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AUTHOR(S): R. E. MacFarlane

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los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

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ENDF/B-IV AND V CROSS SECTION LIBRARIES FOR THERMAL POWER REACTOR ANALYSIS

R. E. MacFarlane
Los Alamos Scientific Laboratory, University of California
Theoretical Division
Los Alamos, New Mexico 87545 USA

The NJOY processing system has been used to produce thermal reactor cross-section libraries from ENDF/B-IV and V evaluations for the fuel cycle codes EPRI-CELL and EPRI-CPM, for the continuous-energy Monte Carlo code MCNP, and for the Los Alamos discrete-ordinates transport codes. This consistent data source has allowed the approximate methods (equivalence theory, B_1, integral transport, P_L-S_N) to be compared with accurate Monte Carlo results. So far, this has resulted in improved methods for space-and-energy self-shielding in the resonance range (e.g., the NJOY flux calculator, epithermal disadvantage factors for EPRI-CELL, shielded elastic removal), it has shown why the newest ENDF-based libraries initially gave results worse than the old libraries, and it has pointed out problems for future study such as resonance interference effects at high burnup. Finally, the results are compared to various criticality benchmarks to evaluate the performance of ENDF/B-V for thermal reactor analysis and to establish the biases introduced by the approximate methods used in the fuel cycle codes.

(Thermal reactor cross sections, ENDF/B-V)

Evaluated Nuclear Data

The fifth version of the Evaluated Nuclear Data Files (ENDF/B-V) has recently been released.[1] It shows improvements in both scope and quality due to the inclusion of new experimental data, to the expanded use of nuclear models, and to the dedicated work of the members of the Cross Section Evaluation Working Group (CSEWG) and the U. S. National Nuclear Data Center. In addition to many updated evaluations, ENDF/B-V includes new materials (e.g., ^{15}N, ^{231}Pa, ^{253}Es), new data types (e.g., gas production, isomer production, and components of energy release in fission), improved representations (e.g., Watt fission spectra, Adler-Adler multilevel resonance representations), and expanded data covariance and photon production files.

Except in its early years, the development of ENDF/B has been most responsive to the needs of its major supporter, the U. S. Fast Reactor Program. The impact of ENDF/B-III and IV on thermal power reactor design and operation has been minimal; various proprietary adjusted cross-section libraries have dominated the field. This situation has begun to change with the advent of the Electric Power Research Institute (EPRI). The existing sets are not always adequate for analyzing the new ideas such as ^{233}U-fueled reactors, thermal breeders, and advanced converters that are so active these days. Even more important is the problem of regulatory accountability. It is becoming increasingly desirable for everyone--vendors, utilities, fuel management companies, and regulatory agencies--to be able to trace their calculations back to a single reference data base without the problems of proprietary rights. Many people in the power reactor industry think that ENDF/B-V could become this standard.

Neutron Cross-Section Processing

For these reasons and others, EPRI has sponsored the development of the Advanced Recycle Methodology Program (ARMP)[2] whose main cross-section-producing components are the reactor cell codes EPRI-CELL and EPRI-CPM. CELL was developed by Nuclear Associates, International (NAI) and uses the B_1 method of GAM[3] and the integral transport method of THERMOS[4] to produce coarse-group cell-averaged cross sections. Its library is an adjusted set based on ENDF/B-I and II. CPM was developed by AB Atomenergi, Studsvik, Sweden, and uses collision probability methods similar to WIMS[5] with a library adjusted from ENDF/B-III to give agreement between CPM and CELL.

With the hope that ultimately no adjustments will be required, EPRI has sponsored the development of new libraries for CELL and CPM based on ENDF/B-IV and V and using the NJOY nuclear data processing system.[6] This code system operates directly from the ENDF/B files. It first reconstructs resonance shapes and linearizes all cross sections, then Doppler broadens them to all desired temperatures, and then adds unresolved self-shielded cross sections where required. Next thermal scattering data is added. Inelastic cross sections and energy-to-energy-by-angle scattering matrices can be produced from ENDF/B scattering functions $S(\alpha,\beta)$ (e.g., H in H_2O, D in D_2O, and graphite) or the free-gas model. Elastic coherent or incoherent cross sections by energy and angle can be produced for hexagonal crystals (C, BeO) as well as for polyethylene and zirconium hydride. The result is a pointwise-ENDF (PENDF) file that can be saved as the starting point for several subsequent procedures. For multigroup codes, the GROUPR module of NJOY is used to average the PENDF cross sections. The results can then be reformatted using the POWR module into the proper forms for the CELL and CPM library maintenance programs, or the MATXSR module can be used to produce a file called MATXS appropriate for later coupling to discrete-ordinates transport codes such as ONETRAN[7] and its diffusion-accelerated successor ONEDA. Alternately, the PENDF file can be processed with the ACER module into a form acceptable to the Los Alamos continuous-energy Monte Carlo neutron and photon code MCNP.[8]

