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VITAMIN E: A MULTIPURPOSE ENDF/B-V COUPLED NEUTRON-GAMMA CROSS SECTION LIBRARY

Barhen, D. G. Cacuci, W. E. Ford III, R. W. Roussin, J. J. Wagschal†, C. R. Weisbin, J. E. White, R. Q. Wright

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830, USA

†On leave from The Hebrew University, Jerusalem, Israel.

The U. S. Department of Energy (DOE) Office of Fusion Energy (OFE) and the Division of Reactor Research and Technology (DRRT) jointly sponsored the development of a coupled fine-group cross section library [VITAMIN-C]. The experience gained in the generation, validation and utilization of the VITAMIN-C library along with its broad range of applicability has led to the request for updating this data set using ENDF/B-V. Additional support in this regard has been provided by the Defense Nuclear Agency (DNA) and by EPRI in support of weapons analyses and light water reactor shielding and dosimetry problems, respectively. The rationale for developing the multipurpose ENDF/B-V based VITAMIN-E library is presented, with special emphasis on new models used in the data generation algorithms. The library specifications and testing procedures are also discussed in detail. The distribution of the VITAMIN-E library is currently subject to the same restrictions as the distribution of the ENDF/B-V data.

[Multigroup Cross Section Libraries, ENDF/B-V, Fusion Neutronics, LMFBR Analysis, LWR Shielding and Dosimetry, Weapons Applications]

Introduction

The U.S. Department of Energy (DOE) Office of Fusion Energy (OFE) and the Division of Reactor Research and Technology (DRRT) jointly sponsored the development of a coupled fine-group cross section library.[1-4] This 171-neutron, 36-gamma-ray group library was based upon ENDF/B-IV and was intended to be applicable to fusion reactor neutronics and LMFBR core and shield analysis. Versions of the library are available from the Radiation Shielding Information Center (RSIC) at the Oak Ridge National Laboratory in both AMPX (DLC-41/VITAMIN-C) and CCCC (DLC-53/VITAMIN-4C) formats. Computer codes for energy group collapsing, interpolation on Bondarenko factors for resonance self-shielding and temperature corrections, and various other useful data manipulations are also available via the PSR-63/AMPX-II and PSR-117/MARS packages.

VITAMIN-C has been utilized in a variety of projects at ORNL[5-7] and at other organizations.[8-10] The experience gained in the generation, validation, and utilization of this library along with its broad range of applicability has led to the request for updating this data set using ENDF/B-V. Additional support in this regard has been provided by the Defense Nuclear Agency (DNA) and by the Electric Power Research Institute (EPRI) in support of weapons analyses and light water reactor shielding and dosimetry problems, respectively. The purpose of this paper is to provide detailed specifications and rationale for the proposed ENDF/B-V update (designated VITAMIN-E) to the VITAMIN-C library, emphasize the changes made to upgrade the data generation algorithms, and discuss the various testing procedures.

Specifications for VITAMIN-E

Materials/Temperatures/Background Cross Sections

All materials on the ENDF/B-V General Purpose file will be processed at 0°, 300°, 900°, and 2100°K. There is a possibility that future Doppler calculations may require higher temperatures for certain selected materials, but this will be treated later on a case-by-case basis. The selection of background cross sections σ_B was modified from VITAMIN-C based upon experience[1,11] and extended to include values of $\sigma_B = 0$ (actually $\sigma_B = 10^{-6}$ is used to avoid problems taking logarithms) and $\sigma_B = 10^{10}$, corresponding to pure concentration and infinite dilution, respectively. The special purpose files (e.g., actinide, dosimetry, activation, etc.) will be processed at room temperature and infinite dilution. The ENDF/B-V fission product library has also been updated; accordingly, the DLC-38/ORYX-E library[12] will be updated with fine-group fission-product cross sections. The ORYX data can be collapsed to the group quantities required by ORIGEN[13] to obtain lumped fission products for fuel calculations. Additional materials not in this issue of ENDF/B include Ar, Ga, and Sn. These will be taken from the ENDL library.[14] All reactions will be processed, including the covariance files.

