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THE IMPACT OF ENDF-6 ON CROSS SECTION PROCESSING CODES

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ABSTRACT

The new ENDF-6 format for evaluated nuclear data provides some important new capabilities, but it was designed to keep many features of the earlier formats. As a result, codes that do not need the new capabilities can be updated with a few key modifications. Other codes will require more extensive changes, but they will become more useful. Some of the new capabilities included in the ENDF-6 format are (1) an extended and more systematic procedure for naming reactions, including complex and and charged-particle reactions; (2) new resonance representations for Reich-Moore and R-Matrix parameters; (3) a capability of giving energy-angle distributions for all the products of a nuclear reaction, including the recoil nucleus; and (4) incident charged-particle data including large-angle Coulomb scattering. The effects of these changes are discussed for three classes of processing code applications: fission reactor codes, fusion neutronics codes, and charged-particle codes.

INTRODUCTION

Times are changing. Up until a few years ago, many reactor analysts could get by using packaged cross section libraries that remained stable over long periods of time. Many of them were working on refinements of light water reactor or liquid-metal breeder reactor designs with fairly standard configurations, and there was lots of critical assembly data or operational experience to normalize to. Now days, people are working on all kinds of unusual fission and fusion systems containing new materials and using unusual configurations, and there is little experimental data do help them. This situation is putting increasing emphasis on accurate evaluated cross section data for a wider variety of materials at to higher energies than ever before. Better photon production, heating, and damage results are needed for exacting shielding calculations. Requests for charged-particle production numbers and charged-particle transport cross sections are becoming more frequent.

Luckily, these needs can be met by a new generation of data fitting codes that are capable of producing very good resonance parameter sets, and a new generation of nuclear model codes with good predictive power that can produce cross sections, angular distributions, and energy distributions for all the particles produced by nuclear reactions at quite high energies in a wide variety of materials. The problem is to make these new data available to reactor analysts. The solution to this problem is an extended format for evaluated nuclear data, and an updated set of processing codes to transform the evaluated data into forms that can be used by nuclear analysis codes.

The U.S., and to an increasing extent, the rest of the world, depends upon the Evaluated Nuclear Data Files (ENDF) format. The newest version of this format is now becoming

available.[1] It is called the "ENDF-6" format, and it will be used for the U.S. ENDF/B-VI evaluated nuclear data library. The ENDF-6 format has a number of new features designed to meet the kinds of new demands described above. They include (1) an extended and more systematic procedure for naming reactions, including complex and and charged-particle reactions; (2) new resonance representations for Reich-Moore and R-Matrix parameters; (3) a capability of giving energy-angle distributions for all the products of a nuclear reaction, including the recoil nucleus; and (4) incident charged-particle data including large-angle Coulomb scattering. There are also new extensions to the cross section covariance files and new ways of arranging the radioactive decay and fission yield data that will not be discussed here.

This paper will discuss the impact of these format changes on the nuclear data processing codes that convert the evaluated data into code-dependent libraries for doing particle transport calculations, dosimetry analyses, radiation damage assessments, and the like. The discussion will be based on ENDF-6 changes made to the NJOY Nuclear Data Processing System,[2] which is widely used all over the world, but the principles should apply equally to many other processing codes.

FISSION REACTOR CODES

Processing codes for fission reactor applications will require the fewest changes because the existing ENDF formats are generally adequate for these problems.

In the ENDF-6 format, most evaluated nuclear data is grouped into "sublibraries" by incident particle; in addition, there are sublibraries for special kinds of data such as radioactive decay, fission product yields, and thermal neutron scattering data. For fission reactor applications, the sublibrary of incident neutron data is of most interest.

First of all, the code designer will find a new card near the beginning of ENDF File 1 (General Information) that specifies the sublibrary and initial particle for this evaluation. In addition, there are a few changes in reaction identifiers, MT. For users who only process simple cross-section data (File 3), these are the only changes needed.

The next set of important changes are in File 2, the resonance parameter data. The ENDF-6 format reinstates the Reich-Moore multi-level representation, which promises important improvements for fissile materials like ^{235}U and for structural materials like Ni. Therefore, most fission reactor codes will have to be updated for this representation. This has already been done for several codes that reconstruct cross sections at 0K and then apply pointwise Doppler broadening (for example, NJOY[2] and RECENT[3]), and the appropriate FORTRAN coding is readily available. Analytic Doppler broadening methods have been developed by Fröhner[4] and by Hwang.[5] The Hwang approach leads directly to the familiar ψ and χ functions used by MC^2-II[6] and many other reactor physics codes. The ENDF-6 format also provides for a new "Hybrid R-Function" format that will possibly be used for structural materials. FORTRAN code is available[7] for reconstructing cross sections at 0K. Still another new format is available for "Generalized R-Matrix" parameters, but its use is not anticipated for the first generation of new evaluations.

