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LA-UR -88-2130

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TITLE THE STATUS OF NUCLEAR DATA EVALUATIONS FOR VERSION VI OF ENDF/B

LA-UR--88-2130

DE88 014410

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SUBMITTED TO Reactor Physics Conf.
Jackson Hole, WY
Sept. 18-22, 1988

Los Alamos
Los Alamos National Laboratory
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THE STATUS OF NUCLEAR DATA EVALUATIONS FOR VERSION VI OF ENDF/B

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ABSTRACT

A new version of the United States national evaluated nuclear data file, ENDF/B-VI, is nearing completion. Major emphasis is being placed on correcting some long-standing nuclear data problems that adversely affect applied calculations for both fission and fusion reactors. This paper reviews some of the evaluation activities of most relevance for fission reactor applications, namely, those involving control, cooling, and shielding materials, structural elements, and the major actinides. Additionally, because of its impact on all the data, work on the Standards Data File for Version VI is also summarized.

INTRODUCTION

Oversight and technical development of the United States national evaluated nuclear data base, ENDF/B, is carried out by the Cross Section Evaluation Working Group (CSEWG), which is an industrial/governmental cooperative effort involving up to some 20 laboratories. Since its formation in 1966, CSEWG has systematically improved the evaluated data base as new experimental and theoretical information became available, periodically issuing new versions of the ENDF/B library. The last major revision of the data base occurred in 1979 with the issuance of Version V of ENDF/B,[1] followed by a significant updating in 1981 that is referred to as Revision 2 of ENDF/B-V.[2] In the time period since ENDF/B-V.2 became available, a number of important differential measurements have been completed, and advances in nuclear theory and evaluation methods have occurred that make updating of the data base again desirable. As a result, CSEWG is now working toward another major revision that is planned for issuance in the 1989-1990 time frame as Version VI of ENDF/B.

Thorough reviews of the fission-reactor-related cross section data in ENDF/B-V.2 were published in 1984.[3-8] While Version V represented a significant improvement over previous versions, deficiencies are known to exist in the data base. Time and space do not permit a detailing of all the problems we are addressing. In very general terms, we expect major improvements to be realized in the ENDF/B-VI standard cross section data as well as other reactions included in the simultaneous standards analysis ((see below), in the resonance region for several key structural materials and the major actinides, in the neutronics data for many materials due to improved representations of energy-angle correlations and improved theoretical model calculations, and in the overall completeness of the data base due to additions in the gamma-ray production, covariance, yield, decay, and delayed neutron data files. Finally, there should be overall improvement in the entire evaluated data file due to the availability of more accurate and comprehensive experimental data with generally higher energy resolution.

In the present paper the status of evaluations for ENDF/B-VI is reviewed with emphasis on materials of most interest for fission reactors, that is, control, cooling, and shielding materials, structural elements, and the major actinides. Also, because of its relevance to the evaluated data in each of these areas, work on the standards data file for ENDF/B-VI is described. For reference, a master list of the isotopes and elements that are expected to be updated for Version VI is included in Table I. It should be noted that at this writing many of the ENDF/B-VI results referred to here are preliminary.

TABLE I

Status of Neutron Cross Section Evaluations for ENDF/B-VI

Material	Major Applications	Target Date	Responsible Laboratory*	Evaluators
^{1}H	Stand.,Cool.	Done	LANL	D. Dodder, G. Hale
^{3}He	Stand.	9/88	LANL	G. Hale
^{6}Li	Stand.,T Breed.	7/88	LANL	G. Hale, P. Young
^{7}Li	T Breed.	7/88	LANL	P. Young, T. Beynon
^{9}Be	Shield.,n-Mult.	Done	LLNL	S. Perkins, E. Plechaty, R. Howerton
^{10}B	Stand.,Control	9/88	LANL	G. Hale, P. Young
^{11}B	Shield.	7/88	LANL	P. Young
C	Stand.,Shield.	6/88	ORNL	C. Fu, E. Axton
^{40}Ca	Shield.	11/88	ORNL	C. Fu, D. Hetrick, D. Larson
V	Struct.	9/88	ANL	A.Smith, D. Smith, R. Howerton et al.
^{50,52,53,54}Cr	Struct.	7/88	ORNL	D. Hetrick, C. Fu, D. Larson, K. Shibata
^{55}Mn	Struct.	Done	JAERI	K. Shibata
^{54,56,57,58}Fe	Struct.	7/88	ORNL	C. Fu, C. Perey, D. Hetrick et al.
Co	Struct.	9/88	ANL	A. Smith, P. Guenther, R. Howerton et al.
^{58,60,61,62,64}Ni	Struct.	7/88	ORNL	D. Hetrick, C. Perey,D. Larson,C. Fu et al.
^{63,65}Cu	Struct.,Cond.	10/88	ORNL	D. Hetrick, C. Fu, D. Larson
^{89}Y	Fiss.Prod.	Done	ANL	A. Smith, D. Smith, R. Rousset et al.
Zr	Struct.,Activ.	11/88	ANL	A. Smith et al.
^{93}Nb	Activ.,Dos.	Done	ANL	A. Smith, D. Smith, R. Howerton
^{151,153}Eu	Activ.,Dos.	9/88	LANL	P. Young
^{165}Ho	Dos.	7/88	LANL	P. Young, E. Arthur
W	Shield.	9/88	LANL	E. Arthur, P. Young, D. Muir
^{197}Au	Stand.,Dos.	9/88	LANL	P. Young, E.Arthur
^{206,207,208}Pb	Shield.,n-Mult.	6/88	ORNL	C. Fu
^{235}U	Fuel Cyc.	9/88	ORNL	G. de Saussure, M. Moore et al.
^{238}U	Fuel Cyc.	9/88	ANL	A. Smith, W. Poenitz, M.Sowerby et al.
^{239}Pu	Fuel Cyc.	9/88	LANL	P. Young, L. Weston, H. Derrien et al.
^{240}Pu	Fuel Cyc.	Done	ORNL	L. Weston, E. Arthur
^{241}Pu	Fuel Cyc.	10/88	ORNL	L. Weston, H. Derrien et al.
^{241}Am	Fuel Cyc.	11/88	CNDC	D. Zhou et al.
^{243}Am	Fuel Cyc.	10/88	ORNL	L. Weston
^{249}Bk	Fuel Cyc.	Done	CNDC	D. Zhou et al.
^{249}Cf	Fuel Cyc.	Done	CNDC	D. Zhou et al.

