

## **Status of the ENDF Project**

**Report to the WPEC Meeting, Port Jefferson, NY, June 25-26, 2009**

Michal Herman for CSEWG  
National Nuclear Data Center, BNL, Upton, NY 11973

### **Abstract**

Since the release of the ENDF/B-VII.0 library in December 2006, the work focused on the validation, identifying deficiencies and preparing improved evaluations for the VII.1 release. Progress was made on developing covariance evaluation and processing capabilities. Support activities include release of the updated ENDF-6 Formats Manual, new version of checking codes and third version of the SIGMA web retrieval.

### **1. Status of the ENDF/B-VII.0 Library**

#### Big paper

The ENDF/B-VII.0 library was released in December 2006 and it was described in detail in the extensive paper by Chadwick, Oblozinsky, Herman *et al.* in the special issue of Nuclear Data Sheets, **107** (2006) 2931. So far, according to Scopus, this paper was cited 115 times.

#### Validation

Validation of ENDF/B-VII.0 continued throughout 2007 and 2008, details can be found in [www.nndc.bnl.gov/exfor/4web/benchmarking.html](http://www.nndc.bnl.gov/exfor/4web/benchmarking.html). The list of benchmarks and testing contain 20 entries with the following three added after the last WPEC meeting in June 2008:

- A code comparison study for the Bigten critical assembly by R.E. MacFarlane et al.
- Analyses of thermal compound low-enriched-uranium systems by E. Kolbe et al.
- Benchmarking against critical assemblies using TRIPOLI by J-Ch. Sublet

Generally, the results of the validation are positive and show improved performance of the ENDF/B-VII.0 library compared to its predecessor ENDF/B-VII.8. Extensive testing discerned, however, a number of issues that need improvement.

McKnight (ANL) has found that control rod worth calculations for the ZPPR-10A assembly are accurately calculated with either ENDF/B-VI or ENDF/B-VII.0 data, but sodium void worth calculations with ENDF/B-VII.0 data are under-predicted and exhibit changes with core loading whereas these worths were over-predicted but displayed a

constant bias with ENDF/B-VI data.

Apparent deficiencies remain to be reported for  $^9\text{Be}$  and the isotopes of nickel and tungsten. While ENDF/B-VII.0 derived cross sections are found to generally produce the most accurate  $k_{\text{eff}}$  results for various ICSBEP benchmarks, there are a number of specific evaluations that require further review, including portions of  $^2\text{H}$ ,  $^9\text{Be}$ ,  $^{63,64}\text{Cu}$ ,  $^{113}\text{Cd}$ ,  $^{232}\text{Th}$ ,  $^{233,235}\text{U}$ ,  $^{237}\text{Np}$  and  $^{239}\text{Pu}$ . ICSBEP benchmark calculations for fast Ti and V reflected HEU systems indicate that current isotopic Ti cross sections in ENDF/B-VII.0 perform worse than the old elemental evaluation available in ENDF/B-VI.8, but new evaluation work at LANL partially eliminates this deficiency.

The ENDF/B-VII.0 based cross-section libraries for SCALE-6 were created with the AMPX code. The related data testing includes  $k_{\text{eff}}$  calculations of more than 1000 ICSBEP benchmarks. While the critical eigenvalues are calculated with good accuracy for the vast majority of these benchmarks, there are a number of instances where the  $k_{\text{eff}}$  calculations are several standard deviations outside the expected value. Given the many accurate results, this suggests that in selected cases there may be deficiencies in the ICSBEP handbook and it was suggested at the CSEWG meeting that these deficient cases be highlighted to the ICSBEP community for further study.

Continuing deficiencies exist in  $^2\text{H}$  cross sections that impact calculated D2O moderated HEU benchmark eigenvalues and ZED-2 coolant void reactivity coefficients.

#### Known deficiencies

The list of known deficiencies of ENDF/B-VII.0 is maintained by the NNDC and made available to the users at [www.nndc.bnl.gov/exfor/4web/VII.0-deficiencies.html](http://www.nndc.bnl.gov/exfor/4web/VII.0-deficiencies.html). It collects comments and observations communicated to the NNDC by the users of the library. Issues compiled in the list will be addressed in the future ENDF/B-VII.1 release.