The multigroup codes account for resonance self-shielding using the background cross-section method.[9] For an accurate representation of the broad and intermediate resonances important for resonance absorption in thermal reactors, GROUPR uses a detailed pointwise calculation of the flux in an homogeneous mixture of the heavy absorber (e.g., ^{238}U) with a light moderator. The moderator can be real, (i.e., ^{1}H, ^{16}O), the ideal moderator that gives a 1/E source, or a combination of the two. Equivalence relations based on an infinite two-region model can then be used to obtain shielded cross sections[9] for CELL, CPM, or ONEDA.

This library generation process has been carried out using ENDF/B-IV and V for the four codes, EPRI-CELL, EPRI-CPM, ONEDA, and MCNP.

Initial ENDF/B Library Testing

As a first test, the ENDF/B-IV libraries were used to analyze the CPTWG benchmark[16] assembly BAPL-UO2-1. This is a simple light-water triangular lattice with a pitch of 1.558 cm fueled by aluminum-clad enriched uranium pins 1.15 cm in diameter. The calculated integral parameters are compared with results obtained using the standard NAI and Studsvik libraries in Table I. The lack of agreement is very disappointing.

The largest difference here is clearly the prediction of ^{235}U resonance absorption using the ENDF-based CELL library (note ρ_{28} and σ_{a3}).

EPRI-CELL Epithermal Disadvantage Factor

A study of the CELL code has shown that it implicitly assumes that the flux in the fuel is equal to the flux in the moderator when preparing cell average cross sections for its epithermal B_1 calculation. On the contrary, near a resonance, the fuel flux is expected to be depressed, putting the fuel at a relative "disadvantage" in competing for absorptions. A correct accounting for this effect would require separate detailed calculations for each different set of cell dimensions, and hence problem-dependent libraries. However, for many purposes, it is possible to define a single disadvantage factor based on two-region equivalence theory.

Following the notation of Ref. 9, the fluxes in fuel f and moderator m are given by

$$V_f\Sigma_f\phi_f = (1-P_f)V_fS_f + P_mV_mS_m \quad , \quad \text{and} \tag{1}$$

$$V_m\Sigma_m\phi_m = P_fV_fS_f + (1-P_m)V_mS_m \quad , \tag{2}$$

where V is volume, Σ is macroscopic total cross section, φ is flux, and S is source. The escape probabilities are assumed to satisfy the reciprocity relation $V_m\Sigma_mP_m = V_f\Sigma_fP_f$, and the fuel escape probability is represented by the Wigner rational approximation

$$P_f = \frac{\Sigma_e}{\Sigma_e + \Sigma_f} \quad , \tag{3}$$

where Σ_e is an effective escape cross section. Assuming further that all fuel resonances are narrow with respect to moderator scattering ($S_m = \Sigma_m/E$) and using the intermediate-resonance approximation for fuel scattering [$S_f = \lambda\Sigma_p/E + (1-\lambda)\Sigma_p\phi_f$], the fuel and moderator fluxes become

$$\phi_f = \frac{\Sigma_e + \lambda\Sigma_p}{\Sigma_e + \lambda\Sigma_p + \Sigma_a}\,\frac{1}{E} \quad , \quad \text{and} \tag{4}$$

$$\phi_m = (1-\beta)\,\frac{1}{E} + \beta\phi_f \quad , \tag{5}$$

where $\lambda\Sigma_p$ is an effective potential scattering and

$$\beta = \frac{V_f\Sigma_e}{V_m\Sigma_m} \quad , \tag{6}$$

Table I. Comparison of Integral Parameters of BAPL-UO2-1 for ENDF/B-IV and Standard Libraries Using Standard Codes

