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VIM: Initial ENDF/B-VI Experience*

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by Roger N. Blomquist

Introduction

The VIM Monte Carlo particle transport code[1] uses detailed continuous-energy cross sections produced from ENDF/B data by a set of specialized codes developed or adapted for use at Argonne National Laboratory[2]. ENDF/B-IV data were used until about 1979, and Version V data since then. These VIM libraries were extensively benchmarked[3] against the MC^2-2 code[4] and against ZPR and ZPPR criticals for fast spectrum calculations, as well as other fast and thermal experiments and calculations. Recently, the cross section processing codes have been upgraded to accommodate ENDF/B-VI files, and a small library has been tested.

Several fundamental tasks comprise the construction of a faithful representation of ENDF data for VIM calculations: (1) The resolved resonance parameters are converted to Doppler-broadened continuous-energy cross sections with energy grids suitable for linear-linear interpolation. (2) The unresolved resonance parameter distributions are sampled to produce many (40-400) resonance ladders in each energy band. These are converted to Doppler-broadened continuous-energy resonance cross sections that are then binned by cross section, accumulating ladders until statistical convergence, the result being probability tables of total cross sections and conditional mean scattering and fission cross sections. VIM samples these tables at run time, and File 3 background cross sections are added. (3) Anisotropic angular distribution data are converted to angular probability tables. All other ENDF data are unmodified, except for format.

Modifications

In the resolved range, Version VI required several changes. The Reich-Moore formalism in the resolved resonance range was implemented using the REICH subroutine of the WHOPPER code[5]. The piecewise resolved resonance ranges in ^{239}Pu and ^{235}U were separately converted to pointwise cross sections, and then combined. Finally, the Doppler broadening algorithm, based on the finite-difference scheme for solving the heat equation for an infinite medium, was not applied at energies far below the lowest resonance.

In the unresolved range, when LSSF=0, the File 3 data are the partial background cross sections to be added to the resonance cross section sampled from the probability table at run time. For Version VI nuclides with LSSF=1, the File 2 data are used to compute the self-shielding factors, and File 3 contains the dilute cross sections on a much finer grid. In VIM, when LSSF=1, we store the probability table average cross sections, $\bar{\sigma}_{x(table)}$, and the potential scattering cross section with each table and self-shield the resonance portion of the total (and elastic) cross sections at run time according to:

$$\sigma_t = (\sigma_{t(file3)} - \sigma_p) \times \frac{(\sigma_{t(table)} - \sigma_p)}{(\bar{\sigma}_{t(table)} - \sigma_p)} + \sigma_p .$$

The fission and capture cross sections are constructed by self-shielding the conditional mean, $\sigma_{x(table)}$, according to:

$$\sigma_x = \sigma_{x(table)} \times \frac{\sigma_{x(file3)}}{\bar{\sigma}_{x(table)}} .$$

Several other features in Version VI required accommodation. Some of the fission neutron yield tables are larger (2726 elements for ^{239}Pu) than in earlier versions. The coupled secondary neutron energy-angle distributions are converted to File 4 equivalents in which anisotropy is ignored.

Results

It was anticipated that the more detailed resolved range and other data would result in a massive increase in the increase in the size of data libraries, but this turned out not to be a serious problem. The largest increases (Version V to VI) were ^{238}U (4300 to 40,000 energy points, and 77,000 to 171,000 total words), Ni (13,000 to 64,000 energy points over all isotopes), and ^{235}U (1,000 to 14,000 points in the secondary energy data).

Verification was accomplished by detailed inspection of the intermediate and final results for several nuclides, including nearly every cross section and distribution, and also by graphical comparison with ENDF data. The Reich-Moore cross sections were compared numerically with those from the multipole method[6]. In addition, two hard-spectrum benchmarks were used to verify the Version VI cross sections. The ^{235}U cross sections were tested by detailed comparison between VIM and a 29-group MC^2-2 calculation using a zero-buckling infinite medium GODIVA composition. The ^{239}Pu cross sections were checked similarly in a Jezebel composition. Finally, idealized critical benchmark calculations for both criticals were used.

References:

1. "VIM Continuous Energy Monte Carlo Transport Code", by R. N. Blomquist, *Proceedings of the International Conference on Mathematics and Computations, Reactor Physics, and Environmental Analyses*, April 30 - May 4, 1995, Portland, OR.
2. VIM - A Continuous Energy Monte Carlo Code at ANL", *A Review of the Theory and Applications of Monte Carlo Methods, Proceedings of a Seminar-Workshop*, ORNL/RSIC-44, April 21-23, 1980.
3. R. E. Prael and H. Henryson, II, A Comparison of VIM and MC^2-2 -- Two Detailed Solutions of the Neutron Slowing Down Problem, *Proc. Conf. on Nuclear Cross Sections and Technology*, NBS SP 425, p.425 (March 3-7, 1975).
4. H. Henryson II, B. J. Toppel, C. G. Stenberg, *MC2-2: A Code to Calculate Fast Neutron Spectra and Multigroup Cross Sections*, ANL-8144 (ENDF-239), Argonne National Laboratory (1976).
5. R. N. Hwang, "An Extension of the Rigorous Pole Representation of Cross Sections for Reactor Applications", *Nucl. Sci. Eng.*, **111**,113 (1992).
6. R. N. Hwang, "Rigorous Pole Representation of Multilevel Cross Sections and Its Practical Applications", *Nucl. Sci. Eng.*, **96**,192 (1987).