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DEVELOPMENT OF ENDF/B-VII.1 AND ITS COVARIANCE COMPONENT

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The US nuclear data community, coordinated by CSEWG, is preparing release of the ENDF/B-VII.1 library. This new release will address deficiencies identified in ENDF/B-VII.0, include improved evaluations for some 50-60 materials and provide covariances for more than 110 materials. The major players in this undertaking are LANL, BNL, ORNL, and LLNL. We summarize deficiencies in the ENDF/B-VII.0 and outline development of the new library. We concentrate on the BNL activities which aim in providing covariances for the materials important for the design of the innovative reactors. Finally we outline a futuristic approach, known as *assimilation* that tries to link nuclear reaction theory and integral experiments.

KEYWORDS : Nuclear Data, ENDF/B library, Covariances, Evaluated reaction data

1. INTRODUCTION

The ENDF/B-VII.0 library, released in December 2006, was the first major release of this major US nuclear reaction data library in 16 years. It represents a coordinated effort by researchers from many US institutions that was extensively documented in the special issue of Nuclear Data Sheets [1].

The ENDF/B-VII.0 has been intensively validated over last four years in US and Europe. Overall performance of the library proved to be very good, considerably better than its predecessor. Below we summarize some results of the validations posted at the NNDC Web site www.nndc.bnl.gov/endl/.

Mosteller reported that ENDF/B-VII.0 shows particular improvement for the ²³³U, HEU, and plutonium cases with fast neutron spectra. Furthermore, there is much greater consistency between the results for the bare spheres and the corresponding Flattop cases. It also produces dramatically better results for BIG TEN, a cylinder of 10% enriched uranium surrounded by natural uranium. In addition, ENDF/B-VII.0 produces better results for the water-reflected spheres of HEU and plutonium. Relative to ENDF/B-VI, ENDF/B-VII.0 also produces significant improvements for several other cases with significant amounts of hydrogen.

Cullen has shown that use the ENDF/B-VII.0 data library, for the first time allows to reproduce the expected k_{eff} values for Godiva (U235), Jezebel (Pu239) and Jezebel23 (U233) assemblies to within the quoted accuracy of the models, namely 1.0 +/- 0.001.

MacFarlane and Kahler analyzed a number of the ICS-BEP U-233 solution criticals, and a few of the U-233 lattice criticals showing that the ENDF/B-VII.0 performs better than ENDF/B-VI.8.

In recent criticality safety evaluation performed for the licensing of a new commercial wet storage pool with the ENDF/B-VII.0 and JEFF-3.1 libraries [2], the maximum permissible initial fuel-enrichment limit was found to be dependent upon the applied library. By performing trend analyses for a set of benchmarks authors shown that negative trends with respect to the size of the thermal neutron flux, observed when using JEFF-3.1 and ENDF/B-VI.8 libraries, vanish when ENDF/B-VII.0 is employed. The authors recommended that ENDF/B-VII.0 be used for criticality safety evaluation of wet storage pools.

2. DEVELOPMENT OF ENDF/B-VII.1

2.1 Needs for Improvements

In spite of unquestionable successes of ENDF/B-VII.0, further improvements still are needed in some areas. At the meeting of the Cross Section Evaluation Working Group (CSEWG) in 2007 McKnight provided the following short list of apparent deficiencies:

- Large discrepancies in ²³⁹Pu in thermal (e.g., solutions) and intermediate spectra systems
- Improvements needed in resolved and unresolved resonance range of Cr as evidenced in Pu/C/SST assembly
- Improvements needed in resolved and unresolved resonance range of Mn as evidenced in Pu/C/SST assembly
- Very poor performance for clean assemblies with W
- Puzzling results with ²³³U data testing
- Some issues remain with Zr isotopes
- Although largely improved, some large discrepancies remain with ⁹Be

- Some discrepancies with ^{238}U capture
- Results for many polyethylene moderated and reflected critical assemblies are very high
- Some Pb biases remain in thermal systems

More ENDF/B-VII.0 deficiencies were revealed in integral testings reported during subsequent CSEWG meetings:

- The sodium void worths are under-predicted and exhibit changes with core loading.
- Mosteller suggested that the fast cross sections for beryllium and thorium be reviewed.
- Descalle noted that apparent data deficiencies remain in ^9Be and in the isotopes of nickel and tungsten.
- Mosteller concluded that there are 18 specific evaluations that require further review, including portions of ^2H , ^9Be , Ti and V isotopes, $^{63,65}\text{Cu}$, ^{113}Cd , ^{232}Th , $^{233,235}\text{U}$, ^{237}Np and ^{239}Pu .
- Kozier reminded of continuing deficiencies in ^2H cross sections and their impact upon calculated D2O moderated HEU benchmark eigenvalues and ZED-2 coolant void reactivity coefficients.
- Mosteller noted significant (1%) decreases in the calculated k_{eff} for HEU-D2O benchmarks attributed to elastic scattering angular distribution changes below 3 MeV.

Additional list of deficiencies, mostly formal ones, is posted on the GForge site ndclx4.bnl.gov/gf/endl7.

At the 2008 CSEWG meeting a decision was made to begin work on a new version of the ENDF/B-VII library. The release date was eventually set for December 2011. The objective is to provide a modern nuclear reaction library that would support design needs of new generation of power reactors, advanced fuel cycle, criticality safety, and national security. The new release will focus on eliminating major deficiencies identified in ENDF/B-VII.0. It is expected that ENDF/B-VII.1 will include new or significantly improved neutron evaluations for some 50-60 materials and provide covariances for more than 110 materials.

2.2 Status of ENDF/B-VII.1

Most of the ENDF/B-VII.0 deficiencies concern minor actinides and structural materials, i.e., the areas that, to a large extent, were set aside when developing ENDF/B-VII.0. Almost all of these evaluations were taken over from ENDF/B-VI.8. On the contrary, many covariance data in ENDF/B-VI.8 were not migrated to the ENDF/B-VII.0 that resulted in a dramatic drop in the covariance coverage in the current library. Accordingly, the majority of changes in ENDF/B-VII.1 will concern neutron sublibrary. Consistent modifications are also expected in the fission yields and decay sublibraries, while interventions in other sublibraries, if any, will be limited to simple corrections.

Update of the ENDF/B-VII.0 library is a cooperative effort of several national laboratories. The leading parties in the evaluation phase are BNL, LANL, LLNL, and ORNL. Los Alamos is responsible for the fast neutron range in major actinides, and some structural materials, and is the only

provider of complete evaluations for light nuclei. The latter are based on simultaneous fitting of adopted experimental data with the R-matrix theory which naturally provides also covariance data. Livermore is evaluating fast neutron range for a number of materials including some minor actinides. The responsibility for the thermal, resolved and unresolved regions, along with the related covariances, traditionally lie with Oak Ridge. As in the past, the development of ENDF/B-VII.1 is benefiting from the collaboration with the IAEA, which is contributing complete new evaluations, including covariances, for the chain of tungsten isotopes. Brookhaven is charged with estimating covariance data for about 70 fission products and structural materials in the full energy range. BNL is also entrusted with collecting new/revised evaluations, final assembly of the library, its verification, and overall coordination of the project.

List of new and/or modified evaluations submitted to BNL by April 1, 2010 as candidates for the ENDF/B-VII.1 release includes 120 materials:

New evaluations: ^9Be , ^{19}F , ^{27}Al , ^{35}Cl , ^{37}Cl , ^{39}K , ^{41}K , ^{46}Ti , ^{47}Ti , ^{49}Ti , ^{50}Ti , ^{52}Cr , ^{53}Cr , ^{55}Mn , ^{58}Ni , ^{60}Ni , ^{74}As , ^{75}As , ^{78}Kr , ^{90}Zr , ^{123}Xe , ^{124}Xe , ^{180}W , ^{182}W , ^{183}W , ^{184}W , ^{186}W , ^{185}Re , ^{187}Re , ^{237}U , ^{239}U , ^{240}Pu , ^{240}Am

New covariances: ^{235}U , ^{238}U , ^{239}Pu

Corrected for ACE library: ^1H , ^{45}Sc , ^{89}Y , ^{96}Zr , ^{97}Mo , ^{242}Am , $^{242m1}\text{Am}$

Simple fixes: ^3H , ^{22}Na , ^{87}Rb , ^{113}Cd , ^{233}U , ^{236}U , ^{241}Am

Taken from other libraries: ^{63}Cu , ^{65}Cu , ^{174}Hf , ^{176}Hf , ^{177}Hf , ^{178}Hf , ^{179}Hf , ^{180}Hf