Group Structure

For the intended range of application (LMFBR core physics and shielding, LWR shielding and dosimetry, weapons analyses, fusion blanket technology), a 174-neutron/37-gamma-ray group structure was adopted. This structure was obtained from the favorably received 171/36 VITAMIN-C specification[2] by making only minor adjustments to formally include energy boundaries of the DNA broad group library[15] and to extend the energy range to ∿ 20 MeV. Synthesis with higher energy libraries (> 20 MeV), primarily for CTR applications, will be performed in a separate step as done previously.[16] Finally, the group boundaries include the break points used to describe the multi-region weighting function. The gamma-ray energy group structure has been extended to 20 MeV and a single minor change to one energy boundary (75 keV → 70 keV) was made, for compatibility with the DNA gamma-ray group structure.

Weighting Function

Several considerations enter into the selection of a smooth weighting function, W(E), to represent the neutron flux spectrum. Experience in Cooperative Processing Methods Testing has shown that the use of a more realistic smooth weighting function would help in assuring computation of proper group constants. In particular, below ∿ 25 keV the weighting function used previously was 1/E while we know that typical LMFBR spectra in this energy range are roughly constant and do not increase with decreasing energy. Similarly, the point at which the 1/E spectrum was joined to the fission spectrum was 821 keV in the VITAMIN-C library, while testing has shown that a higher value might be more reasonable. One must be quite careful with these types of arguments however, since for "typical" shielding situations the flux spectrum is often 1/E and sometimes even $1/E^n$, where $n > 1$. Also, it is perceived that the use of any particular reactor-dependent weighting function may detract from the generality of the resulting shielding factor library. Finally,

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built-in spectral corrections (e.g., elastic removal) are intended to account for some of these effects and the associated theories are currently based on a 1/E model.[17] It is also recognized that in special circumstances other sets of weighting functions may be required.

Thus, the weighting function specified in Table I obviously represents a set of compromises which hopefully can provide adequate accuracies over the range of intended applications. Basically, the energy at which the fission spectrum can be smoothly joined to the 1/E spectrum (i.e., where flux/lethargy is constant) is found to be equal to 3/2 of the fission spectrum temperature (taken here as $\theta \cong 1.4$ MeV). To provide consistency with the selected energy group boundaries, the (1/E)/fission spectrum cutpoint was raised to 2.1225 MeV, a boundary equal to 3/2 θ (θ = 1.415 MeV). Below this energy and above 0.414 eV, the W(E) spectrum is assumed to be 1/E with the knowledge that elastic removal corrections may be used to improve estimates of flux shapes. Shielding and thermal reactor problems also favor this shape. It should also be noted whereas the Maxwellian temperature in the thermal group was fixed at 300°K for the VITAMIN-C library, it will be temperature dependent in the VITAMIN-E library. For the 0° temperature, the smooth flux spectrum temperature is still set at 300°K. However, for the 300°, 900°, and 2100°K cases the spectrum temperature will be changed to the respective temperatures. The cutpoint for the Maxwellian and 1/E shapes is fixed at 0.414 eV independent of temperature (the original 5kT guideline was only nominal).

The weighting function for the gamma ray interaction cross sections is to be constant in energy.

Table I. Specification of neutron interaction weighting function

Functional Form	Energy Limits	Group Range
1) Maxwellian Thermal Spectrum $W_1(E) = C_1 E e^{-E/kT}$	10^{-5} eV to 0.414 eV	173-174
2) "1/E" Slowing-Down Spectrum $W_2(E) = C_2/E$	0.414 eV to 2.12 MeV	48-172
3) Fission Spectrum (θ=1.415 MeV) $W_3(E) = C_3 E^{1/2} e^{-E/\theta}$	2.12 MeV to 10.0 MeV	16-47
4) "1/E" Spectrum $W_4(E) = C_4/E$	10.0 MeV to 12.52 MeV	11-15
5) Velocity Exponential Fusion Peak (E_p = 14.07 MeV) (kT = 0.025 MeV) $W_5(E) = C_5 \exp -\left\{\frac{5}{kT}(E^{1/2}-E_p^{1/2})^2\right\}$	12.52 MeV to 15.68 MeV	5-10
6) "1/E" Spectrum $W_6(E) = C_6/E$	15.68 MeV to 19.64 MeV	1-4

Legendre Order of Scattering

The neutron group-to-group transfer matrices for the following materials are being expanded to P_8: H^1, H^2, H^3, He^3, He^4, Li^6, Li^7, Be^9, B^{10}, B^{11}, C, N^{14}, O^{16}, Na^{23}, Mg, Al, Si, K, Ca, Ti, Cr, Mn^{55}, Fe, Co^{59}, Ni, Cu, Mo Pb, Ta^{181}, Ta^{182}, W^{182} to W^{186}. All other materials are being processed with a P_3 expansion.

