ANL/TD/CP--85106
CONF-9409107--7

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To be presented at the
1994 International Meeting on
Reduced Enrichment for Research and Test Reactors

September 18-23, 1994
Williamsburg, Virginia, USA

*Work supported by the U.S. Department of Energy
Office of Nonproliferation and National Security
under Contract No. W-31-109-38-ENG

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ABSTRACT

The WIMSD4 code has been adopted for cross-section generation in support of the Reduced Enrichment 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 WIMSD4M cross-section libraries for reactor modeling of fresh water moderated cores. The results of calculations performed with multigroup 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 HEU critical spheres, the TRX LEU critical experiments, and calculations of a modified Los Alamos HEU D_2O 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.

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 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 by the RERTR program.

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 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 HEU 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. In addition, the fission and capture rates for each isotope were in excellent agreement. These results demonstrate the capacity of the WIMSD4M code for generating problem-dependent group-collapsed cross-section data for applications in H_2O moderated 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 in WIMS to model spherical geometry. TWODANT and VIM reaction rates are in excellent agreement but the fast neutron leakage is slightly different causing eigenvalues about 1% Δk_{eff} larger than VIM for the smaller bare spheres in cases 1-4. The reactivity bias is reduced to 0.45% Δk_{eff} for the largest sphere (#10) in the DIF3D model.

The benchmark results of the ORNL criticals were for a single-region homogeneous HEU sphere. The H_2O moderated uranium experiments, TRX-1 and TRX-2 hexagonal cores,[4] were analyzed to address the heterogeneous effects for a slightly enriched uranium fuel (e = 1.29%) in two different neutron spectra 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 adequacy of the WIMSD4M cross-section data for the very low enriched water-moderated lattices were accounted for with the measured heavy metal reaction rate ratios, 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. The whole critical core of 764 fuel rods for TRX-1 and 578 fuel rods in TRX-2 lattice were also modeled in VIM, XSDRNPM and DIF3D using WIMSD4M cross sections.

Also included in Tables 3 and 4 are the computed infinite and effective multiplication factors, k_∞ and k_{eff} respectively. As can be seen from a comparison of measured and computed integral parameters, group-collapsed ^{235}U and ^{238}U thermal and epithermal reaction rates are in very good agreement with measured and Monte Carlo Calculations. While the calculated core k_{eff} values are lower than measured using DIF3D and XSDRNPM models, they are in good agreement with the whole core VIM model k_{eff} calculation.

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

Several highly enriched critical assemblies of heavy water moderated core solutions of UO_2-F_2-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. Transport calculations were performed with XSDRNPM. The core and reflector dimensions and k_{eff} values for VIM, XSDRNPM 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.

CONCLUDING REMARKS

The study presented in this paper addressed 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 low enriched TRX criticals and the k_{eff} for the HEU 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.

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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	8.221×10^5
3	5.53×10^3
4	4.0
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	Continuous	10-group	10-group	238-group	Continuous
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[a]
2	1.2089	1.2083±0.0005	1.0100	1.0103	0.9985	0.9991±0.0005
3	1.2022	1.2016±0.0005	1.0066	1.0072	0.9955	0.9965±0.0005
4	1.2025	1.2019±0.0005	1.0080	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.

Note: The critical spherical radius of cases 1-4 is 34.6 cm and sphere 10 radius is 61.0 cm.

TABLE 3
Integral property values for the TRX-1 Lattice

	k_∞	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C*
Measured		1.000	1.320±0.021	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±0.0001	0.0914±0.0001	0.784±0.0010
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.

Note: Integral parameters correspond to thermal cutoff of 0.625eV. The WIMSD4M ENDF/B-V data uses mod. 2 data for ^{235}U and ^{238}U while VIM and MCNP ENDF/B-V data uses mod. 0 data.

ρ^{28} = ratio of epithermal-to-thermal ^{238}U captures.
δ^{25} = ratio of epithermal-to-thermal ^{235}U captures.
δ^{28} = ratio of ^{238}U fissions to ^{235}U fissions.
C^* = ratio of ^{238}U captures to ^{235}U captures.

TABLE 4
Integral Property Values for the TRX-2 Lattice

	k_∞	k_{eff}	ρ^{28}	δ^{25}	δ^{28}	C^*
Measured		1.000	0.8370±0.016[a]	0.0614±0.008	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±0.0014	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.

Note: Integral parameters correspond to thermal cutoff of 0.625 eV. The WIMSD4M ENDF/B-V data uses mod. 2 data for ^{235}U and ^{238}U while VIM and MCNP ENDF/B-V data uses mod. 0 data.

ρ^{28} = ratio of epithermal-to-thermal ^{238}U captures.
δ^{25} = ratio of epithermal-to-thermal ^{235}U captures.
δ^{28} = ratio of ^{238}U fissions to ^{235}U fissions.
C^* = ratio of ^{238}U captures to ^{235}U captures.

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

		k_{eff}			
Inner Core Radius (cm)	Outer Reflector Thickness (cm)	VIM	XSDRNPM	DIF3D	
		Continuous	238-Group	10-Group	18-Group
8.0	71.9	0.9987±0.0007	0.9977	1.0027	1.0009
10.0	39.9	0.9937±0.0007	0.9950	0.9958	0.9937
12.0	27.9	0.9972±0.0007	0.9981	0.9954	0.9943