JENDL Actinoid files: ^{225}Ac , ^{226}Ac , ^{227}Ac , ^{227}Th , ^{228}Th , ^{229}Th , ^{230}Th , ^{231}Th , ^{233}Th , ^{234}Th , ^{229}Pa , ^{230}Pa , ^{231}Pa , ^{232}Pa , ^{230}U , ^{231}U , ^{232}U , ^{234}Np , ^{235}Np , ^{236}Np , ^{238}Np , ^{239}Np , ^{236}Pu , ^{237}Pu , ^{238}Pu , ^{241}Pu , ^{242}Pu , ^{244}Pu , ^{246}Pu , ^{240}Cm , ^{241}Cm , ^{242}Cm , ^{243}Cm , ^{244}Cm , ^{245}Cm , ^{246}Cm , ^{247}Cm , ^{248}Cm , ^{249}Cm , ^{250}Cm , ^{245}Bk , ^{246}Bk , ^{247}Bk , ^{248}Bk , ^{249}Bk , ^{250}Bk , ^{246}Cf , ^{248}Cf , ^{249}Cf , ^{250}Cf , ^{251}Cf , ^{252}Cf , ^{253}Cf , ^{254}Cf , ^{251}Es , ^{252}Es , ^{253}Es , ^{254}Es , $^{254m1}\text{Es}$, ^{255}Es , ^{255}Fm

'New evaluations' refer to brand new work or to significant updates involving large portions of the file, e.g., full reevaluation of the resonance or fast neutron region. Several of the 33 new evaluations replace evaluations that were found to rise concerns in ENDF/B-VII.0 (^9Be , ^{46}Ti , ^{47}Ti , ^{49}Ti , ^{50}Ti , ^{52}Cr , ^{53}Cr , ^{58}Ni , ^{60}Ni , ^{90}Zr , ^{180}W , ^{182}W , ^{183}W , ^{184}W , ^{186}W).

'New covariances' segment includes files with newly developed covariances that apply to the existing ENDF/B-VII.0 cross sections. This part of the library will grow dramatically once the current APCI exercise is completed and its results used to produce ENDF/B-VII.1 files. New are also covariances for the three major actinides $^{235,238}\text{U}$ and ^{239}Pu prepared by ORNL (resonance region) and LANL (fast neutron region).

The subsequent two categories contain ENDF/B-VII.0 files with simple format fixes or localized modifications and corrections done at LANL when generating the official ENDF/B-VII.0 ACE library.

The two final groups contain foreign evaluations proposed for inclusion in ENDF/B-VII.1. $^{63,65}\text{Cu}$ are borrowed from the CENDL-3 library in attempt to improve poor performance of the ENDF/B-VII.0 files. The results of the validation are inconclusive and new JENDL-4 evaluations will be tested when available. Hafnium files, initially evaluated for JENDL and revised in JEFF-3.1 to include γ -production data were updated by R.Q. Wright to comply with the most recent edition of the Atlas of Neutron Resonances [3]. LLNL put forward for consideration consistent set of 59 minor actinide evaluations originating from the JENDL/AC-2008 (Actinoid) file.

2.3 Work in Progress

The most important ENDF/B-VII.1 related tasks that are carried out in the participating laboratories are summarized below.

H3: LANL corrected (n,2n) cross sections.

Li6 & O16: New evaluations completed by LANL.

Be9: New LANL evaluation includes RPI experimental data. Still, it suffers from the same deficiencies as ENDF/B-VI.8.

Na23: New evaluation with covariances has been prepared by BNL. Adjustment of the (n,2n) cross sections to experimental data rather than to ENDF/B-VII.0 is planned in 2010.

Cr isotopes: ORNL is working on SAMMY analysis of resonance region in Cr50 and Cr53.

Mn55: New evaluation is underway by the BNL-IAEA collaboration, with new resonance parameters provided by ORNL.

Fe56: Modification to α -production cross sections is in progress at LANL.

Ni58, 60: New resonance parameters with covariances were evaluated at ORNL. Ni60 resonance range was extended to 812 keV. LANL made new calculations at higher energies, which reproduce α -production data of LANSCE.

Zn62-73: Some apparently too low cross sections need to be investigated in the new LLNL evaluations.