The photon-interaction expansion is truncated at P_5.

Convergence Parameter Requirements

To improve accuracy the tolerance on resonance reconstruction has been reduced from 1% in VITAMIN-C to 0.5% in VITAMIN-E and that for linearization from 0.5% to 0.2%. The linearization tolerance was reduced below 0.5% without significant computational penalty. Thinning and integration convergence parameters were specified as 0.2% and 0.1%, respectively. The cumulative uncertainty is a complex combination of all of these approximations; there is currently no methodology used to systematically combine these various sources of error.

Processing Codes System

The upgraded self-consistent processing codes system has been tested as part of the CSEWG Data Testing Process. Multigroup neutron cross sections are being generated with the updated MINX module[18] and photon production and interaction cross sections are being generated with the LAPHNGAS and SMUG modules of the AMPX-II system.[19] Covariance files are being processed with PUFF[20,21] This system was chosen because of its successful performance in the generation of VITAMIN-C, the experience obtained by ORNL and General Electric as part of the preliminary ENDF/B-V Data Testing, and the improvements to the modules as described in the following section.

Output Formats

Multigroup BRKOXS, ISOTXS, AMPX master, and MATXS libraries are being produced. The pointwise files generated from ENDF/B-V in the process of preparing VITAMIN-E are also available. The covariance files will be output in COVERX format.[22] Special purpose files of elastic removal f-factors will also be provided.

Handling Codes for the Library

Two different sequences of handling codes for retrieving, manipulating, converting, editing, collapsing, self-shielding, etc., the libraries are available depending upon whether one needs to work in the CCCC or AMPX code systems. Codes for handling AMPX format are available in PSR-63/AMPX-II, and codes for handling CCCC format are available in PSR-117/MARS. Both computer code packages are available from RSIC. The various programs and functions are listed in Table II.

Table II. Handling codes from the AMPX and MARS packages of software support

AMPX Module	CCCC Computer Code	Function
AIM	BINX, LASIP-III	BCD-to-binary (or vice-versa) conversion
AJAX	LINX, I2I, B2B	Merging and deleting operations
CHOX		Combining neutron and gamma-ray files
CHOXM		Combining self-shielding factors, neutron files, and gamma-ray files
MALOCS	CINX	Energy group collapsing
BONAMI-2	SPHINX	Compute system-dependent shielded cross sections
NITAWL	I2D	Prepare working libraries for use in transport calculations
RADE		Perform tests on multigroup libraries

A new program has been written[23] to provide a conversion capability between the AMPX-master and MATXS formats.

Upgrading of the Data Processing System

The processing codes system has been upgraded by updating individual modules as described below.

Resonance Reconstruction/Linearization/Doppler Broadening

New editions[24,25] of the LINEAR and SIGMA-1 programs have been installed. In the new SIGMA-1 version, particular care is taken to include a sufficient number of points on the Doppler broadened file, so that linear interpolation is accurate to within a fixed input criterion. In addition, the program allows now for proper broadening of threshold reactions to controlled thermonuclear reactor temperatures.

In future releases of the VITAMIN-E library, the resonance profile reconstruction algorithm will also be upgraded by replacing the standard RESEND techniques by the newly-developed RECENT code.[26]

Finally, by optimizing the computational flow, i.e., thinning the 0°K data before broadening, enormous amounts of computer time are saved.

Unresolved Resonances Treatment

The treatment of the unresolved resonance region in MINX has been updated by replacing the standard UNRESR module with a new treatment largely based on the sophisticated techniques developed by Hwang[27] and implemented in the MC²-2 code[28] for computing flux-weighted effective pointwise cross sections. These techniques were extended at ORNL to allow for the computation of effective pointwise current weighted total cross sections[29], and more generally for the computation of higher order effective pointwise cross sections required for the consistent computation of the shielded scattering matrices.[30] Notice that these algorithms[27-30] include processing of competitive widths, interference scattering, within sequence and sequence-sequence overlap corrections.

