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## Generation of Covariance Files for the Isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI

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Engineering Physics and Mathematics Division

**GENERATION OF COVARIANCE  
FILES FOR THE ISOTOPES OF Cr,  
Fe, Ni, Cu, AND Pb IN ENDF/B-VI**

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## ABSTRACT

The considerations that governed the development of the uncertainty files for the isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI are summarized. Four different approaches were used in providing the covariance information. Some examples are given which show the standard deviations as a function of incident energy and the corresponding correlation matrices.



# 1. INTRODUCTION

Covariance data are required to assess uncertainties in design parameters of fusion reactors and to refine the use of nuclear data in reactor applications. This paper summarizes the considerations which governed the development of the uncertainty files for the isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI. First, some background information for the evaluations is appropriate.

References to experimental data sets used in the evaluations were obtained primarily from CINDA but also from the literature and reports. The nuclear model code TNG (FU88, SH86) was the primary model code used for the evaluations. TNG is an advanced multistep Hauser-Feshbach code which includes precompound and compound contributions to cross sections in a self-consistent manner, provides correlated angular and energy distributions, calculates gamma-ray production, and conserves angular momentum in all steps. For each isotope, extensive model calculations were performed with the goal of simultaneously reproducing measured data (within experimental uncertainties) for all reaction channels with one set of parameters (FU86). This method ensures internal consistency and energy conservation within each evaluation. Thus, evaluations for ENDF/B-VI are based on a combination of experimental data and nuclear model calculations.

The following section reviews the methods used in constructing the covariance files for the evaluations. In Section 3, some examples are given which show the standard deviations as a function of incident energy and the corresponding correlation matrices. A short conclusion is given in Section 4.

## 2. METHODS

Covariances are provided in ENDF/B-VI for all reactions given in file MF = 3, including inelastic scattering (levels and continuum). However, at present, no covariance information is given for distributions included in the evaluations (files MF = 4 and 6), nor for resonance parameters or gamma-ray production. Four approaches were taken to provide covariance information, depending upon the quantity and quality of available experimental data.

In the first approach, when sufficient data were available for a reaction (such as for the  $(n, p)$  reaction in  $^{54}\text{Fe}$ ,  $^{56}\text{Fe}$ , and  $^{58}\text{Ni}$ , the  $(n, 2n)$  reaction for  $^{63}\text{Cu}$  and  $^{65}\text{Cu}$ , and the  $(n, \alpha)$  reaction for  $^{63}\text{Cu}$ ), a Bayesian analysis using the GLUCS code (HE80) was done, using ENDF/B-V as the prior. GLUCS provides updated cross sections and covariances in ENDF/B-VI format. Of the methods used, this is the most rigorous and will not be discussed in this report. In the second approach, if insufficient data were available for a GLUCS analysis on a reaction, the scatter among the data sets selected for evaluation was estimated and used to construct the covariance file. For the third approach, if the evaluated cross section depended primarily on TNG calculations, uncertainties were assigned as shown in Table 1, based on the magnitude of the cross section, in order to construct a covariance file.

Table 1. Assigned uncertainties for calculated cross sections.

Cross Section X (mb)	Standard Deviation
$500 < X$	10%
$100 < X < 500$	15%
$30 < X < 100$	20%
$X < 30$	$\geq 30\%$

This assumes that nuclear model codes are more reliable in their predictions for reactions which have large cross sections than for reactions which have small cross sections. A fourth approach was to describe the covariances in energy ranges where the cross sections in file MF = 3 can be derived in terms of other evaluated cross sections in the same energy range. This is often done to insure that correct correlations are obtained, for example, when the relatively large elastic and nonelastic uncertainties must be combined to be consistent with the relatively smaller uncertainties of the total cross section. Due to the number of evaluations that ORNL is responsible for and resulting time constraints, methods that consider uncertainties of model parameters (e.g., see Kanda and Uenohara (KASS), Zhao et al. (ZH90)) were not used for the first phase of the evaluations.

For most reactions the following algorithm was used to construct the covariance file, starting with the second and third approaches described above. Short-range (i.e., small energy intervals - typically 2 to 4 MeV) correlations using fractional components correlated within each energy interval were assembled using the "NI type" LB=1 sub-subsection in File 33 (PE78). The fractional components were assigned using either available data uncertainties from measurements or the assigned uncertainties listed in Table 1 in the case of calculated cross sections. The energy range of the correlation was based on experimental information, if available, or evaluator judgement. The short-range correlations were used to relay information

primarily on the perceived uncertainty in the shape of the cross sections. An absolute component for the whole energy range from threshold to 20 MeV was included using the "NI type" LB=0 sub-subsection in File 33 if the reaction has cross section values which differ by orders of magnitude, such as often occur at total cross section minima, near thresholds, or at high incident energies. This absolute component was typically taken as a percentage of the smallest cross section value in the file for the reaction. For example, for  $^{56}\text{Fe}$ , this percentage varied from 5% for reactions with large minimum cross sections to over 100% for reactions with very small minimum cross sections ( $\ll 1$  mb). Note that this component provides appropriately larger uncertainties for the smallest cross section values.

