thermal (group 6) and resonance region (groups 3 and 4) captures, for which the overestimation increases with increasing temperature. The difference in the fission cross sections in the thermal groups is more than five times larger (~9 %) in the hot case as compared to the cold case. Again, the largest difference lies in the lower resonance region capture cross section (+15.08 %), as overpredicted by MICROX-2. The MICROX-2-predicted infinite multiplication factor for the hot case is 3.57 % smaller than the corresponding reference value.

Table II. Cross Section Comparison: 296 K

Cross Section	Group #	MCNP	σ^{rel}_{MCNP} (%)	MICROX-2	Diff[a] (%)
Total	1	1.6244E-01	0.02	1.6457E-01	***1.31***
	2	2.4486E-01	0.01	2.4580E-01	***0.38***
	3	2.5313E-01	0.01	2.5392E-01	***0.31***
	4	2.5306E-01	0.02	2.5261E-01	***-0.18***
	5	2.4680E-01	0.05	2.5150E-01	***1.91***
	6	2.5620E-01	0.04	2.5889E-01	***1.05***
Capture	1	2.8341E-05	0.16	2.8574E-05	***0.82***
	2	5.7710E-05	0.02	5.7333E-05	***-0.65***
	3	6.4958E-04	0.06	6.6968E-04	***3.09***
	4	2.4726E-03	0.08	2.7534E-03	***11.35***
	5	2.0842E-04	0.08	2.0666E-04	***-0.84***
	6	7.9889E-04	0.05	8.0250E-04	***0.45***
Fission	1	2.8994E-05	0.04	2.8707E-05	***-0.99***
	2	2.1648E-05	0.01	2.2136E-05	***2.25***
	3	1.6304E-04	0.02	1.6570E-04	***1.63***
	4	3.7038E-04	0.05	3.7939E-04	***2.43***
	5	1.4698E-04	0.07	1.4874E-04	***1.20***
	6	2.9039E-03	0.05	2.9372E-03	***1.15***
k_{inf}		1.51902	0.02	1.49114	***-1.84***

Table III. Cross Section Comparison: 1073 K

Cross Section	Group #	MCNP Hot	σ^{rel}_{MCNP} (%)	MICROX-2 Hot	Diff[a] (%)
Total	1	1.6243E-01	0.02	1.6457E-01	***1.32***
	2	2.4483E-01	0.01	2.4581E-01	***0.40***
	3	2.5351E-01	0.01	2.5426E-01	***0.30***
	4	2.5417E-01	0.02	2.5244E-01	***-0.68***
	5	2.4834E-01	0.06	2.4776E-01	***-0.23***
	6	2.5791E-01	0.04	2.5976E-01	***0.72***
Capture	1	2.8306E-05	0.16	2.8578E-05	***0.96***
	2	5.7720E-05	0.02	5.8096E-05	***0.65***
	3	7.8179E-04	0.06	8.1825E-04	***4.66***
	4	3.1172E-03	0.07	3.5871E-03	***15.08***
	5	2.0852E-04	0.08	2.0683E-04	***-0.81***
	6	5.6599E-04	0.05	6.0657E-04	***7.17***
Fission	1	2.8997E-05	0.04	2.8705E-05	***-1.01***
	2	2.1641E-05	0.01	2.2163E-05	***2.41***
	3	1.6262E-04	0.02	1.6532E-04	***1.66***
	4	3.7007E-04	0.04	3.8158E-04	***3.11***
	5	1.4701E-04	0.08	1.4864E-04	***1.11***
	6	1.9316E-03	0.05	2.1042E-03	***8.93***
k_{inf}		1.41473	0.02	1.36419	***-3.57***

In addition to the cell-homogenized macroscopic cross sections, the spectral indices were calculated, as shown in the formulae below, with the thermal boundary at 0.625 eV.

$$\rho^{28} = \frac{\int_{E>E_T} dE\Phi(E)\sigma_a^{238}(E)}{\int_{E<E_T} dE\Phi(E)\sigma_a^{238}(E)} \qquad \delta^{25} = \frac{\int_{E>E_T} dE\Phi(E)\sigma_f^{235}(E)}{\int_{E<E_T} dE\Phi(E)\sigma_f^{235}(E)}$$

$$\delta^{28} = \frac{\int dE\Phi(E)\Sigma_f^{238}(E)}{\int dE\Phi(E)\Sigma_f^{235}(E)} \qquad C^* = \frac{\int dE\Phi(E)\Sigma_a^{238}(E)}{\int dE\Phi(E)\Sigma_f^{235}(E)}$$

The flux spectrum chosen for the above calculations is simply the lattice-cell-averaged spectrum. The calculated spectral parameters for both the hot and cold case (MCNP and MICROX-2) are presented in Table IV.

Table IV. Spectral Indices

			BCC 61%	
			cold	**hot**
ρ^{28}	**epithermal-to-thermal ^{238}U captures**	**MCNP**	5.91	7.50
		MICROX-2	6.34	8.79
		diff (%)	***7.3***	***17.1***
δ^{25} **x** 10^2	**epithermal-to-thermal ^{235}U fissions**	**MCNP**	9.63	10.99
		MICROX-2	9.43	10.63
		diff(%)	***-2.0***	***-3.3***
δ^{28} **x** 10^4	**^{238}U fissions to ^{235}U fissions**	**MCNP**	28.08	30.14
		MICROX-2	27.60	28.52
		diff (%)	***-1.7***	***-5.4***
C^*	**^{238}U captures to ^{235}U fissions**	**MCNP**	0.360	0.463
		MICROX-2	0.388	0.534
		diff (%)	***7.8***	***15.3***

As can be seen in Table IV, the largest differences between MICROX-2 and MCNP occur for those parameters involving U^{238} captures. The largest difference is seen for ρ^{28}, which is overestimated by 7.3 % for the cold case and 17.1 % for the hot case. The same applies to the parameter C^*, involving U^{238} captures, which is overpredicted by 7.8 % and 15.3 %, respectively, For both of these quantities, the overestimation increases with increasing temperature.

