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Evaluation of Neutron Induced Reactions for 32 Fission Products

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New ENDF/B-VII.0 Library

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Abstract. We describe the new version of the Evaluated Nuclear Data File, ENDF/B-VII.0, of recommended nuclear data for advanced nuclear science and technology applications. The library, produced by the U.S. Cross Section Evaluation Working Group, was released in December 2006. The library contains data in 14 sublibraries, primarily for reactions with incident neutrons, protons and photons, based on the experimental data and nuclear reaction theory predictions. The neutron reaction sublibrary contains data for 393 materials. The new library was extensively tested and shows considerable improvements over the earlier ENDF/B-VI.8 library.

1 Introduction

The new ENDF/B-VII.0 library has been developed by the U.S. Cross Section Evaluation Working Group (CSEWG) over the period 2002-2006. Its release represents the first major revision of ENDF/B after the initial release of the previous ENDF/B-VI library in 1990 (its last upgrade, ENDF/B-VI.8, occurred in October 2001).

The new library, released in December 2006, is described in detail in the extensive “big paper” on ENDF/B-VII.0 by Chadwick *et al.* [1] that appeared in the special issue of Nuclear Data Sheets. The dedicated paper by van der Marck on ENDF/B-VII.0 benchmarking can be found in the same issue [2]. The purpose of the present paper is to give a short overview on ENDF/B-VII.0 to this conference.

2 ENDF/B-VII.0 library

We start with a brief description of the new library, first summarizing its highlights and then its contents.

2.1 Highlights

The principal advances of the ENDF/B-VII.0 library over the previous ENDF/B-VI.8 are the following:

- 1) New cross sections for U, Pu, Th, Np and Am actinide isotopes with improved validation criticality and neutron transmission benchmark tests;
- 2) New standard cross sections for neutron reactions;
- 3) Improved thermal neutron scattering;
- 4) Extensive set of new neutron cross sections for fission products;
- 5) Large suite of photonuclear reactions;
- 6) Extension of many neutron- and proton- induced reactions 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 along with several sample covariance evaluations;
- 11) New actinide fission energy deposition.

Extensive validation, using transport codes to simulate measured critical assemblies, show the following major improvements: 1) Long-standing underprediction of low-enriched uranium thermal assemblies was removed; 2) ²³⁸U, ²⁰⁸Pb and ⁹Be reflector biases in fast systems are largely removed; 3) ENDF/B-VI.8 good agreement for simulation of high-enriched uranium assemblies is preserved; 4) Under prediction of fast criticality of ^{233,235}U and ²³⁹Pu assemblies is removed; and 5) Intermediate spectrum critical assemblies are predicted more accurately.

2.2 Contents

The ENDF/B-VII.0 library contains 14 sublibraries that are summarized in table 1. Although the ENDF/B library is widely known for evaluated neutron cross sections, it can be seen that it contains a considerable amount of non-neutron data. Brief description of each sublibrary is given below.

Table 1. Contents of the ENDF/B-VII.0 library, with ENDF/B-VI.8 shown for comparison. NSUB stands for the sublibrary number in the ENDF-6 format. Given in the last two columns are the number of materials (isotopes or elements).

| No. | NSUB | Sublibrary name | Short name | VII.0 | VI.8 |
|-----|-------|--------------------|------------|-------|------|
| 1 | 0 | Photonuclear | g | 163 | - |
| 2 | 3 | Photo-atomic | photo | 100 | 100 |
| 3 | 4 | Radioactive decay | decay | 3838 | 979 |
| 4 | 5 | Spont. fis. yields | s/fpy | 9 | 9 |
| 5 | 6 | Atomic relaxation | ard | 100 | 100 |
| 6 | 10 | Neutron | n | 393 | 328 |
| 7 | 11 | Neutron fis.yields | n/fpy | 31 | 31 |
| 8 | 12 | Thermal scattering | tsl | 20 | 15 |
| 9 | 19 | Standards | std | 8 | 8 |
| 10 | 113 | Electro-atomic | e | 100 | 100 |
| 11 | 10010 | Proton | p | 48 | 35 |
| 12 | 10020 | Deuteron | d | 5 | 2 |
| 13 | 10030 | Triton | t | 3 | 1 |
| 14 | 20030 | ³ He | he3 | 2 | 1 |