* ANL = Argonne National Laboratory, CNDC = Chinese (Beijing) Nuclear Data Center, JAERI = Japan Atomic Energy Research Institute, LANL = Los Alamos National Laboratory, LLNL = Lawrence Livermore National Laboratory, ORNL = Oak Ridge National Laboratory.

STANDARDS DATA

Earlier ENDF/B standards evaluations generally followed a hierarchical procedure in which the various standard reactions were analyzed *sequentially*, with each new reaction evaluation depending on the previous results. The ENDF/B-VI evaluation, on the other hand, was performed by *simultaneously* analyzing all the standard reactions that are linked through ratio measurements, as well as several other non-standard reactions that are similarly linked to the standards and for which absolute data exist. Although some of the details have changed slightly, the basic approach followed in the analysis is described in a 1985 paper,[9] and a more up-to-date account was given recently at the Mito Conference.[10] Starting from a very accurate $^{1}H(n,n)^{1}H$ reference file, the light element standard reactions were analyzed in a coupled-channel R-matrix framework that permitted inclusion of auxiliary information such as very accurate charged-particle and neutron total cross section data. The heavier element standard cross sections, a portion of the light element data, and the thermal constants were analyzed independently using a generalized least squares program. The results of the R-matrix and least squares analyses were then combined in a manner that took full account of all correlations in the experimental data as well as those introduced by the R-matrix analysis. The standards data file for ENDF/B-VI was completed and made available in the fall of 1987.

The methodology used in the simultaneous standards evaluation is particularly appropriate for fission reactor problems because it facilitates accurate determination of cross sections for several important control and actinide materials. In addition to data for the usual standard cross sections, which include the $^{10}B(n,\alpha)$ and $^{235}U(n,f)$ reactions, absolute cross section measurements and connecting ratio data for the $^{238}U(n,\gamma)$, $^{238}U(n,f)$, and $^{239}Pu(n,f)$ reactions were incorporated in the simultaneous analysis. While this technique is expected to improve absolute cross sections, it should be especially effective in determining relative cross sections and covariances, hopefully eliminating some of the bias that has been evident in the past between uranium and plutonium critical systems.

The results of the simultaneous standards evaluation for the $^{235}U(n,f)$ and $^{239}Pu(n,f)$ cross sections are compared to the ENDF/B-V.2 values in Fig. 1. In addition to the ratios of the Version VI (preliminary) to Version V ^{235}U and ^{239}Pu fission cross sections, the Version VI/V ratio is shown for the $^{239}Pu(n,f)/^{235}U(n,f)$ cross section ratio. It is evident that both the ^{235}U and ^{239}Pu fission cross sections have decreased relative to ENDF/B-V.2 by of the order of 1-2% in the fission spectrum range above 100 keV, although their ratio has generally changed less. The largest cross section change occurs for $^{239}Pu(n,f)$ near 16 MeV, where a decrease of ~13% is seen.

CONTROL, COOLANT, AND SHIELDING MATERIALS

^{10}B is an important control material in many reactor systems. The evaluation of the complete n+^{10}B data file, which includes the $^{10}B(n,\alpha)$ standard data to 250 keV, is being carried out at Los Alamos. Additionally, a new evaluation of n+^{11}B data is being provided. Although ^{11}B is not itself important for reactor control, it is 80% of natural boron and is present in some quantity in reactors, and the existing ENDF/B-V.2 evaluation is among the poorest in the data base. Other control materials such as Cd, Ag, Gd, and Hf are generally thought to be reasonably described in ENDF/B-V.2, and updates are not planned for the first issue of Version VI. The improvements that are needed[6] will be implemented in a future issue of Version VI.

The only ENDF/B-VI activity for coolant materials are the new standards evaluations for ^{1}H and C. From the point of view of reactor calculations, the changes in the evaluated data files are not great. Although existing data files for some other coolants (for example, ^{16}O) need updating, resources are not available to include them in this issue of Version VI.

