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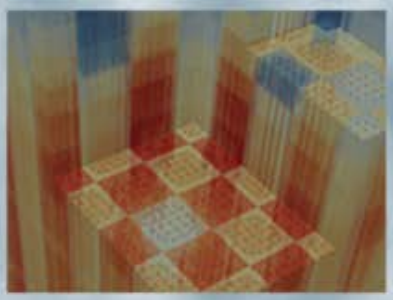

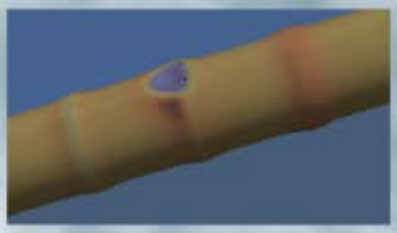

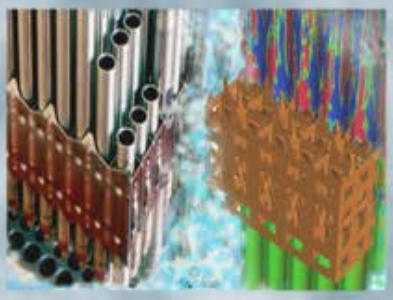

Scott J. Wilderman and William R. Martin
University of Michigan

Forrest B. Brown
Los Alamos National Laboratory

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SIMULATION OF CASL 3D HFP FUEL ASSEMBLY BENCHMARK PROBLEM WITH ON-THE-FLY DOPPLER BROADENING IN MCNP6

Scott J. Wilderman and William R. Martin
University of Michigan
Department of Nuclear Engineering and Radiological Sciences, Ann Arbor, MI 48105
sjwnc@umich.edu and wrm@umich.edu

Forrest B. Brown
Los Alamos National Laboratory
Los Alamos, NM 87545
fbrown@lanl.gov

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ABSTRACT

An On-the-Fly Doppler broadening methodology has been applied in a neutronics simulation of a single fuel assembly (problem 6 of the CASL/VERA Core Physics Benchmark Problems) using MCNP6. HFP temperatures and densities were taken from results of a coupled neutronic-TH computation with the neutron transport code MPACT and the subchannel TH code COBRA-TF. An MCNP6 input file with over 13000 cells with independent temperatures and densities was constructed from a template input file for CASL/VERA problem 3 (3D HZP full assembly). OTF Doppler broadening coefficients for the 54 unique isotopes of the problem were generated using the routines provided in the MCNP6 distribution. HZP OTF MCNP6 results are compared with published benchmark results, and results for 3D HFP assembly simulations are compared with neutronics results from the coupled MPACT/COBRA-TF simulation.

1. INTRODUCTION

Multi-physics calculations which attempt to couple thermal hydraulics (TH) computations and continuous-energy Monte Carlo neutronics codes can require many thousands or even millions of distinct region temperatures. The traditional Monte Carlo approach of using precalculated Doppler broadened nuclear cross-sections at each temperature is not feasible for such large numbers of independent material regions. Previously, we have reported the implementation of an On-the-Fly (OTF) Doppler broadening methodology to provide continuous energy broadened cross sections based on cell temperatures on-the-fly during neutron tracking in the Monte Carlo code MCNP6. In the current work, we apply the MCNP6 OTF methodology to the simulation of a single fuel assembly at hot full power (HFP).

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Problem 6 of the CASL/VERA core physics benchmark progression[1] involves simulation of a 17x17 Westinghouse fuel assembly (including spacer grids, end plugs and core plates, etc.), modeled in 3D and with quarter symmetry at beginning of life at HFP with iterative feedback between coupled thermal hydraulics and neutronics computations. Because of the inherent difficulty in accounting for the variation with temperature of the neutron cross sections required for the neutronics calculation, a reference Monte Carlo solution has yet to be obtained. A recent report[2] detailed the use of the MPACT[3] neutron transport code in conjunction with the COBRA-TF[4] code to determine the HFP beginning of life solution of both a single assembly and full core (problem 7 of the benchmark). The MPACT analysis for the single assembly used a Chebyshev-Gauss quadrature and temperature-dependent multi-group cross section libraries. Neutron transport modeling was performed on a mesh of eight angular and three radial rings in each fuel pin, but temperature (taken iteratively from COBRA-TF runs) varied in only the axial domain within the fuel region in each pin. The exact material and geometry specifications for the assembly for this problem are given by Godfrey[1], and details of the MPACT simulation can be found in the reference cited[2].