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1. The photonuclear sublibrary is new. It contains data for 163 materials (all isotopes), mostly up to 140 MeV. The sublibrary was supplied by LANL and it is largely based on the earlier IAEA photonuclear project. There are new LANL evaluations for actinides including nubar up to 20 MeV.
2. The photo-atomic sublibrary contains data for photons interacting with atoms for 100 materials (all elemental). It was taken over from ENDF/B-VI.8. These data along with the atomic relaxation and electro-atomic data were supplied by LLNL.
3. The decay data sublibrary was completely re-evaluated by BNL. It contains 3838 materials, to be compared with 979 materials in ENDF/B-VI.8. The new evaluations are based on the latest information from the Evaluated Nuclear Structure Data File (ENSDF) and Nuclear Wallet Cards, with some additional adjustments.
4. The spontaneous fission yields, produced by LANL, were taken over from the ENDF/B-VI.8 library.
5. The atomic relaxation data (LLNL) were from over from the ENDF/B-VI.8 library.
6. The neutron reaction sublibrary represents the heart of ENDF/B-VII.0. The sublibrary was considerably updated and extended. It contains 393 materials, including 390 isotopic and 3 elemental (C, V, and Zn) evaluations. Important improvements in actinides were made by LANL, in several key instances in collaboration with ORNL. Evaluations in the fission product range (219 materials) were entirely changed, with 74 new evaluations made largely by BNL. The new covariance evaluations were performed for 13 materials.
7. Neutron fission yields, produced by LANL, were taken over from the ENDF/B-VI.8 library.
8. The thermal neutron scattering sublibrary was extended and updated, it contains $S(\alpha, \beta)$ evaluations for 20 materials out of which 7 were reevaluated or updated by LANL. Notable improvements were made for H in H_2O , D in D_2O , and also for O in UO_2 , U in UO_2 and H in ZrH.
9. The neutron cross section standards sublibrary is new. It is the outcome of the collaboration with the IAEA and WPEC [3].
10. The electro-atomic data (LLNL) are from ENDF/B-VI.8.
11. The proton reaction sublibrary, supplied by LANL, was extended and updated, with data mostly up to 150 MeV.
12. - 14. The deuteron, triton and 3He reactions for altogether 10 materials, important for nuclear astrophysics, were supplied by LANL.

3 Neutron reaction sublibrary

In the following we will discuss in more detail the neutron reaction sublibrary that represents the most important part of the new library.

3.1 Actinides

Considerable attention was given to improvements of actinide evaluations. Newly evaluated, updated and improved were

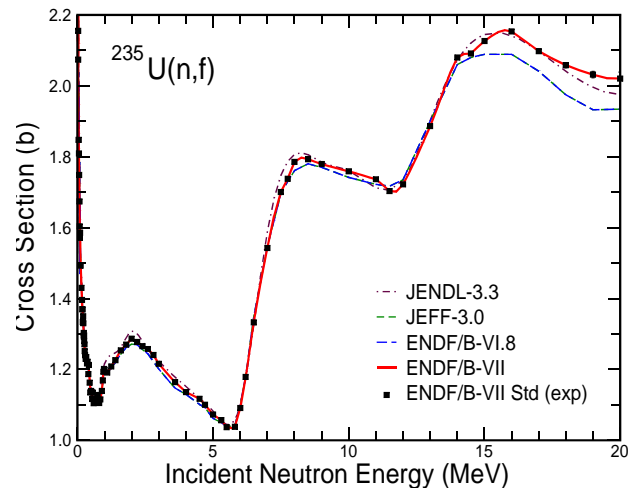


Fig. 1. Evaluated fission cross sections for ^{235}U compared with measured data represented by the ENDF/B-VII Standards. Other evaluations from JEFF and JENDL are also shown.

three major actinides $^{235,238}U$ and ^{239}Pu ; other uranium isotopes, ^{233}U , $^{232,234,236,237,240,241}U$ and ^{241}Pu ; several americium isotopes, $^{241,242g,242m,243}Am$; ^{237}Np . In addition, new ^{232}Th and $^{231,235}Pa$ evaluations, produced by the IAEA project, were adopted.