Of the shielding materials that are being updated, some of the most significant improvements are being made for ^9Be and ^{11}B. In the case of ^9Be, a complete new evaluation has been done with special emphasis on accurately specifying the energy-angle correlated neutron emission spectra from (n,2n) reactions.[11] The distributions were obtained using a Monte Carlo technique and recent new double differential experimental data. The new ^{11}B evaluation is primarily based on improved experimental data, supplemented with Hauser-Feshbach calculations to extend the data to higher energies. The most significant improvement for ^{11}B occurs in the neutron total cross section, which in ENDF/B-V.2 is in error by as much as 40% near E_n = 1 and 2.3 MeV. A comparison of the new evaluation of the ^{11}B total cross section with ENDF/B-V.2 and with experimental data[12] is given over this neutron energy range in Fig. 2.

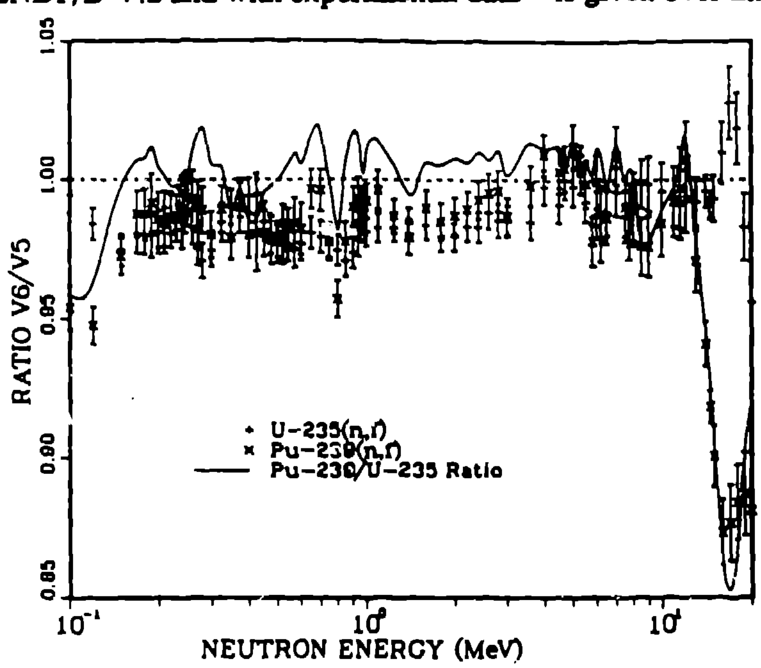

Fig. 1. Comparison of the preliminary ENDF/B-VI fission cross sections of ^{239}Pu and ^{235}U with ENDF/B-V.2. The points indicate the Version VI/Version V (n,f) cross-section ratios and the curve represents the ratio between Versions VI and V of the $^{239}Pu/^{235}U$ cross-section ratio.

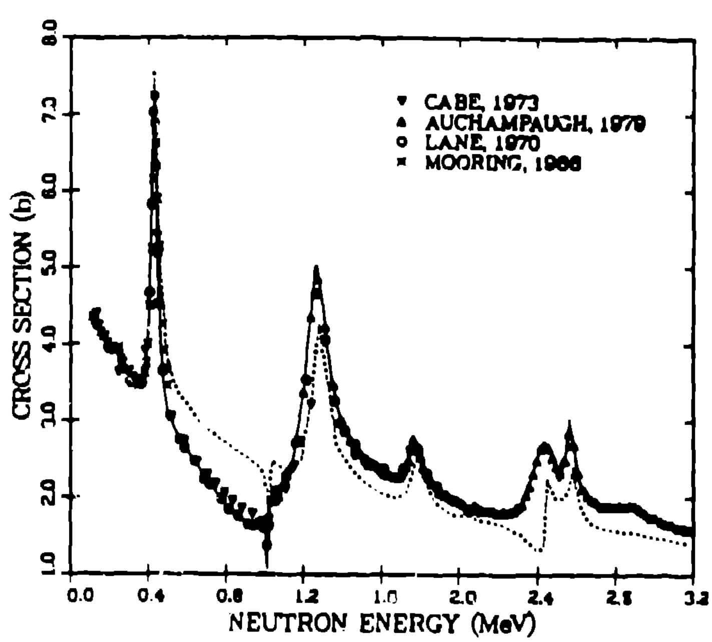

Fig. 2. The ^{11}B neutron total cross section from 0.1 to 3.2 MeV. The solid curve is the preliminary ENDF/B-VI evaluation, the dashed curve is ENDF/B-V.2, and the points are experimental data.[12]

STRUCTURAL MATERIALS

Fe, Ni,and Cr are among the most important structural materials for fission reactors. Separate evaluations are complete or in progress at Oak Ridge National Laboratory (ORNL) for all stable major isotopes of each of these elements. The evaluations are based on analyses of experimental data and extensive new theoretical studies in the MeV region.[13-15] Additionally, new multichannel resonance parameter analyses are being performed for ^{56}Fe and ^{58}Ni (Ref. 16) using recent high resolution transmission, capture, and scattering data. A similar analysis for ^{60}Ni transmission and capture already exists.[17] New evaluations of ^{55}Mn, ^{63}Cu, ^{65}Cu, and ^{206,207,208}Pb will also be available. At Argonne National Laboratory (ANL), a series of new neutron-induced cross section measurements and theoretical analyses have been completed for several structural materials,[18] and evaluations are being performed for V, Co, and Zr that will incorporate the new results, both experimental and theoretical.