Recent progress in modeling the temperature variation in neutron cross sections with OTF cross sections[5,6] gives rise to the possibility of attacking this problem with a more accurate (albeit much slower) Monte Carlo code such as MCNP6[7] rather than a multigroup transport code. It is the goal of this work to demonstrate the utility of the OTF methodology in modeling this problem with MCNP6, using in each region of the assembly the converged temperatures and densities provided from the coupled COBRA-TF/MPACT simulation[2].

2. METHODS

The 3D fuel assembly of the HFP benchmark problem 6 is identical to that used in the HZP (at 600K) benchmark problem 3, for which a reference solution is provided[1]. As initial verification of the OTF methodology for this problem, an OTF simulation was performed on the HZP fuel assembly. A template MCNPX input file for the HZP case provided by Gurecky[8,9] was adapted to use OTF libraries with MCNP6. The OTF data was generated using the routines provided with the MCNP6 distribution and ENDF/B-VII.1 data libraries. OTF coefficients were calculated for the temperature range of 550K to 1500K for 54 unique isotopes, using a maximum order of 8 in the expansion coefficients and a 1 degree Kelvin (1K) temperature grid spacing when determining energy grid endpoints and in computing error tolerances on the fits. Roughly 1.8GB of data was generated for the 54 nuclides, and no cross section tolerance errors greater than 0.1% were reported by the fitting code. To be comprehensive in our validation comparison, MCNP6 simulations for the HZP fuel assembly were run with and without OTF invoked. Additionally, since OTF computations rely on standard MCNP libraries for all physics data other than broadened cross section values, to investigate the impact of any temperature dependences of quantities such as probability table (ptable) data, OTF runs were done using both the 600K and 900K MCNP libraries for non-broadened cross sections.

Since all the fuel pins were equivalent in the HZP case, the problem 3 MCNP input file made extensive use of the lattice geometry building function in defining the assembly geometry. For the HFP case of problem 6, however, each axial region of each fuel pin (and

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also of the cladding and moderator in each pin region) needed to be defined as a unique cell. A script was written to perform this segmentation, and also to insert temperatures and densities taken from the converged COBRA-TF/MPACT results. The MCNP input file required to model the assembly expanded from roughly 450 cards and 50 cells for the HZP case to almost 14,000 cards and 13,500 unique material cell regions for the HFP case. To verify that the segmentation was done correctly, an MCNP6 OTF simulation was performed using the expanded deck but with the original HZP temperatures. Full HFP simulations were then performed using the temperatures obtained from the converged MPACT/COBRA-TF simulation.

3. RESULTS

3.1 Validation of HZP Results

Table 1 below gives results from the HZP simulation of problem 3. KENO-VI[10] results are taken from the appendix of the benchmark problem description[1], the MCNPX results from Gurecky[9] and the MPACT results from Godfrey[11] (converted from pcm relative to the reference KENO-VI result).

Table 1 Computed HZP simulation eigenvalues

Simulation	ENDF/B library	Histories per Cycle	# Active Cycles	keff ± 1σ
KENO-VI (reference)	VII.0	5M	4500	1.175722 +/- 0.000005
MCNPX	VII.1	300k	3250	1.17525 +/- 0.00002
MCNP6	VII.1	500k	950	1.17521 +/- 0.00006
MCNP6 OTF 600K	VII.1	500k	950	1.17519 +/- 0.00006
MCNP6 OTF 900K	VII.1	500k	950	1.17517 +/- 0.00006
MCNP6 OTF 900K 13k cells	VII.1	500k	950	1.17518 +/- 0.00006
MPACT	VII.1	--	--	1.17444