In view of the limited scope of the present paper we restrict ourselves to a few observations and several illustrative examples. We refer the reader to ref. [1] where many more details can be found.

The new ^{235}U evaluation builds upon the previous ENDF/B-VI.8 file with many improvements from Los Alamos in the fast neutron region. These improvements include the new fission standards cross sections, improved nubar values, new (n,2n) and (n,3) data, new prompt fission spectra as well as improved modeling of inelastic scattering. The resulting fission cross sections are shown in fig. 1.

In the unresolved resonance region, improved evaluation for ^{235}U was done by ORNL at the 2.25 keV - 25.0 keV energy range. This built on their earlier ENDF/B-VI.8 evaluation in the resolved resonance region using the multilevel R-matrix analysis by the SAMMY code. The capture cross sections are shown in fig. 2. We note that in the 30 keV - 1 MeV region our evaluation is lower by 10% than the JENDL-3.3 evaluation. In the resolved resonance region the ENDF/B-VI.8 evaluation was adopted.

Major modifications were made to the ^{238}U evaluation, in both the resonance region and in the fast neutron region. We note that thanks to the extensive effort that included WPEC Subgroup 22 [4] the long-standing underprediction of low-enriched uranium thermal assemblies was removed.

Of considerable importance was improved description of fast neutron emission based upon new data and improved modeling. This had impact on both the inelastic scattering where the underprediction below the elastic scattering was removed, as well as on the (n,2n) cross sections. Shown in fig. 3 are (n,2n) cross sections on ^{239}Pu that illustrate quite dramatic change compared to earlier evaluations.

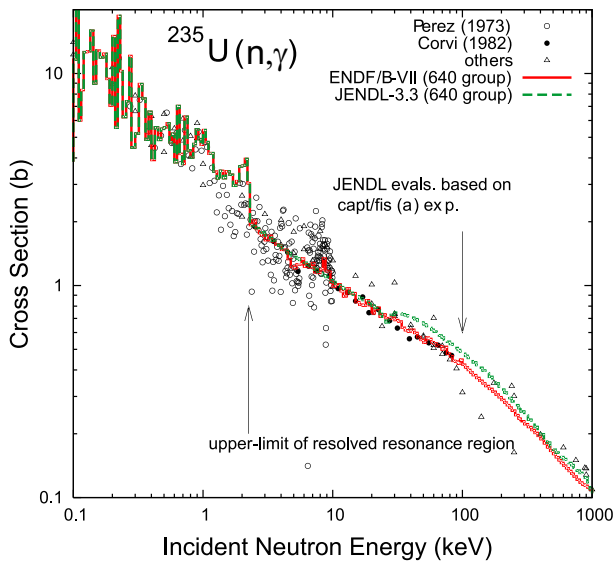


Fig. 2. Evaluated fission cross sections for ^{235}U , including the energy range 2.25 keV - 25.0 keV, compared with the measured data and the JENDL-3.3 evaluation.

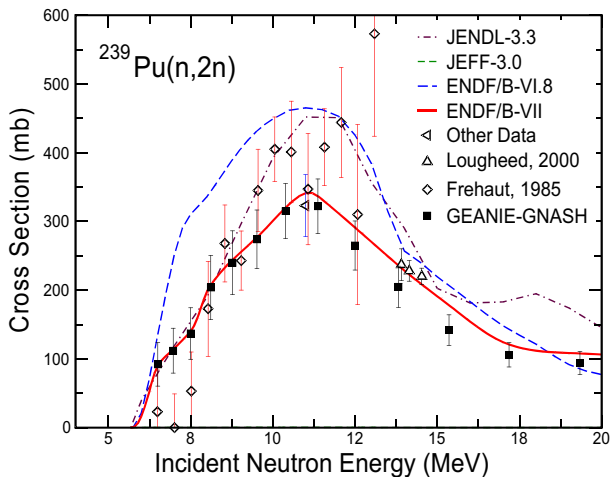


Fig. 3. Evaluated $^{239}\text{Pu}(n,2n)$ compared with measured data and previous evaluations.

