ENERGY-POINTWISE DISCRETE ORDINATES TRANSPORT METHODS

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An accurate determination of the space-dependent flux spectrum throughout an array of fissionable components is one of the most important and basic quantities required in criticality safety analysis. Knowledge of the detailed energy spectrum within the various fissionable and absorber components is needed to determine realistic reaction rates and resonance-shielded multigroup cross sections for subsequent criticality analysis performed with multigroup codes such as KENO. Due to the presence of resonance materials such as uranium and plutonium, the energy spectrum generally exhibits very complex, fine-structure effects within the resolved resonance range that will vary spatially from region to region. Although pointwise Monte Carlo codes such as MCNP can in theory accurately include these effects directly in the transport calculation, multigroup codes such as KENO and all deterministic codes must rely on properly averaged multigroup cross sections to reflect the impact of resonance self-shielding. The great difficulty involved with determining the complicated behavior of the flux spectrum has led to the use of rather simplistic approximations for averaging multigroup cross sections. For instance, equivalence theory and the narrow resonance approximation are inherent in the widely used Bondarenko approach, and the old Nordheim integral method assumes isolated resonances and is limited to only a single absorber component surrounded by moderator. These two methods are currently utilized in the SCALE system to self-shield multigroup cross sections for criticality calculations. Errors introduced into the problem-dependent, self-shielded cross sections by the approximations will propagate into errors in the calculated value of the multiplication factor. Hence, there is strong motivation to develop a more rigorous approach to obtain accurate problem-dependent spectra for multigroup cross section generation.

A new one-dimensional code called "CENTRM" has been developed that computes a detailed, space-dependent flux spectrum in a *pointwise-energy representation* within the resolved resonance range, coupled to a fine-group multigroup calculation above and below the pointwise range. The code uses discrete-ordinates transport theory with an arbitrary angular quadrature order and a Legendre expansion of scattering anisotropy up to P7 for moderator materials and up to P3 for heavy nuclides. The elastic scattering source moments in the pointwise range are evaluated with a new, efficient algorithm called a "sub-moment expansion" developed for s-wave center-of-mass scatter kernels. Pointwise nuclear data is rigorously processed from ENDF/B into a specially formatted CENTRM file, and multigroup data for the non-pointwise range can be obtained from any desired "Working Library" generated by the AMPX code system. For example, the criticality safety libraries in the SCALE system can be used directly in CENTRM.

The CENTRM program provides unprecedented capability to deterministically compute full energy range, space-dependent angular flux spectra in one-dimensional geometries, rigorously accounting for resonance fine-structure and scattering anisotropy effects. The code will become a

component in the SCALE system to improve the computation of self-shielded cross sections used in criticality safety calculations, thereby enhancing the accuracy of such codes as KENO.

Several applications to lattices of low-enriched fuel rods are discussed at the workshop presentation. In these examples, an energy mesh of approximately 15,000-20,000 energy points is used in the flux calculation, with an S8 quadrature and P3 scattering. It is shown that the CENTRM-produced multigroup cross sections give critical eigenvalues that agree within about 0.15% of MCNP calculations. Comparisons of CENTRM results to critical benchmark measurements also show good agreement but suggest that the U-238 capture data in ENDF/B-VI predicts more resonance capture than the experiment.