Y89: Capture cross sections were recalculated at LANL. The upper energy boundary of the resonance region needs to be decreased to avoid missing resonances.

Zr90: New version of the BNL evaluation was successfully tested by KAPL. At the last CSEWG meeting Trkov reported that the ENDF/B-VI.8 performed better in the integral testing, but it might be due to the elastic angular distributions in Zr91.

Gd157: Recent RPI measurement of the thermal cross section is 9% lower than ENDF/B-VII.0. This result is confirmed by testing in BWR assemblies with Gd pins. If the new RPI measurement is to be adopted other six, so far trusted, measurements must be discarded.

Cd113: Thermal capture has been modified by Mughabghab. The entire resonance region, however, might be replaced by the new Geel evaluation.

W isotopes: IAEA is refining the evaluations to improve reproduction of integral experiments. EGAF data will be added in future.

Pu239: New resonance parameters were evaluated in 2008. Tests showed that problems in Pu solution benchmarks persist. CEA made a modification to the resonance parameters in JEFF-3.1.1 to technically solve the issue. ORNL is working on new evaluation which may have a similar fix as JEFF-3.1.1.

Minor Actinides: some of the JENDL/AC actinides data reviewed and submitted by LLNL might be replaced by newer evaluations. In particular, work on Np isotopes is underway at LANL. New EMPIRE based evaluations for Cm isotopes, including covariances, were performed at KAERI. Alternative evaluations might also be produced by BNL.

Fission spectra: LANL is preparing prompt fission spectra on finer energy grid since the current grid turned out to be too coarse.

3. DEVELOPMENT OF COVARIANCES FOR ENDF/B-VII.1

In most cases the general purpose libraries are not accurate enough for a specific application and have to be adjusted to the carefully selected set of integral experiments. In order to perform such adjustment in a meaningful way one needs covariance data for the materials that play significant role in the considered design. The covariances in ENDF/B-VII.0 are scarce and erratic that makes them inadequate for any application.

The ENDF/B-VII.1 will satisfy covariance needs of one particular application - the Advanced Fuel Cycle Initiative (AFCI). This project is seeking to produce adjusted group-wise data suitable for the design of fast reactors. The list of nuclei that are involved in this exercise comprises 110 materials, as shown in Tab. 1. Covariances are requested for elastic, radiative capture, inelastic scattering, fission and (n,2n) cross sections, ν -bars, fission spectra and, in a few particular cases, also for μ -bars. This considerable effort is shared by BNL, LANL, and ORNL with: (i) LANL responsible for light nuclei and actinides in the fast neutron range, (ii) ORNL responsible for the resonance range in a number of selected materials, and (iii) BNL in charge of all the remaining materials in the whole energy range.

There is a general consensus that covariances should be an integral part of the evaluation procedure to reflect actual experimental data and reaction theory modeling adopted by the evaluator and to ensure that the covariances are determined with respect to the current cross sections. Strict adherence to this principle would mean reevaluation and subsequent validation of the 110 materials listed in Tab. 1. Such effort would be impossible before the release of the library that is planned for December 2011, chosen so for the

Table 1. List of isotopes in the AFCI project (priority materials in bold).

