

Comparison of SCALE and MCNP Results for Computational Pebble Bed Benchmarks

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INTRODUCTION

The use of small uranium fuel particles in a graphite matrix, which comprises a fuel element in a pebble bed reactor, results in a double heterogeneity of the fuel that must be taken into account when processing the nuclear cross sections. Version 5.1 of SCALE [1] supports modeling of double-heterogeneity through the use of CENTRM's pointwise resonance processing, which creates 238-group, self-shielded cross sections for use in the Monte Carlo codes KENO V.a and KENO-VI as well as in the two-dimensional lattice physics code NEWT. [2]

Participants in a Gen-IV Physics Colloquium at Idaho National Laboratory on October 5–7, 2003, drafted a suite of benchmarks “for evaluating basic cross section generation methods and for assessing critical issues in the construction of few-group cross sections for VHTR fuel.” Specifically, it calls for the simulation of several increasingly heterogeneous configurations and, for each one, the calculation of the fine-group energy spectrum ϕ , infinite medium multiplication factor k_∞ , and a set of broad-group collapsed microscopic cross sections.

The suite specifies a homogeneous atomic density of carbon and 8% enriched uranium to be used in the seven cases: an infinite homogeneous medium, simple cubic (SC) and body-centered cubic (BCC) lattices of 0.025-cm fuel particles, simple and BCC lattices of 6-cm diameter pebbles consisting of homogenized fuel regions surrounded by a 0.5-cm thick carbon shell, and finally the same pebbles with a lattice of particles in a carbon matrix comprising the fuel region.

The goal of this work is to compare the results from SCALE and MCNP for these benchmark simulations.

ANALYSIS

SCALE 5.1 and MCNP 5 [3] were used to analyze the specified problems. The multiplication factor and energy spectrum result directly from the calculations. The broad-group per-nuclide microscopic homogenized cross sections are computed using the definition in Eq. 1, which preserves the total reaction rates in a way that will be clearly affected by resonance self-shielding.

$${}^i\bar{\sigma}_g^x = \frac{\sum_R V_r \sum_G^i [\phi N \sigma]_{r,g}^x}{\sum_R V_r {}^i N_r \sum_G \phi_{r,g}} \quad (1)$$

The given homogeneous and uranium densities are used to calculate lattice cell widths and carbon matrix densities for each configuration. For the infinite homogeneous case, a 1-cm³ unit cell is used. Each lattice cell has reflecting boundaries on every side.

The SCALE simulation uses its standard ENDF/B-VI.7 cross section library, and the MCNP simulation uses a temperature-dependent ENDF/B-VI.8 library processed at Oak Ridge National Laboratory. Both simulations were run until a high convergence was achieved, yielding low statistical uncertainties for k_∞ and 238-group fluxes with a relative error of, at most, about 0.7% and, on average, about 0.3%.

SCALE Simulation

Using the control sequence CSAS6, each unit cell is described for self-shielding processing in CENTRM. The exact geometry for each configuration is implemented in KENO VI. The KMART6 module processes fluxes from KENO and the cross sections from the AMPX libraries to produce reaction rates for each region in the lattice cell. A Perl script was written to process the output data: using flux disadvantage factors from CENTRM if needed, volumes input into KENO VI, and fluxes and reaction rates from KMART6, it outputs the volume-homogenized flux and per-nuclide collapsed microscopic cross sections.

MCNP Simulation

MCNP uses a continuous-energy Monte Carlo simulation with an explicitly defined lattice of particles to determine the system criticality and individual cell fluxes. Per-cell, per-nuclide, collapsed reaction rates and fluxes are output via F4 path length flux tally cards along with M and E cards. As with SCALE, a script calculates homogenized flux and microscopic cross sections.

RESULTS

KENO and MCNP calculate values of k_∞ that agree to less than one-half of one percent in nearly every case (Table I). However, when examined in more detail, some discrepancies appear, even in the simplest homogeneous case (Figs. 1, 2). Between 100 and 300 keV, KENO's flux differs from MCNP's by up to 5%. The discrepancy at 3 eV is a consequence of neglecting upscattering in SCALE above 3 eV. The final and possibly most

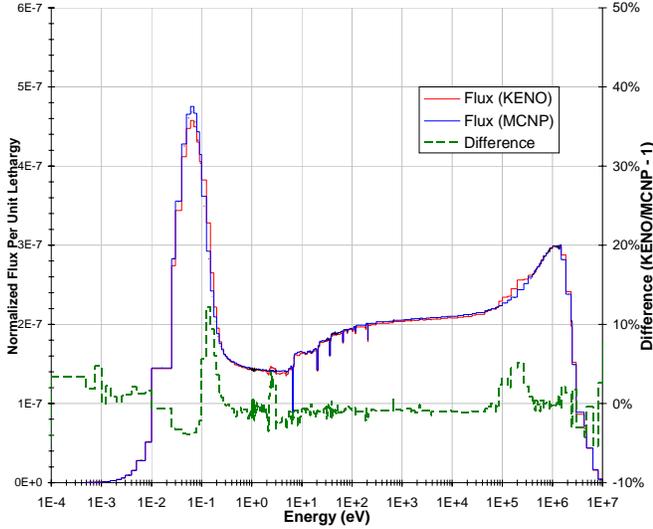


Fig. 1. Infinite homogeneous medium flux generated by KENO and MCNP and relative difference between them.