#### ACE library

The MCNP ENDF70 library has been produced by LANL and released in the beginning of 2009. It contains all ENDF/B-VII.0 except of 3 materials,  $^7\text{Be}$ ,  $^{253}\text{Cf}$ ,  $^{253}\text{Es}$ , which are too incomplete. It was produced at 5 temperatures, between 293.6K and 2500K. This library is available to users through RSICC, Oak Ridge. Several fixes were made to the original ENDF/B-VII.0 files:

- $^1\text{H}$  - a tiny change was made to the capture gamma-ray energy.
- $^{45}\text{Sc}$  - angular distributions were changed to Lab frame and poor excitation function definition was changed.
- $^{89}\text{Y}$  - negative cross sections for the inelastic scattering to the continuum were fixed.
- $^{96}\text{Zr}$  and  $^{97}\text{Mo}$  – typos in the Kalbach parameter were corrected.
- $^{153}\text{Eu}$  - negative distributions in MT91 were corrected.
- $^{242}\text{gAm}$  – lack of angular distribution for MT18, and some strange values in MT51-54 were fixed.

The unofficial version of the ACE library, prepared by the NNDC in December 2006 using the processing code NJOY-99.161, is still available free of charge from RSICC, Oak Ridge. It should be understood, however, that it does not meet the rigor and the quality assurance standard of the official release. The unofficial library contains 392 materials of the neutron sublibrary as well as all 20 materials in the thermal neutron scattering sublibrary.

## 2. Work on ENDF/B-VII.1 Library

Participants of the CSEWG meeting held in November 2008 decided that the next VII.1 version of the ENDF/B library would be released in 2010. The overall emphasis of this release will be on the increase of the number of covariances, and improving structural materials, materials relevant to criticality safety, and minor actinides. Detailed list of related actions has been formulated and reviewed by the mini-CSEWG meeting on June 22, 2009.

### New evaluations

CSEWG re-established the original idea of the ENDF/A library as a depository of updated and new files to be considered for ENDF/B-VII.1. The ENDF/A library currently contains 42 complete files contributed by BNL, LANL, LLNL and ORNL. These files can be grouped into 4 categories:

- Files with fixes to ENDF/B-VII.0 including those introduced when preparing the official ACE library,
- Files containing data from the Evaluated Gamma Activation File, EGAF,
- Files with new evaluations,
- Files with covariances in MF32 and/or MF33.

The list of 42 complete neutron files in ENDF/A is as follows:

0-01\_H\_001-fix0.lanl  
0-21\_Sc\_045-fix0.lanl  
0-39\_Y\_089-fix0.lanl  
0-40\_Zr\_096-fix0.lanl  
0-42\_Mo\_097-fix0.lanl  
0-95\_Am\_242-fix0.lanl  
0-95\_Am\_242m-fix0.lanl  
n-01\_H\_003.RCullen-fix  
n-09\_F\_019+EGAF.llnl  
n-09\_F\_019-new\_MF\_2\_32.ornl-prelim  
n-11\_Na\_022.res-tot-width  
n-17\_Cl\_035\_081111.ornl  
n-17\_Cl\_037\_070307.ornl  
n-19\_K\_039-new\_res-081015.ornl  
n-19\_K\_041-new\_res-081020.ornl

n-22\_Ti\_046-fix-0902xx.lanl  
n-22\_Ti\_047-fix-0902xx.lanl  
n-22\_Ti\_047-fixMF12MT91.llnl  
n-22\_Ti\_048-fix-0902xx.lanl  
n-22\_Ti\_049-fix-0902xx.lanl  
n-22\_Ti\_050-fix-0902xx.lanl  
n-25\_Mn\_055-newRR.ornl  
n-37\_Rb\_087.RCullen-fix  
n-40\_Zr\_90-beta4.bnl  
n-48\_Cd\_113-res-fix.bnl  
n-74\_W\_180-new.iaea  
n-74\_W\_182+EGAF.llnl  
n-74\_W\_182-new.iaea  
n-74\_W\_183+EGAF.llnl  
n-74\_W\_183-new.iaea  
n-74\_W\_184+EGAF.llnl  
n-74\_W\_184-new.iaea  
n-74\_W\_186+EGAF.llnl  
n-74\_W\_186-new.iaea  
n-92\_U\_233-newMF33.ornl-lanl  
n-92\_U\_235-newMF33.ornl-lanl  
n-92\_U\_237\_071211.llnl  
n-92\_U\_238-newMF33.ornl-lanl  
n-94\_Pu\_239-newMF33.ornl-lanl  
n-94\_Pu\_241.za-fixed  
n-95\_Am\_240-new.llnl  
n-95\_Am\_241.za-fixed