¹ H	²⁸ Si	⁹² Mo	¹⁰⁹ Ag	¹⁴⁹ Sm	²³² Th
² H	²⁹ Si	⁹⁴ Mo	¹²⁷ I	¹⁵¹ Sm	²³³ U
⁴ He	³⁰ Si	⁹⁵ Mo	¹²⁹ I	¹⁵² Sm	²³⁴ U
⁶ Li	⁵⁰ Cr	⁹⁶ Mo	¹³¹ Xe	¹⁵³ Eu	²³⁵ U
⁷ Li	⁵² Cr	⁹⁷ Mo	¹³² Xe	¹⁵⁵ Eu	²³⁶ U
⁹ Be	⁵³ Cr	⁹⁸ Mo	¹³⁴ Xe	¹⁵⁵ Gd	²³⁸ U
¹⁰ B	⁵⁵ Mn	¹⁰⁰ Mo	¹³³ Cs	¹⁵⁶ Gd	²³⁷ Np
¹¹ B	⁵⁴ Fe	⁹⁹ Tc	¹³⁵ Cs	¹⁵⁷ Gd	²³⁸ Pu
¹² C	⁵⁶ Fe	¹⁰¹ Ru	¹³⁹ La	¹⁵⁸ Gd	²³⁹ Pu
¹⁵ N	⁵⁷ Fe	¹⁰² Ru	¹⁴¹ Ce	¹⁶⁰ Gd	²⁴⁰ Pu
¹⁶ O	⁵⁸ Ni	¹⁰³ Ru	¹⁴¹ Pr	¹⁶⁶ Er	²⁴¹ Pu
¹⁹ F	⁶⁰ Ni	¹⁰⁴ Ru	¹⁴³ Nd	¹⁶⁷ Er	²⁴² Pu
²³ Na	⁹⁰ Zr	¹⁰⁶ Ru	¹⁴⁵ Nd	¹⁶⁸ Er	²⁴¹ Am
²⁴ Mg	⁹¹ Zr	¹⁰³ Rh	¹⁴⁶ Nd	¹⁷⁰ Er	^{242m} Am
²⁵ Mg	⁹² Zr	¹⁰⁵ Pd	¹⁴⁸ Nd	²⁰⁴ Pb	²⁴³ Am
²⁶ Mg	⁹³ Zr	¹⁰⁶ Pd	¹⁴⁷ Pm	²⁰⁶ Pb	²⁴² Cm
²⁷ Al	⁹⁴ Zr	¹⁰⁷ Pd		²⁰⁷ Pb	²⁴³ Cm
	⁹⁵ Zr	¹⁰⁸ Pd		²⁰⁸ Pb	²⁴⁴ Cm
	⁹⁶ Zr			²⁰⁹ Bi	²⁴⁵ Cm
	⁹⁵ Nb				²⁴⁶ Cm

library to have impact on development of the AFCI project. Therefore, CSEWG decided to relax the strict consistency requirement and the overwhelming majority of covariances will be developed *a posteriori*, i.e., the existing ENDF/B-VII.0 evaluations will be amended with newly developed covariances. This approach presents additional challenge since the uncertainties are to be assigned to the ENDF/B-VII.0 data although the present analysis might suggest different values. These inconsistencies must be accounted for in the final covariances, which implies acceptance of rather conservative uncertainties and necessitates use of some *ad hoc* methods for their determination.

Only in a few instances ENDF/B-VII.1 covariances will result from a consistent evaluation procedure. This is the case of ²³Na that will be discussed separately. This is also true for ORNL analysis of new resonance data for ^{58,60}Ni and ⁵³Cr. Sets of new cross sections and covariances in the full energy range were also submitted for ⁵⁵Mn (ORNL/BNL/IAEA) and ⁵²Cr (ORNL/FZK).

In addition, the ENDF/B-VII.1 library will include covariances for a number of materials that are not in the AFCI list (Tab. 1). To this category belong complete new evaluations for the chain of tungsten isotopes ^{180,182,183,184,186}W (IAEA) and titaniums ^{46,47,49,50}Ti (ORNL/LANL). Furthermore, ORNL has evaluated resonance regions in ^{39,41}K, ^{35,37}Cl, and ¹⁹F providing covariances for the resonance parameters (MF=32).

3.1 Covariance Methodology

The covariance component of the ENDF/B-VII.1 includes various types of the materials, such as light nuclei, structural materials, fission products and actinides. In each of these classes there are priority materials (see bold entries in Tab. 1) and those which are of lesser importance. These

factors influence choice of the methodology chosen for the estimation of covariances.

Light nuclei are evaluated by Hale (LANL) using R-matrix fit to various experimental data including neutron and proton induced reactions. The cross section covariances are based on propagation of the covariances of the R-matrix parameters. The results are given in MF=33 and cover the entire energy range.

The resolved resonance region evaluations performed in ORNL rely on the Bayesian SAMMY code. Although uncertainties of resonance energies and widths are felt to be realistic, the uncertainties of the computed cross sections are dramatically underestimated. Recently, systematic uncertainties of background, normalization, scattering radius and other long-range correlations have been included in the analysis bringing computed cross section uncertainties to a more plausible level.

