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BENCHMARK ANALYSIS OF THE SCALE 5 VERSIONS OF THE KENO-VI AND CENTRM CODES

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ABSTRACT

One of the limitations of the SCALE code system prior to the release of version 5 was the method used to process the multigroup cross-section data. By default the cross-section data are processed by the functional module NITAWL-III, which uses the Nordheim Integral Treatment to self-shield the resolved resonances. This methodology contains several limitations such as processing only one resonance at a time (thus not taking into account resonance overlap), not processing nonresonance data in the resonance region (such as ENDF file 3 data), and not accounting for fissile material in adjacent regions. The CENTRM/PMC (*C*ontinuous *EN*ergy *TR*ansport *M*odule/*P*roduce *M*ultigroup *C*ross sections) cross-section processing codes eliminate these and other limitations by using one-dimensional continuous-energy cross-section data to generate a problem-dependent flux spectrum and then collapsing the continuous-energy data using the calculated flux spectrum into group cross-section data. A comparison of the NITAWL-III and CENTRM/PMC cross-section processing codes using KENO-VI was performed by evaluation of 194 individual cases, derived primarily from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook. These evaluations show that in all cases CENTRM/PMC performs as well as NITAWL-III and in certain problems, where the limitations in NITAWL-III are exceeded, CENTRM/PMC consistently produces excellent results.

Key Words: KENO-VI, validation, CENTRM, ICSBEP, k_{eff}

1 INTRODUCTION

SCALE 5 [1] contains updated versions of all the existing computer codes in the previous version of SCALE plus several new computer codes. CENTRM [2] and PMC [3] are two of the new computer codes designed to perform resolved resonance processing using continuous-energy cross-section data. KENO-VI [4], although used in previous versions of SCALE, has been significantly enhanced. A suite of diverse critical benchmark problems, most from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) handbook [5], one from a Pacific National Laboratory (PNL) report [6], and the rest from an Organization for Economic Cooperation and Development (OECD) calculational benchmark [7], were selected to perform validations of the KENO-VI and CENTRM/PMC computer codes [8,9].

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Both the KENO-VI validation report and the CENTRM validation report include all the cases contained in 16 selected ICSBEP handbook evaluations plus an evaluation from a PNL report, for a total of 164 separate critical configurations. The validation reports contain a wide variety of critical configurations including high-enriched uranium (HEU) thermal, intermediate-enriched uranium (IEU) thermal, low-enriched uranium (LEU) thermal, mixed oxide (MOX) thermal, U-233 thermal and intermediate, and Pu metal fast experiments. The CENTRM validation contained an additional set of cases from the OECD calculational benchmark, which consists of 30 configurations of UO_2 spheres in a solution with varying amounts of uranium and boron. The one-dimensional discrete ordinates computer code XSDRN [10] was used in place of KENO-VI for these 30 configurations.

The results show that the KENO-VI computer code effectively calculates system k_{eff} and other physics parameters such as fluxes, fission densities, and mean free paths. The results are strongly dependent on the cross-section library used and the method used to self-shield the cross-section data. Both the NITAWL-III and CENTRM/PMC cross-section processors produce good results for the 164 cases derived from the ICSBEP benchmarks and the PNL report. None of these cases exceeded the inherent limitations of the Nordheim Integral Treatment used in NITAWL-III. The 20 OECD calculational benchmarks highlight the differences between NITAWL-III and CENTRM/PMC. In the cases where fissile material is contained in the pellet and surrounding solution, those that used NITAWL-III as the resonance processor diverged from those that used CENTRM/PMC, while the CENTRM/PMC cases remained in agreement with the results obtained using MCNP [11].

2 NITAWL-III vs CENTRM/PMC METHODOLOGY

The Nordheim Integral Treatment is the basis for the NITAWL-III module. NITAWL-III numerically solves the integral transport equation using collision probabilities; however, the geometry is limited to a single absorber region surrounded by a single moderator. This method can also be applied to simple lattice geometries by introducing a Dancoff factor into the escape probability from the absorber lump. Prior to the development of CENTRM and PMC, NITAWL-III was the primary module used in SCALE for self-shielding group cross sections in the resolved resonance range. The Nordheim method produces accurate problem-dependent cross sections for many classes of problems. It, however, has several limitations, some of which are listed below:

- The absorber composition in NITAWL-III is limited to a single resonance material combined with two admixed moderators, so that no resonance overlap effects are treated.
- Multiple absorber regions, such as a fuel lump inside a solution of dissolved fuel, cannot be treated, due to the assumed 1/E spectrum in the moderator.
- Space-dependent self-shielding within an absorber cannot be treated by NITAWL-III, nor can the impact of a space-dependent temperature variation be treated rigorously.
- A flat, isotropic neutron source is assumed in computing the absorber body spectrum.
- Anisotropic scattering effects on resonance self-shielding are ignored.
- A flat 1/E spectrum is assumed for the flux spectrum in the external moderator.
- The removal cross sections of nonabsorber materials are not corrected for problem-dependent spectrum effects.

The CENTRM/PMC self-shielding method is able to remove most of the limitations found in the Nordheim methods. Due to the general availability of dramatically improved computer resources, it is now feasible to treat resonance self-shielding with a much more rigorous approach. Multigroup cross sections can be generated directly by integrating the pointwise cross-section data in the CENTRM library, using problem-dependent flux spectra as weight functions for the various regions in the system. It can be shown that if the true flux spectrum in the system of interest is used as the weight function for multigroup averaging, then the resulting reaction rates computed with the processed multigroup cross sections and concomitant group fluxes should theoretically produce *exact* reaction rates. This approach is used by the CENTRM/PMC codes using a simplified one-dimensional system.

CENTRM (*C*ontinuous *EN*ergy *TR*ansport *M*odule) computes a one-dimensional "continuous-energy" neutron flux spectra using the Boltzmann transport equation. The purpose of the code is to provide highly accurate angular fluxes and flux moments for applications that require a detailed description of the fine-structure variation in the neutron energy spectrum. This is done by performing a CENTRM calculation for a simplified system model (e.g., a one-dimensional unit cell either isolated or in a lattice by reflecting the surfaces) and then utilizing the spectrum as a *problem-dependent weight function* for multigroup averaging. The multigroup data processing is done by the PMC code, which reads the CENTRM continuous-energy flux spectra and cross-section data; calculates problem-dependent, group-averaged cross sections over some specified energy range; and then replaces the corresponding data in an input AMPX master library. The resulting application-specific multigroup cross-section library is then passed to higher-dimensional calculations performed with a multigroup Monte Carlo code such as KENO-VI or with discrete ordinates codes such as XSDRN.

A multigroup working library and a CENTRM pointwise library are both required in CENTRM and PMC. Pointwise data in the CENTRM library are processed such that values at any energy can be obtained with a linear interpolation, within some error tolerance specified during the library generation (usually ~0.1% or less). In general, the library contains cross-section data at several temperatures; CENTRM interpolates pointwise cross sections to the desired temperatures using a $\sqrt{T}$ interpolation law.

The CENTRM pointwise calculation assumes s-wave elastic scatter from stationary nuclei; however, the CENTRM multigroup calculation places no restrictions on scattering reactions. For example, discrete and continuum inelastic reactions are included in the high-energy multigroup calculation; and both bound and free molecular motion are accounted for in the thermal portion of the multigroup calculation. CENTRM represents the anisotropy of the pointwise scattering source in the laboratory system by Legendre expansion orders up to P_5. A new technique, called a "submoment" expansion, allows the scatter source moments to be computed efficiently in CENTRM. A problem-dependent energy mesh is determined either internally by CENTRM or externally by a SCALE control module such as CSAS6.

3 ANALYSIS

The 164 cases, derived from the ICSBEP evaluations and the PNL report, contained in the KENO-VI validation report and the CENTRM validation report were set up using KENO-VI as

part of the CSAS26 sequence. They were analyzed using both NITAWL-III and CENTRM/PMC as cross-section data processors. For the cases derived from the ICSBEP handbook, the results from each case using each cross-section processor were then compared with ICSBEP results. The one case from the PNL report was compared with a measured k_{eff} = 1.0. Table I contains a listing of all the cases, their ICSBEP designation or source document, the number of cases derived from each ICSBEP evaluation or source document, and a brief description of the type of critical setup.

