BROOKHAVEN NATIONAL LABORATORY

BNL-93618-2010

ISSUES IN NEUTRON CROSS SECTION COVARIANCES

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Presented at the
International Conference on Nuclear Data for Science and Technology

Jeju Island, Korea, April 26-30, 2010

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International Conference on Nuclear Data for Science and Technology 2010

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Received
Accepted for Publication

We review neutron cross section covariances in both the resonance and fast neutron regions with the goal to identify existing issues in evaluation methods and their impact on covariances. We also outline ideas for suitable covariance quality assurance procedures. We show that the topic of covariance data remains controversial, the evaluation methodologies are not fully established and covariances produced by different approaches have unacceptable spread. The main controversy is in very low uncertainties generated by rigorous evaluation methods and much larger uncertainties based on simple estimates from experimental data. Since the evaluators tend to trust the former, while the users tend to trust the latter, this controversy has considerable practical implications. Dedicated effort is needed to arrive at covariance evaluation methods that would resolve this issue and produce results accepted internationally both by evaluators and users.

KEYWORDS : ND2010, Nuclear Data, ENDF, Neutron Cross Sections, Covariances, Quality Assurance

1. INTRODUCTION

Neutron cross section covariances are receiving renewed attention in response to needs of many real-world applications, including nuclear criticality safety, dosimetry, and design of future nuclear reactors. At the same time, new evaluation techniques, and advances in computing, permit evaluators to produce results more rapidly. Recent efforts have resulted in covariances not only on major reaction channels, but also reaction cross-correlations, angular distributions of emitted neutrons ($\bar{\mu}$), and prompt neutron fission spectra.

The National Nuclear Data Center is profiling itself as a 'covariance lab' with broad range of activities and considerable experience accumulated over last 5 years, including:

- Development of covariance methods and tools in the resonance and fast neutron region (Atlas of Neutron Resonances [1], EMPIRE-KALMAN code system [2])
- Evaluations and estimates of covariances for a number of projects and libraries (ENDF/B-VII.0 [3], BOLNA, Low-fidelity [4], AFCI [5], ENDF/A)
- Assembly, review and testing of these libraries, distribution to users and response to feedback from evaluators and users.

The current focus of the NNDC is on developing a covariance library for the Advanced Fuel Cycle Initiative, AFCI [5]. This latest experience along with our earlier observations lead to our firm conclusion that some serious issues appear in many covariance evaluations and estimates produced today. These issues (particularly very low uncertainties) make the covariances much less useful for applications: users may choose not to trust these results. Care must therefore be taken to assure covariance quality.

In this paper, we describe some of the most commonly observed issues along with possible fixes, and suggest possible criteria for covariance quality assurance.

2. UNREALISTIC UNCERTAINTIES

Unrealistically small uncertainties appear in covariances for many materials, and users frequently challenge them. Low uncertainties, *e.g.,* $\Delta\sigma$(n,inel)< 3 – 5%, are generally not trusted by users. User may typically consult experimental data and spread of evaluations in major data libraries and readily conclude that low uncertainties are far too optimistic. From the practical point of view, if covariances are used (for example) for adjustment of evaluated cross sections to integral experiments, unrealistically small uncertainties would imply that no adjustment is possible.

Low uncertainties arise for several different reasons. One common source is the use of model-based covariances which, otherwise, have several advantages: they can be produced rapidly for most materials of interest; they also permit covariance estimates where little or no experimental evidence is available. These covariances should be treated with considerable caution, however, as they are often contain uncertainties that may be unphysical.

In two recent projects, *en masse* covariances were produced for many materials at once. The US 'low-fidelity' covariance project [4] used simple estimates in thermal and resonance region based on integral values [1], and model-based estimates mostly by EMPIRE-KALMAN in the fast region [2]. TENDL library contains massive amount of covariances produced with the TALYS code and Monte Carlo methods [6]. In both cases, questionable uncertainties are found. Thus, in the low-fidelity library, there is strong uncertainty peak in (n,el) for many materials in the 10 keV to 100 keV region. These peaks result from global optical model parametrization which is not suitable for this region.

In the case of TENDL, unrealistic uncertainties are found in many places. As an example, Fig. 1 shows the important structural material ^{56}Fe: (n,el) displays unrealistically high uncertainties in the MeV range, while in (n,γ) the resonance region uncertainty appears far too low compared to thermal.