Resonance range evaluations at BNL make use of the resonance parameters and their uncertainties compiled in the Atlas of Neutron Resonances [3]. In the original approach, respective Atlas data are formatted in MF=2 and MF=32 and adjustment involving a few initial resonances (including bound states) is performed to reproduce thermal cross sections uncertainties for capture and elastic. The latter adjustment generally introduces correlations among considered resonances. Correlations have also to be assumed among radiative widths in order to prevent collapse of the uncertainties in the upper part of the resonance range when many resonances are contributing to a single energy-group. The uncertainty of the scattering radius can, in principle, be included using the extension of the ENDF-6 format approved by CSEWG-2009. Even with this extension, however, there is no possibility to account for the correlations between scattering radius uncertainty and uncertainties of the resonance parameters. In most cases, this format deficiency destroys agreement with the experimental uncertainty at the thermal energy. To avoid this issue one may simulate the effect of scattering radius uncertainty by invoking energy dependent MF=33 “background”.

An alternative procedure relying on the Atlas of Neutron Resonances, is the so called “kernel approach”. This technique has been recently developed at BNL [4] to avoid difficulties associated with the previous approaches. It makes use of a simplified expression for calculating cross sections integrals over predefined energy groups directly from the resonance parameters in order to propagate resonance parameter uncertainties to the group cross sections. The approximation is excellent for capture, while elastic scattering requires careful choice of the energy group structure tailored to the particular isotope. The method offers several advantages. Analytical formulation enables accounting for any correlations among resonance parameters including the scattering radius. Since cross section covariances are given (File 33) there is no strict requirement for the resonances in File 2 to match exactly those in the Atlas of Neutron Resonances, a feature very useful when adding covariances to an existing evaluation. For capture, positive correlation assumed between radiative widths are usually sufficient to

prevent the decrease of uncertainties. Most of the BNL evaluations in the resonance region are performed using the kernel approach.

In the fast neutron region the methodology employed at BNL and LANL makes extensive use of nuclear theory modeling coupled to the Bayesian code KALMAN [5]. This approach links input parameters to the nuclear reaction codes (e.g., EMPIRE [6], GNASH [7] or CoH [8]) to the experimental data yielding covariances for the input parameters and cross sections. If several reaction channels are treated simultaneously a consistent set of model parameters is obtained together with the parameter covariances. The latter, when propagated to reaction cross sections, provide a full covariance matrix including cross-reaction terms. When many measurements are available for a certain reaction channel (typically for fission) LANL is often invoking the least-square fitting procedure, which being free of the model constrains, is more flexible in reproducing experimental data.

A special type of the least-square fitting, developed by Muir and implemented in the GANDR system [9], is used in the IAEA tungsten evaluations. This approach employs informative prior obtained with the Monte Carlo method, in which the constrains of nuclear theory are introduced by performing a large number of EMPIRE calculations with randomly perturbed input parameters.

All these approaches are being utilized in the preparation of covariances for the ENDF/B-VII.1. The choice depends on the mass range, importance of the material and the origin of the evaluation. For example, recent LANL evaluation of ^{240}Pu covariances uses GLUCS to analyze experimental data for fission and the average number of prompt fission neutrons, while for other reaction channels the KALMAN code, which combines GNASH sensitivity calculations with experimental data, is used to infer cross section covariances. Similar method, with the Madland-Nix model replacing GNASH, was employed for estimating covariance matrix for the prompt fission neutron spectrum.

For less important fission products default EMPIRE calculations with propagation of global parameter uncertainties might be used. In this case the most recent release of the AFCI library will serve as guidance for the uncertainties. Alternatively, the AFCI results might be converted into the ENDF-6 formatted files.

The uncertainties for the minor actinides will rely on the recent parametrization of the fission channel in EMPIRE by Mihaela Sin. This work provides outstanding reproduction of cross sections enabling use of the KALMAN code to infer uncertainties. Two pilot calculations of this type were performed at BNL for ^{242}Pu and ^{237}Np . Simultaneous modeling of all reactions channels permits to estimate cross reaction correlations that turn out to be significant.