Integral Parameter[a]	Standard CELL	Standard CPM	ENDF/B-IV CELL	ENDF/B-IV CPM
k_∞	1.133[illegible]	1.136[illegible]	1.162[illegible]	[illegible]
k_{eff}	0.997[illegible]	0.997[illegible]	0.97[illegible]	[illegible]
ρ_{28}	1.37[illegible]	1.36[illegible]	1.61[illegible]	1.47[illegible]
δ_{25}	0.0[illegible]	0.08[illegible]	0.08[illegible]	0.08[illegible]
δ_{28}	[illegible]	0.0716	0.073[illegible]	[illegible]
σ_{a3}	[illegible]	[illegible]	[illegible]	[illegible]
σ_{f3}	25.4[illegible]	24.97[illegible]	25.49[illegible]	24.9[illegible]

[a] ρ_{28} is ^{238}U epithermal to thermal capture ratio.
δ_{25} is ^{235}U epithermal to thermal fission ratio.
δ_{28} is ^{238}U to ^{235}U fission ratio.
σ_{a3} and σ_{f3} are ^{238}U absorption and ^{235}U fission for the 0.625 eV to 5.53 keV group.

is an heterogeneity parameter (β = 1 gives the close-packed limit where $\phi_f = \phi_m$ as assumed in CELL, while β = 0 gives an isolated rod with ϕ_m = 1/E); β = [illegible] is appropriate for the BAPL-UO2-1 cells.

It is now easy to define disadvantage factors for the fuel and moderator regions based on flux and volume weighting:

$$\xi_f = \frac{V_f\phi_f}{V_f\phi_f + V_m\phi_m} = \frac{V_f}{V_f + V_m}\,\frac{1}{1 + d\Sigma_a} \quad , \tag{7}$$

where d can be called the "disadvantage coefficient" (d = 0.257 cm for BAPL-1),

$$d = \frac{(1-\beta)V_m}{(V_f+V_m)\,(\lambda\Sigma_p+\Sigma_e)} \quad . \tag{8}$$

Equation (7) clearly leads to a reduction in fuel cross sections for an energy group containing a large absorption resonance. The moderator factor is given by

$$\xi_m = \frac{V_m\phi_m}{V_f\phi_f + V_m\phi_m} = \frac{V_m}{V_m + V_f}\,\frac{1 + \frac{V_f + V_m}{V_m}\,d\Sigma_a}{1 + d\Sigma_a} \quad . \tag{9}$$

Coding to implement this correction has been added to EPRI-CELL for use with ENDF/B-IV and V libraries. Table II shows a comparison of the modified CELL with MCNP, ONEDA, and EPRI-CPM for a simplified infinite model of BAPL-UO2-1 using ENDF/B-IV libraries. The new method together with consistent libraries clearly reduces the absorption discrepancy between the codes (note that this CPM library has not been adjusted).

Since the MCNP calculation is nearly a correct solution to this problem, the results in Table II cast severe doubt on the validity of the original CELL and CPM libraries. It is suspected that the original NAI

Table II. Comparison of EPRI-CELL with Disadvantage Factor Against Several Other Codes for Infinite BAPL-1[a] Using ENDF/B-IV

Parameter	CELL	CPM	ONEDA[b]	MCNP
k_∞	1.1373	1.1284	1.1241	1.1394
f^{25}	1.1422	1.424	1.443	1.427
f^{28}	0.0826	0.0797	0.0821	0.0824
f^{49}	0.0693	0.0681	0.0682	0.0686
$\bar{\nu}\Sigma_f$	1.261	1.297	1.297	1.303
	1.644	1.670	1.673	1.685
	25.5-	24.32	25.31	21.58
	366.1	367.0	366.5	369.4
$^{238}\delta_f$	0.453	0.436[c]	0.459	0.458[d]
	0.25	0.25	0.253	0.266[d]
	2.062	2.063	2.075	2.049
	1.791	1.795	1.795	1.800

[a] Infinite cylinder (zero buckling) with white boundary conditions on outer radius.

[b] f_∞, f_{28}, 28 fine mesh intervals, CPM 69-group structure.

[c] n,2n subtracted.