A sample of results from the new Reich-Moore simultaneous analysis[16] of transmission, capture, and scattering data for n+^{58}Ni reactions is shown in Fig. 3. These fits were made with the SAMMY[19] code, which utilizes Bayes' theorem in its fitting routines. In order for this technique to be used most effectively, it is necessary that very high resolution data be available on an accurate energy grid, such as the ORELA results shown in Fig. 3.

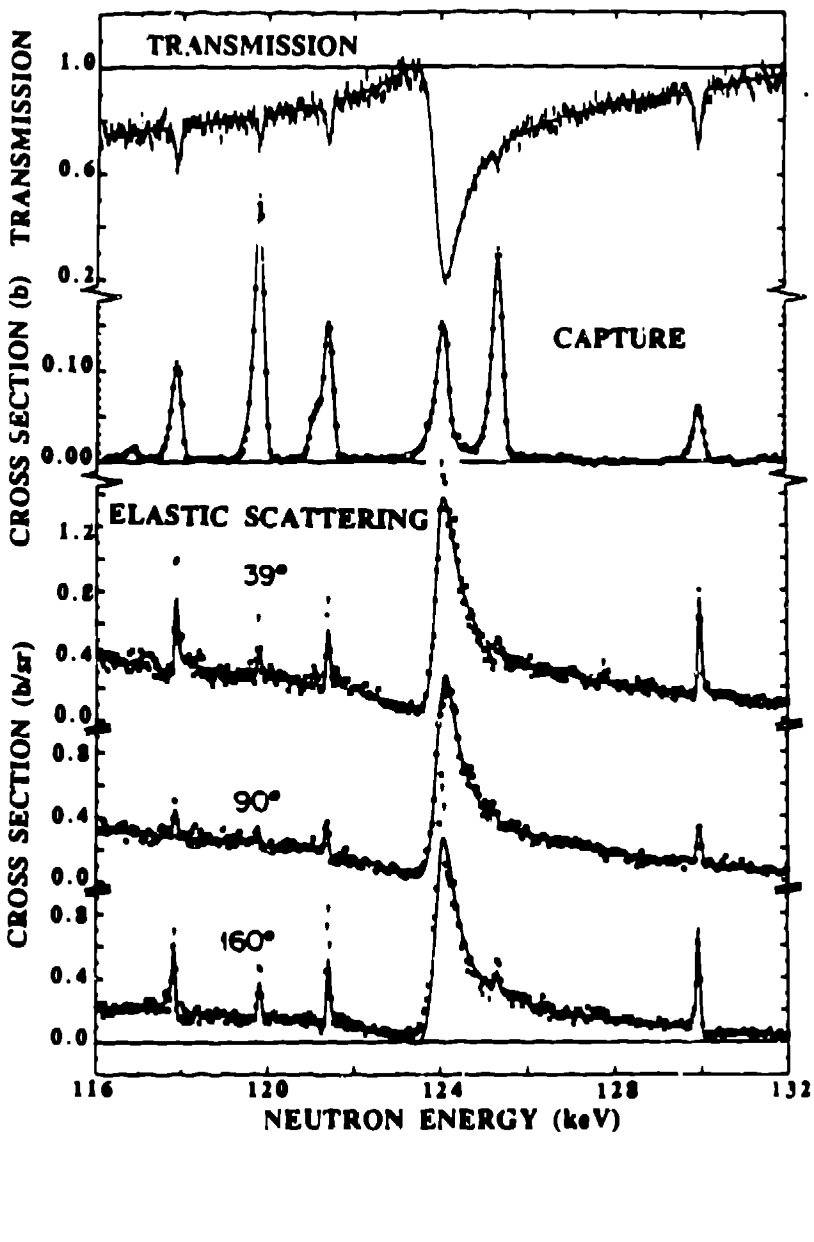

Fig. 3. Simultaneous multichannel Reich-Moore fits from 116 to 132 keV of n+^{58}Ni transmission, radiative capture, and differential elastic scattering data at three angles. The figure is provided courtesy of C. M. Perey.[16]

To illustrate the capability of modern theoretical analyses, a comparison is given in Fig. 4 (left side) of ^{60}Ni(n,n') cross section measurements and a calculated curve using Hauser-Feshbach statistical theory with corrections for width fluctuations and including preequilibrium and direct reaction contributions.[14] In the right side of Fig. 4 the ^{60}Ni(n,n') angular distribution for the first excited state of ^{60}Ni with 6.5-MeV incident neutrons that is *predicted* from the analysis is compared to experimental data.[12]