Discrepancies between the various MCNP6 runs were all within a single standard deviation, demonstrating the accuracy of the OTF method and the negligible effect (for this problem) of the temperature dependence of the ptables. The difference between the MCNPX (ENDF/B-VII.0) and MCNP6 (ENDF/B-VII.1) results were also within a single standard deviation. Relative to the reference result, the MCNP6 runs showed a systematic underestimation in k-eff of -46 pcm, while the MPACT discrepancy was -109 pcm. A plot of the axial power distribution comparing the OTF results and the MCNPX results of Gurecky results and the KENO solution is shown in figure 1 below. Godfrey[11] reports RMS differences between MPACT and the KENO reference axial power distribution of 0.19%, with a slight underestimation of power at the top and bottom of the assembly, and over-estimation near the center, with the largest variations (up to .45%) near the spacer grids. The RMS difference between MCNPX and KENO was 0.77%, and between MCNP6 OTF and KENO 0.69%. The larger RMS differences found for the MCNP runs (relative to the reported MPACT differences) are almost certainly from insufficient histories.

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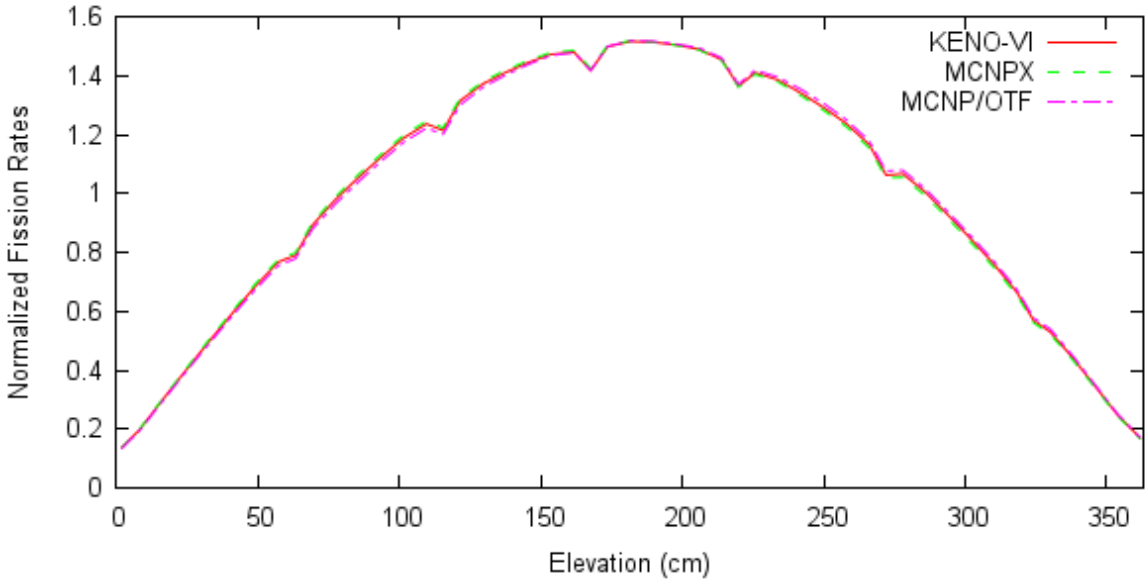

Fig. 1 Comparison of MCNP/OTF, MCNPX, and KENO reference results for the HZP Case

3.2 HFP Results

For the HFP case, MPACT[2] reported a value of k-eff of 1.16459, while the OTF MCNP6 result was 1.16500, a difference of -32 pcm, which is in the expected direction and consistent with the -63 pcm difference between the two codes for the HZP case. A plot comparing MPACT axial pin power/fission rate distributions with MCNP6 OTF results is shown in figure 2 below. While there is no reference data for comparison, it is instructive to