On the other hand, low uncertainties may also come from a detailed analysis that includes many experimental data. The methods used in this case are a source of disagreement between evaluators and users. Users tend to prefer what may be called a 'common-sense' approach, such as assigning uncertainties with 1 σ approximately reproducing the spread of experimental data. Evaluators prefer mathematically rigorous treatments, where the biggest challenge seems to be proper inclusion of systematic uncertainties and related correlations. Even though these methods are widely considered to be formally correct, the lower uncertainties they produce are often rejected by users as unphysical.

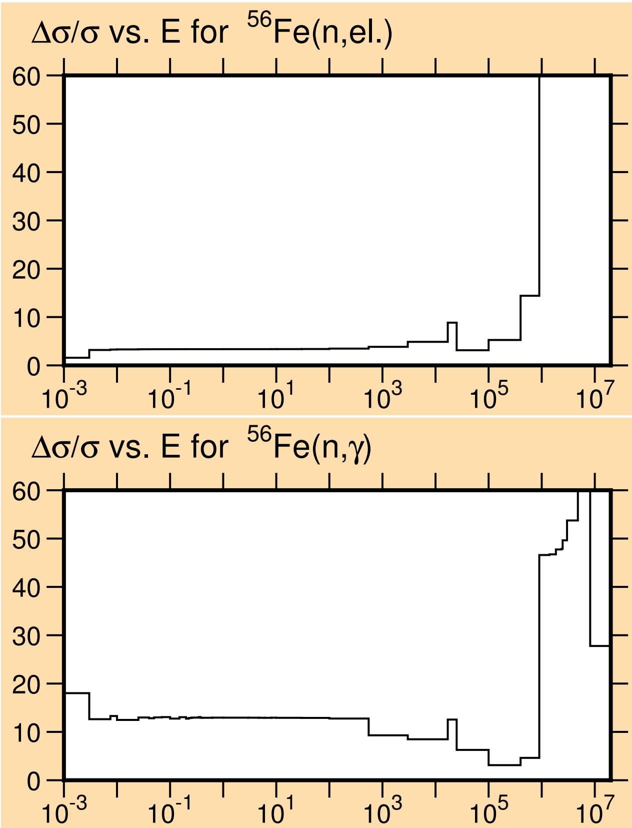

Fig. 1. ^{56}Fe+n uncertainties in TENDL-2009 library [6]. In (n,el) huge uncertainties above 1 MeV are unrealistic based on optical model considerations. In (n,γ) the decrease through 1 MeV is unphysical: the thermal cross section of 2.6 b is much better known than tiny 6 mb at 10^5 eV. Units are in eV and %.

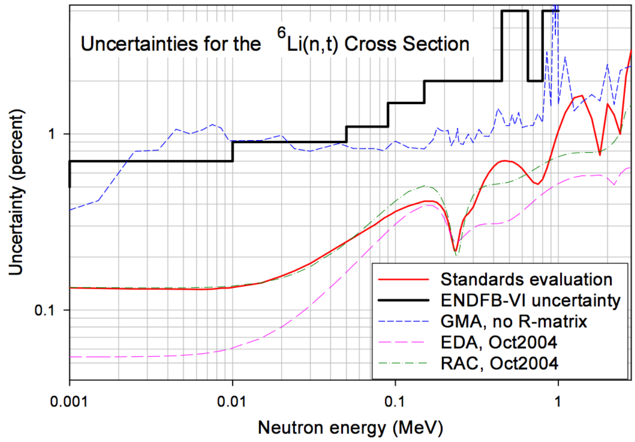

Fig. 2. Uncertainties of ^{6}Li(n,t) neutron cross section standard. Common-sense results of the earlier release (black) were replaced by much lower values for ENDF/B-VII (bold red), but certain unease still remains [8].

This disagreement between users and evaluators was highlighted during the production of the neutron cross section standards. The standards are produced by a large international effort, with great attention to detail, using carefully analyzed experimental data and different evaluation procedures. Uncertainties resulting from this approach are in general quite low. In the previous release (1990, part of ENDF/B-VI), evaluators eventually agreed to expand the low uncertainties in accordance with the guideline by a group of CSEWG experts [7]. As an example, uncertainties for the ^6Li (n,t) are shown in Fig. 2. The bold black curve shows the expanded uncertainties adopted in 1990, about a factor of 5 larger than 'rigorous' results (bold red curve) adopted by ENDF/B-VII in 2006 [8].