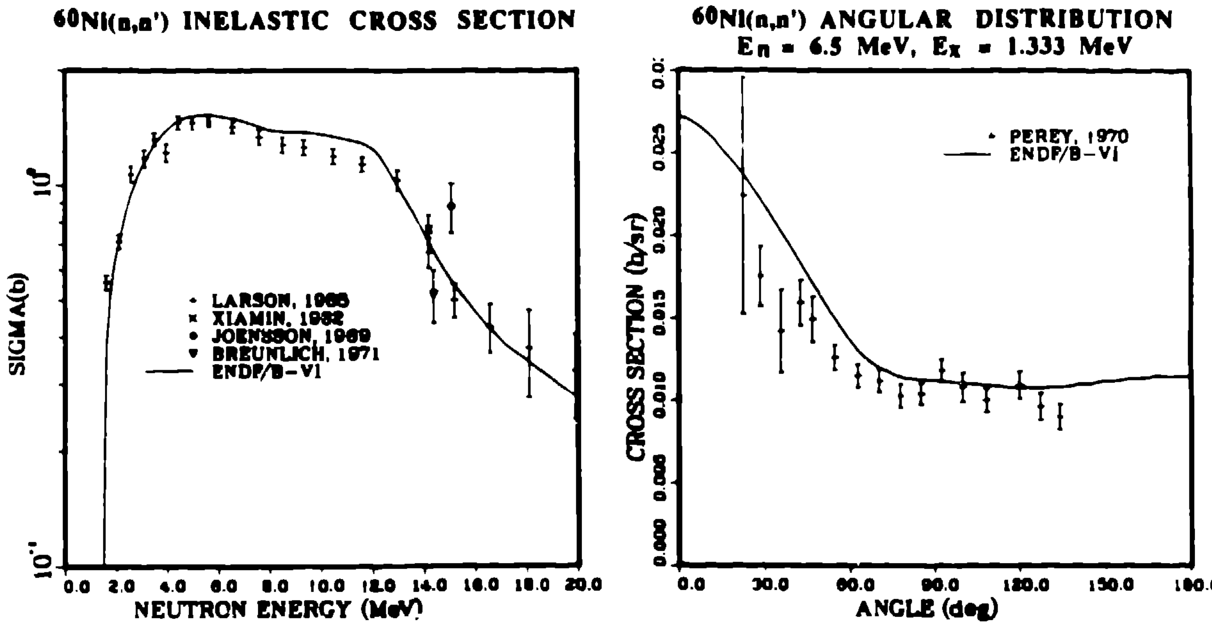

Fig. 4. Calculated and measured data for ^{60}Ni(n,n') reactions. The solid curves were calculated with the TNG code,[14] and the points represent experimental data.[12] The energy dependence of the ^{60}Ni total inelastic cross section is shown on the left side; the neutron angular distribution from the ^{60}Ni(n,n') reaction to the 1.333-MeV state in ^{60}Ni with 6.5 MeV incident neutrons is shown on the right side of the figure.

MAJOR ACTINIDES

New evaluations of resolved resonance parameters using the Reich-Moore multilevel formalism will be provided for ^{235}U, ^{238}U, ^{239}Pu, and ^{241}Pu. Each of these resonance evaluations covers a considerably larger energy range than does the current version of ENDF/B, and will thereby reduce difficulties and uncertainties in calculating self-shielding effects. It is expected that the ^{235}U evaluation will extend up to approximately 1-2 keV, ^{238}U to ~15 keV, and ^{239}Pu to 1 keV. Of these, only the ^{239}Pu and ^{241}Pu evaluations are complete, the products of French/ORNL collaborations. The ^{235}U and ^{238}U analyses are being carried out in ORNL/LANL and ORNL/ANL/Harwell collaborations, respectively.

An example of the results of such a multilevel Reich-Moore/SAMMY analysis for the ^{239}Pu(n,f) reaction is shown in Fig.5. Here the results of Derrien et al.,[20] which will be used for ENDF/B-VI, are compared to the measurements of Weston and Todd[21] and to the existing ENDF/B-V.2 evaluated data for neutron energies between 150 and 200 eV. Again, the availability of high resolution experimental data is crucial to such an analysis.

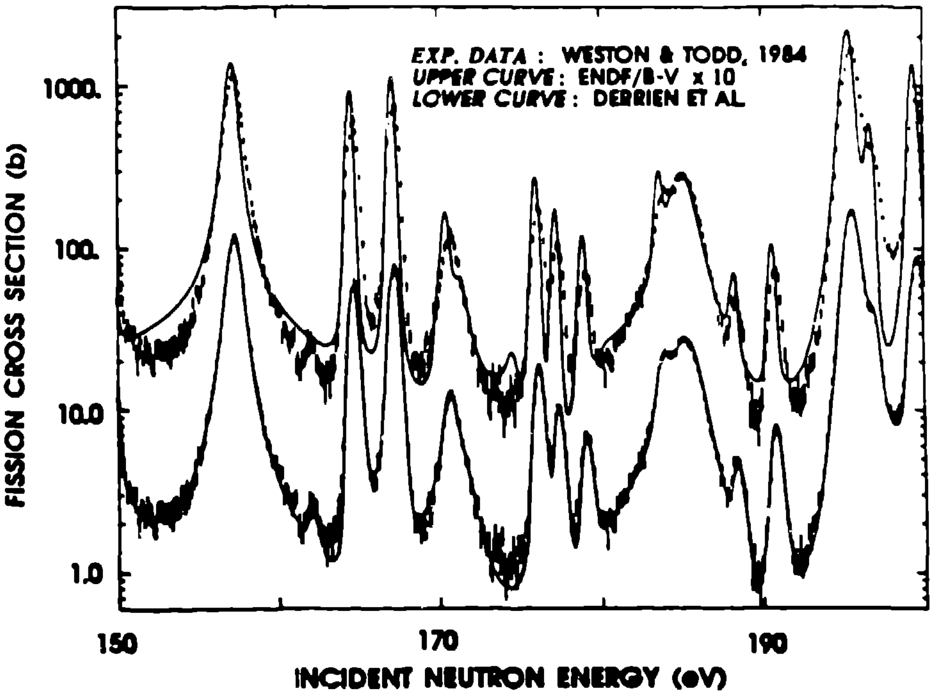

Fig. 5. Comparison of the $^{239}Pu(n,f)$ cross section between 150 and 200 eV from a multilevel Reich-Moore resonance analysis[20] with ENDF/B-V.2 and with experimental data.[21] The lower part of the figure shows the new analysis (curve) with the experimental data and the upper half compares ENDF/B-V.2 to the same data, both displaced by a factor of 10.