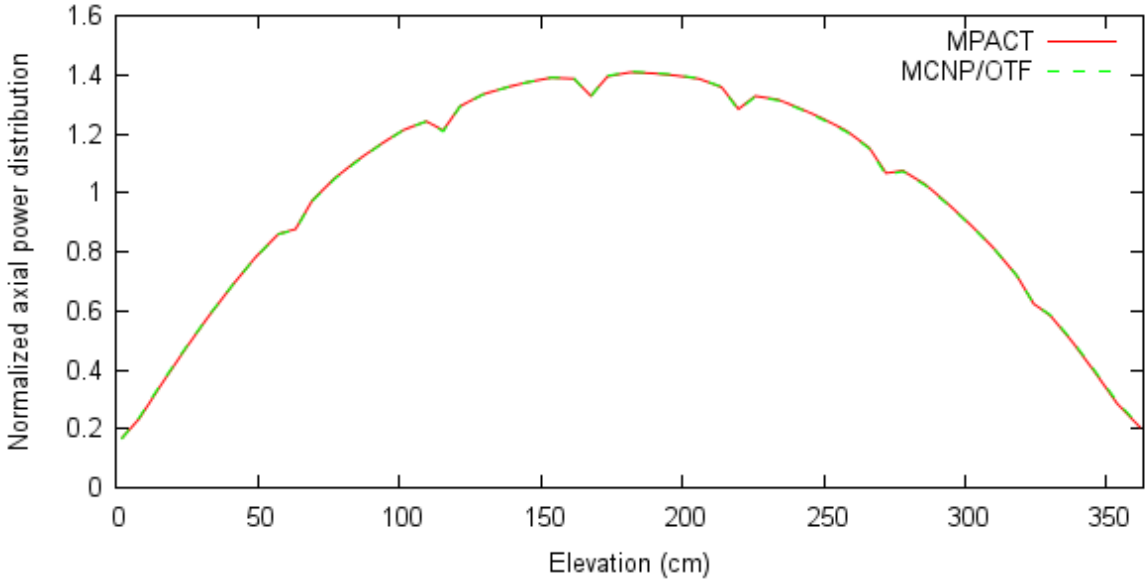

Fig. 2 MCNP/OTF and MPACT HFP axial power distributions

examine the differences between MCNP6 OTF and MPACT, which we present in figure 3, below. The primary features of this figure are the discrepancies between the two codes at the spacer grids, at which the MPACT results overestimate the power relative to the MCNP6 OTF results. These differences between MPACT and MCNP6 OTF are similar both in direction and in magnitude (up to 0.5%) to the discrepancies between MPACT and the KENO reference results reported by Godfrey for the HZP case (figure 3-1 of that work)[11].