Table I. List of evaluations used in this validation report

ICSBEP designation [5]	No. of cases	Description
HEU-COMP-THERM-010	21	U(62.4)O_2 and BeO fuel pins surrounded by water, borated water, or uranyl nitrate
HEU-SOL-THERM-025	18	uranyl nitrate solution (89.0 wt % ^{235}U) with gadolinium nitrate in a 40-cm-diameter tank
HEU-SOL-THERM-035	9	uranyl nitrate solution (89.0 wt % ^{235}U) in a 110-cm-diameter tank w/ and w/o boron carbide absorber rods
HEU-SOL-THERM-037	9	uranyl nitrate solution (89.0 wt % ^{235}U) in a 160-cm-diameter tank w/ and w/o boron carbide absorber rods
IEU-COMP-THERM-002	6	SS-clad UO_2 annular fuel rods (17 wt % ^{235}U) in H_2O w/ and w/o gadolinium and cadmium absorbers
IEU-SOL-THERM-001	4	uranyl sulfate solution (~20.9 at. % ^{235}U) with graphite reflector
LEU-COMP-THERM-031	6	UO_2 rods (5 wt % ^{235}U), water moderated, hexagonally pitched (0.8 cm), zirconium clad
LEU-COMP-THERM-032	9	UO_2 rods (5 wt % ^{235}U), water moderated, varied temps., hexagonally pitched (0.7, 1.4, 1.852 cm)
LEU-SOL-THERM-005	3	uranyl nitrate solution (5.64 wt % ^{235}U) in a 110-cm-diameter tank w/ and w/o boron carbide absorber rods
LEU-SOL-THERM-006	5	uranyl nitrate solution (10.0 wt % ^{235}U) in a 110-cm-diameter tank w/ and w/o boron carbide absorber rods
MIX-COMP-THERM-002 (PNL)	6	UO_2(nat.) + PuO_2 fuel, square pitched (1.778, 2.20914, 2.51447 cm), varied array size, water moderated
MIX-COMP-THERM-003 (SAXTON)	6	UO_2(nat.) + PuO_2 fuel, square pitched, varied pitch and array size, water moderated
MIX-COM-THERM-004 (TCA)	11	UO_2(nat.) + PuO_2 fuel, square pitched, varied pitch and array size, water moderated
PNL-4976 [6]	1	2 wt % PuO_2 + UO_2(nat.) fuel interspersed with 4.3 wt % UO_2 fuel, hexagonally pitched, water moderated
PU-MET-FAST-045 (LCX-I)	7	Pu (w/Ni coating) disks with Ta and Al disks stacked to form a core of varying heights
U233-SOL-INTER-001	33	Be, CH_2, and Be-CH_2 reflected spherical SS tanks of ^{233}U uranyl nitrate solutions
U233-SOL-THERM-003	10	paraffin-reflected 5-, 5.4-, 6-, 6.6-, 8-, 8.5-, 9-, and 12-in.-diameter cylinder of ^{233}U uranyl nitrate solutions
OECD Calculational Benchmarks [7]	30	partially dissolved UO_2 pellets in a borated solution containing uranium

The 30 OECD calculational benchmarks are not based on critical experiments but were designed to test the capability of the cross-section resonance processor to properly account for fissile material and/or a strong neutron absorber in a solution surrounding fuel pellets. This was

intended to mimic the type of system one would expect in a fuel reprocessing plant. The uranium in the system ranged from 100% in the pellet and 0% in the solution (variation A and B from Table IV) to 50% in the pellet and 50% in the solution (variation E and F from Table IV). The boron concentration was either 1500 or 3500 ppm. Also the pellets were arranged in both square- and triangular-pitched arrays with cell pitches ranging between 0.9747 and 1.1788 cm. The 30 cases were evaluated using both NITAWL-III and CENTRM/PMC as cross-section resonance processors and then XSDRN PM [10] to calculate the system k_{eff}. These results were compared against MCNP [11] results. Tables III and IV list the characteristics of each OECD case.

4 RESULTS

There are two distinct sets of results: (1) the ICSBEP and PNL benchmarks and (2) the OECD calculational benchmarks. Table I contains a list of all the ICSBEP and PNL benchmarks used in this paper, the number of unique critical configurations in each benchmark, and a brief description of each benchmark. Table II contains the average k_{eff} and range of average fission energies (EALF) of all the critical configurations in each benchmark, using both NITAWL-III and CENTRM/PMC as the resonance processor. Finally a Δk_{eff}, which is the absolute value of the difference between the NITAWL-III results and the CENTRM/PMC results, is calculated. The average differences between the NITAWL-III and CENTRM/PMC results is well under 0.5% for all benchmark cases, although the individual critical configurations in a benchmark may vary by as much as 1.0%. Since the limitations associated with the Nordheim Integral Treatments are not violated in any of these benchmark cases, good agreement between the NITAWL-III and CENTRM/PMC results is expected.