Since the standards evaluations have received most detailed attention, the NNDC uses the associated uncertainties as a baseline for judging other evaluations. The underlying assumption is that these other evaluations are unlikely to achieve the same precision and we compare uncertainties of major reaction channels (capture, elastic, fission) to standards. Several new evaluations with questionable, low uncertainties have been found. For example, ^{232}Th(n,γ) in ENDF/B-VII.0 has a very low uncertainty in the region from approximately 10 keV to 1 MeV, covering the unresolved and fast neutron regions. The uncertainty is about 1.5%, comparable to the uncertainties assigned to the ^{197}Au(n,γ) standard. Another, more dramatic case is ^{233}U (n,el) as seen in Fig. 3. The uncertainty in the unresolved region, 1 keV to 20 keV, is 0.2-0.3%, which is substantially less than 0.5% uncertainty on the ^{nat}C(n,el) standard.

These low uncertainties raise the question: were the evaluations done in such a way as to achieve uncertainties similar to or better than the standard? Unless the answer is 'yes', which is very unlikely, comparing to the standards is a valuable way to quickly judge which new evaluations have suspiciously low uncertainties that warrant further attention.

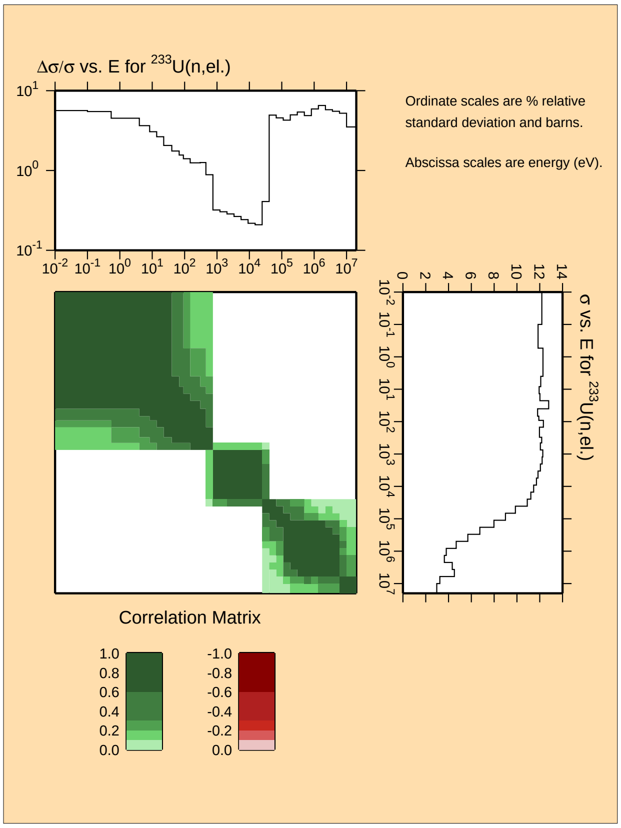

Fig. 3. ^{233}U (n,el) in ENDF/A, with uncertainties of 0.2-0.3% in the unresolved region are unrealistic when compared to 0.5% uncertainty of the ^{nat}C(n,el) standard.

3. ISSUES IN RESOLVED RESONANCE REGION

Covariances in the resonance region are mostly in the form of resonance parameter covariance matrix stored in ENDF file 32 (MF32). This matrix should be converted to cross section covariances using the processing codes NJOY [9] or PUFF [10]. Another possibility is to directly produce a cross section covariance matrix in MF33. There are several important issues that need to be addressed.

3.1 Resonance-Resonance Correlations

Decrease of cross section uncertainties at the top of the resonance region, where the density of resonances increases, indicates lack of resonance-resonance correlations. This can be best illustrated on capture for structural materials (Cr, Fe, Ni) which are almost pure scatterers, $\Gamma_n >> \Gamma_\gamma$. Resonance strength can be expressed through kernel [11]

$$A_\gamma = \frac{g\Gamma_n\Gamma_\gamma}{\Gamma_{\rm tot}} \approx g\Gamma_\gamma, \quad \text{implying} \quad \Delta A_\gamma \approx \Delta\Gamma_\gamma, \qquad (1)$$

where Γ_n, Γ_γ and $\Gamma_{\rm tot}$ are partial and total widths. Neglecting some variation of $\Delta\Gamma_\gamma$ along with energy dependence, collapsing N uncorrelated resonances into one energy group