The differences in the results obtained with the two codes might arise from an incomplete absorption treatment of U^{238} in the resonance range. The authors speculate that inappropriate treatment of U^{238} capture comes from one of two possible sources, or a combination of both.

One of these sources cold be due to the fact that the NJOY/MICROR [10] system used to create the fine-group library for MICROX-2 does not completely reconcile the dilution-*dependent* unresolved resonance data (U^{238}, U^{235}) with dilution-*independent* resolved resonance data. The most proper way to process the point data would be from the General Atomics GAND processing code [14] for the resonance data. The other possible source of error for the U^{238} capture is that the method used to calculate the flux self-shielding factors at the fuel grain level, the Wälti method [1] outlined in the manual, makes certain questionable assumptions regarding the spatial and angular distribution of the flux in the vicinity of the grains. The central premise of the method is that a many-grain problem may be reduced to a two-region transport problem with a white boundary condition [1]. It may not be reasonable to suppose that these same assumptions apply to a grain in the vicinity of the outer shell boundary. It has been shown that the average grain Dancoff factor [9], hence the resonance integral, can vary significantly over the radius of a fuel pebble. Thus, the calculation carried out in MICROX-2 is truly for an infinite-medium, many-grained problem, with no account being taken of the effect of the finiteness of the pebble dimensions on the granular self-shielding.

4 CONCLUSIONS

The MICROX-2 code was tested as a cross section generator for a particular configuration of a PBR lattice at both hot and cold temperatures. It was found that MICROX-2 underestimates the infinite-medium multiplication factor. Large differences were observed in the spectral indices that involve U^{238} captures and in the capture cross sections in the resonance energy range. The causes for the discrepancy are still under investigation, but preliminary investigations with different lattice configurations [13] lean toward the cross section errors being due to the overprediction with MICROX-2 of the neutron capture resonances of U^{238}.

There are several future directions for this work. The authors would like to make a similar assessment of the homogenized cross sections, but for different energy-group structures. Also, assessing the applicability of MICROX-2 to lattices in which more moderation is present would be of interest, as some PBR designs consider fuel and pure moderator pebble mixtures. As noted, the PBR lattice cell studied in this paper is under-moderated (no graphite pebbles). The authors are also interested in completing a similar evaluation for a finite medium.

5 ACKNOWLEDGMENTS

The work was performed as part of a Nuclear Engineering Research Initiative project. The primary author was supported under appointment to the U.S. Department of Energy Nuclear Engineering and Health Physics Fellowship Program sponsored by the U.S. Department of Energy's Office of Nuclear Energy, Science, and Technology. The authors would like to acknowledge Dan Ilas's helpful suggestions on generating the continuous-energy library for use with MCNP.

6 REFERENCES

1. D. Mathews, “An Improved Version of the MICROX-2 Code", *PSI Bericht Nr. 97-11* (1997).
2. R. Mphahlele and K. Ivanov, “Cross Section Generation for Pebble Bed Reactors,” *Transactions of the ANS 2003 Winter Meeting,* New Orleans, LA, USA, November 16-20, Vol. 89, pp. 605-607 (2003).
3. J.F. Briesmeister, "MCNP - A General Monte Carlo Code for Neutrons, Photons, and Electrons Transport, Version 4B", *LA-12625-M, LANL* (1997).
4. M. Ougouag and W. K. Terry, “A Preliminary Study of the Effect of Shifts in Packing Fraction on K-Effective in Pebble-Bed Reactors,” *M & C 2001*, Salt Lake City, Utah, USA, September 2001.
5. H. Gougar, Private Communication (2003).
6. Z. Karriem, C. Stoker, and F. Reitsma, “MCNP Modeling of HTGR Pebble-Type Fuel,” *Proceedings of the Monte Carlo 2000 Conference*, Lisbon, 23-26 October 2000.
7. R. E. MacFarlane and D. W. Muir, “The NJOY Nuclear Data Processing System,” *LA-12740-M*, Los Alamos National Laboratory, Los Alamos (1999).
8. R.M.Westfall, "Cosine Current Transmission Probabilities for Spherical Shells," *Trans. Am. Nucl. Soc.,* **18**, 147 (1974).
9. E.E. Bende, A.H. Hogenbirk, J.L. Kloosterman, and H. van Dam, “Analytical Calculation of the Average Dancoff Factor for a Fuel Kernel in a Pebble Bed High-Temperature Reactor”, *Nuclear Science and Engineering* **133**, pp.147-162 (1999).
10. S. Pelloni, “Edition 2 of the MICROR Interface Code,” *PSI technical memorandum TM-41-92-27*, 12 August (1992).
11. H. Gougar, Private Communication (2004).
12. E. Teuchert, K. A. Haas, H. J. Rutten, H. Brockman, H. Gerwin, U. Ohlig, W. Scherer, “V. S. O. P. (’94) Computer Code System for Reactor Physics and Fuel Cycle Simulation Input Manual and Comments, April 1994.
13. N. Hudson, Private Communication (2004).
14. R. J. Archibald and D. R. Mathews, “The GAF/GAR/GAND Fast Reactor Cross Section Preparation System, Volume II, GAND2 and GFE2, Computer Programs for Preparing Input Data For the GAFGAR, GGC, and MICROX codes from and ENDF/B Format Nuclear Data File,” *Gulf General Atomic Report GA-7542*, Volume II (1973).