An alternative to updating the resonance section of a fission reactor processing code is conversion. Reich-Moore parameters can be converted into Adler-Adler parameters to a good degree of approximation using the POLLA code.[8] For some of the more approximate methods, multi-level parameters can be used in the single-level formulas without introducing excessive

additional error. This kind of conversion should be installed as a preprocessing step in the code being updated to ENDF-6 format so that the approximations are explicitly accepted by the code designer as being appropriate for his range of applications. Converted ENDF-6 format tapes should not be circulated.

In previous versions of the ENDF format, angular distributions were given in File 4 and energy distributions were given in File 5. This representation may still be used in the ENDF-6 format, but a better coupled energy-angle representation using File 6 will be found for many important materials. In most fission reactor applications, the energy-angle coupling is not very important. Therefore, it is appropriate to convert File 6 into File 5 "arbitrary tabulated function" format, preserving only the isotropic part of the secondary energy distribution. FORTRAN subroutines for doing this conversion are available from the author; they can be used as the basis of a preprocessor to be installed in the processing code being converted to ENDF-6 format.

For code designers interested in processing ENDF-6 directly, here is an outline of the conversion process. In File 5, the secondary-energy distribution for a given incident energy is represented by a series of $E', g(E, E')$ pairs, where E, E', and g are the incident energy, secondary energy, and emission probability, respectively. In File 6, the energy-angle distribution is represented by a series of multiplets containing E', $g(E, E')$, and angular parameters for E, E'. It is easy to simply copy File 6 to File 5 leaving out the angular parameters, thus obtaining the P_0 part of the neutron distribution with very little effort. If the energy-angle distribution is given in the CM system and the mass of the target is small, or the phase-space law is used, it is necessary to convert to the LAB system using the method described below. If the "angle-energy" option is used (LAW=7), the distribution is represented by giving secondary energy distributions at a number of scattering angles for each incident energy. For each E, integrals over scattering angle are performed on the union grid of secondary energies by simple trapezoidal integration. While performing the integrals, the secondary energy grid is thinned to obtain a linearly interpolable result in $E', g(E, E')$ form.

In a few cases, File 6 may contain discrete-level scattering data for neutrons. The format of this data is almost identical to the File 4 format, and the existing two-body scattering logic in the processing code can probably be adapted to process these cases.

FUSION NEUTRONICS CODES

Fusion reactor applications will gain important new capabilities from the ENDF-6 format, and codes processing data for these applications will need additional changes. File 6 for important materials will contain energy-angle distributions for all of the outgoing particles, including the recoil nucleus. Most such evaluations will be prepared with nuclear model codes that enforce energy balance. Thus, there will be a great improvement in the ability to compute heating and radiation damage. Any code that computes KERMA or DPA will have to be updated to cope with the multiple subsections used to describe the different outgoing particles in File 6. Fusion codes will also have to take advantage of the energy-angle correlations expected to be available for neutron emission. This new data should allow significant improvements in the ability to compute the transport of high-energy neutrons through fusion systems. The following will discuss how these new capabilities are implemented in NJOY.

If the File 6 data is expressed as a continuous energy-angle distribution (LAW=1) in the LAB system, it is fairly easy to generate the multigroup transfer matrix. The only problems

are handling the new ENDF-6 interpolation laws for two-dimensional tabulations (for example, unit base) and converting tabulated angle functions into Legendre coefficients. If the File 6 data is given in the angle-energy form (LAW=7), NJOY converts it to the LAW=1 form for processing using a Gauss-Legendre quadrature of order 8.

