CONF-950420--14

VALIDATION OF THE WIMSD4M CROSS-SECTION GENERATION CODE WITH BENCHMARK RESULTS

L. C. Leal
Oak Ridge National Laboratory*
P. O. Box 2008
Oak Ridge, Tennessee 37831

and

J. R. Deen and W. L. Woodruff
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

To be presented at
International Conference on Mathematics and Computation, Reactor Physics, and Environmental Analyses
April 30-May 4, 1995
Portland, Oregon

*Managed by Martin Marietta Energy Systems, Inc., under contract DE-AC05-84OR21400 with the U.S. Department of Energy.

VALIDATION OF THE WIMSD4M CROSS-SECTION GENERATION CODE WITH BENCHMARK RESULTS

L. C. Leal
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, Tennessee 37831

(615)574-5281

J. R. Deen
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

(708)252-4853

W. L. Woodruff
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

(708)252-8634

ABSTRACT

The WIMSD4 code has been adopted for cross-section generation in support of the Reduced Enrichment for Research and Test Reactor (RERTR) program at Argonne National Laboratory (ANL). Subsequently, the code has undergone several updates, and significant improvements have been achieved. The capability of generating group-collapsed micro- or macroscopic cross sections from the ENDF/B-V library and the more recent evaluation, ENDF/B-VI, in the ISOTXS format makes the modified version of the WIMSD4 code, WIMSD4M, very attractive, not only for the RERTR program, but also for the reactor physics community.

The intent of the present paper is to validate the procedure to generate cross-section libraries for reactor analyses and calculations utilizing the WIMSD4M code. To do so, the results of calculations performed with group cross-section data generated with the WIMSD4M code will be compared against experimental results. These results correspond to calculations carried out with thermal reactor benchmarks of the Oak Ridge National Laboratory (ORNL) unreflected critical spheres, the TRX critical experiments, and calculations of a modified Los Alamos highly-enriched heavy-water moderated benchmark critical system. The benchmark calculations were performed with the discrete-ordinates transport code, TWODANT, using WIMSD4M cross-section data. Transport calculations using the XSDRNPM module of the SCALE code system are also included. In addition to transport calculations, diffusion calculations with the DIF3D code were also carried out, since the DIF3D code is used in the RERTR program for reactor analysis and design. For completeness, Monte Carlo results of calculations performed with the VIM and MCNP codes are also presented.

I. INTRODUCTION

The cross-section generation capability for the RERTR program is based on a modified version of the WIMSD4[1] code, which has been named WIMSD4M.[2]

Problem-dependent group-collapsed cross-section libraries generated with the WIMSD4M code are based on a fine-group microscopic cross-section library containing 98 materials in which 69 neutron energy groups are utilized. The basic 69-group cross-section library, presently available at ANL, was created by processing the ENDF/B-V library with the NJOY system[3] with the modules RECONR, BROADR, UNRESR, THERMR, GROUPR,and WIMSR. In contrast to other modules of the NJOY system, extensive work was required to make WIMSR produce reliable multigroup cross-section data for the WIMSD4M code.

In addition to the NJOY modules, a utility code, LIBUPD, for adding and replacing isotopes and maintaining the libraries, was also created. This supplementary code makes it possible to edit the WIMSD4M library file into a readable ASCII form.

The NJOY capability of processing the latest version of the ENDF/B file, ENDF/B-VI, has been considered, and in the near future a WIMSD4M fine-group library processed from the ENDF/B-VI file may be added for use with the RERTR program.