For the total (MT=1), nonelastic (MT=3), and capture (MT=102) cross sections, long-range (i.e., large energy intervals — typically 1 to 3 intervals from threshold to 20 MeV) correlations taken from available data (e.g., normalization effects, boundaries between different data sets, etc.) were assembled using the LB=1 sub-subsection. The long-range correlations were used to relay information about uncertainty in the absolute value of a cross section. In the absence of experimental information, the short-range uncertainties were compiled (as explained above) first and the long-range covariance component (one energy interval from threshold to 20 MeV) was derived by using one-half of the minimum value of the short-range components. The short range uncertainties were then divided by two to compensate for the effective removal of the estimated long-range correlations. That is, it was desired to have long-range correlations when no experimental information was available, and experience with measured data led to this method of estimating the long-range uncertainties from the assigned short-range uncertainties. See Appendix A for an example showing how the covariance file was generated for the  $^{60}\text{Ni}(n, 2n)$  reaction.

To ensure that processed covariance matrices are positive-definite, the required LB=8 sub-subsection (see RO90) was derived from the resulting short-range correlations. This was done by taking a fraction  $F$  from the short-range covariance component (for each energy interval) and multiplying this value by the square of the cross section for the appropriate energy interval (from file MF = 3) for inclusion into the LB=8 sub-subsection format. The resulting short-range values were then finalized by taking  $(1 - F)$  times the initial short-range components (see Appendix A). After testing this algorithm extensively by comparing results from this ad-hoc method to calculations from the GLUCS code (FUS2), the fraction  $F$  chosen for the method was 0.01 for the total, elastic, nonelastic, and capture cross sections and 0.10 for all other reactions. The smaller fraction was used for the total, elastic, nonelastic, and capture because of problems caused by the small energy intervals and resulting discontinuities in the cross section file. That is, recognize that the variance contribution  $VAR_{jj}$  from an LB=8 sub-subsection to the processed group variance for the energy group  $(E_j, E_{j+1})$  is inversely proportional to its width  $\Delta E_j$  and is obtained from

$$VAR_{jj} = F_k \Delta E_k / \Delta E_j ,$$

where  $E_k \leq E_j < E_{j+1} < E_k + 1$  and where the  $E_k$ 's and  $F_k$ 's come from file 33 and the  $E_j$ 's come from file 3 (if one desires the processed covariance matrix on the  $E_j$  grid), or from group boundaries. Thus, if the energies in file 3 are very close together and the energies in file 33 are far apart, an unreasonably high standard deviation can result. Choosing the fraction  $F$  as 0.01 in these cases helped to minimize this problem. Again, see Appendix A for an example.

## 4 METHODS

In the fourth approach, the covariances for portions of the total, elastic, and nonelastic reactions are derived using the "NC type" sub-subsections (PE78). That is, a combination of explicit and derived uncertainties were used. The uncertainties for the total inelastic cross section ( $MT = 4$ ) were totally derived. Derived is used here in the context that a reaction type (and therefore its uncertainties) may be determined by summing other reaction types. The "NI type" sub-subsections are the basis for the construction of the "NC type" sub-subsections. The use of the "NI type" sub-subsections for the production of the "NC type" derived redundant cross section covariances is demonstrated by Smith (SM80). Note that for all reactions with  $MT$  greater than four, we use explicit uncertainties only, no derived uncertainties.

There are several ways to form uncertainty files for  $MT = 1, 2, 3,$  and  $4$ . One option is to give them all explicitly, but this does not take advantage of the constraints among the various cross sections. They cannot all be derived since a derived file cannot be used in another derived file. In general, we used the following scheme to obtain  $MT = 1, 2, 3, 4$  uncertainty files, consistent with the given considerations:

- a. The total cross-section ( $MT = 1$ ) uncertainties are generally well known at thermal, in the resonance region, and up to 20 MeV.
- b. The elastic-scattering cross-section ( $MT = 2$ ) uncertainties are generally well known at thermal and in the resolved resonance region, but not from the end of the resolved resonance region to several MeV due to structure (experimentally undefined) in the cross section (which occurs as a result of obtaining  $3/2$  from  $3/1 - 3/3$ ).
- c. The nonelastic cross-section ( $MT = 3$ ) uncertainties up to the threshold of the first reaction are given by the capture cross-section uncertainties, and above the threshold are defined by data and optical model uncertainties to 20 MeV.
- d. The total inelastic cross-section ( $MT = 4$ ) uncertainties may be estimated more accurately from the uncertainties for the nonelastic and other partial components of the nonelastic than obtained simply by summing uncertainties given for  $MT = 51-91$ , which may be large.