If the File 6 data is expressed in the CM system, or if the phase-space option is used, more processing is necessary to convert to the LAB system. In NJOY, this conversion is done for each incident energy E given in the file. The grid for laboratory secondary energy E'_L is obtained by doing an adaptive reconstruction of the emission probability $p_{L\ell}(E, E'_L)$ such that each Legendre order can be expressed as a linear-linear function of E'_L. The values for $p_{L\ell}(E, E'_L)$ are obtained by doing an adaptive integration along the contour E'_L=const in the E'_C, μ_C plane using μ_L as the variable of integration:

$$p_{L\ell}(E, E'_L) = \int_{\mu_{min}}^{+1} p_C(E, E'_C, \mu_C)\, P_\ell(\mu_L)\, J\, d\mu_L, \tag{1}$$

where μ is a scattering cosine and L and C denote the LAB and CM systems, respectively. The Jacobian of the transformation is given by

$$J = \sqrt{\frac{E'_L}{E'_C}} = \frac{1}{\sqrt{1 + c^2 - 2c\mu_L}}, \tag{2}$$

and the cosine transformation is given by

$$\mu_C = J(\mu_L - c). \tag{3}$$

The constant c is given by

$$c = \frac{1}{A+1}\sqrt{\frac{E}{E'_L}} \tag{4}$$

where A is the ratio of the atomic weight of the target to the atomic weight of the projectile. The lower limit of the integral depends on the maximum possible value for the CM secondary energy as follows:

$$\mu_{min} = \frac{1}{2c}\left(1 + c^2 - \frac{E'_{Lmax}}{E'_L}\right), \tag{5}$$

where

$$E'_{Lmax} = E\left(\sqrt{\frac{E'_{Cmax}}{E}} + \frac{1}{A+1}\right)^2. \tag{6}$$

The CM energy-angle distribution will probably be given as a set of Legendre coefficients for each possible energy transfer $E \rightarrow E'$, parameters for a phase-space distribution, or as a "precompound fraction" $r(E, E')$ for use with the Kalbach-Mann[9] or Kalbach[10] angular distributions. This last option leads to a very compact representation. Kalbach and Mann examined a large number of experimental angular distributions for neutrons and charged particles. They noticed that each distribution could be divided into two parts: an equilibrium part symmetric in μ, and a forward-peaked preequilibrium part. The relative amount of the two parts depended on a parameter r that varied from zero for low E' to 1.0 for large E'. The shapes of the two parts of the distributions depended most directly on E'. This representation is very useful for

preequilibrium statistical-model codes like GNASH[11], because they can compute the parameter r, and all the rest of the angular information comes from simple universal functions. More specifically, Kalbach's latest work says that

$$f(\mu) = \frac{a}{2\sinh(a)}\left[\cosh(a\mu) + r\sinh(a\mu)\right], \tag{7}$$

where a is a simple function of E, E', and B_b, the binding energy of the emitted particle from the liquid-drop model.

Codes that compute photon production, energy deposition (KERMA), and radiation damage production (DPA) are important for fusion neutronics. The new feature for photon production codes is that gammas can now be given in File 6 for some reactions in addition to the conventional Files 12, 13, 14, and 15. Continuum gammas in File 6 use a format very similar to that of File 15, and some of the methods in an existing code can be adapted to process the new file. In some cases, discrete photons can be given together with the tabulation of the continuum photons using a kind of "delta-function interpolation." This representation is very compact for capture gammas, and the additional processing is easy to do.

Previous versions of the ENDF format had difficulty in calculating energy deposition, or "kinetic energy release in materials" (KERMA), and radiation damage production, or "displacements per atom" (DPA), because spectral information for emitted charged particles and residual nuclei was not included. KERMA and DPA codes had to resort to simplified models for complex reactions, or to using energy-balance considerations to deduce how much of the available energy appeared as charged particles. The first failed because of not knowing enough about the physics of the reactions, and the second failed because the neutron and photon files in ENDF/ν evaluations were often not consistent. Now, with the ENDF-6 format, the evaluator can put in his best estimate for the spectrum of each emitted charged particle and residual or recoil nucleus. The KERMA and DPA can be computed directly by the processing code. Most such evaluations will be done with nuclear model codes that enforce a high degree of energy balance. The result should be an order-of-magnitude improvement in the accuracy of KERMA factors for 14 MeV neutrons.

CHARGED-PARTICLE CODES

Finally, the ENDF-6 format allows for the introduction of a new generation of processing codes that generate data for coupled neutron, charged-particle, and photon transport calculations.