The OECD calculational benchmarks were derived to test the ability of resonance-processing computer codes to properly self-shield group cross sections of fissile material lumps in a solution containing fissile material. The cases are divided by volume fraction of the cell containing the UO_2 pellet, array type, pitch, pellet diameter, percent of fissile material (UO_2) in the pellet, and amount of boron in the solution. Tables III and IV contain the data needed to construct the physical cell for each case. Cases are labeled using a number from Table III and a letter from Table IV. XSDRN PM was used in place of KENO-VI to produce the results of an infinite array of each cell type using both NITAWL-III and CENTRM/PMC as resonance processors. To check the results, each case was then modeled using MCNP. The results of each case are listed in Table V, along with the difference between the NITAWL-III and MCNP results and the CENTRM/PMC and MCNP results. The CENTRM/PMC results compare very well with the MCNP results in all cases, with differences in all but five cases being within 0.5%. Only the NITAWL-III results from the cases having no fissile material in the surrounding solution agreed with the CENTRM/PMC and MCNP results. When fissile material was present in the solution, the results varied by as much as 2.5%. This is due to the violation of the NITAWL-III limitation involving fissile material in more than one region in a cell.

Table II. Average results for each benchmark evaluation

ICSBEP designation [5]	NITAWL-III		CENTRM		% Δk_{eff}
	Range of EALF (eV)	Average k_{eff} (±σ)	Range of EALF (eV)	Average k_{eff} (±σ)	
HEU-COMP-THERM-010	0.0767 0.7930	1.00070 (0.00066)	0.0858 0.793	1.00321 (0.00076)	0.251
HEU-SOL-THERM-025	0.0405 0.1840	1.00943 (0.00057)	0.040 0.184	1.00785 (0.00055)	0.158
HEU-SOL-THERM-035	0.0369 0.0832	1.00635 (0.00066)	0.0369 0.0831	1.00360 (0.00066)	0.275
HEU-SOL-THERM-037	0.0378 0.0539	1.01059 (0.00069)	0.0378 0.0538	1.00965 (0.00069)	0.094
IEU-COMP-THERM-002	0.0894 0.1300	0.99403 (0.00066)	0.0889 0.133	0.99569 (0.00063)	0.166
IEU-SOL-THERM-001	0.0487 0.0774	0.98455 (0.00067)	0.0487 0.0772	0.98334 (0.00065)	0.121
LEU-COMP-THERM-031	0.3040 0.3550	0.99067 (0.00064)	0.304 0.356	0.98918 (0.00067)	0.149
LEU-COMP-THERM-032	0.0542 1.2260	0.99991 (0.00058)	0.0542 1.232	0.99992 (0.00058)	0.001
LEU-SOL-THERM-005	0.0402 0.0403	0.99887 (0.00044)	0.0401 0.0402	0.99844 (0.00045)	0.043
LEU-SOL-THERM-006	0.0477 0.0488	1.00503 (0.00058)	0.0477 0.0489	1.00078 (0.00061)	0.425
MIX-COMP-THERM-002 (PNL)	0.13761 0.77395	0.99991 (0.00060)	0.137 0.772	0.99961 (0.00055)	0.030
MIX-COMP-THERM-003 (SAXTON)	0.10101 0.89019	0.99920 (0.00060)	0.101 0.895	0.99895 (0.00062)	0.025
MIX-COM-THERM-004 (TCA)	0.07928 0.14560	1.00206 (0.00056)	0.0793 0.145	1.00216 (0.00055)	0.010
PNL-4976 [6]	4.68099	0.98192 (0.00049)	4.609	0.98530 (0.00051)	0.338
PU-MET-FAST-045 (LCX-I)	735,242 931,712	1.00963 (0.00065)	559,695 895,608	1.00690 (0.00064)	0.273
U233-SOL-INTER-001	1.18710 9.74552	0.98267 (0.00084)	1.209 9.929	0.98339 (0.00080)	0.072
U233-SOL-THERM-003	0.04520 1.01219	1.00502 (0.00076)	0.0455 1.014	1.00886 (0.00076)	0.384

