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SCALE 5: New Cross-Section Processing Features and Capabilities

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Executive Summary

A new version of SCALE is being prepared for release in 2002. This new version, SCALE5, has many new features and capabilities. It has been reprogrammed using FORTRAN90, which provides more portability, reliability, and ease in updating for the code package. One of the major enhancements is the inclusion of the new resolved resonance processor modules CENTRM and PMC. CENTRM produces a problem dependent point-wise continuous energy flux profile at discrete geometric intervals. PMC uses this flux profile to collapse point-wise continuous energy cross-sections into multi-group cross-sections. Three sets of problems were examined to compare the results from this new resolved resonance processor, CENTRM/PMC, and KENO V.a (or XSDRNPM) with those from the multi-group resonance processor, NITAWL-III, and KENO V.a (or XSDRNPM) and the continuous energy code, MCNP. In all cases the CENTRM/PMC results were as good or significantly better than the NITAWL results. In all but one case, the CENTRM/PMC and MCNP results were within a few tenths of a percent. CENTRM/PMC enables problem-dependent multi-group cross-sections to have the flexibility and accuracy of point-wise continuous cross-sections.

1. Introduction

A new version of the SCALE [1] code package is being prepared for release in 2002. This paper discusses its new cross-section processing capabilities as well as some new and expanded features. The capabilities of new computer hardware and software enable more precise calculations for the resonance processing of nuclides. To take advantage of the increased speed and memory in current computers, the codes in SCALE5 have been updated and new modules added.

In addition to presenting some of the more important changes to SCALE5, this paper discusses and compares the new SCALE5 cross-section processor sequence, CENTRM/PMC/KENO V.a [2] (or XSDRNPM), to both NITAWL/KENO V.a [1] (or XSDRNPM), and MCNP [3]. Three different classes of problems are examined: (1) fuel pellets partially dissolved in a solution, (2) a subset of the Falstaff experiments, and (3) the temperature profile of a pressurized water reactor (PWR) pin cell. The CENTRM/PMC [2] processor is shown to produce good results in all cases.

2. SCALE5 Modifications

Our first consideration was to reprogram all modules using FORTRAN90. This change allows the modules to incorporate many features that were previously not possible. For example, in many modules the code now calculates and dynamically allocates the amount of memory needed. Data is stored in linked lists as it is read, eliminating the need to read through input data multiple times. The data previously stored in common blocks in each subroutine are now stored in modules referenced by the subroutines. Data can be passed between subroutines using modules, thus making it possible to shorten or, in some cases, remove the subroutine argument list. These types of changes make SCALE5 more robust, efficient, and easier to update.

Significant changes have also been made to the Standard Composition input format used by many modules in SCALE5 that are invisible to the user. Most of these changes were necessitated by the addition of the option to specify multiple unit cells. Currently in SCALE4.4a, only one unit cell can be specified and all other materials are treated as infinite homogeneous medium. Data must be added to the MORE DATA block to account for the geometry and lattice effects of the materials not specified in the unit cell. In SCALE5, each unit cell specification contains the cell type (infhommedium, multiregion, latticecell), cell geometry type (squarepitch, sphsquarep, symmslabcell, etc.), and appropriate material and geometry data. As many unit cells as required may be specified, but each material may only appear in one unit cell. All materials not in a unit cell are still processed as infinite homogeneous medium.

The search capabilities in SCALE5 have been expanded to allow each unit cell to be explicitly tied to either a unit or a material that is being modified in KENO V.a. Since multiple unit cells are now allowed, a search may now be done on lattices containing more than one fuel pin type. As the geometry or material in KENO V.a is modified, the unit cell is similarly modified thus ensuring that the cross-sections for the material are appropriately processed. A search case may alter the material densities, the pitch of the cells in a lattice, or simple geometry boundaries. Cell-weighted materials may now be included in the searches, updating the geometry, material, and cross sections as the search progresses.

In SCALE4.4a the specified control module (e.g. CSAS or CSAS6) produces a binary input file for every functional module (e.g. BONAMI, NITAWL, XSDRNPM) to be called prior to running the set of modules. These files are created in the temporary directory that executes the sequence. In SCALE5, because some modules must be executed once for every unit cell specified, multiple inputs for the same module may exist in this directory. To distinguish the input files, the unit cell number associated with the input file is appended to the end of the file name. In SCALE5 these input files are ASCII files, which allows a user to directly read and modify the input files for individual modules.