The first problem here was to define a new reaction naming scheme that preserved as much of the old ENDF structure as possible. It was decided to let the MT number determine the outgoing particles for the reaction. Therefore, MT=16 is used for both (n,2n) and (p,2n), and MT=112 is used for both (n,pα) and (α,pα). An exception is made for elastic scattering, which is always MT=2. To make the assignment of an MT number unique, it is necessary to impose two conditions: (1) the list of emitted particles must be in ascending order of particle ZA, and (2) there must be a residual nucleus. This means that the reaction d+t$\rightarrow$n+α must be classified as the reaction ^{3}H(d,n$_0$)^{4}He (MT=50, see below) rather than the reaction ^{3}H(d,nα) (MT=22).

Discrete levels that emit neutrons use MT numbers in the 50 series; that is, MT=51 is used for both (n,n$_1$) and (p,n$_1$). Of course, MT=50 is used for (p,n$_0$), but MT=50 is not allowed for incident neutrons, because that particular cross section uses MT=2. As before, MT=91 is used

for continuum inelastic neutron emission. Discrete levels that emit protons use numbers in the 600 series; for example, MT=601 for (n,p_1). Continuum inelastic proton emission is represented using MT=649. These reactions used MT=701 and 719 before; the numbering was changed to allow up to 48 discrete levels for each particle (600-649 for p, 650-699 for d, 700-749 for t, etc.). One consequence of this is that the old photoatomic absorption cross section, MT=602, had to be changed to 522.

Many charged-particle reactions can be interpreted as "breakup" reactions, where the first particle out leaves an unstable compound nucleus that later breaks up into 2 or more additional materials. An example is, ^{9}Be(α,n_3)^{12}C(3α), which is denoted by MT=53. The fact that the residual ^{12}C breaks up into three alpha particles can be expressed by giving an "LR flag" of 23 as in previous ENDF versions, or by using File 6 with an explicit subsection describing the alphas. For breakup reactions, the list of particles in each set of parentheses must be in ZA order, but the reaction can go through different intermediate states, and the residual nucleus can break up in different ways. Examples are ^{12}C(n,n)^{12}C(3α) vs ^{12}C(n,α)^{9}Be(n2α), or ^{6}Li(d,p_4)^{7}Li(tα) vs ^{6}Li(d,p_4)^{7}Li(n^{6}Li).

At high energies, so many reaction channels open up that it becomes difficult to construct enough MT numbers. It becomes convenient to define a single "complex reaction", MT=5, that simply gives yields and distributions for all the particles emitted for a superposition of many reactions. However, an evaluator will usually want to keep elastic scattering, and maybe some discrete levels, in separate MT numbers. Therefore, MT=5 has the following unusual definition: it represents all reactions not included in another MT number in the evaluation.

This naming scheme has been tested on a very long list of important charged-particle reactions for light targets, and it works.

All charged-particle transport data is given using File 3 and File 6. Except for elastic scattering, all the different particles behave in similar ways. And photons behave like particles. Therefore, the same processing tools developed to handle neutrons in File 6 (as described above) can be used to handle protons, alphas, or gammas, either incident or emitted. It is only necessary to take care to use generalized kinematic formulas that allow the mass ratios of the incident and outgoing particles to be different from unity.

The other unique feature of charged-particle evaluations is Coulomb scattering. This reaction is always given in MT=2. The actual Coulomb scattering is represented using the Rutherford formula, but several different representations are allowed for the nuclear scattering and the interference between the Coulomb and nuclear terms. The most complete format is the "nuclear amplitude expansion." It provides a full representation of the nuclear and interference scattering terms, but it can only be constructed if a phase-shift or R-Matrix analysis of the experimental data can be performed. When only experimental data is available, a nice representation is the "residual cross section expansion." It is obtained by calculating

$$\sigma_R(\mu, E) = (1 - \mu)[\sigma_e(\mu, E) - \sigma_c(\mu, E)], \tag{8}$$

where σ_e is the experimentally observed cross section and σ_c is the Rutherford cross section, and fitting σ_R with Legendre polynomials. The residual cross section σ_R will normally show oscillations at small angles, but if the coefficients are chosen properly, the effect of this region will be small because the Coulomb term is large. The third option is "nuclear plus interference", where $\sigma_e - \sigma_c$ is given directly in the file, and the ill-behaved region near $\mu = 1$ is eliminated by using a cut-off cosine, μ_{max}.

In all three cases, special formulas apply for identical particles (for example, p+^{1}H elastic scattering).

