Working Party on International Nuclear Data Evaluation Cooperation, ENDF Project

Status of the ENDF Project

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Abstract

The new ENDF/B-VII.0 library was released in December 2006. The library contains 14 sublibraries, including the neutron sublibrary with 393 materials. The new library was extensively tested and shows considerable improvements over the earlier ENDDF/B-VI.8 library.

1. Introduction

Since October 2001, when ENDF/B-VI.8 was released, the CSEWG has been working on the new version of the library, ENDF/B-VII.0. A considerable attention was paid to the library performance and four preliminary versions were distributed for testing and validation in 2005-2006.

Table 1. Testing versions of the ENDF/B-VII.0 library

Version	Date	Comment
beta0	March 2005	1 sublibrary (neutron)
beta1	October 2005	11 sublibraries
beta2	April 2006	14 sublibraries
beta3	October 2006	Became VII.0 in December 2006

The new library, released in December 2006, is described in detail in the extensive paper ('Big Paper') on ENDF/B-VII.0 by Chadwick, Oblozinsky, Herman *et al*. in the special issue of Nuclear Data Sheets, **107** (2006) 2931.

2. ENDF/B-VII.0 Library

2.1 Highlights and contents

Highlights. The principal advances of the new library over the previous ENDF/B-VI.8 library are the following:

1. New cross sections for U, Pu, Th, Np and Am actinide isotopes, with improved performance in integral validation criticality and neutron transmission benchmarks,
2. More precise standard cross sections for neutron reactions on H, ^{6}Li, ^{10}B, Au and for ^{235,238}U fission (IAEA and WPEC SG6 collaboration),

3. Improved thermal neutron scattering,
4. Extensive set of neutron cross sections for fission products (WPEC SG23 collaboration),
5. Large suite of photonuclear reactions,
6. Extension of many neutron- and proton-induced evaluations up to 150 MeV,
7. Many new light nucleus neutron and proton reactions,
8. Post-fission beta-delayed photon decay spectra,
9. New radioactive decay data,
10. New methods for uncertainties and covariances, together with covariance evaluations for some sample cases, and
11. New actinide fission energy deposition

Contents. ENDF/B-VII.0 contains 14 sublibraries summarized in Table 2. Compared to ENDF/B-VI.8, the neutron sublibrary was considerably updated and extended. Two sublibraries (photonuclear, neutron cross section standards) can be considered as new. Major update and extension was made for the decay data sublibrary. For 6 other sublibraries quite considerable updates and extensions were made. The remaining 5 sublibraries (2 fission yields and 3 atomic data) were taken over from ENDF/B-VI.8.

Table 2. Contents of the ENDF/B-VII.0 library compared to ENDF/B-VI.8

No.	Sublibrary	Short name	Materials in VII.0	Materials in VI.8	Comment
1	Photonuclear reactions	g	**163**	-	**New sublibrary**
2	Photo-atomic	photo	**100**	100	Taken from VI.8
3	Radioactive decay	decay	**3838**	979	**New evaluations**
4	Spont. fission yields	s/fpy	**9**	9	Taken from VI.8
5	Atomic relaxation	ard	**100**	100	Taken from VI.8
6	Neutron reactions	n	**393**	328	**Many new evaluations**
7	Neutron fission yields	n/fpy	**31**	31	Taken from VI.8
8	Thermal scattering	tsl	**20**	15	**Some new evaluations**
9	Standards	std	**8**	8	**New evaluations**
10	Electro-atomic	e	**100**	100	Taken from VI.8
11	Proton reactions	p	**48**	35	**Some new evaluations**
12	Deuteron reactions	d	**5**	2	**Some new evaluations**
13	Triton reactions	t	**3**	1	**Some new evaluations**
14	He-3 reactions	he3	**2**	1	**Some new evaluations**

2.2 Neutron reaction sublibrary

The sublibrary contains 393 materials, majority of which was updated or newly evaluated. There are 390 isotopic evaluations, and 3 elemental evaluations (C, V and Zn). All evaluations except for ^{253}Es are complete, meaning that they cover all reaction channels needed for neutronics calculations.

