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# AFCI-2.0 Library of Neutron Cross Section Covariances

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## INTRODUCTION

Neutron cross section covariance library has been under development by BNL-LANL collaborative effort over the last three years. The primary purpose of the library is to provide covariances for the Advanced Fuel Cycle Initiative (AFCI) data adjustment project, which is focusing on the needs of fast advanced burner reactors. The covariances refer to central values given in the 2006 release of the U.S. neutron evaluated library ENDF/B-VII.0 [1].

The preliminary version (AFCI-2.0beta) has been completed in October 2010 and made available to the users for comments. In the final 2.0 release, covariances for a few materials were updated, in particular new LANL evaluations for $^{238,240}$Pu and $^{241}$Am were adopted.

BNL was responsible for covariances for structural materials and fission products, management of the library and coordination of the work, while LANL was in charge of covariances for light nuclei and for actinides.

## CONTENTS AND FORMAT OF THE LIBRARY

The AFCI-2.0 library [2] contains neutron cross section covariances for 110 materials, including 12 light nuclei (coolants and moderators), 78 structural materials and fission products, and 20 actinides. Covariances are given up to 19.6 MeV for elastic, inelastic, capture, (n,2n) and, for actinides, fission cross sections processed into 33-energy groups with 1/E flux. In addition, the library contains 20 files with nu-bar covariances, 3 files with covariances for fission neutron spectra ($^{238,239,240}$Pu), and 2 files with mu-bar covariances ($^{23}$Na, $^{56}$Fe).

The library is released in the multigroup format for AFCI reactor analysts and also for the Working Party on International Nuclear Data Evaluation Co-operation (WPEC) Subgroup 33 for the international data adjustment exercise.

## COVARIANCE METHODOLOGY

Several methods of different complexity were used for estimating covariances depending on the mass number A, energy region, priority, and availability of the differential experimental data:

- Low A: R-matrix analysis in the full energy range.
- Resonances, intermediate A: kernel approximation [3]; estimates based on uncertainties of integral quantities, developed for the low-fidelity project [4].
- Resonances, actinides: full scale SAMMY [9] analysis and retroactive SAMMY analysis adopted from ORNL; estimates based on integral quantities.
- Fast region: EMPIRE/GNASH-KALMAN method [5] including experimental data; least-squares fitting of data; propagation of model parameter uncertainties (low-fidelity); dispersion analysis - assessment of differences among evaluations and among measurements. Detailed description can be found in the report of the WPEC Subgroup 24 [5].

### Light Nuclei

Two distinct approaches have been used at LANL to provide covariance matrices for light elements. The full R-matrix formalism has been used in a few cases, and the covariance matrices obtained with this method can be considered of the highest possible quality. This method was used for $^{1}$H, $^{4}$He, $^{6}$Li and $^{10}$B ($^{16}$O was evaluated for ENDF/B-VII.1, but not retro-fitted for ENDF/B-VII.0). For the remaining light nuclei, covariances were inferred from the survey of available experimental data.

### Structural Materials and Fission Products

This group contains 78 materials. For the structural materials including isotopes of Mg, Al, Si, Cr, Mn, Fe, Ni, Zr, Mo, Pb, and Bi covariances for scattering are most important. In the resonance region covariances were determined using the newly developed kernel approach [3]. In the fast region, EMPIRE-KALMAN system has been used, the representative experiments were included in this analysis and nuisance parameters were marginalized to account for neglected cross experiment correlations, systematical uncertainties and data spread. For several important structural materials (Si, Cr, Fe, Ni) decent fast neutron covariances in ENDF/B-VI.8 are available, and these were adopted after the revision based on the dispersion analysis. ENDF/B-VII.0 contains few covariances and whenever possible these were adopted (isotopes of Gd, and $^{99}$Tc). Particular attention was given to the important coolant material, $^{23}$Na, which was evaluated at BNL in the full energy range in the frame of the Assimilation project.