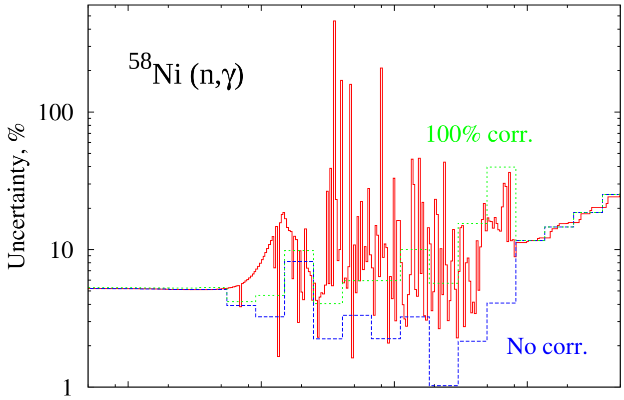

Fig. 4. Uncertainties of ^{58}Ni (n,γ), with resonances extended up to about 1 MeV, and file MF32 processed into fine and broader group structures. The uncertainties for the latter decline strongly if radiative widths of resonances are uncorrelated.

can be done readily,

$$\Delta A_\gamma^{\rm group} \approx \frac{1}{\sqrt{N}}\Delta\Gamma_\gamma\,, \qquad (2)$$

showing considerable decrease of the group uncertainty. This may eventually mean that the high end of the resonance region would claim better precision than the thermal capture cross section which is usually the best-known value for most materials.

Correlations between resonances are essentially due to data reduction. Assume, for example, that the data reduction involved subtraction of a background $b \pm \Delta b$ and multiplication by a calibration factor $c \pm \Delta c$. This means that the data reduction recipe to get count α_j from raw count a_j was

$$\alpha_j = (a_j - b)c. \qquad (3)$$

To get covariance matrix elements one should compute sensitivities and apply quadratic summation. For off-diagonal terms the statistical component vanishes and

$${\rm cov}(\alpha_j, \alpha_k) \approx c^2(\Delta b)^2 + (a_j - b)(a_k - b)(\Delta c)^2 \quad \text{for} \quad j \neq k, \quad (4)$$

confirming that these terms and hence also correlation coefficients are indeed due to data reduction and positive. Strong role of background subtraction and normalization was recognized also in the recent evaluation of ^{239}Pu [12].

As an example in Fig. 4 we show ^{58}Ni(n,γ). One can see that adding a strong (Γ_γ,Γ_γ) correlation between resonances prevents the decrease in uncertainties.

3.2 Scattering Radius Uncertainty

Another issue in the resolved resonance region arises from improper treatment of the uncertainty on the scattering radius R'. The scattering radius arises from the potential (hard-sphere) scattering of neutrons from nucleus. Potential scattering makes an important, sometime dominant contribution to the elastic cross sections, so the uncertainty on R' cannot be neglected.