Actinides. Actinide evaluations, representing the backbone of the new library, were evaluated mostly by LANL. In several instances new MF2 data were supplied by ORNL (RRR for ^{233,238}U and ^{241}Pu; URR for ^{233,235}U). New evaluations include the following materials:

- ^{235}U, ^{238}U, ^{239}Pu,
- ^{233}U, ^{232,234,236,237,239,240,241}U and ^{241}Pu, and
- ^{241,242,243}Am, ^{237}Np, and also ^{232}Th, ^{231,233} Pa from the IAEA CRP project

Delayed neutrons and photons. Delayed neutrons (MT=455) were taken over from ENDF/B-VI.8 with some modifications (^{235}U thermal nubar). Delayed photons for ^{239}Pu and ^{235}U were provided, for the first time, by LLNL.

Fission products. A full set of 219 materials in the fission products range (Z = 31 – 68) was taken from the WPEC SG23 library, representing a massive update of ENDF/B-VI.8. Altogether 72 materials were evaluated for ENDF/B-VII.0 by BNL and 2 materials by LLNL, using RRR and URR data derived from the Atlas of Neutron Resonances (2006) and fast neutron data based on the nuclear reaction model code EMPIRE-2.19.

High-energy extensions up to 150 MeV. The high-energy data from the Los Alamos LA150 library were recalculated and included to ENDF/B-VII.0 for both neutron and proton induced reactions for more than 40 materials.

Light nuclei. Several updates were done by LANL, for ^{1}H, ^{3}H and ^{9}Be. In addition, important modification was done for ^{16}O(n, α_0) cross sections that were reduced by 32% in the 2.4-8.9 MeV laboratory energy range.

Covariances. Sample cases for new covariance evaluations were produced, including 9 materials with MF=32, 33 data, and 4 other materials with MF=33 data in the entire energy range:

- ^{152,153,154,155,156,157,158,160}Gd with MF = 32, 33
- ^{232}Th with MF = 31, 32, 33 (supplied by the IAEA CRP project)
- ^{89}Y, ^{99}Tc, ^{191,193} Ir with MF=33.

2.3 Other sublibraries

Thermal neutron scattering sublibrary. The thermal neutron scattering sublibrary was extended and updated, it contains S(α, β) evaluations for 20 materials. LANL using recent results from IKE Stuttgart made notable improvements for H in H_2O and D in D_2O by IKE Stuttgart and LANL. Some improvements were also done for O in UO_2, U in UO_2, H in ZrH and several other materials.

Neutron cross-section standards sublibrary. Neutron cross-section standards are given in the Standards Sublibrary (NSUB=19). The data, produced by the WPEC-IAEA-CSEWG collaboration, are new evaluations, except for ^{3}He(n,p) and C(n,n). Full files, to be found in the neutron sublibrary, were adjusted to the new standards.

Photonuclear sublibrary. This is entirely new sublibrary containing 163 materials (isotopes only), mostly up to 150 MeV. The sublibrary was supplied by LANL, with new evaluations of actinides including nu-bars up to 20 MeV. The rest is largely based on the IAEA photonuclear project completed in 2000.

Charged-particle sublibraries. These sublibraries were extended and updated. The proton sublibrary contains data for 48 materials up to 150 MeV, while the other three sublibraries contain altogether 10 materials for fusion and nuclear astrophysics applications.

Decay data sublibrary. The radioactive decay sublibrary contains entirely new evaluations for 3838 materials, to be compared with 979 materials in ENDF/B-VI.8. New evaluations were performed by BNL using the latest information from the Evaluated Nuclear Structure Data File (ENSDF) and Nuclear Wallet Cards, with some additional adjustments.