Another considerable improvements were made to ^{233}U evaluation. It is true for both the fission and capture cross sections. This is illustrated in fig. 4 that compares evaluated capture cross sections with data and previous evaluations.

Data on americium are especially important for applications involving transmutation and advanced reactors with high minor actinide burn up. As an example of new evaluation by LANL we show in fig. 5 branching ratios for $^{241}\text{Am}(n,\gamma)$ reaction.

The ENDF/B-VII.0 library includes new information for the energy released in fission for the major actinides, $^{235,238}\text{U}$ and ^{239}Pu . This is based on the recent work by Madland [5] that was implemented into the recent version of the processing code NJOY. The results, summarized in table 2, show important improvements.

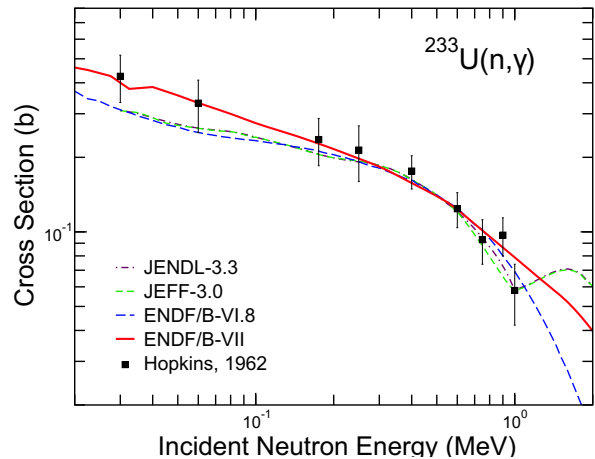


Fig. 4. Evaluated $^{233}\text{U}(n,\gamma)$ cross sections compared with experimental data and with previous evaluations.

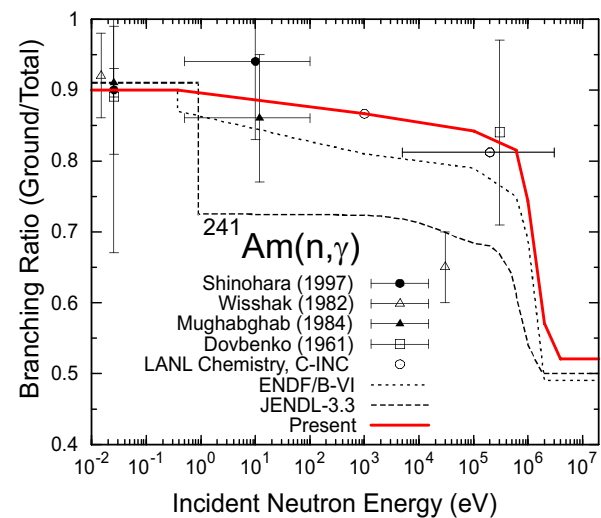


Fig. 5. $^{241}\text{Am}(n,\gamma)$ branching ratios for $^{242g}\text{Am}/^{242g+m}\text{Am}$ compared with experimental data and previous evaluations.

3.2 Fission products

A massive improvement was undertaken in the range of fission products, $Z = 31 - 68$. The new International Fission Product Library, produced by the collaborative effort of the NEA WPEC Subgroup 23, contains 219 evaluations judged to be the best from all available evaluations. This set includes 74 new complete evaluations plus 74 evaluations in the resonance region developed for ENDF/B-VII.0. This new fission product library was fully adopted by ENDF/B-VII.0. As an example of the new ENDF/B-VII.0 evaluation in fig. 6 we show capture cross sections for a full set of 8 isotopes of neodymium, produced by the BNL-KAERI collaboration.