The numerical procedure employed in MINX to obtain the infinitely dilute group averaged cross section in the unresolved energy region has also been improved.[31]

Elastic Removal

In the current version of MINX fully shielded scattering transfer matrices are generated as functions of the temperature T and the Bondarenko parameter σ_B

$$\sigma^{g\to h}_{e,\ell}(\sigma_B,T) = \frac{\int_g W_\ell(E)\,\frac{\sigma_e(E,T)}{[\sigma_B+\sigma\ (E,T)]^{\ell+1}}\,A^h_\ell(E)dE}{\int_g \frac{W_\ell(E)}{[\sigma_B+\sigma_t(E,T)]^{\ell+1}}\,dE} \quad (1)$$

$A^h_\ell(E)$ denotes the integral of the scattering transfer probability moment over group h.

Particular care has to be exercised in the unresolved resonance region, where Eq. (1) becomes

$$\sigma^{g\to h}_{e,\ell}(\sigma_B,T) = \frac{\int_g W_\ell(E^*)A^h_\ell(E^*)\bar{\sigma}_{e,\ell}(E^*,\sigma_B,T)\prod_{k=0}^{k=\ell}\frac{1}{\sigma_B+\bar{\sigma}_{t,k}(E^*,\sigma_B,T)}\,dE^*}{\int_g W_\ell(E^*)\prod_{k=0}^{k=\ell}\frac{1}{\sigma_B+\bar{\sigma}_{t,k}(E^*,\sigma_B,T)}\,dE^*} \quad (2)$$

The higher order effective pointwise cross sections are defined as

$$\bar{\sigma}_{x,\ell}(E^*,\sigma_B,T) = \frac{\int_{\Delta E}\frac{\sigma_x(E,T)dE}{[\sigma_B+\sigma_t(E,T)]^{\ell+1}}}{\int_{\Delta E}\frac{dE}{[\sigma_B+\sigma_t(E,T)]^{\ell+1}}} \quad (3)$$

In the above expressions $W_\ell(E)$ describes the slow varying broad energy behavior of the weighting function. E* denotes the energy point, contained in the interval ΔE at which average resonance parameters are specified. The computational procedure is based upon the transformation

$$\sigma_B+\sigma_t(E,T) = \sigma_p + \sum_\lambda x_\lambda(E,T) \quad (4)$$

where x_λ refers to resonance component λ (i.e., resonance i in sequence ν) of the total cross section, expressed in terms of the usual symmetric and anti-symmetric line shape functions

$$x_\lambda = \sigma_{o,\lambda}[\psi_\lambda+a_\lambda\chi_\lambda] \quad (5)$$

According to the ENDF specifications, the "effective" potential cross section σ_p includes the smooth corrections contributions (σ^x_{F3}) from scattering, fission (if relevant), and capture, but not from the competitive reaction

$$\sigma_p = \sigma_{pot}(E^*) + \sum_{\substack{x\\ x\neq comp}}\sigma^x_{F3}(E^*) + \sigma_B \quad (6)$$

Since existing spectral correction procedures [TDOWN[17,32], SPHINX[33], BONAMI-2[19], etc.] are based on elastic removal treatments, elastic removal shielding factors will be provided with VITAMIN-E. These are computed according to the standard definition

$$f^g_{er}(\sigma_B,T) = \frac{\sigma^g_{er}(\sigma_B,T)}{\sigma^g_{er}(\infty,o)} \quad (7)$$

where the shielded elastic removal cross section is obtained from the shielded outscatter matrix

$$\sigma^g_{er}(\sigma_B,T) = \sum_{h>g}\sigma^{g\to h}_{el,\ell=0}(\sigma_B,T) \quad (8)$$

The elastic removal shielding factors will be stored on special purpose files.

Temperature-Dependent Thermal Weighting

A change was made in MINX to permit the smooth energy weighting Maxwellian in the thermal range to be temperature dependent.

Computation of Analytical Bounds for the Cross Section Self-Shielding Factors

A fundamental problem regarding the applicability of the shielding factor method is to determine the limits of the range of values within which a cross section shielding factor is restricted, and whether these limits are physically meaningful. Using functional analysis techniques, a general methodology for computing strict upper and lower bounds for self-shielding factors has been developed.[34,38] The complete range of f-factors computed by cross section processing codes was addressed, and ENDF/B specified cross section

discontinuities were taken into account. The resulting formalism was implemented into BRINE[35], a stand-alone module easily incorporable into existing cross section processors. BRINE is being used to check the VITAMIN-E shielding factors.