Covariances for the major structural materials (such as ^{52}Cr , ^{56}Fe , and ^{58}Ni) require special attention. Due to the critical role of these materials default global estimates are not acceptable. On the other hand, full reevaluation of these isotopes would be impossible in the available timeframe. After considering various options the BNL team decided

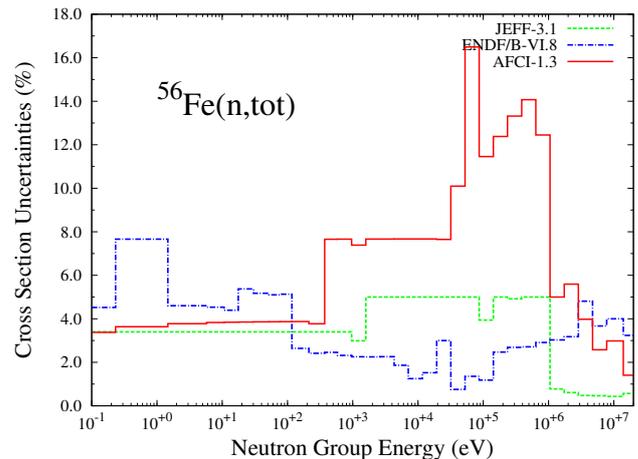


Fig. 1. Comparison of uncertainties for $^{56}\text{Fe}(n,\text{tot})$ in JEFF-3.1, ENDF/B-VI.8 and AFCI-1.3 (ENDF/B-VII.1 candidate) in the full energy range using AFCI 33-group structure.

to adopt the 'kernel method' in the resonance range, and restore ENDF/B-VI.8 covariances in the fast neutron range. The latter were authored by the same group that developed the basic files.

In the resonance range our uncertainties are considerably higher than those of JEFF-3.1 and ENDF/B-VI.8 (see Fig. 1). We retain that being based on the recent edition of the Atlas of Neutron Resonances they are more reliable than those reported in the other two evaluations. In the fast neutron region we increased ENDF/B-VI.8 uncertainties for inelastic in the threshold region as shown in Fig. 2. This increase is justified by the dispersion of the cross sections in existing evaluations and much higher uncertainties reported by JENDL-3.3 as seen in Fig. 3. We conclude that JEFF-3.1 uncertainties in the fast neutron region, although resulting from a very detailed analysis, are too small to be associated with ENDF/B-VII.0 cross sections. This conclusion is supported by the AFCI users' findings.

4. CONSISTENT ADJUSTMENT (ASSIMILATION)

Consistent adjustment, also called assimilation, is a collaborative attempt by BNL and INL to build up a link between precise integral experiments and basic theory of nuclear reactions. Recent advances in reaction modeling and transport calculations, combined with the sensitivity analyses methods offer a possibility of de-convoluting results of the integral experiments to obtain feedback on parameters of nuclear reaction models. Essential ingredients of such procedure are covariances for model parameters and sensitivity matrices propagating parameter variations to the integral quantities. The resulting evaluation is constrained by the differential as well as integral experiments assimilating nuclear reaction theory and systematics of model parameters.

We use nuclear reaction code EMPIRE, and Bayesian code KALMAN to reproduce differential experiments and

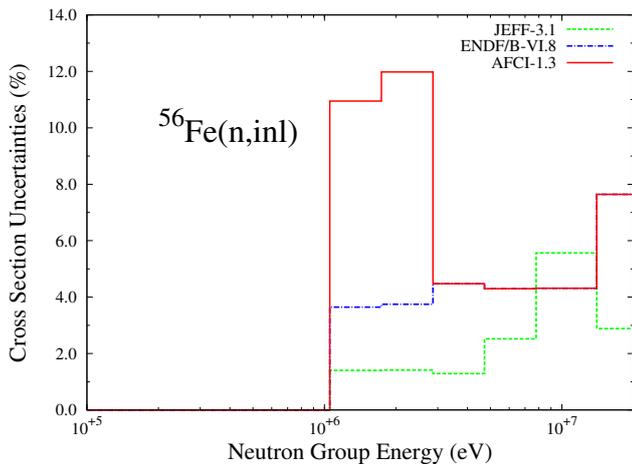


Fig. 2. Comparison of uncertainties for $^{56}\text{Fe}(n,n')$ in JEFF-3.1, ENDF/B-VI.8 and AFCI-1.3 using AFCI group structure.

