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Combining MC^2-2 and SCALE cross section methods to process nuclear data for GNEP

M. L. Williams[a*], J. C. Gehin[a], Won Sik Yang[b]

[a]*Oak Ridge National Laboratory, Oak Ridge, TN USA*
[b]*Argonne National Laboratory, Argonne, IL USA*

Abstract

This paper describes a joint project by Oak Ridge National Laboratory and Argonne National Laboratory to merge components of the SCALE nuclear analysis system with the MC2-2 code to obtain a more general tool for producing problem-dependent MG cross sections for GNEP and other advanced reactor applications. The complementary aspects of the two methods are described, and the procedure used to couple the codes is outlined. The combined system was used to compute problem-specific self-shielded cross sections for a model of the Advanced Burner Reactor.

1. Description of Work

The processing of problem-specific multigroup (MG) cross section data is one of the primary factors affecting the reliability of reactor physics calculations for the Global Nuclear Energy Partnership (GNEP) project. Much emphasis has been placed on design of a liquid metal reactor (LMR) to serve as the Advanced Burner Reactor (ABR). The ABR will have a hard spectrum efficient for burning long-lived transuranic actinides. In this energy range the most important data are actinide fission and capture cross sections in the unresolved – and to a lesser extent, the upper resolved – resonance range. Resolved resonance data for structural materials are also important. Hence accurate self-shielding methods are required for analysis of fast reactors. In addition, the detailed composition of recycled fuel and waste products must be accurately predicted for evaluation of radiation sources and criticality safety at reprocessing and fabrication plants. This requires calculating detailed fission product distributions beyond what is needed exclusively for core physics.

The complete GNEP vision also requires improvements in reactor physics methods for thermal systems. Advanced thermal reactors are envisioned for the grid of international power plants that form the basis of the global partnership. The thermal reactor nodes will most likely utilize reprocessed fuel and will produce much of the high level waste stream to be transmuted in the ABR. Analysis of advanced thermal reactors requires processing nuclear data in the resolved resonance and thermal ranges of actinide materials as well as treating moderation, thermal scattering, and heterogeneous lattice effects that are much different from those of the ABR. Hence a wide spectrum of reactor physics methods is needed to address the overall performance of the closed global fuel cycle as proposed for GNEP.

Oak Ridge National Laboratory (ORNL) is currently working with Argonne National Laboratory (ANL) to examine the feasibility of establishing a unified set of neutronic methods to address the full

[*] Corresponding author, WilliamsML@ornl.gov
Tel. +865-576-5565; Fax +865-574-9619.

range of reactor physics and transmutation issues anticipated for GNEP and other advanced reactor concepts. The initial effort has focused on self-shielding methods for fast reactor calculations but later may be extended into other areas such transmutation -depletion data and methods, advanced thermal reactor physics, sensitivity/uncertainty analysis, and core modeling and simulation using high performance computing techniques. The basic idea is to merge the capabilities of two existing code systems: MC^2-2 and SCALE. The MC^2-2 code was developed at ANL during the 1970's to generate problem-specific MG cross sections for liquid metal fast breeder reactor (LMFBR) design calculations and for analysis of fast critical integral experiments. MC^2-2 is still the standard method being used by ANL and other organizations for multigroup transport calculations supporting ABR analysis. On the other hand the SCALE code system was developed at ORNL mainly for thermal reactor physics, criticality safety, and shielding applications. The latest version, SCALE-6.0, is scheduled to be released during 2008. Hence, the uses of MC^2-2 and SCALE are somewhat complementary. This paper describes initial work to integrate the two systems into a unified, robust procedure for processing problem-specific multigroup data for applications in the GNEP program.