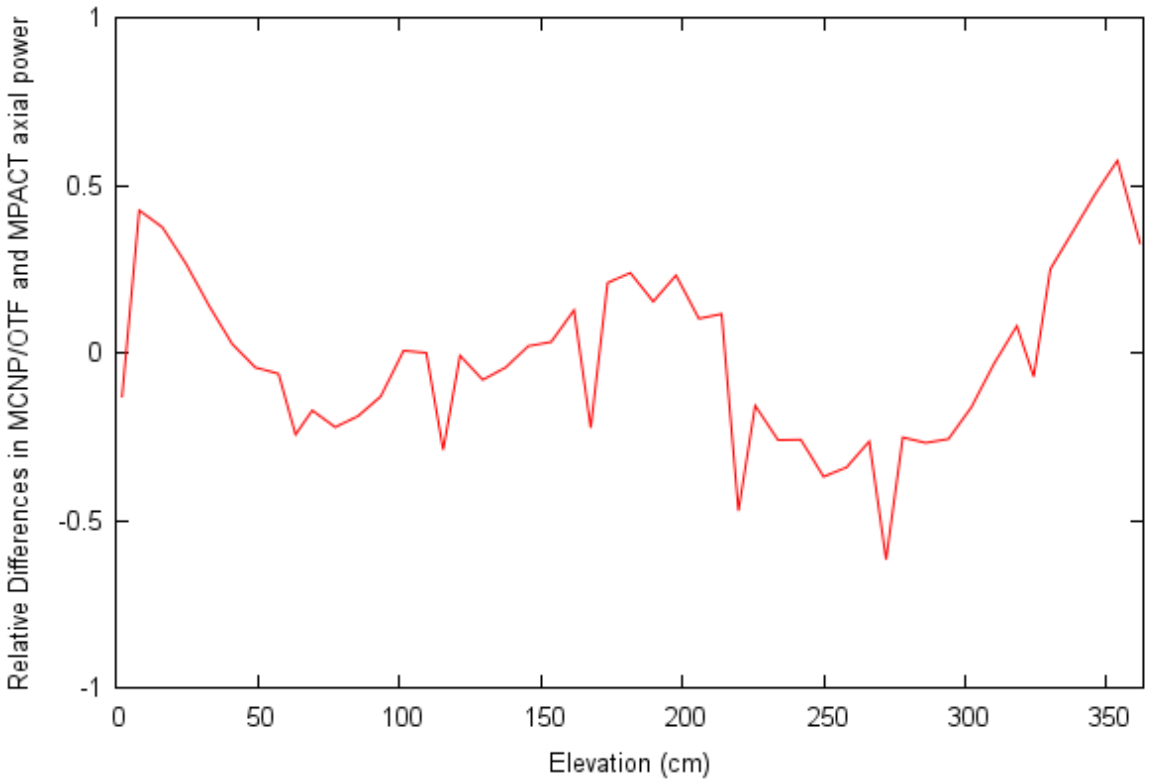

Fig. 3 Differences (%) in MCNP/OTF and MPACT axial power distributions

Figure 4 below shows the relative difference (in %) between the MCNP6 OTF and MPACT radial power distribution. The MCNP6 OTF results are consistently higher than the MPACT results at the assembly edges (recall that the simulation was performed on a ¼ assembly). While there are some minor differences in the modeling of the problem for the two cases (for example, the spacer regions are treated exactly in MCNP6 OTF, but homogenized with the moderator in MPACT), the inter-assembly gap was modeled identically in the two simulations here, and so it is not believed that modeling differences account for the differences in the results. The cause of this systematic discrepancy is still under investigation.

4. CONCLUSIONS

An OTF methodology for MCNP6 has been applied to the hot full assembly CASL/VERA Core Physics Benchmark Problem (problem 6), using individual cell

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temperatures and densities taken from converged thermal hydraulics feedback runs. The methodology and fidelity of the ~14000 card MCNP input deck was validated by comparison with KENO-VI HZP benchmark data. While no reference data exists for problem 6, differences between MCNP6 OTF and MPACT eigenvalue results were consistent in direction with results from the HZP benchmark. MCNP6 OTF and MPACT HFP axial power distributions agreed within roughly 0.4%, with greater differences at spacer grid elevations, again consistent with previously published MPACT errors relative to benchmarks. MCNP6 OTF and MPACT radial power distributions agreed within 0.25%, with some systematic differences at the inter-assembly gaps.