With these caveats, the uncertainties for  $MT = 3$  from  $1.E-5$  eV to the end of the resolved resonance region (or to the threshold of the first reaction in some cases) are given as derived (33/102). From the end of the resolved resonance region to 20 MeV the uncertainties for  $MT = 3$  are given explicitly based on uncertainties estimated from data and the optical model.

Next, the uncertainties for  $MT = 4$  are derived from threshold to 20 MeV as (33/3 - 33/16 - 33/22 - 33/28 - 33/102 - 33/103- ...).

Then, looking at the elastic cross-section ( $MT = 2$ ) uncertainties, from  $1.E-5$  eV to some arbitrary energy  $E$  between thermal and the first resonance (determined by where the smooth cross-section shape begins to be affected by the lowest resonance), the uncertainty is given explicitly which insures the correct thermal uncertainty. From  $E$  to the first reaction threshold the uncertainties are derived as (33/1 - 33/102), and from threshold to 20 MeV the uncertainties are derived as (33/1 - 33/3).

Finally, the uncertainties for the total cross-section ( $MT = 1$ ) from  $1.E-5$  eV to  $E$  are derived (33/2 + 33/102). This insures the correct uncertainties at thermal.

From  $E$  to 20 MeV, the uncertainties are explicitly given, based on experimental data.

The above method of obtaining uncertainties for  $MT = 1, 2, 3, 4$  generally achieves the desired goals noted above, and uses the concepts of derived and explicit uncertainties in a consistent manner. However, it is surely not the only way of representing uncertainties for these cross sections.

### 3. RESULTS AND DISCUSSION

Tables 2-5 show results for the  $^{56}\text{Fe}(n,p)$ ,  $^{56}\text{Fe}(n,2n)$ ,  $^{60}\text{Ni}(n,2n)$ , and  $^{56}\text{Fe}$  nonelastic cross sections, respectively. The first approach (using GLUCS) described above was used in constructing the covariances for the  $^{56}\text{Fe}(n,p)$  cross sections. The second approach was used for  $^{56}\text{Fe}(n,2n)$ , while the third approach was used for  $^{60}\text{Ni}(n,2n)$ . For the  $^{56}\text{Fe}$  nonelastic cross sections, both the second and fourth approaches were used. Note that for clarity selected points have been deleted from the cross sections for these tables.

The  $^{56}\text{Fe}(n,p)$  covariances are taken from the GLUCS calculation (FU82) in which this reaction was studied simultaneously with 13 other dosimetry reaction cross sections correlated by ratio data (see Table 2). The standard deviations at high incident energies seem low, but are due to high-precision absolute cross sections for energies from 14.67 to 18.95 MeV for this reaction from the National Physical Laboratory in Great Britain (PA79).

The  $^{56}\text{Fe}(n,2n)$  covariances shown in Table 3 are estimated from the scatter of the measured data and the file was constructed according to the method described above. The effect of the absolute component can be seen at energies close to threshold.

The  $^{60}\text{Ni}(n,2n)$  cross section was calculated by TNG and no data were available, thus the uncertainties were assigned as a function of cross section magnitude from those listed in Section 2. The covariance file was constructed according to the method described above and the results are given in Table 4.

Note that in Table 5 the standard deviations for the  $^{56}\text{Fe}$  nonelastic cross sections are large when the incident energy intervals are small. This characteristic is directly related to the variance contribution from the LB=8 sub-subsection (see explanation above). In this case, if the fraction  $F$  that was used ( $F = 0.01$ ) were higher, the standard deviations for  $E_n$ 's of 1.012, 1.013, and 1.298 MeV would be even larger than those shown in Table 5. Also, note that the covariances for the nonelastic cross section from  $1.0\text{E}-5$  to  $8.6227\text{E}+5$  eV are derived from the capture covariances. The blocks of zero correlations in the matrix reflect the fact that the experimental data are uncorrelated in these regions.