Table III. Benchmark case description

Case	Cell UO_2 volume fraction	Array type	Cell pitch (cm)
1	0.6	Triangular	1.0297
2	0.5	Triangular	1.0943
3	0.4	Triangular	1.1788
4	0.5	Square	0.9747
5	0.4	Square	1.0501

Table IV. Benchmark variation description

Variation	Pellet diameter (cm)	% UO_2 in pellet	Boron in solution (ppm)
A	0.96	100	3500
B	0.96	100	1500
C	0.872	75	3500
D	0.872	75	1500
E	0.762	50	3500
F	0.762	50	1500

Table V. EALF and lambda for the OECD calculational benchmarks

Case	EALF (eV)	CENTRM/ XSDRN k_{eff}	NITAWL-III/ XSDRN k_{eff}	MCNP k_{eff} (±σ)	CENTRM/ MCNP % Δk_{eff}	NITAWL-III/ MCNP % Δk_{eff}
1a	3.137	1.0096	1.0061	1.0056 ± 0.0012	0.40	0.05
1b	2.225	1.0968	1.0929	1.0954 ± 0.0012	0.13	0.22
1c	3.329	0.9906	0.9613	0.9842 ± 0.0011	0.64	2.29
1d	2.371	1.0738	1.0412	1.0663 ± 0.0011	0.75	2.50
1e	3.386	0.9858	0.9563	0.9792 ± 0.0011	0.66	2.29
1f	2.425	1.0669	1.0340	1.0571 ± 0.0012	0.98	2.31
2a	1.264	0.9974	0.9974	0.9982 ± 0.0012	0.08	0.08
2b	0.836	1.1283	1.1283	1.1299 ± 0.0012	0.16	0.16
2c	1.327	0.9752	0.9560	0.9703 ± 0.0012	0.49	1.43
2d	0.881	1.0998	1.0775	1.0962 ± 0.0012	0.36	1.87
2e	1.330	0.9710	0.9516	0.9664 ± 0.0012	0.46	1.48
2f	0.889	1.0926	1.0701	1.0882 ± 0.0012	0.44	1.81
3a	0.627	0.9438	0.9441	0.9411 ± 0.0011	0.27	0.30
3b	0.390	1.1242	1.1245	1.1250 ± 0.0011	0.08	0.05
3c	0.648	0.9210	0.9080	0.9174 ± 0.0011	0.36	0.94
3d	0.405	1.0924	1.0766	1.0920 ± 0.0012	0.04	1.54
3e	0.641	0.9185	0.9053	0.9137 ± 0.0011	0.48	0.84
3f	0.404	1.0860	1.0699	1.0796 ± 0.0012	0.64	0.97
4a	1.264	0.9974	0.9981	0.9973 ± 0.0012	0.01	0.08
4b	0.836	1.1283	1.1292	1.1318 ± 0.0011	0.35	0.26
4c	1.327	0.9752	0.9561	0.9724 ± 0.0012	0.28	1.63
4d	0.881	1.0998	1.0776	1.0970 ± 0.0011	0.28	1.94
4e	1.330	0.9710	0.9515	0.9655 ± 0.0011	0.55	1.40
4f	0.889	1.0926	1.0699	1.0874 ± 0.0012	0.52	1.75
5a	0.628	0.9439	0.9444	0.9438 ± 0.0013	0.01	0.06
5b	0.390	1.1243	1.1249	1.1272 ± 0.0011	0.29	0.23
5c	0.649	0.9210	0.9081	0.9145 ± 0.0012	0.65	0.64
5d	0.405	1.0924	1.0766	1.0887 ± 0.0012	0.37	1.21
5e	0.641	0.9185	0.9052	0.9134 ± 0.0012	0.51	0.82
5f	0.404	1.0861	1.0698	1.0832 ± 0.0012	0.29	1.34

5 CONCLUSIONS

CENTRM/PMC has been shown to produce excellent results for a wide range of problems when used in conjunction with KENO-VI or XSDRN PM. NITAWL-III also produces excellent results as long as its limitations are not violated. The major limitation to CENTRM/PMC is its ability to model only a one-dimensional system. As a result, two- or three-dimensional effects cannot be explicitly taken into account. Other than this limitation, CENTRM/PMC can generate multigroup cross sections that produce results that are equivalent to those obtained by using continuous-energy cross sections.

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