3.3 Covariances

New methods were developed to evaluate uncertainties and covariances for neutron cross sections. These methods include

Table 2. Prompt fission Q-values in MeV obtained with ENDF/B-VII.0 data. To get total energy deposition, add the incident energy to total Q-values tabulated here.

| Nuclide | Incident energy e_n | ENDF/B VII.0 | Madland ref. [5] | NJOY old | NJOY new |
|-------------------|-----------------------|--------------|------------------|----------|----------|
| ^{235}U | 0.0253 eV | 180.65 | 180.57 | 180.65 | 180.65 |
| | 1.0 MeV | 180.19 | 179.68 | 179.84 | 180.19 |
| | 14.0 MeV | 169.07 | 168.14 | 164.24 | 169.14 |
| ^{238}U | 0.0253 eV | 181.28 | 181.04 | 181.30 | 181.30 |
| | 1.0 MeV | 181.02 | 180.15 | 180.68 | 181.03 |
| | 14.0 MeV | 169.59 | 169.37 | 164.86 | 169.76 |
| ^{239}Pu | 0.0253 eV | 188.38 | 188.42 | 189.37 | 188.37 |
| | 1.0 MeV | 187.58 | 187.42 | 187.24 | 187.59 |
| | 14.0 MeV | 175.98 | 174.12 | 171.10 | 176.00 |

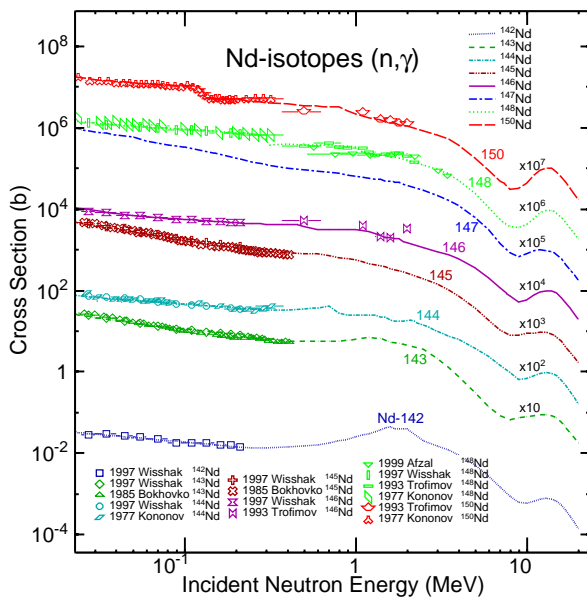


Fig. 6. Neutron capture cross sections for Nd isotopes. The neighboring curves and data are scaled by factors indicated in the legend. Good fit to the available data endorses our prediction of cross sections for the radioactive ^{147}Nd .

the retroactive SAMMY method in the resolved resonance region as well as the methods by BNL-LANL utilizing the information in the new Atlas of Neutron Resonances [6] and the nuclear reaction model code EMPIRE, coupled with the Bayesian code KALMAN. Altogether 12 new covariance evaluations were included to ENDF/B-VII.0. The most prominent among them is a complete set of covariance evaluations for 8 isotopes of Gd. As an example, in fig. 7 we show relative uncertainties for energies above 1 keV for the total, elastic scattering and capture cross sections on ^{157}Gd . The minima for total and elastic scattering at high energies stem from the optical model. For the capture cross sections the uncertainties are fairly small at energies below 1 MeV and they increase substantially at higher energies.