3. New Cross-Section Processing in SCALE5

The cross-section processing capabilities in SCALE5 have been expanded over the capabilities currently in SCALE4.4a. The cross-section data in the unresolved resonance range are still stored as Bondarenko factors and processed using BONAMI. The BONAMI input file contains all the data for all materials in all unit cells so this module is only called once for each non-

search problem. No significant changes have occurred in BONAMI from the user's perspective. However there are two new resolved resonance range cross-section processors: NITAWL-III and CENTRM/PMC.

NITAWL-III, based on NITAWL-II, has the capability to process multi-pole data, thus enabling it to process an ENDF/B-VI cross-section library with the Reich-Moore resonance parameters converted to multi-pole parameters. NITAWL uses the Nordheim Integral Treatment to process cross-section data in the resolved resonance range. Each resonance is processed individually, not accounting for the change in the background cross section due to other overlapping resonances. Also, a flux spectrum in the fuel lump is calculated based on the moderators and absorbers in the fuel lump and assuming a 1/E flux spectrum outside the lump as well as the slowing-down source above each resonance. As a result, if fuel is present outside the fuel lump, in the surrounding moderator, the external flux profile will be incorrect; resulting in improperly processed problem-dependent cross sections. There are certain classes of problems where these restrictions can lead to poor results such as the dissolver cases presented in this paper.

A second resolved resonance processor methodology has been developed and included in SCALE5 that does not have the limitations of NITAWL. This second methodology uses the modules CENTRM and PMC. CENTRM uses a point-wise continuous energy cross-section library to produce a set of point-wise continuous energy fluxes at calculated spatial intervals for each unit cell. Using these fluxes, PMC collapses the point-wise continuous energy cross-sections into multi-group cross sections for each nuclide in each material in the unit cell. Subsequent modules in SCALE5 can then use these multi-group cross sections. Discrete-level inelastic cross-section data can also be processed by CENTRM/PMC. Down scattering from inelastic continuum data and thermal up scattering are planned for future releases of CENTRM/PMC. CENTRM/PMC avoids many of the inherent assumptions in NITAWL by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment. Effects from overlapping resonances, fissile material in the fuel and surrounding moderator, and inelastic level scattering are explicitly handled in CENTRM/PMC.

A separate set of CENTRM and PMC input files are required for each unit cell, plus an additional set containing all the nuclides not specified in a unit cell. For a given SCALE sequence, such as the new CSASC5, the control module produces the input files for CENTRM and PMC based on the unit cell data specified in the problem. If a latticecell is specified, the code converts the cell description to an equivalent Wigner-Seitz cell for processing. When the CENTRM/PMC option is specified, WORKER, CENTRM and PMC are run for each unit cell specified plus one more time to process all the nuclides contained in materials not specified in a unit cell. When all nuclides have been processed WORKER is called one last time to convert the final master format library to a working format library.

Changes have also been made to the Standard Composition Library. A value of $\nu\sigma_f$ for each isotope has been added to the library for use in CENTRM. Also, the number of compositions, nuclides, and isotopes are now automatically tracked so the user does not enter this value when adding or subtracting something from the library. This change makes it easier for a user to add new compositions or nuclides to the Standard Composition Library as needed.

4. Analytical and Benchmark Calculations

The first set of calculations involves a subset of the OECD Criticality Working Group Benchmark 20 Problems [4]. These cases represent fuel pellets partially dissolved in a borated solution. These cases are modeled as infinite arrays of 2.5 wt % enriched UO_2 spheres in a borated solution where the spheres represent the UO_2 pellets. The boron concentration, UO_2 volume fraction, and percent of UO_2 in the pellet are varied. The 6 analyzed cases represent 1.0297 cm triangular pitched infinite 3-D arrays having a 0.6 UO_2 volume fraction. Cases 1a and 1b contain 100% of the UO_2 in the pellet, cases 1c and 1d contain 75%, and cases 1e and 1f contain 50%, with the remaining UO_2 in the surrounding solution. Cases 1a, 1c, and 1e contain 3500 ppm boron and cases 1b, 1d, and 1f contain 1500 ppm boron in the solution.