The simultaneous standards evaluation should provide significantly improved average (n,f) cross sections above E_n ~ 10 keV for $^{235,238}U$ and ^{239}Pu, and improved (n,γ) cross sections in the same range for ^{238}U. Additionally, it is expected that new or updated theoretical analyses of the elastic scattering, (n,n'), (n,2n), and (n,3n) reactions will be available for the major actinides, which should provide improved data for outgoing neutron cross sections, angular distributions, and emission spectra. A preliminary analysis of this nature for n+^{235}U reactions was reported for E_n = 0.01 to 20 MeV at the Mito Conference.[22] Although ENDF/B-VI will rely on the simultaneous standards results for the (n,f) cross section above E_n = 0.1 MeV, it is necessary that the theoretical analysis fit the fission cross section reasonably well in order to predict the neutronics data. Figure 6 shows a comparison of the $^{235}U(n,f)$ cross section calculated via the multibarrier fission model used in the analysis with both the ENDF/B-V.2 evaluation and with the results from the Version VI simultaneous standards analysis. The fitted theoretical curve generally agrees with the evaluated data to better than ±10%. In Fig. 7 the resulting theoretical calculations of $^{235}U(n,n)$ and (n,n') angular distributions at E_n=3.4 MeV are compared with experimental data[23] and with the existing ENDF/B-V.2 evaluation. At this energy the new calculations and data clearly show more forward peaking of the angular distributions and probably will result in a somewhat harder spectrum.

In addition to better elastic, inelastic, and (n,xn) data, ENDF/B-VI will also provide improved evaluations of $\bar{\nu}_p$ (prompt fission neutron multiplicity) and fission neutron spectra. One area where such improvement is needed is in $\bar{\nu}_p(E_n)$ for ^{239}Pu at neutron energies below 0.1 MeV. Figure 8 compares the measurements of Gwin et al.[24] (and older data)[12] with the ENDF/B-V.2 evaluation and with a new evaluation by Frehaut.[25] Current plans are to utilize the Frehaut evaluation below 100 keV for ENDF/B-VI, perhaps with some modifications.

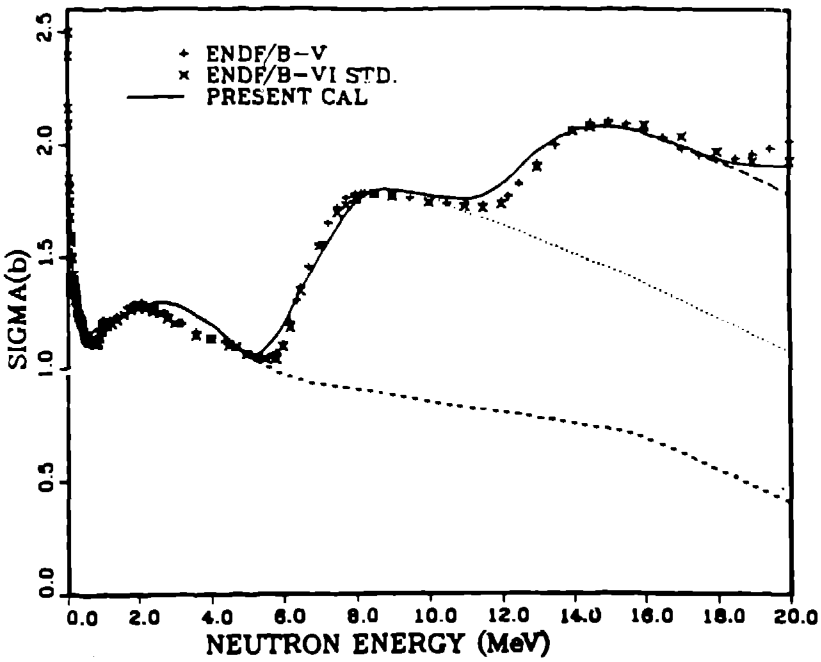

Fig. 6. Comparison of the calculated (n,f) cross sections from a new theoretical analysis of n+^{235}U reactions[22] (smooth curves) with results from the ENDF/B-VI simultaneous standards analysis and with ENDF/B-V.2. The dashed and dotted curves indicate the contributions from first, second-, and third-chance fission.