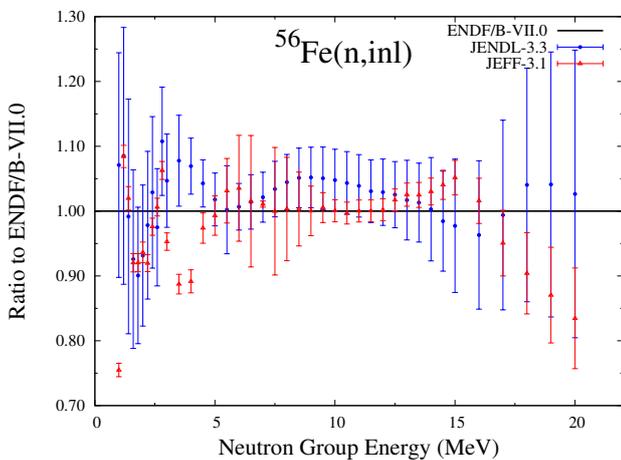


Fig. 3. Ratio of $^{56}\text{Fe}(n,n')$ cross sections in JEFF-3.1 and JENDL-3.3 to the respective values in ENDF/B-VII.0. Shown are the original JEFF-3.1 and JENDL-3.3 uncertainties.

obtain covariances of model parameters. Resonance parameters from Ref. [3] are used construct MF=32. Then, the cross section sensitivities in the 33 energy-group structure are generated by perturbing model parameters (including resonance parameters). These sensitivities are combined with the sensitivities of the integral quantities to the group cross sections in order to link nuclear reaction theory and integral experiments. Finally, the sensitivity analysis code ERANOS is used to adjust model parameters. More details regarding the procedure are given in the contribution by Pigni [10]. The first assimilation results for ^{23}Na are reported in the contribution by Palmiotti [11].

5. CONCLUSIONS

The US nuclear data community is working on the update of the ENDF/B-VII library to be released in December

2011. The major contributor to this endeavor are LANL, BNL, ORNL and LLNL cooperating under auspices of the CSEWG. The development focuses on removing deficiencies in the ENDF/B-VII.0 library, improving evaluations for structural materials, and providing a consistent set of covariances responding to the needs of fast reactor design. In particular, the new set of covariances for 110 materials should enable adjustment of cross sections to meet the exigencies of the AFCI. The new library will also include several improved fission neutron spectra along with their covariances and the revised fission product yields resulting from the meticulous effort by LANL and LLNL. Overall, about one third of the evaluations in the library will be modified or replaced.

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REFERENCES

- [1] M.Chadwick, P.Obložinský, M.Herman, et al, "ENDF/B-VII.0: Next generation evaluated nuclear data library for nuclear science and technology", *Nuclear Data Sheets*, **107**, 2931(2006).
- [2] E.Kolbe, A.Vasiliev, and H.Ferroukhi, "The effect of modern thermal neutron scattering sublibraries on criticality safety evaluations of wet storage pools". *Annals of Nuclear Energy*, **37**, 371(2010).
- [3] S.F. Mughabghab, "Atlas of Neutron Resonances: Thermal Cross Sections and Resonance Parameters", Elsevier, Amsterdam, 2006.
- [4] P. Obložinsky, Y.-S. Cho*, C.M. Mattoon, and S.F. Mughabghab, "Formalism for neutron cross section covariances in the resonance region using kernel approximation", BNL-91287-2010, Brookhaven National Laboratory, 2010.
- [5] T. Kawano and K. Shibata, "Covariance evaluation system", JAERI Data/Code, JAERI, Tokai, Japan, 1997.
- [6] M.Herman, et al, "EMPIRE: Nuclear Reaction Model Code System for Data Evaluation", *Nuclear Data Sheets*, **108**, 2655(2007).
- [7] P.G. Young, E.D. Arthur, and M.B. Chadwick, "Comprehensive nuclear model calculations: Theory and use of the GNASH code", *Proc. of the IAEA Workshop on Nuclear Reaction Data and Nuclear Reactors*, Trieste, Italy, April 15 - May 17, 1996.
- [8] T. Kawano, unpublished.
- [9] A.Trkov. "Summary report of the IAEA technical meeting", INDC(NDS)-471, IAEA, Vienna, 2005.
- [10] M.T. Pigni, et al, "Evaluation of ^{23}Na neutron cross sections for nuclear data assimilation", *ibid*.
- [11] G.Palmiotti, "Use of Covariance Matrices in a Consistent (Multiscale) Data Assimilation for Improvement of Basic Nuclear Parameters in Nuclear Reactor Applications", *ibid*.