Table 2. Covariance information for the  $^{56}\text{Fe}(n,p)$  cross section

	$E_n$ (MeV)	$\sigma$ (mb)	St. Dev. (%)	Correlation Matrix														
				1	2	3	4	5	6	7	8	9	10	11	12	13		
1	2.9655	0.00																
2	3.0	7E-6	18.75	100														
3	4.5	0.14	14.42		100													
4	5.0	1.07	12.33			100												
5	6.0	12.73	7.38				100											
6	8.0	41.73	3.40					100										
7	11.0	82.41	3.64						100									
8	12.0	103.35	3.76							100								
9	13.0	115.23	3.18								100							
10	14.6	109.34	1.81									100						
11	17.0	71.63	1.47										100					
12	18.0	61.30	1.51											100				
13	20.0	50.55	1.51												100			

Table 3. Covariance information for the  $^{56}\text{Fe}(n,2n)$  cross section

	$E_n$ (MeV)	$\sigma$ (mb)	St. Dev. (%)	Correlation Matrix														
				1	2	3	4	5	6	7	8	9	10	11	12	13		
1	11.402	0.00																
2	11.5	2.24	282.52	100														
3	11.6	7.59	83.87		100													
4	11.8	25.04	27.08			100												
5	12.0	49.93	17.48				100											
6	12.4	111.59	11.71					100										
7	13.5	317.68	9.97						100									
8	14.0	402.04	10.84							100								
9	15.5	556.52	10.33								100							
10	16.0	582.71	10.78									100						
11	17.5	611.45	10.69										100					
12	18.0	609.92	10.77											100				
13	20.0	575.40	10.89												100			

Table 4. Covariance information for the  $^{60}\text{Ni}(n,2n)$  cross section

	$E_n$ (MeV)	$\sigma$ (mb)	St. Dev. (%)	Correlation Matrix								
				1	2	3	4	5	6	7		
1	11.581	0.00										
2	12.0	19.74	22.78	100								
3	13.0	168.96	13.60		100							
4	14.5	385.90	12.56			100						
5	16.0	496.33	12.46				100					
6	17.5	519.55	10.00					100				
7	20.0	480.89	10.04						100			

Table 5. Covariance information for the nonelastic cross section of  $^{56}\text{Fe}$ 

$E_n$ (MeV)	$\sigma$ (mb)	St. Dev. (%)	Correlation Matrix																		
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
1	1E-11	1.3E5	7.19	100																	
2	1E-7	1300.	15.21	15	100																
3	1E-4	40.0	8.19	27	13	100															
4	0.1	10.0	7.64	0	0	0	100														
5	0.8	4.0	21.62	0	0	0	22	100													
6	0.863	20.3	5.13	0	0	0	0	0	100												
7	1.012	270.9	43.24	0	0	0	0	0	2	100											
8	1.013	287.9	40.70	0	0	0	0	0	2	1	100										
9	1.014	322.8	6.94	0	0	0	0	0	11	7	7	100									
10	1.298	596.7	20.03	0	0	0	0	0	4	2	2	14	100								
11	1.299	598.5	4.81	0	0	0	0	0	16	10	10	59	21	100							
12	1.583	791.1	4.60	0	0	0	0	0	17	10	11	62	22	90	100						
13	2.235	953.3	4.47	0	0	0	0	0	17	2	2	13	4	19	19	100					
14	7.500	1441.3	5.11	0	0	0	0	0	0	0	0	0	0	0	0	0	100				
15	10.00	1423.1	5.24	0	0	0	0	0	0	0	0	0	0	0	0	0	34	100			
16	14.50	1378.0	5.88	0	0	0	0	0	0	0	0	0	0	0	0	0	30	29	100		
17	17.50	1295.4	5.20	0	0	0	0	0	0	0	0	0	0	0	0	0	34	33	81	100	
18	20.00	1239.8	5.22	0	0	0	0	0	0	0	0	0	0	0	0	0	34	33	81	91	100

## 4. CONCLUSIONS

The methods described in this note were used for the initial ENDF/B-VI release to construct the covariance files for most of the reactions for the isotopes of Cr, Fe, Ni, Cu, and Pb; a GLUCS analysis was used on relatively few reactions. Admittedly, the method is quite simple, but the goal for the first phase of these evaluations was reasonableness and consistency across isotopes and reactions for the structural materials, and this goal has been met. There are problems such as the idiosyncrasies caused by the LB=8 sub-subsection, a fix that was imposed in order to make the processed covariance matrices positive-definite. It appears that including the LB=8 sub-subsection should be reconsidered in the future for some reactions. However, the method is a significant improvement over what was commonly done in the past when only LB=1 sub-subsections were used, resulting in fully-correlated submatrices in the correlation matrix.