Following either NITAWL-III or CENTRM/PMC, XSDRNPM uses the processed cross-sections to calculate the λ, neutron multiplication, for the system. MCNP results using both ENDF/B-V and ENDF/B-VI cross-section libraries are provided for comparison. MCNP4C makes use of probability tables in the unresolved resonance region if they are present in the cross-section library. These tables are present in the ENDF/B-VI libraries but not in the ENDF/B-V libraries. The assumptions inherent to the Nordheim Integral Treatment, used in NITAWL-III, are not valid for the problems having fuel in the surrounding solution. CENTRM resolves this limitation by explicitly calculating a problem dependent point flux from point cross-sections. This flux is then used by PMC to create multi-group cross sections.

Table 1 contains the results for this subset of OECD Criticality Working Group Benchmark 20 problems. The results from processing the cross-sections using CENTRM/PMC are significantly different than those using NITAWL-III for the cases with uranium in the surrounding solution. The results using CENTRM/PMC are up to 3% higher than those using NITAWL-III as the resolved resonance processor. Also, The CENTRM/PMC/XSDRNPM results are in all cases within 0.2% of the MCNP results and are much closer to the MCNP ENDF/B-VI than the ENDF/B-V results, which indicate unresolved resonance processing is important.

Table 1. Comparison of Results Using the NITAWL, CENTRM, and MCNP for a Subset of the Criticality Working Group Benchmark 20 Problems

Case	wt % UO_2 in Pellet	Boron Concentration (ppm)	NITAWL-III XSDRNPM ENDF/B-V (λ)	CENTRM XSDRNPM ENDF/B-V (λ)	MCNP ENDF/B-V σ = 0.0004 k_{eff}	MCNP ENDF/B-VI σ = 0.0004 k_{eff}
1a	100	3500	1.0066	1.0080	1.0120	1.0090
1b	100	1500	1.0934	1.0950	1.0993	1.0969
1c	75	3500	0.9618	0.9887	0.9899	0.9885
1d	75	1500	1.0417	1.0718	1.0734	1.0708
1e	50	3500	0.9566	0.9838	0.9849	0.9827
1f	50	1500	1.0343	1.0647	1.0655	1.0634

The second set of calculations involves a subset of the U233-SOL-INTER-110 Falstaff set of experiments found in the International Handbook of Evaluated Criticality Safety Benchmark Experiments [5]. This series of criticality experiments, performed at the Lawrence Livermore National Laboratory in the late 1950s, used aqueous ^{233}U in the form of UO_2F_2 stabilized with 0.3 wt % HF in a stainless steel spherical container surrounded by a reflector. The ^{233}U concentration for this subset of experiments was 0.866 g/ml and the six type 347 stainless steel spherical vessels had inner radii ranging from 7.87 cm to 10.80 cm. The sphere was surrounded by either a Be, CH_2, or combination Be+CH_2 reflector. The systems were brought to criticality by sequentially adding additional reflector shells in 0.5 cm steps.

Table 2 contains NITAWL-III/KENO V.a, CENTRM/PMC/KENO V.a, and MCNP results of 11 cases from the Falstaff set of experiments. Even though these are critical experiments, in all but one case the system k_{eff} was calculated more than 1% low by all three sets of codes. In all but one case CENTRM produced results closer to critical than NITAWL-III, varying by as much as 1.9% greater than the NITAWL-III results. For all but one case, CENTRM/PMC/KENO V.a and MCNP results agreed within 0.3%. The energy of the average lethargy causing fission (EALF) for these 11 problems is between 3.4 eV and 10 eV. Consequently, the majority of fissions occur by neutrons having energies in the resolved resonance range, which makes resonance cross-sections and resonance processing extremely important. CENTRM/PMC and MCNP process continuous energy cross sections in very different manners but still achieve similar results.

Table 2. Sample k_{eff} Calculational Results of the U233-SOL-INTER-001 Experiment

			EALF (eV)	KENO V.a 238-Group ENDF/B-V		MCNP ENDF/B-VI Continuous Energy
				NITAWL-III	CENTRM/PMC	
Sol'n No.	Sphere No.	Reflector		$\sigma = 0.0003$ k_{eff}	$\sigma = 0.0003$ k_{eff}	$\sigma = 0.0002$ k_{eff}
1	1	Be	7.43	0.9724	0.9909	0.9894
1	2	Be	8.33	0.9715	0.9844	0.9848
1	3	Be	8.80	0.9744	0.9836	0.9854
1	3	Be+CH_2	3.46	1.0001	1.0050	0.9953
1	4	Be	9.27	0.9790	0.9858	0.9885
1	4	Be+CH_2	4.06	0.9878	0.9901	0.9876
1	5	Be	9.60	0.9778	0.9822	0.9853
1	5	CH_2	4.36	0.9782	0.9785	0.9819
1	5	Be+CH_2	6.99	0.9814	0.9841	0.9824
1	6	Be	9.97	0.9753	0.9781	0.9820
1	6	Be+CH_2	7.40	0.9804	0.9815	0.9825
1	Mean $\pm \sigma$			0.9798 ± 0.0081	0.9858 ± 0.0075	0.9859 ± 0.0041