II. CALCULATIONS OF THE ORNL AND TRX THERMAL BENCHMARK WITH WIMSD4M GROUP CROSS SECTIONS

The first series of validation tests of the WIMSD4M cross-section code was carried out with the ORNL homogeneous unreflected critical spheres of ^{235}U and H_2O, ORNL -1, -2, -3, -4, and -10, and the TRX-1 and TRX-2 lattices.[4]

To verify the adequacy of the WIMSD4 generated cross sections, it was decided to rely on the results of transport calculations to avoid possible errors which could be attributed to transport effects. In this regard, the multigroup discrete-ordinates transport codes, TWODANT[5] and XSDRNPM,[6] were used in the calculations. In addition to the transport calculations, diffusion calculations have also been performed with the DIF3D code.[7]

Fine-group cross sections used in the transport and diffusion calculations with the TWODANT and DIF3D codes were obtained from calculations performed based on the built-in 69-group structure of the WIMSD4M library and, subsequently, these fine group cross-section data were collapsed to a 10-group structure used in the benchmark calculations. The collapsed 10-group boundaries are shown in Table 1. The spatial dependence of the neutron spectrum was accounted for in the calculations by using 100 fine spatial intervals. Other parameters which are required in a transport calculation are the angular quadrature and the order of scattering. Calculations performed with 16 quadrature points and the first order scattering ($S_{16}P_1$) proved to be sufficient to reproduce k_{eff} in good agreement with experimental results. The unreflected sphere implies that no particle leaving the system at the sphere surface will return to it, a requirement fulfilled by the vacuum boundary condition option of the TWODANT and DIF3D codes. Prior to the transport calculations with the one-dimensional (1-D) discrete-ordinates transport code XSDRNPM, the CSASN sequence of the SCALE4.2 code system[8] was used to calculate Bondarenko factors and Nordheim resonance integrals with the codes BONAMI and NITAWL, respectively. The cross- section library used in the calculations is a 238-group library processed from ENDF/B-V.

The continuous-energy Monte Carlo codes VIM[9] and MCNP[10] were also used to calculate the ORNL unreflected spheres and the TRX heterogeneous critical lattices.

The benchmark results of the ORNL critical spheres are very useful to test the performance of the cross-section library as to the neutron scattering in H_2O, the absorption cross section of the fissile material, ^{235}U, and the capture cross section of hydrogen. To assess the performance of the WIMSD4M problem-dependent cross-section library, the infinite and effective multiplication factors for the five spheres were computed. These results are displayed in Table 2. The basic cross-section data used in the calculations are taken from the ENDF/B-V files. The results shown in Table 2 indicate that the infinite multiplication factor calculated by WIMSD4M and VIM codes are in excellent agreement. Likewise, the effective multiplication results computed with the TWODANT code using WIMSD4M 10-group cross-section data are very good. These results demonstrate the capacity of the WIMSD4M code for generating problem-dependent group-collapsed cross-section data for applications in reactor calculations.

In addition to the transport and Monte-Carlo calculations, Table 2 also includes results from the diffusion calculations carried out with the DIF3D code. A homogeneous infinite medium was used in WIMSD4M to obtain broad group cross sections for DIF3D and TWODANT since there is no capability to model spherical geometry. The assumption of an infinite medium fuel composition becomes a better approximation as the size of the sphere increases. The slight improvement in the DIF3D k_{eff} prediction computed for ORNL-10 should be noted..

The benchmark results of the ORNL criticals were for a single-region homogeneous sphere. The water-moderated uranium experiments, TRX-1 and TRX-2 lattices,[4] were analyzed to address the heterogeneous effects on the WIMSD4M group-collapsed cross sections. The results presented here are calculations of integral properties performed with the WIMSD4M, VIM,and MCNP codes. The calculations performed with both VIM and MCNP codes were performed with 2 million histories in an infinite lattice. The effectiveness of the WIMSD4M cross-section data for the water-moderated lattices were accounted for with the measured lattice parameters ρ^{28}, δ^{25}, δ^{28}, and c^*. Measured and calculated integral property values for the TRX-1 and TRX-2 lattices are presented in Tables 3 and 4, respectively. Also included in these tables are the computed infinite and effective multiplication factors, k_∞ and k_{eff}, respectively. As can be seen from Tables 3 and 4, the integral parameters calculated with the WIMSD4M group-collapsed cross sections are in very good agreement with measured and Monte Carlo calculations.

