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STATUS OF THE ENDF/B SPECIAL APPLICATIONS FILES

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Abstract

The newly formed SAFE Subcommittee of the Cross Section Evaluation Working Group is charged with the responsibility for providing, reviewing, and testing several ENDF/B special purpose evaluated files. This responsibility currently encompasses dosimetry, activation, hydrogen and helium production, and radioactive decay data required by a variety of users. New formats have been approved by CSEWG for the inclusion of the activation and hydrogen and helium production cross-section libraries. The decay data will be in the same format as that already employed by the Fission Product and Actinide Subcommittee of CSEWG. While an extensive dosimetry file was available on the ENDF/B-IV library for fast reactor applications, other data are needed to extend the range of applications, especially to higher incident neutron energies. This Subcommittee has long-range plans to provide evaluated neutron interaction data that can be recommended for use in many specialized applications.

Introduction

The Cross Section Evaluation Working Group has the responsibility for providing evaluated data sets for neutron-induced reactions for user needs in a variety of applications. About a year ago, a new Subcommittee was formed to evaluate, update, and test data sets for several special purpose applications. The new Subcommittee is called the Special Application Files Subcommittee (SAFE) and is chaired by Benjamin A. Magurno of Brookhaven National Laboratory. Currently, the Subcommittee responsibilities are divided into four subgroups with the following assignments:

1. Activation Data: Robert E. Schenter (HEDL), Chairman
2. H and He Production: Leona Stewart (LASL), Chairman
3. Dosimetry: Benjamin A. Magurno (BNL), Chairman

   William N. McElroy (HEDL), User Needs and Phase II Testing
4. Radioactive Decay Data: Charles W. Reich (EG&G, Idaho), Chairman

   (Bowen R. Leonard, Jr.(BNW) was appointed as a member-at-large.)

The evaluation and Phase I review assignments for the various files will be coordinated by the Chairman of each subgroup, who will also take the responsibility for coordination with the principal evaluator of each general purpose file affected by the individual or partial evaluations provided by the SAFE Subcommittee. It is therefore important to note that extensive interaction among the four subgroups of the SAFE Subcommittee will be required to insure consistency among the various parts of the data files.

While the membership of the SAFE Subcommittee is small, many different people from several institutions will contribute evaluated data and perform Phase I and Phase II reviews for ENDF. Each Sub-Group Chairman, for example can call meetings to delineate problems within his particular application area and extend invitations to each and every contributor. Before proceeding further, however, it should be mentioned that another Subcommittee of CSEWG, the Fission Product and Actinide Subcommittee, retains the responsibility for fission product yields (MT = 454) and several actinide files which may, in some cases, be incomplete insofar as general purpose usage is concerned.

Development of the SAFE Files

A special purpose file is herein defined as one which contains the minimal information required for one specific application. For example, a particular (Z,A) evaluation may contain only half-life and branching ratio data while another may contain the radiative capture or (n,2n) cross section. Still another may contain (n,p) and (n,α) cross sections, such as the Dosimetry File for ^{27}Al. However, the general purpose evaluations must provide, as a minimum, enough information for the user to apply in a neutron transport (and often) gamma-ray transport problem; therefore, energy and angular distributions of the neutrons and gammas must be placed in a general purpose file for all reaction indices.

All special purpose files will be evaluated for isotopic targets. If an elemental evaluation is required, or an evaluation for an enriched sample, then the required information can be obtained by summing the individual contributions weighted by the isotopic abundances.

The n + ^{9}Be $\rightarrow$ p + ^{9}Li reaction outlined in Fig. 1 shows the significance of the overlapping areas of the four subgroup tasks, even though this reaction is not particularly useful in dosimetry due to the short half-life of ^{9}Li. Due to the use of ^{9}Be in fusion reactor design, the residual radioactivity would be of interest. Since two alphas are emitted as the end product, this reaction contributes to the helium production cross section and, finally, in order to calculate the activity, all of the decay information would be needed for design studies. This reaction also produces a delayed neutron and the high-energy betas (up to 13.6 MeV) contribute significantly to local heating, providing still another user application. It is obvious, therefore, that development of the SAFE files