In the remaining lower priority cases, covering almost some 35 fission products, low-fidelity estimates [4] were used after inspection by BNL. This decision was facilitated by reasonable quality of low-fidelity capture covariances, which are primarily needed for these materials. The revision usually extended the resonance region from 5 keV (used by low-fidelity) to values more appropriate for the individual isotopes. In addition, elastic uncertainties were limited to 20% to avoid unrealistic values resulting from propagating uncertainties of optical model parameters at low energies.

Average scattering cosine (mu-bars) covariances for $^{23}$Na and $^{56}$Fe are modified ENDF/B-VII.0 and JENDL-3.3 values.

### Actinides

Covariances of $^{233,235,238}$U, $^{239}$Pu previously evaluated for ENDF/B-VII.0 have been included in the AFCI-2.0 library; covariances in the thermal and resonance regions are those of ORNL using the SAMMY code. The ENDF/B-VII.0 standards' covariances were incorporated in $^{235}$U.

A new covariance evaluation was performed for $^{241}$Am, based largely on the ENDF/B-VII.0 file except for the resonance parameters adopted from JENDL-4.0.

New complete evaluations were performed for $^{238,240}$Pu, with the covariances retro-fitted to ENDF/B-VII.0. Discrepancies between the cross sections were larger and new uncertainties had to be increased to embrace the difference in central values between ENDF/B-VII.1 and ENDF/B-VII.0. The correlations, however, were deemed to be reasonable. The methodology in most of these cases was based on the reaction modeling with GNASH combined with the experimental data through the Bayesian code KALMAN.

For $^{241}$Pu, only the fission cross-section covariances were evaluated, using a least-square fit of experimental data. The large discrepancies observed between evaluations and the recent LANSCE dataset [6] were neglected, and will be revisited in the near future.

BNL contributed $^{242}$Pu and $^{237}$Np up to 20 MeV. In the fast neutron range these estimates were obtained with EMPIRE-KALMAN using parameterization by Sin. Thermal and resonance region follow the low-fidelity data revisited by Mughabghab. The IAEA ENDF/B-VII.0 covariances for $^{232}$Th, revised by Trkov for ENDF/B-VII.1, were adopted.

The remaining actinides $^{234,236}$U, $^{242,243}$Am, and $^{242,243,244,245,246}$Cm make use of the low-fidelity data, with low energy region based on the thermal cross section, resonance integral and scattering radius uncertainties, fast region uncertainties resulting from the assessment of Maslov [7] and correlations from a simple propagation of model parameter uncertainties for WPEC SG26.

Beside nu-bar covariances for $^{232}$Th and $^{235}$U, available in ENDF/B-VII.0, the AFCI-2.0 library contains nu-bar covariances for $^{233,238}$U and $^{238,239,240}$Pu evaluated by LANL, while for the remaining 13 minor actinides Maslov's estimates [7] were adopted.

Covariance matrices for prompt fission neutron spectra have been provided by LANL for $^{238,239,240}$Pu, for incident neutron energy of 0.5 MeV. They were obtained using the Madland-Nix model and the KALMAN code to incorporate experimental data [8].

## QUALITY ASSURANCE (QA)

The AFCI-2.0 library has undergone QA testing designed to disclose formal deficiencies, enforce mathematical correctness and ensure that the uncertainties are reasonable. Two practical tools have been developed at BNL: the unCor code [10], which performs several tests on the entire library, and the Web based system that allows visual comparisons including plots of cross sections along with their uncertainties and experimental data. In addition, calculated values and uncertainties of the integral quantities (thermal cross sections, Maxwellian averages, resonance integrals and $^{252}$Cf spectra integrals can be compared with the measurements).

Because of the QA the AFCI-2.0 data are regarded to be more reliable than other large-scale covariance projects. They are also tailored to meet needs of a certain class of users. The AFCI covariance work provides a foundation for the ENDF/B-VII.1 library, to be released in December 2011. We are fully aware, however, that many of AFCI covariances were still obtained by simplified methods and considerable amount of work is needed to produce more robust covariances that could be used with full confidence in reactor applications.

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