LA-UR-12-00423

Approved for public release;
distribution is unlimited.

Title:	Progress with On-The-Fly Neutron Doppler Broadening in MCNP
Author(s):	Forrest B. Brown, William R. Martin, Gokhan Yesilyurt, Scott Wilderman
Intended for:	2012 American Nuclear Society Summer Meeting Chicago, IL, 24-28 June 2012

Form 836 (7/06)

Progress with On-The-Fly Neutron Doppler Broadening in MCNP

Forrest B. Brown[1], William R. Martin[2], Gokhan Yesilyurt[3], Scott Wilderman[2]

[1]*Los Alamos National Laboratory, PO Box 1663, Los Alamos, NM, 87544, fbrown@lanl.gov*
[2]*University of Michigan, Ann Arbor, MI*
[3]*Argonne National Laboratory, Argonne, IL*

INTRODUCTION

The University of Michigan, ANL, and LANL have been collaborating on a US-DOE-NE University Programs project "Implementation of On-the-Fly Doppler Broadening in MCNP5 for Multiphysics Simulation of Nuclear Reactors." This paper describes the project and provides results from the initial implementation of On-The-Fly Doppler broadening (OTF) in MCNP and testing.

BACKGROUND

The MCNP Monte Carlo code [1,2] is used extensively for high-fidelity analyses of reactor physics problems due to its extensive capabilities for faithfully representing geometry and nuclear cross-sections. MCNP uses nuclear data prepared by the NJOY code [3], which reads ENDF/B nuclear data files, Doppler broadens the neutron cross-sections, and performs many other operations to prepare the data for use in MCNP. Data libraries at several temperatures were prepared using NJOY and included with the standard MCNP distribution package, and problem-specific data at additional temperatures can be generated using NJOY when needed.

In the past, when nuclear data was needed at only a few temperatures, the NJOY-MCNP arrangement was acceptable. Today there are many efforts to link MCNP with CFD codes, to provide multiphysics calculations including temperature feedback. The strong temperature feedback in nuclear reactors, due to Doppler broadening of the resonance cross sections, poses a challenge for the coupled neutronic-thermal-hydraulic analyses. For these multiphysics calculations, 1000s or more temperatures may be needed, and providing NJOY-generated datasets at all required temperatures is infeasible due to computer limitations.

OTF METHODOLOGY

Recent research [4-6] has shown the feasibility of replacing the current cross section files that are generated for Monte Carlo codes such as MCNP5 with a small number of constants that represents the detailed energy and temperature dependence of the cross sections. These constants are the expansion coefficients of a temperature dependent regression model for the cross sections at neutron energy grid points. In essence, these coefficients allow the determination of a given cross section for all neutron energies and all temperatures in the range 250-3200K. Therefore, Doppler broadened cross sections of any type can be calculated during the random walk of the neutrons for an unlimited number of material/temperature regions. In other words, if a neutron enters a material region that is at some temperature T, the Doppler broadened cross sections for that material are *immediately* generated "on-the-fly" by the regression model. Moreover, OTF broadening has minimal impact on computational time.

The OTF methodology involves high precision fitting of Doppler broadened cross-sections over a wide temperature range (the target for reactor calculations is 250-3200K). The fitting process uses NJOY-derived Doppler routines, least squares with singular value decomposition, adaptive energy grid generation for each nuclide, and a physics-based fitting model. Accuracy to the 0.1% level in cross-section linearization is preserved (similar to NJOY). The basic methodology described in [4-6] has been consolidated in a single stand-alone code *fit_otf*, with multicore parallel threading to reduce computer run times. Note that this code does not replace NJOY, but supplements it, providing a convenient mechanism for extending the Doppler broadening to a wide range of temperatures. The temperature dependent fits prepared by *fit_otf* are then used within MCNP during the neutron transport, for OTF broadening based on cell temperatures.

Creating a Union Energy Mesh for a Nuclide

The first step is to construct a union energy grid over a predefined temperature range of interest for each of the isotopes separately, due to the variations in the number of energy grid points with temperature. Here, "union" refers to a common energy grid structure (for a single nuclide) that can be used for all of the predefined temperature points to satisfy a given fractional tolerance for all cross section types for a given nuclide.

Fitting Doppler Broadened Cross-sections

As a next step, cross sections of all types are calculated on the union energy grids for each nuclide at every 1K of the temperature range of interest, using only 0K cross-sections from NJOY. Doppler broadening of the cross sections is performed, using NJOY-derived routines for Cullen's exact Doppler broadening equation. The third step is to determine expansion coefficients at every energy point and every cross section type for each isotope, using the pre-generated temperature dependent nuclear data described in the previous step.

OTF Implementation in MCNP

Then, the regression model is implemented into MCNP, involving only a few routines that retrieve and interpolate cross-section data. The regression model constants are read into memory prior to random walk of the neutrons.

INITIAL TESTING AND RESULTS

Table 1 provides a comparison of the OTF results (where Doppler broadening was performed on-the-fly during the MCNP calculations) with results using NJOY-generated data with MCNP. The calculations were done for a standard "Doppler Reactivity Benchmark" [7], comparing k-effective for HZP (hot, zero power) and HFP (hot, full power) conditions for a unit fuel cell typical of a PWR. It should be noted that this benchmark is strictly a computational benchmark (i.e., no experimental results) used internationally for comparing codes.