$$n + {}^{9}_{4}Be \longrightarrow p + {}^{9}_{3}Li - .12.836 \text{ MeV}$$

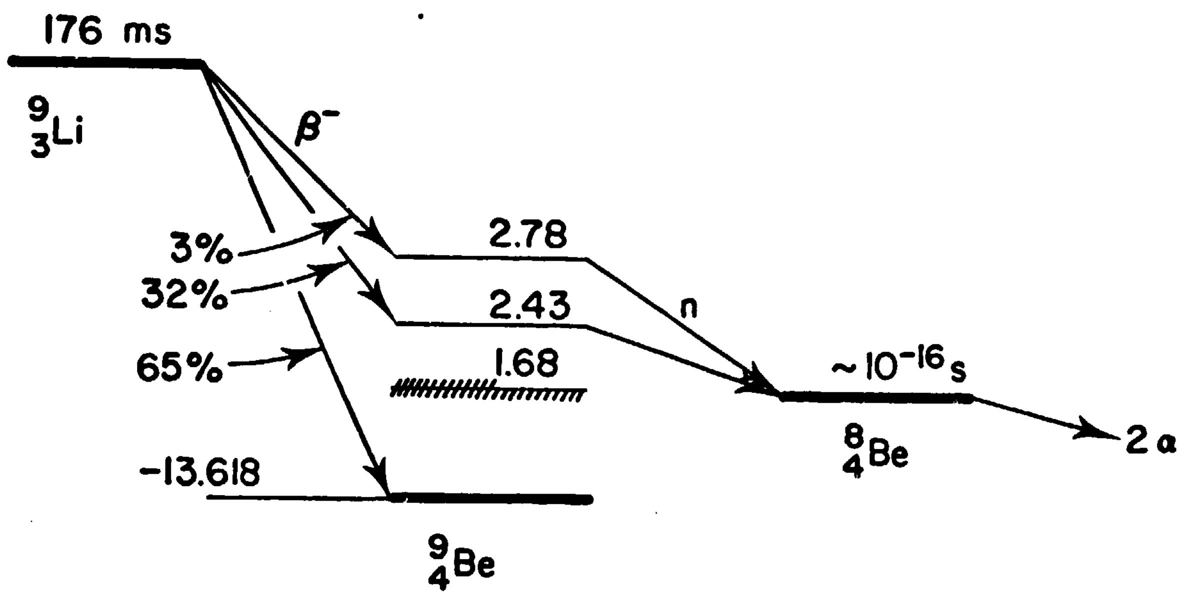

Fig. 1. The chain representing the decay of the radioactive product (^{9}Li) formed in the $^{9}Be(n,p)^{9}Li$ reaction.

should extend the uses of ENDF to a wider variety of applications, not presently allowed in ENDF/B-IV.

Activation (R. E. Schenter, HEDL)

For ENDF, the major difference between the dosimetry and activation files is that the complete decay chain is required for all reaction indices in the activation library, whereas energy dependent cross sections (only) are currently in the dosimetry files. For the study of radiation effects as a function of time and operating history, however, designers require more detailed information than the energy dependent cross sections. For depletion and buildup calculations, the reaction chains must be complete. Of some importance, perhaps, local energy deposition is also time dependent and the total energy may change significantly when the energies of the delayed products are included. The activation library for each (Z,A) will have a minimum of File 1 and File 8 information and those that have cross sections will also have File 10; if multiplicities instead of cross sections are chosen for representation, then data for File 1, File 3, File 8, and File 9 are required (for resonance materials, File 2 must also be included). A brief description of these files follows:

File 1: Descriptive information that includes a minimal amount of information on the evaluation and a list of all the files and reaction indices in the evaluation. File 1 also includes data for $\bar{\nu}$.

File 2: Resonance parameters.

File 3: Energy dependent cross sections; E in MeV and σ in barns.

File 8: For (Z,A) and (MAT); that is, for the evaluation that contains the energy dependent cross sections for (Z,A); this file includes a minimal amount of information for each reaction (MT) for which a radioactive nuclide is produced. For example, each design application may be interested in only a small range of half-lives of the product, therefore, the half-life and first decay are given.

For (ZAP) and (MATP); the complete decay data (only MT = 457) are found in this file.

File 9: File 9 can only be used when cross sections are given in File 3 since the multiplicities in File 9 must be multiplied by the cross sections in File 3. For those cases in which resonance parameters are found in File 2, only multiplicities are allowed. That is, Files 2, 3, and 9 are required.