Remaining sublibraries. Two sublibraries with fission yields (LANL) and three atomic data sublibraries (LLNL) were taken over from ENDF/B-VI.8 without any change.

3. Validation of ENDF/B-VII.0

Data verification consisted of checking of all 14 sublibraries, followed by processing of 7 sublibraries) and subsequent use of ACE files in simple test neutronics calculations of 4 sublibraries. The whole process included checking by CHECKR-7.03, FIZCON-7.04 and PSYCHE-7.02; processing by NJOY-99.161; Monte Carlo neutronics test calculations by MCNP5 and MCNPX; and processing of new covariances by ERRORJ or PUFF.

Extensive validation, using radiation transport codes to simulate measured critical assemblies, show major improvements in ENDF/B-VII.0. These are:

1. The long-standing under-prediction of low enriched uranium (LEU) thermal assemblies is removed,
2. The ^{238}U and ^{208}Pb reflector biases in fast systems are largely removed,
3. ENDF/B-VI.8 good agreement for simulations of thermal high-enriched uranium assemblies is preserved,
4. The under-prediction of fast criticality of ^{233,235}U and ^{239}Pu assemblies is removed
5. The intermediate spectrum critical assemblies are predicted more accurately.

3.1 Testing before release

Validation of neutron data against integral benchmark experiments was done using mostly continuous energy Monte Carlo transport calculations and benchmarks from the ICSBEP Handbook for nuclear criticality safety. Other validation work included delayed neutron testing, reaction rates in critical assemblies, shielding and pulsed-sphere testing, as well as comparison of thermal cross sections and capture resonance integrals with the recently published Atlas of Neutron Resonances.

C/E values for keff were calculated for hundreds of criticality benchmarks using the MCNP code, version 4c3 or 5. An example for fast U and Pu benchmarks given in Fig.1 illustrates an excellent performance and considerable improvement over the earlier ENDF/B-VI.8.

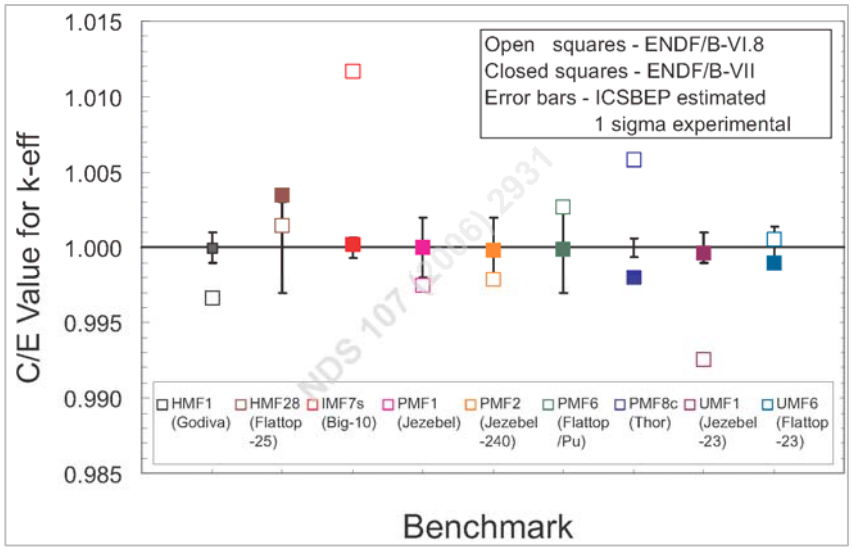

Fig.1. Fast benchmarks: C/E values of keff for HEU, Pu and ^{233}U.

Steven van der Marck [2] analyzed 730 benchmarks. His results, summarized in Table 3, show considerable improvement in low-enriched uranium (LEU) systems. IEU benchmarks as well as Pu and HEU fast ones are modeled more accurately. Low energy PU systems were modeled poorly for ENDF/B-VI.8 and continue so in ENDF/B-VII.0.