2. Methodology

MC^2-2 computes "ultrafine group" asymptotic spectra in 2082 energy groups for homogeneous regions representing the inner core, outer core, reflector, within a fast reactor. Resolved and unresolved resonances are treated explicitly by the generalized J^* integral formulation. This approach determines shielded resonance integrals using the narrow resonance approximation and the single-level Breit Wigner (SLBW) resonance formulae. A multipole method allows the SLBW expressions to be used with the more accurate Reich-Moore resonance formalism in ENDF/B-VII. Alternatively the hyperfine group integral transport option (RABANL) based on collision probabilities can be used for homogeneous or heterogeneous (pin or slab) unit cell calculations. The strengths of MC^2-2 are its treatment of: (a) the rapidly varying elastic scattering cross sections of intermediate nuclides, (b) the unresolved resonance ranges of fissile and fertile materials, (c) the fast energy range where various transport approximations (e.g., consistent/inconsistent-P_N) are available for processing total and transport cross sections weighted by Legendre flux-moments – providing the capability to address high-leakage regions using diffusion or low order transport theory.

In this work MC^2-2 is used to obtain self-shielded cross sections for the unresolved resonance range of all materials; and the ultra-fine group calculation provides an asymptotic flux spectrum to collapse fast nuclear data, using the P_N transport-corrections in the energy range above ~500 keV where neutron leakage effects are important.

SCALE is a modular code system in which a driver program performs a sequence of calculations with executable modules. For example in the TRITON lattice physics sequence (DeHart, 2006b) the modules BONAMI, CENTRM, and PMC (Williams and Hollenbach, 2006) process self-shielded MG cross sections for the unresolved and resolved ranges, respectively. These are passed to the NEWT two-dimensional arbitrary transport code (DeHart, 2006a; Williams et al., 2006) which computes space-dependent microscopic reactions rates for assembly lattices. The ORIGEN-S depletion code uses the reaction rates to calculate the transmutation of ~1500 nuclides versus exposure. This series of calculations is repeated for multiple burnup-steps and for any specified branch states (e.g., step variations in temperature, water density, etc.) to generate a tabulation of assembly-homogenized broad-group cross sections. The tabulated MG data can be interpolated to obtain state-specific cross sections for full core calculations. This procedure of course is well established for thermal reactor physics, but is not usually utilized for fast reactors, where problem-specific/self-shielded cross sections are usually generated once at some reference configuration and then used for all burnup steps. Therefore at this time only the SCALE resolved resonance self-shielding methodology performed with the CENTRM and PMC codes has been integrated with MC^2-2 to process problem-dependent MG data for fast reactor analysis.

Although CENTRM/PMC has been developed primarily for criticality safety analysis and thermal reactor lattice physics, the basic approximations are also applicable to fast systems. CENTRM computes neutron flux spectra on a tailored mesh of ~30,000 to 70,000 energy points, as a function of space and direction, using one-dimensional (1D) discrete ordinates or other transport approximations homogeneous medium with buckling; 1D collision probability, or P_1 (Williams and Asgari, 1995). A linear variation of the flux is assumed between energy points, so that a continuous-energy solution is generated over the entire energy range. The high resolution flux spectra from CENTRM are passed to PMC, where they are used as weighting functions to average pointwise (PW) nuclear data into problem-specific MG cross sections. The CENTRM transport solution accounts for temperature-dependent self-shielding effects due to resonance absorption, cross-shielding from overlapping resonances of different materials, space-dependent slowing-down with anisotropic scattering, and bound-thermal scattering reactions. Discrete level inelastic scattering also is treated rigorously within the assumption of s-wave scattering, but continuum inelastic scattering is approximated crudely.

The CENTRM solution is subdivided arbitrarily into three computational ranges designated Upper Multigroup (UM), Pointwise (PW), and Lower Multigroup (LM), which are coupled by the slowing-down sources. Fine-group MG transport calculations are performed for the UM and LM ranges while a PW solution is done in the energy interval between these two. The energy boundaries between the three ranges are controlled by input; thus the PW solution can extend over the entire energy range if desired; or alternatively, MG solutions can be specified where a detailed PW description of the flux spectrum is not needed. MG cross sections for the UM and LM calculations are taken from the SCALE 238 group ENDF/B-VI and VII libraries. The PW calculation uses tabulated cross sections processed directly from ENDF/B data, with a linear tolerance of 0.1%. For example, the ^{238}U capture cross section at room temperature is represented by about 120,000 energy points at this tolerance. For thermal reactors the PW calculation is typically specified from 0.001 20 keV, which encompasses the resolved resonance ranges of all important actinide nuclides. This can be modified as desired for fast reactors but CENTRM currently assumes that downscatter sources coupling the UM and PW ranges are mainly due to elastic reactions. This assumption becomes less accurate as the PW range is extended significantly above the inelastic threshold of major materials. Therefore in this work the PW calculation is limited to the range below 500 keV, and the CENTRM solution in the UM range is replaced by the ultrafine group MC^2-2 asymptotic solution.