File 10: Cross sections for the production of the radioactive nuclide produced via the reaction mechanism (MT).

Each reaction cross section which produces a radioactive product (ZAP) must have the product identified in File 8 under the specific MT number which defines the energy dependent cross section. The decay data (MT = 457) will then appear in a different evaluation specified by the (ZAP) of the radioactive nuclide produced. Note that the (n,n') reaction is no exception to this rule since the stable and metastable states of a target nuclide will have different MAT numbers. Therefore, several decays and several (Z,A) MAT numbers must often be provided for a single reaction cross section--in order to reach stability.

Using the example in Fig. 1, the $^{9}Be(n,p)^{9}Li$ cross section would appear under the MAT for ^{9}Be, and the complete decay chain for ^{9}Li would be given under a different MAT number, designated as MATP, or the MAT number of the radioactive product produced.

The new formats needed to implement these additions are described in ENDF-102, available from the NNDC at BNL. Also the Version V extensions to Files 8, 9, and 10 have been discussed in detail at the October 27-28, 1976 CSEWG Meeting (see enclosure 10 of the minutes). Time and space prohibit inclusion of the many details here; however an example is outlined below:

FILE 8 DATA REQUIRED FOR EACH CROSS SECTION (MT) THAT PRODUCES A RADIOACTIVE NUCLIDE (ZAP)

Target Description

ZA = Z,A of Target

LIS = State #

LISØ = Isomeric State #

→ THROUGH REACTION TYPE (MT) →

Radioactive Product

ZAP = Z,A of Product

LFS = Level Number

ELFS = Energy of Level

HL = Half-Life (s)

THEN

ZAP(LFS) DECAYS TO ZAN VIA

RTYP

DESCRIBED BY

BR = Branching Ratio

ER = End Point (total) Energy

CT = Chain Terminator (to denote stability of ZAN)

NDND = Number of Branches of LFS

MATP = MAT # for ZAP (for MAT = 457)

LMF = File # (9 for Multiplicities; 10 for Cross Sections)

CARD IMAGE FORMAT (FILE 8)

Field(1)	(2)	(3)	(4)	(5)	(6)	(7) MAT	(8) MF	(9) MT
ZA	AWR	LIS	LISØ	NS	0	4009	8	XXX
ZAP	ELFS	LMF	LFSI	6*ND	MATP	4009	8	XXX
HL	RTYP	ZAN	BR	ER	CT	4009	8	XXX

FILE 8 DATA UNDER (ZA, MAT) FOR EXAMPLE IN FIGURE 1

4.009+03	8.9348	0	0	1	0	4009	8	103
3.009+03	0.0	10	0	18	3009	4009	8	103
0.176	1.0	4.009+03	0.65	13.618+06	1.00	4009	8	103
0.176	1.544	4.009+03	0.32	11.188+06	2.02	4009	8	103
0.176	1.544	4.009+03	0.03	10.838+06	2.03	4009	8	103

THEN

FOR EXAMPLES WITH MORE THAN ONE ZAP(LFS), CONTINUE WITH EACH RTYP UNTIL ALL DIFFERENT HALF-LIVES ARE COMPLETED.

THEN

PREPARE MT=457 DECAY DATA FOR EACH NEW ZAP(LFS) FORMED IN A NEW MATP. THIS MATP CAN CONTAIN ALL DETAILED SPECTRA FOR ALL DELAYED PARTICLES INCLUDING GAMMA RAYS.

A list of activation data required for Version V has been prepared by Fred Mann (HEDL) and is currently being circulated for consideration and review. Since the list is already extensive in the number of requests (although by no means yet complete), it may be impossible to include all of the individual requests in Version V. Examples of a few high-priority requests have been tabulated from Mann's list in Table I. For convenience, the reaction product, half-life, and the application for which the data will be used are included.

Hydrogen and Helium Production (L. Stewart, LASL)

Although helium production has been used as a dosimeter for several years, wide-spread requests for hydrogen and helium production cross sections have grown significantly in the past few years due primarily to the need to study radiation effects of high-energy neutrons on various structural materials for fission and fusion reactor applications.