III. CALCULATIONS OF THE GEOMETRICALLY MODIFIED LOS ALAMOS HIGHLY-ENRICHED HEAVY-WATER MODERATED BENCHMARKS

Several highly enriched critical assemblies of heavy-water solutions and uranium metal D_2O were measured at Los Alamos National Laboratory.[11] Six of these spherical critical assemblies were modeled using VIM and found k_{eff} values of $\approx 1.000 \pm 0.005$ for each measured configuration. These comparisons verified the reliability of VIM to model these D_2O critical systems. Unfortunately, it was not possible to model these measured data in WIMSD4M, since all critical assemblies were in spherical form. Therefore it was decided to use the uranyl-fluoride heavy-water composition in a cylindrical geometry along with the D_2O reflector for a more precise modeling. Each cylinder was assumed to have infinite height. A vacuum boundary condition was used at the outer boundary to specify no return current to the D_2O reflector. Diffusion calculations using DIF3D were performed with cross sections computed with WIMSD4M. The dimensions and k_{eff} values for VIM and WIMSD4M-DIF3D are presented in Table 5. The core solution was assumed to have a stainless-steel container of 1.0 mm thickness. Each DIF3D calculation was made using 10-broad groups collapsed from a 69-fine group WIMSD4M transport solution. The results for three cases are shown in Table 5. They indicate good agreement between VIM and DIF3D k_{eff} values. The modeling of the smallest core radius sphere of 8.0 cm was performed in the DIF3D calculations with 10- and 18-group cross sections. The addition of eight thermal groups in the DIF3D calculation provided a k_{eff} closer to VIM results.

IV. CONCLUDING REMARKS

The study presented in this paper addresses the adequacy of the WIMSD4M multigroup cross sections in the calculation of experimental and computational benchmark results. Existing light- and heavy-water homogeneous and infinite lattice benchmark data were modeled to verify the adequacy of the WIMSD4M transport generated group constants. The integral properties of the TRX criticals and the k_{eff} for the light- and heavy-water assemblies calculated with broad-group cross sections computed with the WIMSD4M code and subsequently used in the WIMSD4M/DIF3D models showed good agreement with measured, and with Monte Carlo calculations.

REFERENCES

1. "WIMSD4 Winfrith Improved Multigroup Scheme Code System," Radiation Shielding Information Center, CCC-576, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (1990).

2. J. R. Deen, W. L. Woodruff and C. I. Costescu,"New ENDF/B-V Nuclear Data Library for WIMSD4M," *Proc. 1993 Int. Mtg. on Reduced Enrichment for Research and Test Reactors,* October 3-7, 1993, Oarai, Japan (to be published).

3. R. E. MacFarlane,"The NJOY Nuclear Data Processing System, Version 91.0," Documentation for NJOY91.13 code package, Radiation Shielding Information Center, PSR-171, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (1991).

4. "Cross Section Evaluation Working Group Thermal Reactor Benchmark Compilation," CSEWG Data Testing Subcommittee, Thermal Data Testing Group, BNL-19302, Brookhaven National Laboratory (1974).

5. "TWODANT: One- and Two-Dimensional, Multigroup Discrete-Ordinates Transport Code System," Documentation CCC-547, Radiation Shielding Information Center, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (1990).

6. N. M. Greene, W. E. Ford III, L. M. Petrie, and J. W. Arwood, "AMPX-77: A Modular Code System for Generating Couple, Multigroup Neutron-Gamma Cross-Section Libraries from ENDF/B-IV and/or ENDF/B-V," ORNL/CSD-283, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory (October 1992).

7. K. L. Derstine,"DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems," ANL-82-64, Argonne National Laboratory (1982).

8. "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (draft November 1993). Available from Radiation Shielding Information Center at Oak Ridge National Laboratory as CCC-545.

9. R. N. Blomquist,"VIM: A Continuous Energy Neutron and Photon Transport Code," *Proc. Topl. Mtg. Advances in Reactor Computations,* Salt Lake City, Utah, March 1983, p. 222, American Nuclear Society.

