Recent Enhancements to the SCALE 5 Resonance Self-Shielding Methodology

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INTRODUCTION

All versions of SCALE (Standardized Computer Analyses for Licensing Evaluation) [1] prior to release 5 have used the same two computation modules for resonance self-shielding. BONAMI, [2] based on Bondarenko's shielding-factor method, performs self-shielding corrections for the unresolved range, and NITAWL [3] applies the Nordheim treatment for the resolved-resonance range. These two codes have changed relatively little over the last 20 years. Although this historical approach was also retained in SCALE 5, a significant extension to the resolved-resonance shielding capability has been provided by the introduction of two new codes, CENTRM [4] and PMC.[5]

CENTRM solves the discrete-ordinates approximation to the Boltzmann transport equation in one-dimensional geometries, using tabulated pointwise (PW) nuclear data. Neutron spectra are typically computed by CENTRM on a grid of 30,000-40,000 energy points tailored to the macroscopic cross-section energy structure for the mixtures in the problem geometry. In this manner the spectral fine structure due to resonance reactions is calculated accurately, taking into account the impact of level-level interference, resonance overlap, and material interface effects. The resulting "continuous-energy" spectra for each material zone are input to the PMC code for averaging PW nuclear cross sections to obtain self-shielded multigroup (MG) data. The problem-dependent MG cross sections can be used in higher-dimensional calculations with the KENO [6] or NEWT [7] modules of SCALE.

RESONANCE-SHIELDING IMPROVEMENTS FOR SCALE 5.1

In the initial 2004 release of SCALE 5.0, NITAWL continued to be the default code for resolved-resonance shielding in all CSAS, SAS, and TRITON sequences. The new CENTRM/PMC approach was optional and typically has been selected when the assumptions inherent in NITAWL fail (e.g., in treating cases with significant resonance interference or overlap effects, for arrays of fissionable bodies contained in a fissionable solution, or for leakage-dominated systems that require self-shielding based on the neutron current rather than the flux spectrum). However, CENTRM/PMC will play a more central role in the next release of SCALE 5, version 5.1, and will be the default resonance-shielding method for many types of cases. For example, because the NITAWL approach does not work well for the Reich-Moore resonance formalism, CENTRM will be utilized for all calculations performed with the new ENDF/B-VI libraries. Several enhancements also are being made to the self-shielding procedures within SCALE 5.1 to provide a broader range of functionality for criticality safety and lattice physics applications. Some of the major improvements being made for the next release of SCALE include:

1. Extension of the PW thermal flux solution in CENTRM to utilize bound thermal-scattering kernels based on ENDF/B S(α, β) data. The original code could use only free-gas kernels.
2. Implementation of an efficient two-region solution method in CENTRM. The two-region approximation usually runs much faster than the discrete-ordinates solution, and is similar to the NITAWL model with fewer limitations. The new option is adequate for a wide range of "standard" applications. Table I shows a comparison of eigenvalue results obtained by the various self-shielding options for several benchmark criticals.
3. Implementation of an improved method to compute MG elastic removal data in PMC.
4. Development of improved techniques to treat nonuniform arrays of absorber bodies. This includes developing a method based on Monte Carlo to compute Dancoff factors and a new approach to determine Dancoff-equivalent cells for CENTRM calculations.
5. Addition of the capability to compute PW disadvantage factors and to obtain cell-homogenized PW cross sections. This provides a technique to "smear" small heterogeneities such as micrograins in fuel pellets or pebbles during the resonance-shielding computation. Figures 1 and 2 show cell-homogenized PW cross sections for a sample case.
6. Development of a new calculation sequence to address doubly heterogeneous cells by applying sequential CENTRM/PMC resonance calculations for the low- and high-level heterogeneities, respectively.

TABLE I. KENO k_{eff} Values, as a Function of Self-Shielding Method (SN = PW discrete ordinates, 2R = PW two-region, NITAWL = Nordheim).

ENDF/B-V				
Case	EALF*	CENTRM-SN	CENTRM-2R	NITAWL
hst25-18	1.55E-01	1.0022	1.0028	1.0032
ict02m-6	1.27E-01	0.9929	0.9890	0.9906
cas09.i	9.83E-02	0.9988	0.9951	0.9956
cas17.i	3.09E-01	0.9953	0.9984	0.9999
cas29.i	3.55E+00	0.9950	0.9998	0.9984
cas40.i	1.47E+00	0.9954	0.9947	0.9925
pnl-35	1.82E-01	1.0056	1.0053	1.0051
ENDF/B-VI				
Case	EALF*	CENTRM-SN	CENTRM-2R	
hst25-18	1.61E-01	0.9983	0.9993	
ict02m-6	1.30E-01	0.9921	0.9902	
cas09.i	9.75E-02	0.9915	0.9908	
cas17.i	3.10E-01	0.9928	0.9958	
cas29.i	3.53E+00	0.9931	0.9930	
cas40.i	1.42E+00	0.9913	0.9921	
pnl-35	1.82E-01	0.9987	1.0002	

*EALF = energy of average lethargy for fission.