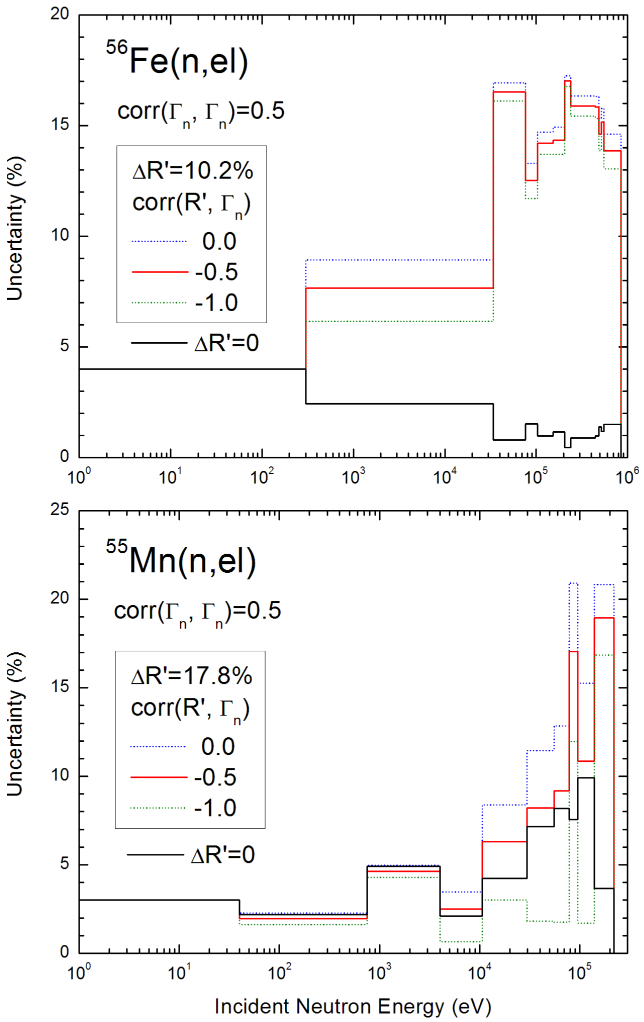

Fig. 5. Importance of $\Delta R'$ to (n,el) uncertainties. In ^{56}Fe uncertainties change dramatically if $\Delta R'$ is included. In ^{55}Mn the impact is smaller, but there is considerable sensitivity to (R',Γ_n) (anti)correlations [11].

Surprisingly, the ENDF-6 format had no provision for $\Delta R'$. This has been noted already in early 1990s by F. Fröhner [13] as a serious deficiency, but his proposal got lost. Only in 2009 CSEWG adopted simple extension, which may not be sufficient since correlations between R' and resonance parameters have not been included.

The impact of scattering radius uncertainty can be illuminated using the recently developed 'kernel approximation' [11]. Average elastic cross section can be expressed as sum of potential and resonance terms,

$$\bar{\sigma}_{el} \approx \bar{\sigma}_{el}^{\rm pot} + \bar{\sigma}_{el}^{\rm res}, \qquad (5)$$

where interference terms are not shown since they approximately cancel out if averaging is done over broad energy bins. To the first order

$$\bar{\sigma}_{el}^{\rm pot} \approx 4\pi R'^2 \quad \text{and} \quad \Delta\bar{\sigma}_{el}^{\rm pot} \approx 2\Delta R'/R' . \qquad (6)$$

Two examples are shown in Fig. 5. In case of ^{56}Fe, potential scattering dominates high resonance energies, hence impact of $\Delta R'$ is particularly dramatic. Consequently, however, impact of anticorrelation between the two terms is small. In case of ^{55}Mn the two contributions are approximately equal, so the (R',Γ_n) anticorrelation is an important factor in final uncertainties.

3.3 Processing Code Issues

Issues have also been encountered with processing of resonance parameter covariances (file MF32) into cross section covariances. Two processing codes, NJOY [9] and PUFF [10], are used at the NNDC, making the processing more robust. The results are nearly identical in most cases, but sometimes significant disagreement is observed. These disagreements appear to be related to evaluations using the Reich-Moore formalism for resonances including several recent evaluations submitted to ENDF/A:

- ENDF/A library contains 24 new MF32 evaluations as candidates for inclusion into future ENDF/B-VII.1. Of these, 7 materials show discrepancies between NJOY and PUFF multigroup covariances [14].
- As an example, in 33-energy groups ^{55}Mn(n,γ) uncertainty at the high resonance end of about 100 keV by NJOY-99.305 is 2.2% while PUFF-IV gives only 0.6%.

It is most desirable that these discrepancies are resolved soon. NJOY and PUFF play an important role in covariance work both for evaluators and users.

4. FAST NEUTRON REGION

In the fast neutron region, least-squares fitting procedures are typically used to produce covariances based on experimental data alone or on combination of data and models. These fitting procedures result in improved values for the cross sections, but frequently produce low uncertainties.

For example, a sophisticated evaluation of ^{56}Fe was performed around 1995 by the reputed group of Vonach, Pronyaev *et al* [15] and included in the JEFF-3.1 library. The evaluation used GLUCS code and employed a detailed approach based on careful analysis of an extensive amount of experimental data. As an important innovation, all reaction channels were fit simultaneously. The resulting precision was unprecedented and viewed by evaluators as a considerable achievement, see Fig. 6. However, these low uncertainties have led users and also experimentalists to question the covariance file.

Since rigorous evaluation procedures produce low uncertainties, the resulting controversy is preprogrammed. The evaluators defend the low uncertainties as being the natural result of their evaluation procedure, but users would challenge them as far too optimistic.