Formats

The code system was upgraded to handle Version V formats. Major new features included the processing of competitive widths, uncertainty files and energy-dependent Watt fission spectra. Note that, as in VITAMIN-C, only the 1-MeV spectrum will be placed in the VITAMIN-E library, since MINX does not currently process fission matrices.

Photon Production Processing

Experience with ENDF/B-IV gamma ray production processing led to linearization and normalization of the weight function to help improve the precision of the LAPHNGAS calculation.

A coding change was made to the LAPHNGAS code to allow better precision when an input weighting spectrum is used (the case for VITAMIN-E). The change improves the integration scheme by incorporating the weighting function energy grid into the energy grid used by LAPHNGAS to calculate the group averaged multiplicities or gamma ray production cross sections.

A feature was also added to LAPHNGAS to allow calculation of multigroup multiplicities for materials without resonance parameters.[19] This permits self-shielding of gamma ray production cross sections, e.g., from capture, using the Bondarenko scheme.

Processing ENDF/B-V Uncertainty Data Into Multigroup Covariance Matrices

A capability for processing ENDF/B-V uncertainty data into multigroup covariance matrices has been developed[21] and implemented in the PUFF-II module. Specifically, the new module allows processing of all "NI-type" uncertainty relationships[36], required to describe explicitly the various components of the covariance matrix. In addition, explicit cross reaction and cross material relationships and derived uncertainties can be treated. Finally, the infinitely dilute cross section covariances due to uncertainties in the resolved resonance parameters can be computed.

First Order Data Checks

Processed VITAMIN-E data are undergoing an extensive series of first order data checks.

The RADE module of the AMPX-II system[19] is used to check each AMPX master data set for partial cross section consistencies. The BRINE module[35] is used to check the shielding factors against analytically computed upper and lower bounds. Finally, plots of point versus multigroup data for specified materials and reactions are being produced.

Testing Program and Anticipated Schedule

The testing program will be intimately associated with feedback from sponsor application and participation in various cooperative national testing programs. Anticipated application includes continued analysis of the OFE integral experiments, analysis of LMFBR critical experiments and Large Plant Design Studies, analysis of experiments relevant to pressure vessel surveillance, and weapons related applications. Benchmark validation will include cooperative testing in the framework of the CSEWG Data Testing Subcommmittee, the CSEWG Processing Methods Testing Subcommittee, ANS-6.1.2 (LWR Shield Standard Cross Sections), and the OFE Validation Group.

In order to initiate the testing procedures, some of the more important materials for the above-mentioned applications are being processed with high priority. Of particular importance is a comprehensive feedback to CSEWG's fast reactor benchmark program, in order to address the following questions: How do Version V data compare to experiment, as compared to Version IV data? If major changes were observed, could one trace their origin? Are there still outstanding discrepancies?

For the initial phase of testing, the available VITAMIN-E data have been augmented, where necessary, with multigroup data generated in adherence to the VITAMIN-E specifications using preliminary ENDF/B-V evaluations and with VITAMIN-C data. The cross section sets were then collapsed to a 100-group structure, and were used to calculate performance parameters of CSEWG fast reactor benchmarks.

Specifically, the effective multiplication factors and central core reaction rate ratios were calculated for the Pu-fueled JEZEBEL, ZPR-3/48, -3/56B, -9/31, and -6/7 benchmarks and for the U-fueled GODIVA, ZPR-3/6F, -3/12, -3/11, and -6/6A benchmarks. Results indicate[37] a general improvement in the ratio of the calculated/experimental values of the parameters calculated with VITAMIN-E data versus parameters calculated with the ENDF/B-IV based VITAMIN-C library.

Our current estimate of the VITAMIN-E schedule is that the first release of the complete library will not be available until mid-1980, although preliminary issues will be used in the context of CSEWG testing and cooperative nuclear data and methods development. Extensions to the current effort will include the dosimetry, activation and gas production data, kerma factors, response functions, and delayed neutron data. Processing refinements and library improvements are thus expected to continue for at least 2-3 more years.

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