The first seven files in the above table (those with names starting with ‘0’ rather than ‘n’) contain corrections introduced by the MCNP team preparing the official ACE library. The total number of materials in ENDF/A is 36 since six materials show up in the list twice. Typically, files constituting such pairs contain complementary information and will be merged in the final release.

### Covariances

Covariances are expected to represent major improvement in the VII.1 release of the ENDF/B library. Most of the covariance evaluations will be prepared in support of the data adjustment for the Advanced Fuel Cycle Initiative (AFCI). Recent activities include:

- Evaluation of MF32, MF33 covariances for the individual materials (ORNL, LANL).
- The low-fidelity covariance project - a full set of simple estimates for all VII.0 materials, has been completed (BNL, LANL, ORNL and ANL).
- AFCI/GNEP project (BNL, LANL) is building upon early covariance estimates (SG26, low-fidelity) that are gradually scrutinized and improved. This scheduled for three years project is in its second year of development. It is expected to provide more than 100 covariance evaluations of which many might be suitable for inclusion to ENDF/B-VII.1.

- Work continues on improvement of covariance evaluation methodology and on validation of the processing codes PUFF and NJOY.
- Workshop on Neutron Cross Section Covariances has been held in Port Jefferson, NY, June 24-27, 2008 attended by 53 participants from 11 countries who presented 39 contributions.

### 3. Support Activities

In general, support ENDF activities are performed by the National Nuclear Data Center, BNL as part of its responsibilities towards CSEWG.

#### Update of ENDF-6 Formats Manual

This important manual has been revised, modernized and updated. The manual was converted into LaTeX with a number of modern features to speed-up navigation etc. The manual was revised with emphasis on the correction of known errors, removal of inconsistencies, clarification of ambiguous text passages and adding format updates approved by CSEWG. Several CSEWG members reviewed various sections of the manual introducing numerous corrections. The manual has been posted on the NNDC web portal in June 2009.

#### ENDF checking codes

The new set of the ENDF Checking & Utility Codes corrects all bugs reported to NNDC as of February 1, 2009 and supersedes all previous releases. A detailed log of changes can be found at the beginning of the respective FORTRAN sources. The suite of ENDF utility codes includes:

CHECKR-8.01 - Format Checking

FIZCON-8.01 - Procedures & Simple Physics Checking

PSYCHE-8.0 - More complicated physics checking

INTER-7.01 - Calculates selected cross sections and integrals

STANEF-8.01 – Standardizes formatting, creates directory list, adds tape label & converts numeric fields.

Provided are FORTRAN95 sources as well as Linux and MS Windows binaries compiled and statically linked using GFORTRAN in case of Linux and Compaq Visual Fortran 6.1.A in case of Windows. Each code can be run in a command mode with an ENDF file as an argument. Machine dependent constructs were eliminated leading to standard FORTRAN95 sources suitable for any architecture (Linux, Mac, and Windows were tested).

## SIGMA retrieval interface

Sigma web retrieval & plotting system tailored to the needs of users of the new ENDF/B-VII.0 library was further improved in its third release. The new features of SIGMA-3 released in April 2009 allow:

- Plotting energy-angle distributions (MF=6).
- Visualization of covariances (MF=33 with LB=1,5; applies to ~80% of cases).
- Retriving thermal neutron cross sections & resonance integrals for neutron capture and fission.

These features add to the existing capabilities to retrieve and plot angular distributions of emitted neutrons (MF4), retrieve and plot energy spectra of emitted neutrons and photons (MF5), and mathematical operations on cross sections (MF3) already available in the release 2.

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