In the determination of gas-production cross sections at high energies, the contributions from (n,p) and (n,α) reactions often do not represent the total cross section, since (n,n'p) and (n,n'α) processes may be important. Experiments are presently underway at LLL and AI to measure total gas production cross sections for various materials for neutrons around 14 MeV. Since these measurements will probably not cover the entire energy region of interest or the complete list of isotopes, heavy reliance will be placed on model code predictions to provide total production cross sections for the evaluated sets. For light isotopes the situation is often very complex. For example, the total helium production cross section for ^{10}B is found from the following sum:

$$\sigma = \sigma(n,\alpha_0) + \sigma(n,\alpha_1) + \sigma(n,n'\alpha) + 2\sigma(n,t2\alpha) + 2\sigma(n,n'd2\alpha) + 2\sigma(n,2n).$$

The above example clearly shows the need for specific reaction indices (MT numbers) for total hydrogen and helium production cross sections. In ENDF/B-V, new MT numbers are already approved for this special gas production file. The new MT numbers can be obtained by simply adding one hundred

TABLE I. EXAMPLES SHOWING A FEW OF THE HIGH-PRIORITY ACTIVATION CROSS SECTIONS REQUESTED FOR INCLUSION IN ENDF/B-V

	Reaction	Product	Half-Life	Applications
1.	$^{23}_{11}$Na(n,γ)	$^{24}_{11}$Na	14 h	LMFBR Dosimetry Shielding for Na piping
		$^{24}_{11}$Na^{m}	∿20 msec	
2.	$^{27}_{13}$Al(n,α)	$^{24}_{11}$Na	14 h	LMFBR, Dosimetry Fusion Structural activation
		$^{24}_{11}$Na^{m}	∿20 msec	
3.	$^{56}_{26}$Fe(n,p)	$^{56}_{25}$Mn	2.58 h	LMFBR, Fusion Dosimetry
4.	$^{56}_{26}$Fe(n,2n)	$^{55}_{26}$Fe	2.7 yr	LMFBR, Fusion Structural activation
5.	$^{58}_{28}$Ni(n,p)	$^{58}_{27}$Co	70.8 day	LMFBR, Dosimetry Fusion Structural activation
6.	$^{60}_{25}$Ni(n,p)	$^{60}_{27}$Co	5.27 yr	LMFBR, Dosimetry Fusion Structural activation
		$^{60}_{27}$Co^{m}	∿10.5 min	
7.	$^{63}_{29}$Cu(n,α)	$^{60}_{27}$Co	5.27 yr	LMFBR, Dosimetry Fusion Structural activation
		$^{60}_{27}$Co^{m}	∿10.5 min	

to the MT number presently used in Version IV for (n,p), (n,d), (n,t), (n,^{3}He), and (n,α) reactions thus giving MT numbers of 203, 204, 205, 206, and 207, respectively, for the hydrogen and helium production cross sections. Note that this assignment is consistent with the ENDF procedures in that the 200 Series MT numbers represent derived cross sections.

A special meeting[1] of the CSEWG Standards Subcommittee was held at Los Alamos on August 3-5 (1976) to discuss plans for preparation of Version V hydrogen and helium production and activiation files. Table II gives the list of principal evaluators and the evaluations planned for Version V for hyrdogen and helium production.

Dosimetery (B. A. Magurno, BNL)

The dosimetry files for ENDF were evaluated for Version III, updated for Version IV, and Version V will include the planned updates outlined in Table III. This file is already widely used for fast reactor applications and was discussed in great detail by Magurno at a recent international meeting.[2] Since that meeting, little new information has been provided on the energy dependent cross sections for Version V.

The emphasis of the new Subcommittee will be to insure the consistency of the dosimetry cross sections with the activation, gas production, and general purpose files, where applicable. In addition, some effort will be needed to extend the file sets for better coverage of fusion reactor applications. This extension already indicates the necessity for new reaction indices for different isotopes and a more detailed examination of some of the high-energy cross sections.

Decay Data (C. W. Reich, EG&G Idaho)

Detailed decay data will be needed for many structural materials including spectra and branching ratios. For Version-IV, extensive work was entailed in providing detailed decay data for the fission product files and this effort has been continued and expanded for Version-V. With the transfer of the responsibility of the decay data to the SAFE Subcommittee, the effort will be extended to include data for structural materials, in particular, those of interest in fission and fusion reactor design. Some decay information will also be provided which are of interest in the plasma and/or blanket regions which are not necessarily considered as structural components. The formats to be employed for the SAFE files will be the same as those used for fission products. It should be remarked, however, that the formats used for the radioactive decay data (MT = 457) used in Version IV have been changed for the Version V input (see ENDF-102 for details).