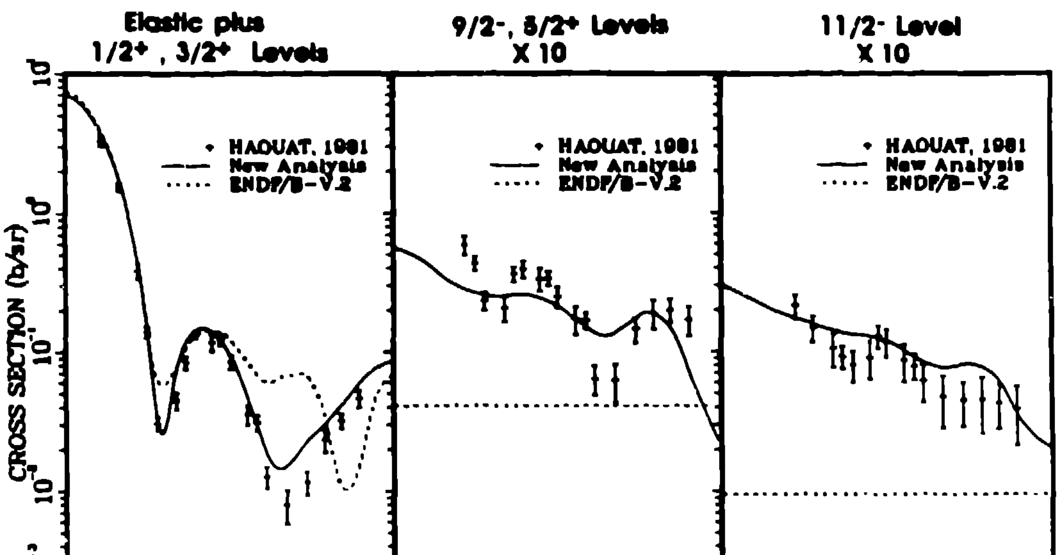

Fig. 7. Comparison of calculations[22] of ^{235}U(n,n) and (n,n') angular distributions (solid curves) with experimental data[23] and with the ENDF/B-V.2 evaluation (dashed curves) at $E_n = 3.4$ MeV. Because it was not possible to resolve all the ^{235}U states in the measurements, the calculated and evaluated angular distributions have been combined for unresolved states to match the experiment, as indicated.

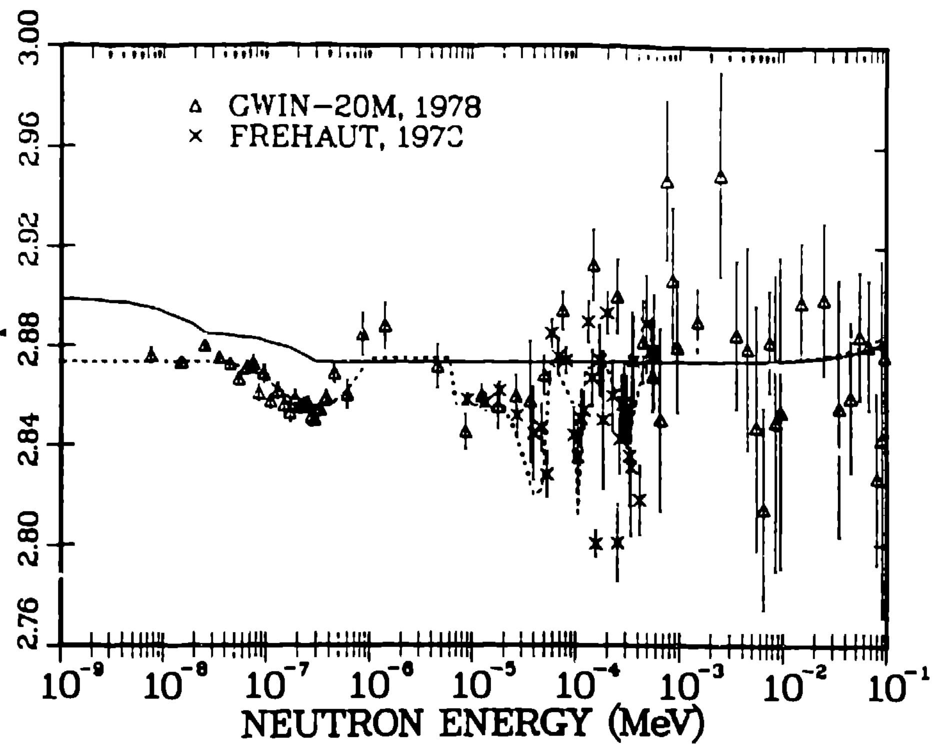

Fig. 8. The prompt fission neutron multiplicity ($\bar{\nu}_p$) of ^{239}Pu from 10^{-3} eV to 100 keV. The points are experimental data,[12,24] the solid curve is ENDF/B-V.2, and the dashed curve is an evaluation by Frehaut[25] that will be adapted for ENDF/B-VI.

Finally, it should be mentioned that the first actinide evaluation completed, fully documented[26], and approved in initial CSEWG data testing for Version VI is that for ^{240}Pu. The major neutron cross sections for ^{240}Pu in the ENDF/B-VI evaluation are given as functions of incident neutron energy in Fig. 9.

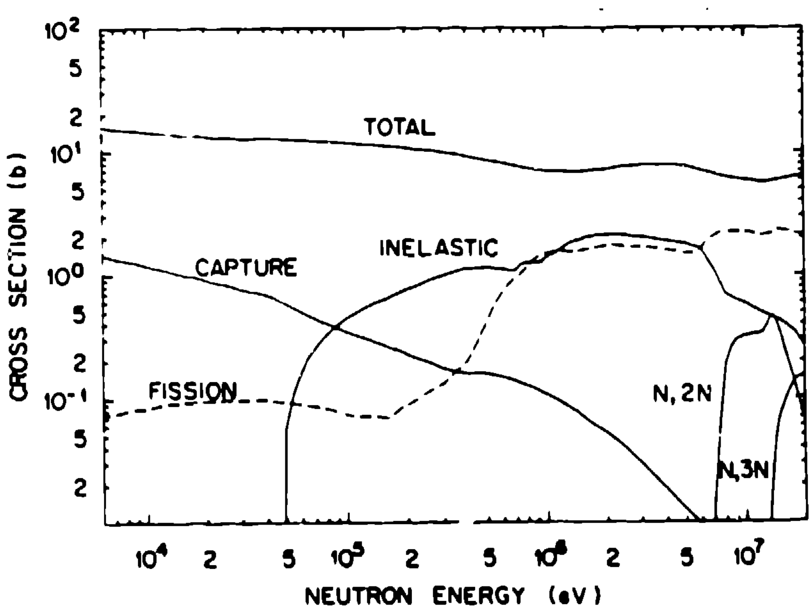

Fig. 9. Evaluated cross sections[26] for n+^{240}Pu reactions that will be used for ENDF/B-VI. This figure is provided courtesy of L. W. Weston, Oak Ridge National Laboratory.