Table 3. The average values of C/E keff -1 in pcm for ENDF/B-VII.0, given in italics are the corresponding values for ENDF/B-VI.8.

	COMP				MET				SOL
	ther	inter	fast	mix	ther	inter	fast	mix	ther
LEU	17 *-452*				-41 *-270*				123 *107*
IEU	103 *-299*	219 *-238*					182 *712*		
HEU		1744 *1442*		104 *-273*	-51 *-411*	88 *-42*	147 *186*	812 *462*	108 *142*
MIX	428 *377*		110 *978*				193 *69*		-254 *-257*
PU		1110 *967*				4565 *4654*	229 *375*	936 *745*	620 *531*
^{233}U	146 *-380*						-364* *-338*		66 *-292*

*) This becomes -64 pcm versus *-254 pcm* if we restrict ourselves to the well understood UMF-001 and UMF-006 assemblies.

Only limited validation with multi-group deterministic codes was done by the time of the ENDF/B-VII.0 release.

3.2 Testing after release

Since the release in December 2006, more validation results are available, including those reported by MacFarlane and Kahler (LANL), by Mosteller (LANL), Huria (Westinghouse), Brown (LLNL) and Sublet (CEA Cadarache).

For example, MacFarlane and Kahler extended their keff suite to about 700 benchmarks, calculated with much better statistics than van der Marck, and in general supporting his findings. Mosteller concluded that ENDF/B-VII.0 produces significantly better overall results for the cases in the MCNP Criticality Validation Suite than do ENDF/B-VI.8, JENDL-3.3, or JEFF-3.1, but pointed out that the fast cross sections for Be and Th be reviewed before the next version of ENDF/B-VII is issued.

4. Future Work

The new ENDF/B-VII.0 library has been released in December 2006. The testing performed so far indicates that the library has superior performance, although much more testing needs to be done and some deficiencies have already been identified.

The following issues should be resolved in future:

- Plutonium thermal solution benchmarks are modeled poorly,
- Inelastic scattering for ^{235}U and ^{239}Pu should be improved,
- ^{235}U capture in the 30 keV – 1 MeV region is about 10% lower than JENDL-3.3 and this should be resolved,
- Contradictory trends were observed in the benchmarks involving ^{233}U and Zr and this should be resolved,
- Considerable reduction of thermal capture for ^{157}Gd suggested by the recent measurement should be resolved,
- Neutron scattering angular distribution on D in the energy range 1-3 MeV should be addressed,
- Reflected assemblies indicate deficiencies in scattering cross sections of Pb, Be.

References

1. M.B. Chadwick, P. Oblozinsky, M. Herman, N.M. Greene, R.D. McKnight, D.L.Smith, P.G. Young, R.E. MacFarlane, G.M. Hale, S.C. Frankle, A.C. Kahler, T. Kawano, R.C. Little, D.G. Madland, P. Moller, R.D. Mosteller, P.R. Page, P. Talou, H. Trellue, M.C. White, W.B. Wilson, R. Arcilla, C.L. Dunford, S.F. Mughabghab, B. Pritychenko, D. Rochman, A.A. Sonzogni, C.R. Lubitz, T.H. Trumbull, J.P. Weinman, D.A. Brown, D.E. Cullen, D.P. Heinrichs, D.P. McNabb, H. Derrien, M.E. Dunn, N.M. Larson, L.C. Leal, A.D. Carlson, R.C. Block, J.B. Briggs, E.T. Cheng, H.C. Huria, M.L. Zerkle, K.S. Kozier, A. Courcelle, V.Pronyaev and S.C. van der Marck, *"ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology"*, Nuclear Data Sheets, vol. **107**, pp. 2931-3060, 2006
2. Steven C. van der Marck, *"Benchmarking ENDF/B-VII.0"*, Nuclear Data Sheets, vol. **107**, pp. 3061-3117, 2006