This extension of the decay data files is just getting underway and the materials will be governed, primarily, by the activation request list. The above description, however, again points out the close cooperation and

TABLE II. HYDROGEN AND HELIUM PRODUCTION CROSS SECTIONS

Element*	Evaluator†	Lab	Element*	Evaluator†	Lab
$_{3}Li^{6}$	Stewart	LASL	$_{3}Li^{7}$	Stewart	LASL
$_{4}Be$	Howerton	LLL	$_{5}B^{10}$	Hale	LASL
$_{5}B^{11}$	Young	LASL	$_{6}C$	Fu	ORNL
$_{7}N$	Young	LASL	$_{9}F$	Larson	ORNL
$_{13}Al$	Arthur	LASL	$_{14}Si$	Larson	ORNL
$_{22}Ti$	Smith	ANL	$_{23}V$	Smith Mann	ANL HEDL
$_{24}Cr$	Prince Burrows	BNL BNL	$_{25}Mn$	Mughabghab	BNL
$_{26}Fe$	Perey Schenter	ORNL HEDL	$_{27}Co$	Mughabghab Model Codes Sub.	BNL
$_{28}Ni$	Divadeenam	BNL	$_{29}Cu$	Fu Mann	ORNL HEDL
$_{40}Zr$	Gardner	LLL	$_{41}Nb$	Smith Arthur	ANL LASL
$_{42}Mo$	Schenter	HEDL	$_{74}W$	Arthur	LASL

*Includes all important isotopes.

†The evaluators volunteered to try to meet the Version V deadline.

TABLE III. DOSIMETRY PLANNED UPDATES FOR VERSION V

Reactions	Evaluator	Lab
${}_{3}Li^{6}$ & ${}_{5}B^{10}$ (total helium production)	Stewart	LASL
${}_{11}Na^{23}$ (n,γ)	Larson	ORNL
${}_{21}Sc^{45}$ (n,γ)	Magurno	BNL
${}_{22}Ti^{46,47,48}$ (n,p)	Magurno Smith	BNL ANL
${}_{25}Mn^{55}$ (n,2n)	Mughabghab	BNL
${}_{26}Fe^{54,55}$ (n,p) and ${}_{26}Fe^{58}$ (n,γ)	Perey Schenter	ORNL HEDL
${}_{27}Co^{59}$ (n,γ), (n,α), and (n,2n)	Prince Model Code Sub.	BNL
${}_{28}Ni^{58}$ (n,p), (n,2n), and ${}_{28}Ni^{60}$ (n,p)	Divadeenam	BNL
${}_{49}In^{115}$ (n,n')	Smith	ANL
${}_{49}In^{115}$ (n,γ)	Schmittroth	HEDL
${}_{53}I^{127}$ (n,2n)	Sher	Stanford
${}_{79}Au^{197}$ (n,γ)	Mughabghab Standards Sub.	BNL
${}_{90}Th^{232}$ (n,γ) and (n,f); < 50 keV (only)	Leonard	BNW
${}_{92}U^{235}$ (n,f)	Bhat Standards Sub.	BNL
${}_{92}U^{238}$ (n,γ) and (n,f)	Pennington Task Force	ANL
${}_{93}Np^{237}$ (n,f)	Mann Stein	HEDL LASL
${}_{94}Pu^{239}$ (n,f)	Kujawski Task Force	GE

${}_{16}S^{32}$ (n,p), ${}_{29}Cu^{63}$ (n,γ), and ${}_{29}Cu^{65}$ (n,2n) are still unassigned involvement required of the four sub-groups of this Subcommittee. A list of MAT numbers for every (Z,A) present in Version V for materials other than fission products will be compiled as each set is evaluated and received by this Subcommittee.

Conclusions

The status of the four sets of the SAFE files for ENDF have been briefly reviewed. Much of the work has just begun, and it is hoped that the overview presented here will allow the interested user to obtain more detailed information from the sources cited in this paper.

References

1. See Appendix C of Enclosure 9 of the CSEWG Minutes of the October 27-28 (1976) Meeting of CSEWG.

2. B. A. Magurno, Proc. of IAEA Consultants' Meeting on Integral Cross-Section Measurements in Standard Neutron Fields, Vienna, Nov. 15-19 (1976), to be published.