This dilemma has led the NNDC to consider the *dispersion* between evaluations when estimating covariances. The idea is that the spread between cross sections evaluated independently or semi-independently for major data

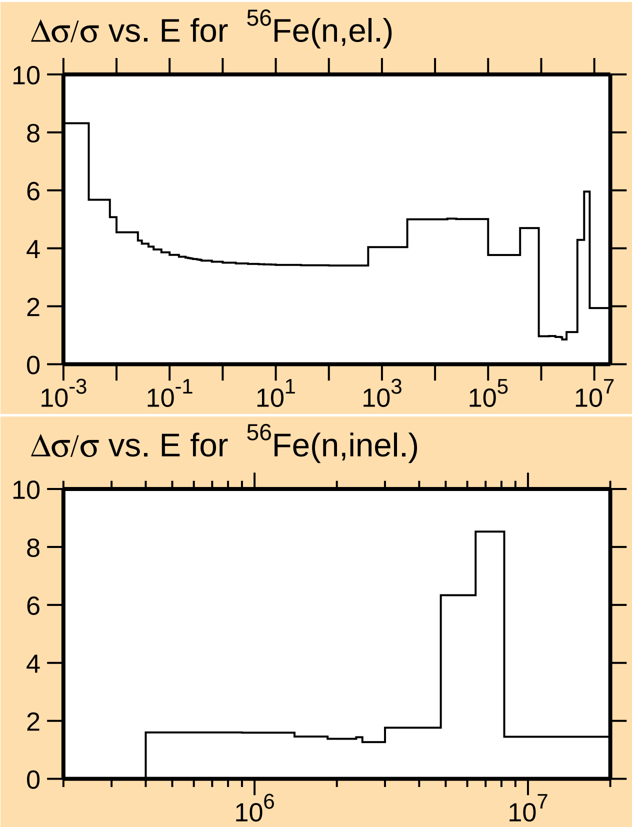

Fig. 6. ^{56}Fe (n,el) and (n,inel) uncertainties from JEFF-3.1. Low uncertainties are generally defended by the evaluators; reactor analysts believe that ^{56}Fe(n,el) should be around 8-10% and (n,inel) 10-15%. Units are in eV and %.

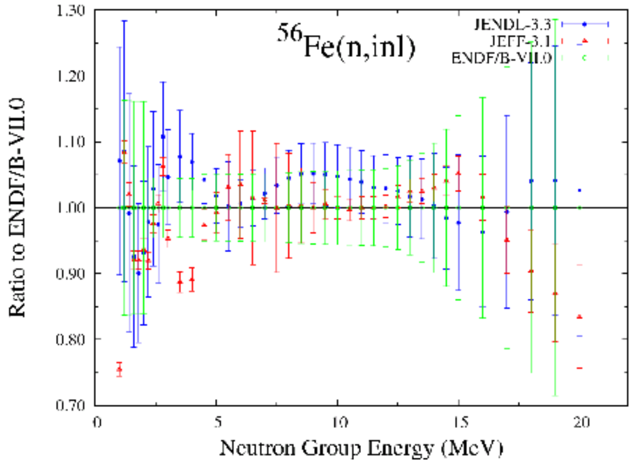

Fig. 7. Dispersion between ^{56}Fe(n,inl) cross sections in JENDL-3.3, JEFF-3.1 and ENDF/B-VII.0. Expanded uncertainties were assigned to AFCI-1.3 covariances based on the observed dispersion [16].

libraries reflect true opinion of the evaluator community about precision of these data. In a dispersion analysis, evaluations from major data libraries are compared, and the uncertainties expanded to reflect the spread between them.

This method has been used before, and has the advantage of being relatively simple and transparent. From the practical point of view it generally produces uncertainties more in line with expectations of users. In reality, users would often do the same, comparing evaluated cross sections in different libraries and consulting experimental data to get a plausible estimate of uncertainties.

On the other hand, we recognize that the dispersion method is controversial. This is mainly because evaluators expect covariances to reflect the evaluation procedure rather than the spread between evaluated libraries.