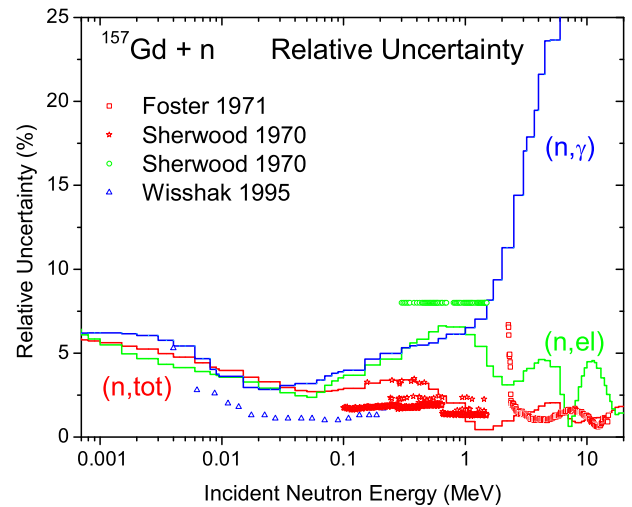


Fig. 7. Relative uncertainties in the unresolved resonance and fast neutron region for the total, elastic scattering and capture cross sections on ^{157}Gd . The capture data do not include the uncertainty from the normalization to Au standards.

4 Other sublibraries

In this section we highlight improvements achieved in several other ENDF/B-VII.0 sublibraries.

4.1 Thermal neutron scattering

The thermal neutron scattering sublibrary is important for applications where thermal neutrons play a role. It contains 20 evaluations out of which 7 were added, reevaluated or updated due to the combined effort of MacFarlane, Los Alamos and Mattes and Keinert, IKE Stuttgart. The remaining evaluations were taken over from the ENDF/B-VI.8 library.

4.2 Neutron cross section standards

The neutron cross section standards sublibrary is new. Out of 8 standards materials (9 reactions, see table 3), six materials were newly evaluated, while the $^3\text{He}(n,p)$ and $^{nat}\text{C}(n,n)$ standards were taken from ENDF/B-VI.8. These new evaluations come from the international collaboration coordinated by the IAEA Nuclear data Section and NEA WPEC Subgroup 7, the US effort was led by NIST and LANL. For more details see Carlson *et al.* [3].

The new standards cross sections were completely adopted by the neutron reaction sublibrary except for the thermal cross section for $^{235}\text{U}(n,f)$ where a slight difference occurs to satisfy thermal data testing.

4.3 Photonuclear reactions

The photonuclear sublibrary is new, with data for 163 materials, largely taken from the IAEA photonuclear project

Table 3. List of neutron cross section standards and their energy ranges.

| Reaction | Energy range |
|-------------------------------------|-------------------------------|
| H(n,n) | 1 keV to 200 MeV |
| ³ He(n,p) | 0.0253 eV to 50 keV |
| ⁶ Li(n,t) | 0.0253 eV to 1 MeV |
| ¹⁰ B(n,α) | 0.0253 eV to 1 MeV |
| ¹⁰ B(n,α ₁ γ) | 0.0253 eV to 1 MeV |
| C(n,n) | 0.0253 eV to 1.8 MeV |
| Au(n,γ) | 0.0253 eV, 0.2 MeV to 2.5 MeV |
| ²³⁵ U(n,f) | 0.0253 eV, 0.15 to 200 MeV |
| ²³⁸ U(n,f) | 2 MeV to 200 MeV |

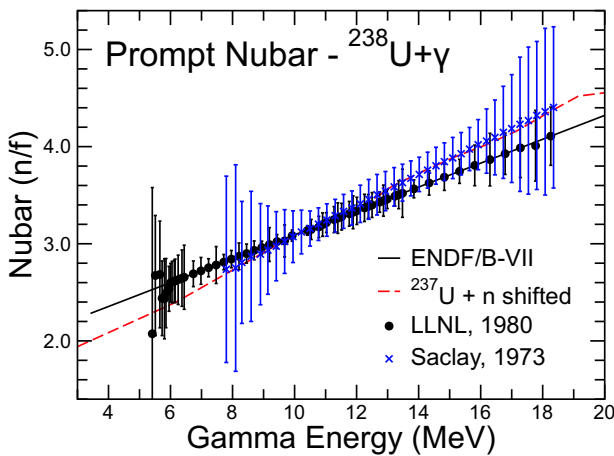


Fig. 8. Prompt nubar for photons incident on ²³⁸U compared to the Livermore experimental data and to the nubar for ²³⁷U+n shifted by the neutron separation energy.

completed in 2000. LANL made important improvements and reevaluated all actinide cross sections, including photofission nubar. The evaluations for the prompt fission neutron multiplicities (nubar) were based on the measured data from Livermore. As an example, in fig. 8 we show prompt nubar for photons incident on ²³⁸U compared with these data. We also show the results that would be obtained if one took the ENDF neutron evaluation for the A-1 system, ²³⁷U+n, shifted by the neutron separation energy.