The basic model for this benchmark is a PWR fuel pin cell with reflecting boundary conditions. For the HZP cases, the fuel is at 600K, and the cladding and moderator are also at 600K. For the HFP cases, the fuel is at 900K, while the cladding and moderator remain at 600K. A uniform temperature is assumed within each of the fuel, cladding, and moderator regions. The number densities and dimensions were adjusted in the MCNP input for the HFP cases to account for thermal expansion. All results

Table 1. On-The-Fly Doppler Broadening in MCNP5 vs. Standard NJOY Broadened Data in MCNP5 for Doppler Reactivity Defect Benchmark

	HZP	HFP	Doppler Coefficient pcm/K
UO2 fuel pin - 0.711% enrichment			
NJOY+MCNP	0.66556 (18)	0.65979 (19)	-4.38 (.20)
OTF+MCNP	0.66567 (18)	0.66022 (19)	-4.13 (.20)
UO2 fuel pin - 1.60% enrichment			
NJOY+MCNP	0.96094 (26)	0.95293 (25)	-2.92 (.13)
OTF+MCNP	0.96026 (24)	0.95283 (23)	-2.71 (.13)
UO2 fuel pin - 2.40% enrichment			
NJOY+MCNP	1.09912 (27)	1.08997 (26)	-2.55 (.10)
OTF+MCNP	1.09923 (27)	1.08975 (28)	-2.64 (.10)
UO2 fuel pin - 3.10% enrichment			
NJOY+MCNP	1.17718 (27)	1.16744 (27)	-2.36 (.09)
OTF+MCNP	1.17703 (30)	1.16767 (30)	-2.27 (.10)
UO2 fuel pin - 3.90% enrichment			
NJOY+MCNP	1.23967 (27)	1.22920 (30)	-2.29 (.09)
OTF+MCNP	1.23953 (29)	1.22979 (29)	-2.13 (.09)
UO2 fuel pin - 4.50% enrichment			
NJOY+MCNP	1.27501 (30)	1.26526 (27)	-2.01 (.09)
OTF+MCNP	1.27534 (29)	1.26552 (29)	-2.03 (.09)
UO2 fuel pin - 5.00% enrichment			
NJOY+MCNP	1.29901 (31)	1.28920 (29)	-1.95 (.08)
OTF+MCNP	1.29907 (28)	1.28938 (29)	-1.93 (.08)

were obtained using 5M active neutron histories for each of the 28 MCNP runs, using ENDF/B-VII.0 nuclear data.

For the "NJOY-MCNP" results, standard MCNP data libraries from NJOY at 600K and 900K were used in MCNP5-1.60.

For the "OTF-MCNP" results, NJOY datasets at 293.6 K were used in *fit_otf* to prepare OTF data covering 300-1000K for ^{16}O, ^{234}U, ^{235}U, and ^{238}U. (In *fit_otf*, 100K increments were used for the union grid generation, and 10K increments were used for the fitting. While these temperature increments were adequate for testing, more precision is expected to be necessary for production use.) The OTF data was then used in a modified version of MCNP5-1.60 for ^{16}O, ^{234}U, ^{235}U, and ^{238}U in the fuel region, while standard NJOY-generated data at 293.6 K was used for non-broadened reactions in the fuel region in MCNP5. Standard NJOY-generated data at 600K was used for the clad and moderator regions, for convenience so that the only changes in comparing the two methodologies were well-defined and confined to the fuel region.

The results in Table 1 clearly indicate that the OTF methodology is effective, providing results that agree with standard NJOY-MCNP calculations within statistics.

CONCLUSIONS

Much more refinement is needed in the fitting process and MCNP implementation, but the initial success is encouraging. Further investigation is needed to: Provide variable fitting orders for different energies, to reduce the computer storage needed for the OTF data; Investigate alternate formulations of the OTF model, and improved numerical methods for the fitting process; Either determine optimal fitting orders for each nuclide, or modify the *fit_otf* code to perform regression on the number of fitting coefficients; Streamline the MCNP implementation of OTF to reduce overhead; Create a library of OTF coefficients suitable for use over all temperatures for reactor applications, so that users never need to generate OTF data. In addition, extensive thorough testing and verification for a wide variety of reactor applications is needed to provide confidence in the OTF methodology. All of this work is planned and in progress.

It is relatively straightforward to extend this capability to cover any temperature range of interest, allowing the Monte Carlo simulation to account for a continuous distribution of temperature ranges throughout the problem geometry.

ACKNOWLEDGEMENTS

The work reported in this summary was supported by DOE NEUP contract DE-AC07-05ID14517.

REFERENCES

1. X-5 MONTE CARLO TEAM, "MCNP – A General N-Particle Transport Code, Version 5 – Volume I: Overview and Theory", LA-UR-03-1987, Los Alamos National Laboratory (April, 2003).
2. F.B. BROWN, B.C. KIEDROWSKI, J.S. BULL, "MCNP5-1.60 Release Notes", LA-UR-10-06235, Los Alamos National Laboratory (2010).
3. R.E. MACFARLANE and D.W. MUIR, ""NJOY99.0 - Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data,"" *PSR- 480/NJOY99.00*, Los Alamos National Laboratory, Los Alamos (2000).
4. G. YESILYURT, "Advanced Monte Carlo Methods for Analysis of Very High Temperature Reactors: On-the-Fly Doppler Broadening and Deterministic / Monte Carlo Methods," *PhD thesis*, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI (2009).
5. G. YESILYURT, W.R. MARTIN, F.B. BROWN, "On-The-Fly Doppler Broadening for Monte Carlo Codes", accepted for publication, *Nuclear Science & Engineering.*
6. F.B. Brown, B.C. Kiedrowski, W.R. Martin, G. Yesilyurt, "Advances in Monte Carlo Criticality Methods", Invited Workshop for M&C-2009, Saratoga Springs, NY, May 3-7 [also, LA-UR-09-02442] (2009)
7. R.D. Mosteller, "Computational Benchmarks for the Doppler Reactivity Defect", ANS Joint Benchmark Committee [LA-UR-06-2968] (2006).