The next step towards improvement of the uncertainty files is to use methods that consider uncertainties of the most sensitive model parameters based on the scatter of measured data around the theoretical curves and the long-range correlation error of the data, such as the methods proposed by Kanda and Uenohara (KA88) and as was done for the  $^{19}\text{F}$  evaluation (ZH90). Also, covariances should be included for the distributions in files MF = 4 and 6, and options to accomplish this need to be studied. Finally, covariances for the important resonance parameters as well as for gamma-ray production need to be included.

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## APPENDIX A. EXAMPLE OF HOW A COVARIANCE FILE WAS GENERATED

The following example demonstrates how the covariance file was generated for the  $^{60}\text{Ni}(n, 2n)$  reaction. The cross sections for this reaction were taken from the TNG calculation as no data were available. The (neutron energy (MeV), cross section (mb)) pairs are:

(11.581, 0.0) (12.0, 19.739) (13.0, 168.96) (14.5, 385.9)  
(17.5, 519.55) (20.0, 480.89).

The total uncertainties for the cross sections, given initially as short-range components, were generated from Table 1. That is, from threshold to 13.0 MeV was assigned a 30% standard deviation, from 13.0 MeV to 17.5 MeV was assigned a 15% standard deviation, and from 17.5 MeV to 20.0 MeV was assigned a 10% standard deviation. These short-range components are given as  $(E_n, (\Delta\sigma)^2)$  pairs using the LB=1 sub-subsection format:

(11.581, 0.09) (13.0, 0.0225) (17.5, 0.01) (20.0, 0.0).

Note that the format dictates an uncertainty of 0.0 be used at 20.0 MeV. Next, the long-range component was generated by taking one-half of the minimum of the short-range components (i.e.,  $0.01/2.0 = 0.005$  at 17.5 MeV). Thus the long-range component in LB=1 format is:

(11.581, 0.005) (20.0, 0.0).

To preserve the total uncertainty at the energy where the uncertainty is the smallest (i.e., at 17.5 MeV), the short range components given above are divided by 2.0 to compensate for the removal of the long-range component:

(11.581, 0.045) (13.0, 0.01125) (17.5, 0.005) (20.0, 0.0).

Thus, combining the short- and long-range components retain the total uncertainty of 10% at 17.5 MeV. Finally, the LB=8 components are "backed out" from the reduced short-range components by taking 10% from the LB=1 short-range values and multiplying by the appropriate cross section value from file 3, squared. The final results for the short-range components in LB=1 format are:

(11.581, 0.0405) (13.0, 0.010125) (17.5, 0.0045) (20.0, 0.0).

The results for the LB=8 sub-subsection are (the cross sections are in barns):

(11.581, 1.7533E-6) where  $1.7533\text{E-}6 = (0.019739)^2 * 0.10 * 0.045$   
(13.0, 3.2116E-5) where  $3.2116\text{E-}5 = (0.16896)^2 * 0.10 * 0.01125$   
(17.5, 1.3497E-4) where  $1.3497\text{E-}4 = (0.51955)^2 * 0.10 * 0.005$   
(20.0, 0.0)

Note that the cross section used to calculate the component at threshold (11.581 MeV) was taken from the energy closest to the threshold energy (i.e., 12.0 MeV).

The resulting standard deviations and correlation matrix for the  $^{60}\text{Ni}(n, 2n)$  cross section are as follows:

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	$E_n$ (MeV)	$\sigma$ (mb)	St. Dev. (%)	Correlation Matrix						
				1	2	3	4	5	6	7
1	11.581	0.00								
2	12.0	19.739	22.778		100					
3	13.0	168.960	13.601		16	100				
4	14.5	385.900	12.559		17	89	100			
5	16.0	496.330	12.456		18	89	97	100		
6	17.5	519.550	10.000		22	37	40	40	100	
7	20.0	480.890	10.042		22	37	40	40	95	100

The smallest assigned uncertainty was 10% at 17.5 MeV, and we note that this value is retained, even though it has been divided into three components.

The use of the LB=8 sub-subsection can result in unreasonably high standard deviations if the energy grid for the cross sections is much finer than the energy grid in the covariance file. For example, if the file 3 and 33 energy grids are

```
file 3  ... 5.0 5.05 5.10 ...
file 33 ... 5.0 10.0 15.0 ...
```

then the variance contribution at 5.0 MeV is

$$VAR_{jj} = Fk\Delta Ek/\Delta E_j = Fk * (10.0 - 5.0)/(5.05 - 5.0) = Fk * 100.0$$

Thus, one must be careful in these cases to choose a finer energy grid in file 33, or use a smaller fraction than 10% when backing out the LB=8 components (e.g., use 1% or less), or both.

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