[d] Unresolved self-shielding.

resonance absorption shielding factors were reduced incorrectly, and do not reflect the ENDF/B evaluation used at that time.[11]

Part of the remaining discrepancy in ^{238}U resonance absorption is probably due to the rather coarse group structure used in CPM and ONEDA. Two other differences between CPM and CELL are yet to be explained: the CPM ^{235}U resonance fission is too low, and the CPM transport cross section is larger than the EPRI-CELL value. The first has little impact except on δ_{25}, but the second causes CPM to predict low values of k_{eff}.

Resonance Overlap and Scattering

Comparisons between the fine-group cross sections used in the CELL and MCNP runs described above show that the resonance interference correction used in CELL does not represent ^{235}U fission well (the results quoted here did not use this option). Resonance interference should become more important at high burnup, and methods to correct for it should be studied. Similar comparisons show that it is important to self-shield resonance scattering from ^{238}U in the fuel pin.[9] Since neither CELL nor CPM allows for this effect, the ENDF/B-IV and V libraries were prepared containing elastic scattering matrices using 50 barns of background cross section for ^{235}U and ^{232}Th but infinite dilution for all other materials. This problem also needs further study.

Thermal Lattices Using ENDF/B-V

As an example of the application of ENDF/B-V to thermal reactor analysis, results for the integral parameters of several lattices are given in Table III. These numbers are generally closer to experiment than the same numbers obtained using ENDF/B-IV. However, the models are fairly crude when compared to full-core Monte Carlo, and these results shouldn't be interpreted as "benchmarks" of ENDF/B-V. They do show that the quality of the results produced by EPRI-CELL and EPRI-CPM is close to that required for engineering studies of reactor fuel cycles. Additional "tuning" of the approximate methods by comparison with Monte Carlo and, perhaps, some small cross-section adjustments, should produce an accurate tool for many practical problems.

This positive result combined with the reasons discussed above (i.e. up-to-date evaluations, open access, analysis of advanced systems, regulatory accountability) provide a strong case for working toward a wide application of ENDF/B-V in the thermal power reactor industry.

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References

1. Information and tapes for ENDF/B-V can be obtained from the National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973.

2. Additional information on ARMP can be obtained from the Electric Power Research Institute, P. O. box 10412, Palo Alto, CA 94303.

3. G. D. Joanou and J. S. Dudek, "GAM-II: A Consistent P_1 Multigroup Code for the Calculation of Fast Neutron Spectra and Multigroup Constants," GA-1850 (1961).

4. H. C. Honeck, "THERMOS, A Thermalization Transport Theory Code for Reactor Lattice Calculations," BNL-5826 (1961).

5. J. R. Askew, F. J. Fayers, and P. B. Kemshell, J. Brit. Nucl. En. Soc. 5, 564 (1966).

6. R. E. MacFarlane et al., "The NJOY Nuclear Data Processing System: User's Manual," LA-7584-M (1978).

7. T. R. Hill, "ONETRAN: A Discrete Ordinates Finite Element Code for the Solution of the One-Dimensional Multigroup Transport Equation," LA-5990-MS (1975).

8. "MCNP - A General Monte Carlo Code for Neutron and Photon Transport," LA-7396-M (1978).

9. R. E. MacFarlane, "Data Processing for Power Reactor Fuel Cycle Codes," in Symposium Proceedings: Nuclear Data Problems for Thermal Reactor Applications, NP-1098 (ENDF-270) (1979).

10. "Cross Section Evaluation Working Group Benchmark Specifications," BNL19302 (ENDF-202) (1974).

11. O. Ozer, Electric Power Research Institute, personal communication (August 1979).

Table III. EPRI-CELL [illegible] Results for Some CSEWG Thermal Benchmarks

Parameter[a]	TRX-2	TRX-1	BAPL-2	BAPL-1
k_∞	[illegible]	[illegible]	[illegible]	[illegible]
k_{eff}	[illegible]	[illegible]	[illegible]	[illegible]
δ^{28}	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible]	[illegible]	[illegible]	[illegible]
δ^{25}	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible]	[illegible]	[illegible]	[illegible]
δ^{49}	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible]	[illegible]	[illegible]	[illegible]

[a] Experimental numbers in parentheses.