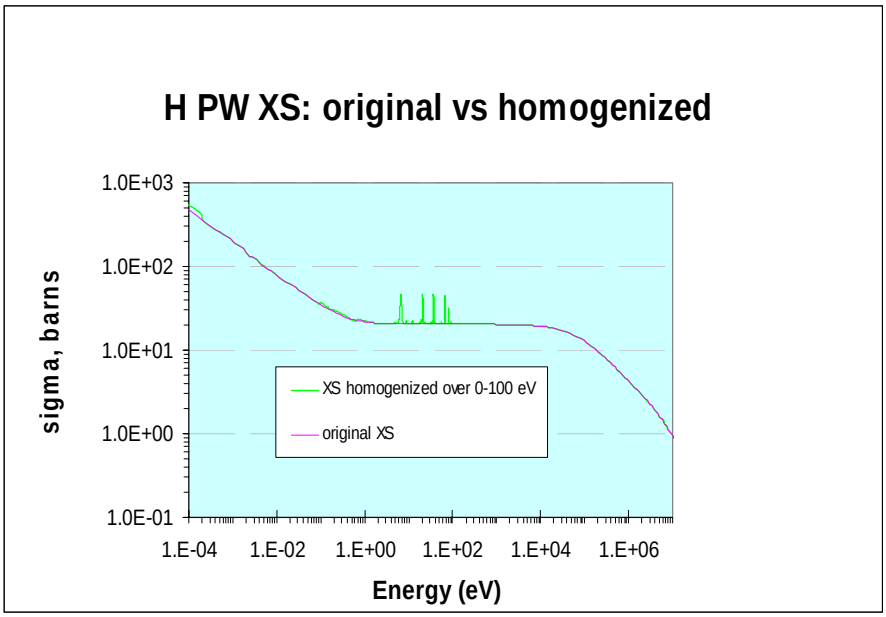

Fig. 1. Point cross sections for hydrogen, cell homogenized over range 0.1–100 eV.

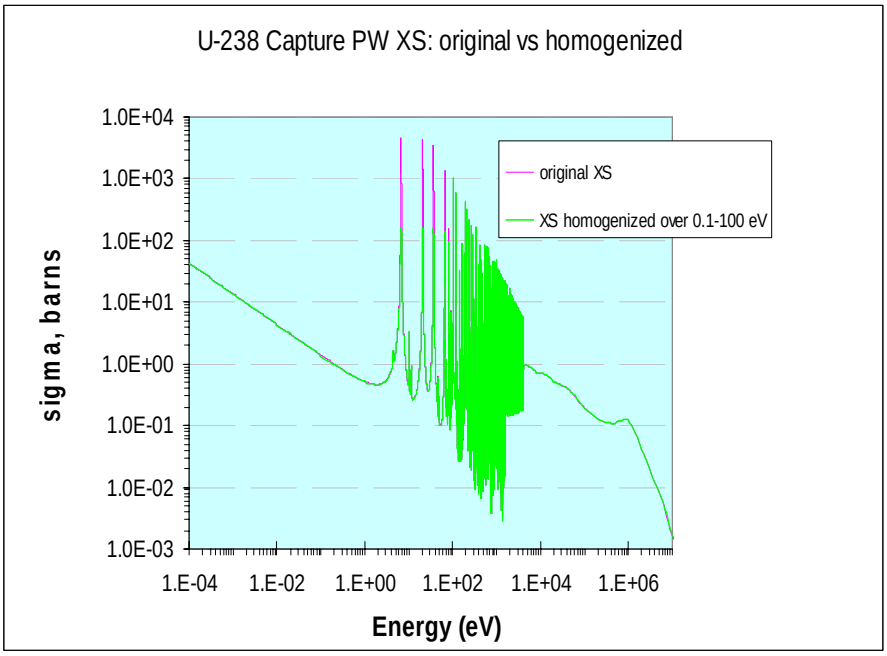

Fig. 2. Point cross sections for U-238, cell homogenized over range 0.1–100 eV.

SUMMARY

The release of SCALE 5.1 will rely heavily on using PW transport calculations for resonance self-shielding calculations. In conjunction with this approach, several important improvements are being made to the CENTRM/PMC codes and the SCALE computation sequences. The enhancements include improved physics approximations and numerical procedures, more accurate techniques to treat nonuniform arrays and doubly heterogeneous fuel lumps, and a new two-region approximation allowing faster self-shielding computations for many conventional types of problems.

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