The final calculation examines the effect of the temperature distribution on the results of an infinite lattice of hot fuel pins. This problem is a simplified representation of a fuel pin from the Takahama-3 PWR reactor reported in Ref. [6]. The cell consists of 4.1% enriched UO_2 fuel rods, a helium filled gap, Zircalloy-4 cladding, and a water moderator on a 0.6555 cm pitch, having the isotopic number densities and dimensions specified in Table 3. The Zircaloy-4 cladding was replaced with zirconium to make it easier to model identical SCALE5 and MCNP versions of the problem. The temperatures were chosen based on available temperatures in the MCNP library. Except for the He in the gap these temperatures are within 10 K of those used in the report.

Table 3. Description of Takahama-3, SF95 Cell

Region	Radius (cm)	Material	Number Density (atoms/bn-cm)	Temperature (K)
Fuel	0.4025	UO_2	^{235}U: 9.64154E-4 ^{238}U: 2.22670E-2 O: 4.64622E-2	900
Gap	0.411	He	1.50456E-4	294
Clad	0.475	Zr	4.28457E-2	587
Coolant	0.739716	H_2O	H: 6.67692E-2 O: 3.33846E-2	587

The cell (consisting of the fuel, gap, clad, and moderator) was reflected on all sides to represent an infinite array of infinitely long cylinders. Results were then obtained for the system using NITAWL-III/KENO V.a, CENTRM/PMC/KENO V.a, and MCNP. The results for the three cases are within 0.9%, as shown in Table 4, with the CENTRM results being about 0.6% lower than the MCNP results. The fuel region was then divided into 10 equally thick regions and given the temperature profile listed in Table 5, which is representative of fresh fuel in a reactor. The cladding was also divided into 2 equally thick regions. The k_{eff} of the multiple fuel temperature region case decreased about 0.6% compared to the single fuel temperature region CENTRM case. The rise in temperature seems to have only a small negative effect on the worth of the fuel. Also, moving from the outermost to the innermost fuel region, the fission density decreases about 14% and the neutron spectrum becomes harder, with a larger percentage of fissions occurring due to fast neutrons. Table 5 contains the fuel temperature, fission density and percent of fissions occurring in each of the 10 regions, where region 1 is the innermost fuel region and region 10 is the outermost fuel region.

Table 4. Results for Temperature Profile Fuel using ENDF/B-V cross-sections in MCNP and the 238groupndf/B-V multigroup cross-section library

Case	Number of fuel regions	k_{eff} ($\pm \sigma$)
NITAWL-III/KENO V.a	1	1.4386 (0.0006)
CENTRM/PMC/KENO V.a	1	1.4414 (0.0006)
MCNP	1	1.4493 (0.0005)
CENTRM	10	1.4320 (0.0005)

Table 5. Fission Density for Fuel Divided Into 10 Equally Thick Regions

Region	Temperature K	Fission Density	% Total Fissions
1	1525	0.0951	0.93
2	1510	0.0965	2.83
3	1485	0.0965	4.72
4	1440	0.0973	6.66
5	1370	0.0984	8.66
6	1290	0.0994	10.69
7	1215	0.1005	12.78
8	1130	0.1027	15.06
9	1000	0.1048	17.45
10	900	0.1088	20.22

5. Conclusions

SCALE5 is a very significant improvement over the existing version of SCALE. It contains many enhancements that add to its flexibility and reliability. Many new features have been added to existing modules and several new modules have been added to the code package. One of the more important additions is the new resolved resonance processor, CENTRM/PMC. This addition enables the code to properly process cross-sections for configurations that do not fit the limiting assumptions of NITAWL. For the problems presented in this paper, CENTRM/PMC/KENO V.a (or XSDRNPM) produces results comparable to those from MCNP. This new resonance processor enables a problem being modeled using multi-group cross-sections to have the accuracy of point-wise continuous cross-sections.

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