Figure 1 shows a flow chart of the procedure for combining MC^2-2 and CENTRM/PMC methodologies to produce a problem-specific ISOTXS formatted library. The method consists of initial MC^2-2 calculations performed by ANL to obtain problem-specific MG cross sections in the ANL 2082 group structure. The resulting MC^2-2 libraries in ISOTXS format have been corrected for unresolved self-shielding, and include total cross sections weighted by Legendre moments of the asymptotic flux. These are required for applying transport corrections to improve the calculation of leakage effects in the fast energy range.

Next a CENTRM calculation is performed using either a 1-D core model, or an asymptotic homogeneous medium. CENTRM PW fluxes, along with the MC^2-2 ISOTXS data, are input to a modified version of PMC, called PMC^2. This code uses the PW flux to process MG data over a specified energy interval, typically including the resolved resonance ranges of all important nuclides, and the new MG data replace the corresponding MC^2-2 values within the designated energy range. The problem-specific 2082 group library can be collapsed further for subsequent broad-group diffusion or low-order transport calculations. Aside from the initial MC^2-2 calculation, the procedure is automated and requires little input by the user.

3. Application

The methodology was tested for several cases based on the projected equilibrium core for the 250 MWt metallic fuel design of the ABR (Yang et al., 2007). MC^2-2 asymptotic calculations were performed for the core compositions and for other homogeneous regions in the system, which provided the fast cross sections above 100 keV. This was followed by a CENTRM space-dependent S_6-P_1 transport calculation using a 1-D cylindrical model of the ABR inner and outer core, reflector, and shield regions. The CENTRM PW range extended up to 100 keV and included about 34,000 energy points. ENDF/B-VI.8 cross sections were used.

Figures 2 and 3 show the CENTRM continuous-energy flux spectra for the energy intervals 5-10 keV and 10-100 keV, respectively, in the inner core region. The general shape of energy spectrum in Figure 2 is caused by the s-wave cross sections of structural material such as iron and chromium, with superimposed fine-structure due to reactions with the narrower p-wave resonances. Self-shielding from capture in the resolved resonances of ^{238}U is apparent in Figure 3. The ^{238}U resolved range extends to 10 keV in ENDF/B-VI.

Because the CENTRM calculation is space-dependent, it is possible to obtain nonasymptotic spectra, for example at the core-reflector interface, which can be used to process space-dependent MG cross sections. Figure 4 illustrates the differences in ^{238}U self-shielded cross sections computed with

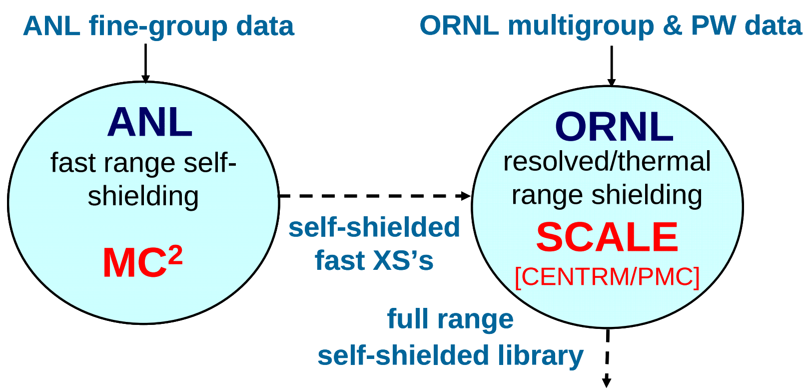

Fig. 1. Flowchart for Combined MC[2]-SCALE Cross Section Processing.