5 Validation

Testing of the new ENDF/B-VII.0 library consisted of phase 1 data verification step that included checking by the ENDF checking codes to ensure compliance with formats and physics, followed by processing with NJOY-99.161 and simple test runs with the MCNP code. This ensured that the files can be used in the neutronics calculations. The second step included validation against integral benchmark experiments.

5.1 Criticality testing

Integral data testing of the ENDF/B-VII.0 cross sections plays an essential role for validation purposes. We note that the

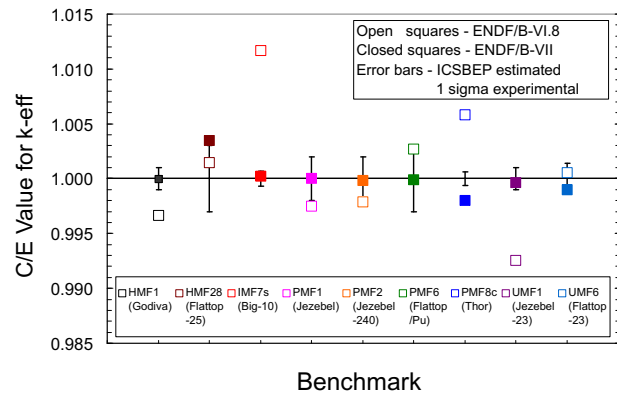


Fig. 9. C/E values for k_{eff} for fast U and Pu benchmarks. Shown by closed squares are ENDF/B-VII.0 results, open squares show ENDF/B-VI.8.

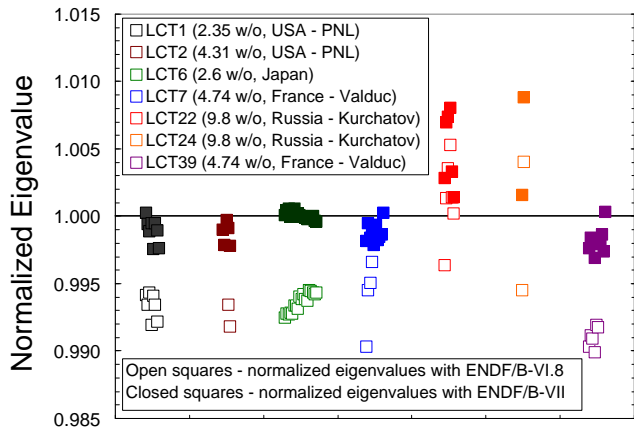


Fig. 10. C/E values for k_{eff} for low-enriched U benchmarks, showing considerable improvements except for LCT22 and 24 (Russia).

validation of the ENDF/B-VII.0 files included some first-ever features, such as almost total reliance on continuous-energy Monte Carlo methods. This was coupled heavily to the ICSBEP handbook [7] of integral data for criticality safety.

C/E values for k_{eff} (also known as normalized eigenvalues) were calculated for hundreds of critical benchmarks using the MCNP code, version 4c3 or 5. Fast neutron U and Pu benchmarks were examined carefully and the results, shown in fig. 9, demonstrate an excellent performance.

The improvements to the ²³⁸U cross section data in ENDF/B-VII.0 have led to major upgrade in our ability to accurately calculate thermal low-enriched uranium C/E values for k_{eff} . The summary is shown in fig. 10 where considerable improvements can be seen for most of LCT benchmarks.

S. van der Marck, NRG Petten, performed extensive independent criticality data testing for ENDF/B-VII.0 [2]. He used impressive amount of 730 benchmarks criticality experiments from the ICSBEP Handbook. Table 4 summarizes his results in terms of average values for different benchmark cate-

Table 4. The average value of $C/E k_{\text{eff}} - 1$ in pcm (100 pcm = 0.1%) for ENDF/B-VII.0 per main ICSBEP benchmark category. Shown in *italics* are the values for the ENDF/B-VI.8 library.