YIELD, DECAY, AND DELAYED NEUTRON DATA

Substantial efforts are underway to improve the fission-product yield data files for Version VI of ENDF/B. New or updated evaluations of independent, cumulative, and mass chain yields with uncertainties will be given for 34 fissioning nuclides at one or more incident neutron energies, as summarized in Table II. Evaluated yields for spontaneously fissioning nuclides are also included, so that a total of 50 nuclide-energy combinations will be available, resulting in the formation of approximately 1100 different fission products. Some 10 additional yield evaluations are in progress and might be completed for the initial release of ENDF/B-VI. Recent reviews of the status of fission yield data and evaluations are given in Refs. 27 and 28.

TABLE II

Evaluated Yield Data Sets+ for ENDF/B-VI

Fissionable Nuclide		Fissionable Nuclide		Fissionable Nuclide		Fissionable Nuclide	
^{227}Th	(t)*	^{237}U	(f)	^{241}Am	(t,f,h)	^{250}Cf	(s)
^{229}Th	(t)	^{238}U	(s,f,h)	^{242m}Am	(t)	^{251}Cf	(t)
^{232}Th	(f,h)	^{237}Np	(f,h)	^{243}Am	(f)	^{252}Cf	(s)
^{231}Pa	(f)	^{238}Np	(f)	^{242}Cm	(f)	^{253}Es	(s)
^{232}U	(t)	^{238}Pu	(f)	^{244}Cm	(s)	^{254}Es	(t)
^{233}U	(t,f,h)	^{239}Pu	(t,f,h)	^{245}Cm	(t)	^{254}Fm	(s)
^{234}U	(f,h)	^{240}Pu	(f,h)	^{248}Cm	(s)	^{255}Fm	(t)
^{235}U	(t,f,h)	^{241}Pu	(t,f)	^{249}Cf	(t)	^{256}Fm	(s)
^{236}U	(f,h)	^{242}Pu	(f)				

+ In progress: ^{240}Pu (t), ^{242}Pu (t,h), ^{237}Np (t), ^{243}Cm (t,f), ^{244}Cm (f), ^{246}Cm (s,f), ^{248}Cm (f)

* s = spontaneous fission, t = thermal, f = fast, h = high (14 MeV)

The decay data (average decay energies, decay spectra and, to a lesser extent, cross sections) for many of the present ~900 fission product and 60 actinide nuclides in ENDF/B-V are being improved for Version VI. New experimental measurements are being factored into the evaluations, and nuclear model calculations are being used to supplement the experimental data base. The status of decay data for fission products, primarily those important for decay heat calculations, was recently reviewed.[29]

Delayed neutron data will be vastly improved for ENDF/B-VI as compared to ENDF/B-V. In particular, individual decay spectra and emission probabilities will be included for some 271 delayed neutron precursors. Additionally, temporal six-group data (total $\bar{\nu}_d$, group spectra, halflives, abundance) will be provided for most of the fissionable nuclides. A more detailed discussion of delayed neutron data is given in another paper at this conference.[30]

CONCLUDING REMARKS

As indicated in Table I, the time frame for completion of the various evaluations is Fall, 1988. A meeting is planned by CSEWG in December, 1988, to continue reviewing and testing the various evaluations for physics consistency, numerical errors, energy balance, and consistency with differential measurements. Such "differential" data testing will continue into the spring of 1989, when final testing of the major evaluations against integral data will begin. Concurrently, incorporation of the fission-product and decay data evaluations into the general cross section files will begin. It is hoped that the entire tested file will be available for issue in the late 1989 time frame with documentation to continue in 1990.

To conclude, significant new experimental data and improved theoretical analyses are being included in evaluations for ENDF/B-VI. For Version VI we have attempted to focus our attention on the most important data problems for applications, and the new information is expected to result in a significantly improved nuclear data base for fission reactor applications. At the same time, however, it should be recognized that there are a number of important omissions from the list in Table I of materials being updated. To cite specific examples, updates or new evaluations are not planned for N, O, Na, Al, Cl, K, Ti, Mo, Re, or Bi, and general updating of fission-product, actinide, dosimetry and activation cross sections is not possible for this first issue of ENDF/B-VI. In some cases significant deficiencies are known to exist in these data. It is hoped that these omissions will be corrected in a future issue of the file.

ACKNOWLEDGMENTS

I wish to thank C. Perey for providing me with advance copies of figures prior to publication of the ^{58}Ni multichannel resonance parameter analysis,[16] and T. England, D. Larson, and L. Weston for several useful discussions.

This work was performed under the auspices of the U. S. Department of Energy.

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