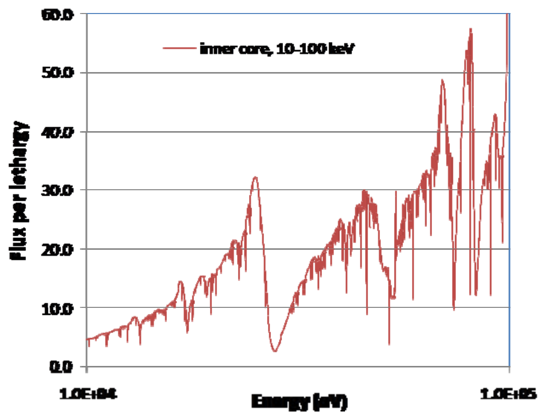

Fig. 2. CENTRM PW Flux Spectrum 10-100 keV for ABR Inner Core.

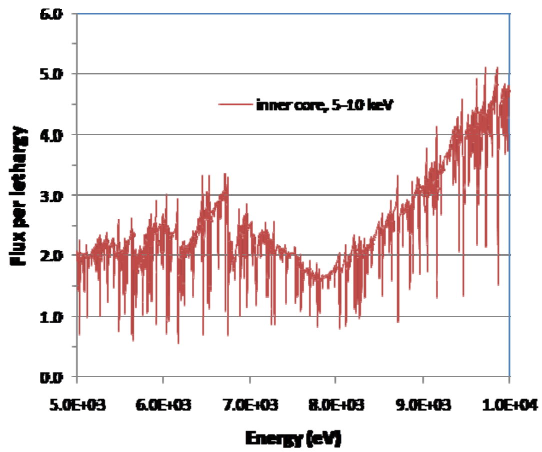

Fig. 3. CENTRM PW Flux Spectrum 5-10 keV for ABR Inner Core.

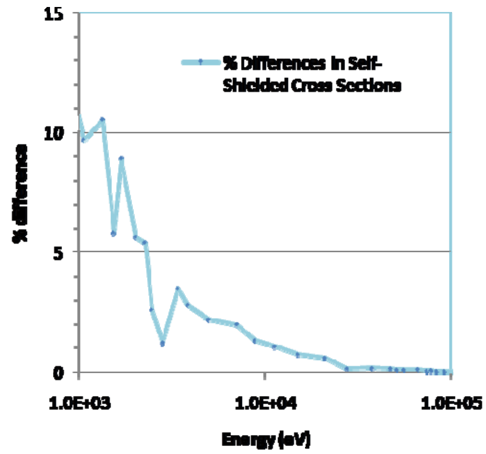

Fig. 4. Difference in ^{238}U self-shielded cross sections: boundary location vs average value for outer core.

the average flux for the outer core region, compared to using the flux spectrum at the outer boundary of the region. Differences of 2-10% are seen in the shielded group cross sections for the resolved resonance range below 10 keV. For ABR designs that use metallic fuel produces a hard spectrum, these differences do not have much overall impact on criticality, but can affect ^{238}U capture rate (and Pu production) near the reflector. However, designs that use oxide fuel have a softer spectrum and are more sensitive to these differences.

4. Conclusions

The key to the GNEP concept is establishing alliances between organizations to resolve problems related to designing and eventually deploying advanced reactors and reprocessing facilities. In this work ORNL and ANL have collaborated to combine features of the MC^2-2 and SCALE computational procedures for analysis of the ABR and other advanced reactor types. The initial phase of the work as described in this paper has focused on processing problem-specific MG cross sections by integrating capabilities of the CENTRM/PMC resolved resonance self-shielding modules from SCALE, with the MC^2-2 treatment of the unresolved and fast range data. A prototypic methodology has been established and applied to a ABR model. Future work will examine the impact of applying this approach to different reactor designs and to a wider range of performance parameters.

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