10. J. F. Briesmeister, Editor, MCNP - A General Monte Carlo Code for Neutron and Photon Transport," Version 3a, LA-7396-M, Rev. 2, Los Alamos National Laboratory (September 1986).

11. H. P. Paxton, "Los Alamos Critical Mass Data," LA-3067-MS, Los Alamos National Laboratory (December 1975).

TABLE 1
The 10-Broad-Group Structure Used in
the Transport and Diffusion Models

Collapsed 10-Group Structure	
Broad Group	Energy Upper Boundaries (eV)
1	10^7
2	8.21×10^5
3	5.53×10^3
4	4
5	2.1
6	1.097
7	0.972
8	0.625
9	0.3
10	0.14[a]

[a]Lower energy boundary is 10^{-5} eV.

TABLE 2
Infinite and Effective Multiplication Factors for the ORNL Critical Spheres

	k_∞		k_{eff}			
	69-group		10-group	10-group	238-group	
ORNL Sphere	WIMSD4M	VIM	TWODANT	DIF3D	XSDRNPM	VIM
1	1.2131	1.2131±0.0005[a]	1.0086	1.0106	0.9987	0.9991±0.0005
2	1.2089	1.2083±0.0005	1.01	1.0103	0.9985	0.9991±0.0006
3	1.2022	1.2016±0.0005	1.0066	1.0072	0.9955	0.9965±0.0005
4	1.2025	1.2019±0.0005	1.008	1.0087	0.9969	0.9977±0.0005
10	1.0724	1.0722±0.0005	1.0039	1.0045	0.9980	0.9998±0.0006

[a]Represents 1 σ standard deviation.

TABLE 3
Integral Property Values for the TRX-1 Lattice

TRX-1

	k_∞	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C*
Measured		1.000	1.320±0.021[a]	0.0987±0.0010	0.0946±0.0041	0.797±0.008
WIMSD4M	1.1755	-[b]	1.347	0.097	0.0941	0.797
DIF3D	1.1728	0.9916	-	-	-	-
XSDRNPM	1.1733	0.9902	1.399	0.1010	0.0989	0.813
VIM	1.1814±0.0005[a]	0.9907±0.0006	1.306±0.002	0.09660±0.0010	0.0914±0.0001	0.784±0.001
MCNP	1.1802±0.0003	-[c]	1.330±0.002	0.0974±0.0001	0.0892±0.0001	0.7880±0.0007

[a]Represents 1 σ standard deviation.
[b]Not possible in WIMSD4M.
[c]The whole core was not modeled in MCNP, only infinite lattice.

TABLE 4
Integral Property Values for the IRX-2 Lattice

TRX-2

	k_∞	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C^*
Measured		1.000	0.8370±0.016[a]	0.0614±0.0008	0.0693±0.0035	0.647±0.006
WIMSD4M	1.1627	-[b]	0.8420	0.0597	0.0675	0.642
DIF3D	1.1594	0.9977	-	-	-	-
XSDRNPM	1.1621	0.9944	0.8710	0.0616	0.0702	0.650
VIM	1.1652±0.0005[a]	0.9938±0.0006	0.8190±0.0014	0.0596±0.0001	0.0661±0.0001	0.6350±0.0008
MCNP	1.1660±0.0003	-[c]	0.8310±0.0013	0.0599±0.0001	0.0643±0.0001	0.6390±0.0005

[a]Represents 1 σ standard deviation.
[b]Not possible in WIMSD4M.
[c]The whole core was not modeled in MCNP, only infinite lattice.

TABLE 5
UO_2-F_2-D_2O Core Solution with Stainless-Steel Container and
Larger D_2O Reflector in Cylindrical Geometry

Core Radius (cm)	Reflector Thickness (cm)	k_{eff}		
		VIM	DIF3D	
			10-group	18-group
8.0	72.0	0.9987±0.0007	1.0027	1.0009
10.0	40.0	0.9937±0.0007	0.9958	-
12.0	28.0	0.9972±0.0007	0.9954	-