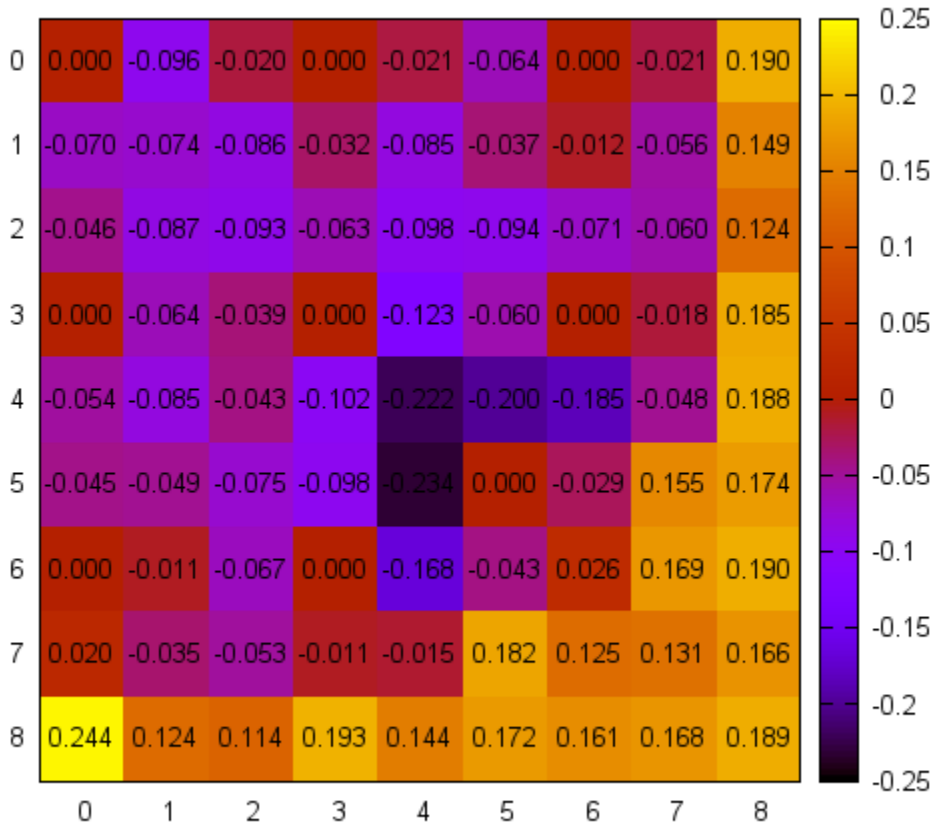

Fig. 4 Difference between OTF and MPACT radial power distributions

REFERENCES

1. A. GODFREY, "VERA Core Physics Benchmark Progression Problem Specifications," CASL Technical Report, CASL-U-2012-0131-004, Revision 4, August (2014).

2. B. D. KOCHUNAS, D. JABAAY, B. COLLINS, and T. DOWNAR, *"*Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using COBRA-TF/MPACT,*"* CASL Technical Report, CASL-U-2014-0051-000, April (2014).

3. B. KOCHUNAS, B. COLLINS, T. J. DOWNAR, and W. R. MARTIN, "Overview of Development and Design of MPACT: Michigan Parallel Characteristics Transport Code," *Proc. ANS Topical Meeting M&C2013, American Nuclear Society,* Sun Valley, Idaho, May 2013.

4. M. N. AVRAMOVA, "CTF: A Thermal Hydraulic Sub-Channel Code for LWR Transient Analyses," User's Manual, Pennsylvania State University, February 2009.

5. W. R. MARTIN, F. B. BROWN, S. WILDERMAN and G. YESILYURT, " On-the-Fly Doppler Neutron Broadening in MCNP," *Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA + MC 2013)* La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013.

6. G. YESILYURT, W. R. MARTIN, and F. B. BROWN, "On-The-Fly Doppler Broadening for Monte Carlo Codes", *Nucl. Sci. Eng.*, **171**, 239-257 (2012).

7. J. T. GOORELY, et al., "Initial MCNP6 Release Overview - MCNP6 version 1.0", Los Alamos National Laboratory report, LA-UR-13-22934 (2013).

8. W. GURECKY, A GODFREY, and E SCHNEIDER, "Watts Bar Unit 1 MCNPX Simulations with KENO-VI Comparisons," *American Nuclear Society Winter Meeting*, Anaheim, CA, November 2014.

9. W. GURECKY, *private communication.*

10. D. F. HOLLENBACH, L. M. PETRIE, and N. F. LANDERS, "KENO-VI: A General Quadratic Version of the KENO Program," Vol. II, Sect. F17 of SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation, NUREG/CR-0200, Rev. 7 (ORNL/NUREG/CR/CSD-2R7), 3 vols., April 2004. Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

11. A. GODFREY, "MPACT Testing and Benchmarking Results," CASL Technical Report, CASL-U-2014-0045-000, March (2014).