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

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

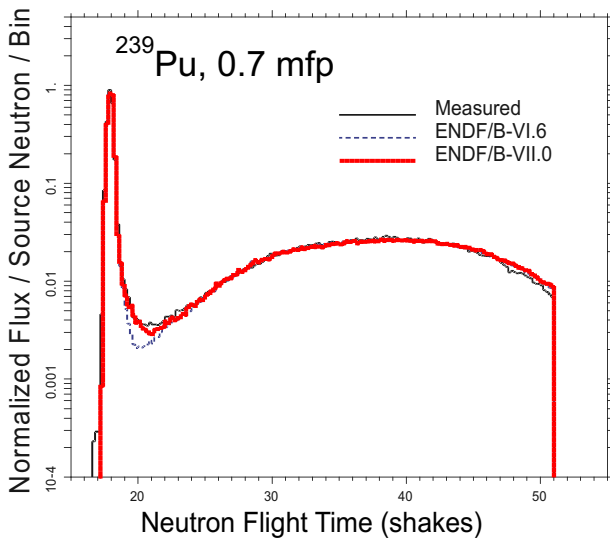


Fig. 11. Comparison of the simulated results using ENDF/B-VII.0 and ENDF/B-VI.6 data for the 0.7 mfp sphere of ²³⁹Pu in the units of shakes (shake = 10⁻⁸ sec). The improvement in the neutron scattering energy close to the elastic peak is clearly visible.

gories. One can see that the low-enriched U (LEU) compound benchmarks, the intermediate-enriched U (IEU) as well as the high-enriched U (HEU) fast benchmarks are modeled more accurately. This is also true for ²³³U thermal benchmarks. Lower energy Pu (PU) benchmarks are modeled poorly in ENDF/B-VI.8 and continue to be modeled poorly also in the new library.

5.2 Other data testing

Improved modeling of inelastic neutron scattering already discussed above can be demonstrated on improved modeling of fast pulsed benchmarks measured by LLNL. This is shown in fig. 11 that provides important confirmation of the better agreement with microscopic data.

Important quantities at low neutron energies are thermal capture cross sections and capture resonance integrals

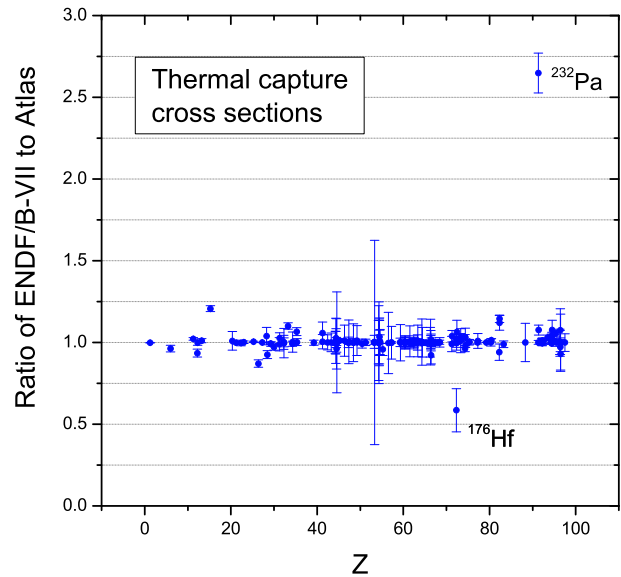


Fig. 12. Thermal neutron capture cross sections in ENDF/B-VII.0 compared to the Atlas of Neutron Resonances [6].

that were compared with the recent Atlas of Neutron Resonances [6]. Ratios of thermal capture cross sections shown in fig. 12 demonstrate good overall agreement.

6 Conclusions

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 results reported in this paper represent an outcome of a considerable multi-year effort of many scientists organized in the U.S. Cross Section Evaluation Working Group. We acknowledge several important contributions from the international activities by the NEA WPEC, the IAEA as well as numerous scientists across the world.

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