In charged-particle transport calculations, particles that scatter through very small angles are normally treated by a continuous slowing-down calculation. The Coulomb potential in this region is screened by the atomic electrons, but ENDF-6 does not provide these continuous slowing-down parameters. Large angle scattering can be computed from the ENDF-6 data for $\mu < \mu_{max}$ using methods similar to those used for neutron elastic scattering. FORTRAN versions of the non relativistic Coulomb formulas are available.

The ENDF-6 format charged-particle files will allow the processing code to prepare a wide variety of multigroup transfer matrices, for example, np, pγ, αn, and so on. For actual calculations, it will often be convenient to combine these blocks into large "coupled sets." For example, an "npγ" coupled set would be convenient for a fusion plasma calculation because high-energy protons would be present. In such a case, the heavier charged particles, including residual nuclei, could be included in the energy deposition cross section (KERMA). For a more detailed calculation, an "npdt^{3}He$\alpha\gamma\beta$ coupled set might be used. Needless to say, the bookkeeping problems will be severe. The MATXS format, which can be produced by NJOY, already has provisions for storing partial transfer or production matrices like np or αn. The TRANSX[12] code, which is currently used for producing multigroup transport sets from libraries in MATXS format has been modified to produced coupled sets that included charged particles.

CONCLUSION

Most of the features discussed above have been implemented in the NJOY Nuclear Data Processing System. Some of the changes were difficult, but the new processing capabilities combined with new ENDF-6 format evaluations should lead to significant improvements in processed nuclear data libraries for many applications.

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REFERENCES

1. The current draft of the ENDF-6 format can be requested from C. L. DUNFORD, National Nuclear Data Center, Bldg. 197-D, Brookhaven National Laboratory, Upton, NY 11973 U.S.A.

2. R. E. MACFARLANE, D. W. MUIR, and R. M. BOICOURT, "The NJOY Nuclear Data Processing System, Volume I: Users' Manual" and "The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THERMR Modules", LA-9303-MS Vols I and II (ENDF-324), Los Alamos National Laboratory (1982). R. E. MACFARLANE and D. W. MUIR, "The NJOY Nuclear Data Processing System, Volume

III: The GROUPR, GAMINR, and MODER Modules" LA-9303-MS Vol III (ENDF-324) Los Alamos National Laboratory (1987). D. W. MUIR and R. E. MACFARLANE, "The NJOY Nuclear Data Processing System, Volume IV: The ERRORR and COVR Modules". LA-9303-MS Vol. IV (ENDF-324), Los Alamos National Laboratory (1985).

3. D. E CULLEN, "Program RECENT (version 79-1): Reconstruction of Energy Dependent Neutron Cross-Sections from Resonance Parameters in the ENDF/B Format," UCRL-50400, Vol. 17, Part C, Livermore National Laboratory (1979).

4. F. H. FRÖHNER, "New Techniques for Multi-Level Cross Section Calculation and Fitting," KFK-3081 (1980).

5. R. N. HWANG, "A Rigorous Pole Representation of Multilevel Cross Sections and Its Practical Applications," Nucl. Sci. Eng. 96, 192 (1987).

6. H. HENRYSON, B. J. TOPPEL and C. G. STENBERG, "MC^2-II: A Code to Calculate Fast Neutron spectra and Multigroup Cross Sections," ANL-8144 , Argonne National Laboratory (1976).

7. C. L. DUNFORD, Brookhaven National Laboratory, Private Communication (1988).

8. G. DESAUSSURE and R. B. PEREZ, "POLLA, A FORTRAN Program to Convert R-Matrix-Type Multilevel Parameters into Equivalent Kapur-Peierls-Type Parameters," ORNL-2599, Oak Ridge National Laboratory (1969).

9. C. KALBACH and F. M. MANN, "Phenomenology of Continuum Angular Distributions. I. Systematics and Parameterization," Phys. Rev. C. 23, 112 (1981).

10. C. KALBACH, "Systematics of Continuum Angular Distributions: Extensions to Higher Energies," LA-UR-87-4139. Los Alamos National Laboratory (1987). To be published in Phys. Rev. C.

11. P. G. YOUNG and E. D. ARTHUR, "GNASH: A Preequilibrium Statistical Nuclear Model Code for Calculation of Cross Sections and Emission Spectra," LA-6947, Los Alamos National Laboratory (1977).

12. R. E. MACFARLANE, "TRANSX-CTR: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes for Fusion Systems Analysis," LA-9863-MS, Los Alamos National Laboratory (1984).