An example of dispersion analysis for ^{56}Fe(n,inl) [16] is shown in Fig. 7. This analysis was used to provide covariances for AFCI-1.3 library. Evaluated cross sections along with uncertainties from three major data libraries are shown relative to ENDF/B-VII.0. We note that ENDF/B-VII.0 cross sections are identical with ENDF/B-VI.8, from which we also took uncertainties even though they were not taken over by ENDF/B-VII.0. One can see considerable differences between evaluations, especially below about 5 MeV. Thus, AFCI-1.3 evaluators adopted ENDF/B-VI.8 covariances as the basis and expanded the uncertainties taking into account dispersion with the other libraries.

5. QUALITY ASSURANCE

The many issues found in current covariance analyses demonstrate that suitable quality assurance procedures (QA) are clearly required. Currently, there is no consensus on these procedures, though CSEWG in the United States has already begun to consider them.

5.1 QA Procedures at the NNDC

With no agreed-upon standard for covariance QA, the NNDC is using internally developed criteria and tools. These tools include codes STANEF and CHECKR, Sigma retrieval and plotting system, processing codes NJOY and PUFF, and the dedicated code unCor. QA is performed in 4 steps:

1. Checking by STANEF and CHECKR. Files are checked for compliance with the ENDF-6 format including covariances in MF31, 32, 33 and MF35.
2. Processing with NJOY and PUFF. Files are processed to ensure that they can be collapsed into fine as well as coarse energy grids.
3. Visual inspection of major reaction channels. MF33 can be visualized using the Sigma web interface; processed covariances are plotted by NJOY. Plots reveal low, high, and strongly discontinuous uncertainties which likely indicate problems in the covariance.
4. Checking with 'unCor'. Processed covariances for *all* materials and all reaction channels are checked. The code reads the covariances produced by NJOY and raises warnings when they fall outside adopted criteria.

Table 1. Minimal acceptable uncertainties used in unCor-1.1.

Reaction	Min. uncertainty
(n,tot)	1%
(n,el)	2%
(n,γ)	2%
(n,inel)	3%
(n,f)	0.7%
$\bar{\nu}$	0.7%
Other	3%

5.2 Covariance Checking Code 'unCor'

'unCor' (uncertainties and correlations) is a dedicated code developed by the NNDC, designed to check the entire processed covariance library. It performs systematic testing of all available data and issues warnings to be analyzed by reviewer and/or evaluator. The code performs two types of tests:

Uncertainties

- Small uncertainties. The criteria are summarized in Table 1. While some uncertainties below these thresholds may be justified, they warrant further attention.
- Large uncertainties. Criterion: $\Delta\sigma > 100\%$. In some cases these may be warranted, but may cause problems for users not ready to handle asymmetric uncertainties.
- Completeness. Criterion: if $\sigma > 0$, then $\Delta\sigma > 0$; this criterion is obligatory.
- Shape of uncertainty curve. Sudden discontinuities may arise from problems in the analysis, or from merging two or more sections produced by different methods to a full covariance matrix.

Matrices

- Basic properties. A symmetric matrix with diagonal = 1.0 and off-diagonal between -1.0 and +1.0 is required for correlations.
- Positive-definiteness. This is important test for eigenvalues of covariance matrices. Problems should be identified and fixed. However, the limited precision used in the ENDF-6 format may mean that some negative eigenvalues in processed results are unavoidable [17].
- Sum rule for MF35. The rows and columns of a covariance matrix for a normalized distribution should sum to zero. Adopted criteria: the absolute value of the sum should be 10^{-6} or less for each row.

New additions to the code are under consideration. Thus, some materials, such as threshold fissioners, may be treated as special cases with different values for acceptable uncertainties. It might be useful to check uncertainties against absolute values of cross sections. The code should also be extended to check cross-reaction covariances.

6. CONCLUSIONS

Robust neutron cross section covariances are required by several users' communities. Probably the major challenge faced by the evaluators lies in the lack of suitable quality covariance assurance procedures. Such methods would help to produce evaluations that are better suited to the needs of users. Specific problems, particularly low uncertainties, cause users to question current evaluations.

The purpose of this paper was to initiate an effort to establish basic quality assurance guidelines for covariance matrices, that should be agreed upon by all major nuclear data evaluation projects. This may be best accomplished by a new WPEC subgroup devoted to quality of covariances.

ACKNOWLEDGMENTS

We are grateful to our NNDC colleagues for numerous discussions on the subject. Brookhaven National Laboratory is sponsored by the Office of Nuclear Physics, Office of Science of the U.S. Department Energy under Contract No. DE-AC02-98CH10886 with Brookhaven Science Associates, LLC.

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