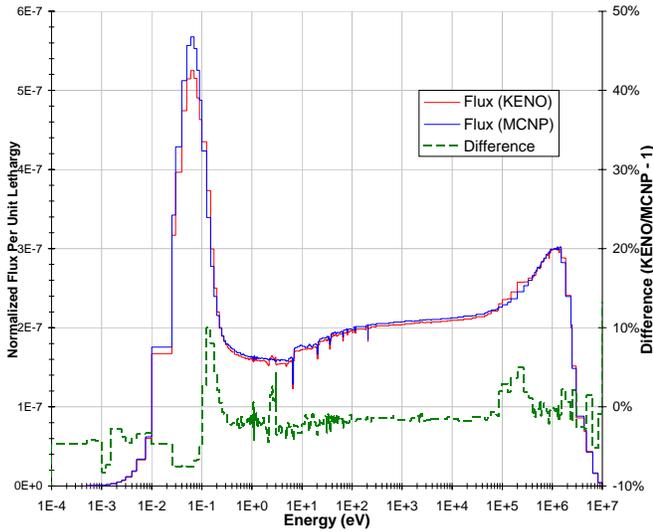


Fig. 2. Homogenized flux of a body-centered, double-heterogeneous pebble generated by KENO and MCNP.

significant discrepancy occurs in the thermal region of the spectrum. At 300K, MCNP calculates a Maxwellian peak that is higher and at a lower energy than KENO calculates.

KENO's microscopic cross sections for each nuclide in capture and fission are about a full percentage lower in the thermal group of the collapsed broad-group cross sections (Table II). Additionally, the group at 100 keV has consistent 1~3% differences. Finally, in only the doubly heterogeneous cases, there are differences on the order of 1% in both uranium isotopes' capture and fission

CONCLUSIONS

Several consistent differences are common to all levels of heterogeneity: the difference in the lowest energy broad-group cross section is a result of the weighting caused by the shifted thermal flux spectrum, the consistent discrepancies in the second-highest broad-group cross sections appear to be an effect of how the hump in KENO's flux in the 100 to 300 keV range weights the cross sections in those energies, and the differences in the small values of the high-energy carbon cross section are likely a result of the nuclear data processing.

The small incongruence of the resonance cross sections in the double-heterogeneous pebbles may be a result of SCALE's resonance processing. Even with these differences, the k_{∞} for each simulation match very closely, demonstrating the good agreement between MCNP and SCALE for doubly heterogeneous pebble bed simulations.

FUTURE WORK

The simple simulations specified in the test suite are insufficient to fully compare the simulation capabilities of SCALE and MCNP; a more thorough benchmark should be developed. The differences revealed by the test suite are under investigation.

TABLE I. Infinite multiplication factor for homogeneous, heterogeneous particle, heterogeneous pebble, and double heterogeneous simulations at 300K. The final two rows show the relative difference and the absolute difference divided by the higher of the standard deviations.

Configuration	Homogeneous	Particle	Particle	Pebble	Pebble	Doublehet	Doublehet
Lattice	--	Simple Cubic	BCC	Simple Cubic	BCC	Simple Cubic	BCC
KENO VI							
k_{∞}	1.3808	1.5075	1.5041	1.4146	1.4149	1.5262	1.5267
σ	0.0009	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010
MCNP							
k_{∞}	1.3816	1.5145	1.5155	1.4182	1.4184	1.5247	1.5300
σ	0.0008	0.0010	0.0010	0.0011	0.0011	0.0010	0.0010
Comparison:							
$KENO/MCNP - 1$	-0.06%	-0.46%	-0.75%	-0.25%	-0.24%	0.10%	-0.22%
$(KENO - MCNP)/\sigma_{max}$	-0.8	-7.0	-11.4	-3.3	-3.2	1.5	-3.4

TABLE II. Comparison of six-group collapsed cross sections for a body-centered cubic lattice of double-heterogeneous pebbles. Boldfaced entries are those with a greater than 0.50% difference.

U-238					
Upper Energy	Relative Difference, KENO/MCNP – 1 (percent)				
	σ_c	σ_{es}	σ_{is}	σ_f	σ_{tot}
20 MeV	0.8	0.3	-0.4	-3.0	0.1
128 keV	-1.4	-0.9	2.9	---	-0.9
8.03 keV	-1.2	-0.3	---	---	-0.5
30.0 eV	-1.6	-0.4	---	---	-1.2
2.38 eV	0.0	0.0	---	---	0.0
1.86 eV	-1.0	0.0	---	---	-0.2
C					
Upper Energy	Relative Difference, KENO/MCNP – 1 (percent)				
	σ_c	σ_{es}	σ_{is}	σ_f	σ_{tot}
20 MeV	19.2	0.6	5.1	---	0.6
128 keV	0.2	0.0	---	---	0.0
8.03 keV	-0.2	0.0	---	---	0.0
30.0 eV	-0.1	0.0	---	---	0.0
2.38 eV	-0.1	0.0	---	---	0.0
1.86 eV	-1.1	0.0	---	---	0.0
U-235					
Upper Energy	Relative Difference, KENO/MCNP – 1 (percent)				
	σ_c	σ_{es}	σ_{is}	σ_f	σ_{tot}
20 MeV	0.8	0.2	-0.3	0.0	0.1
128 keV	-0.3	-0.1	2.9	-0.2	-0.1
8.03 keV	-0.1	-0.1	0.0	-0.1	-0.1
30.0 eV	-0.6	-0.1	---	-0.6	-0.5
2.38 eV	-0.8	0.0	---	-0.2	-0.4
1.86 eV	-1.0	-0.1	---	-1.2	-1.2

REFERENCES

1. *SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluations, Version 5.1*, ORNL/TM-2005/39, Oak Ridge National Laboratory, 2006.
2. S. GOLUOGLU, M. L. WILLIAMS, "Modeling Doubly Heterogeneous Systems in SCALE." *Trans. Am. Nucl. Soc.*, **93**, 963-965, 2005.
3. *MCNP5—A General Monte Carlo N-Particle Transport Code, Version 5*, LA-UR-03-1987, Los Alamos National Laboratory, 2003.