Nuclear Data and Integral Measurements
Correlation for Fast Reactors.
Part 3: the Consistent Method

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1. **FORWORD**

One of the major difficulties encountered in the adjustment procedure of cross-sections relevant to fast reactor analysis has resulted the proper assessment of their dispersion matrix. Attempts in this direction have been made by a few authors and reviewed in the second part (see Ref. [2]). The covariant terms relative to intercorrelations between different cross-sections should result directly from the theoretical assumptions and experimental peculiarities of the differential data adopted in the cross-section group reduction. There seem to be, however, a number of drawbacks within this procedure, a major one consisting in the lack of flexibility of the adjusted group cross-section library. In other words if, for instance, a calculation with an higher number of groups would be required, a somehow arbitrary redistribution of corrections and errors should be made with a consequent loss of reliability of the adjusted data. In order to avoid all these difficulties, a consistent method of correlation is proposed which is based on correcting directly the nuclear parameters in a way which should result consistent with the more or less sophisticated theoretical models adopted by the code used for the group cross-section generation. These adjusted parameters should then replace the older ones so that any type of adjusted cross-section library may thereafter be formed. Assuming, as references,
the ENDF/B library files and the algorithms for group cross-
section generation of the ETOX type [3] (as used by the MC
2 code [47]), in the present paper it is shown how the procedures
to be adopted with this method are all reasonably feasible. A
few simplifying assumptions are made which appear, however, to
amount, on the whole, to a considerable improvement in com-
parison with the methods of correlation previously considered.

For simplicity, references to formulations to be
found in the first and second part of this paper (Ref.[1]
and [2]) are made directly and distinguished by the roman
numbers I and II, respectively (for example: Eqn.(15/I)).
2. **THE CONSISTENT CORRELATION METHOD**

As mentioned before, it consists in estimating directly the parameters which are present in the data file and processed by means of the algorithms for group cross-section generation. Therefore, for the generic group cross-section \( \sigma_i \) we may write

\[
\sigma_i = \sigma_i(q_1, q_2, \ldots) \quad (1.1)
\]

where \( q_k \) represent a given number \( K \) of nuclear parameters. Supposing we know the derivatives

\[
\frac{q_{ok}}{\sigma_{oi}} \frac{\partial \sigma_i}{\partial q_k} = z_{ik} \quad (2.1)
\]

where \( q_{ok} \) and \( \sigma_{oi} \) are given values close to the true ones, the relative difference \( (\sigma_i - \sigma_{oi})/\sigma_{oi} \), between the expected (or true) and given values may be expressed, along with Eqn. (2.1), by the linear expansion

\[
\frac{\sigma_i - \sigma_{oi}}{\sigma_{oi}} = \sum_{k=1}^{K} z_{ik} \frac{q_k - q_{ok,k}}{q_{oi,k}} \quad (3.1)
\]

The formulations derived so far for the cross-section adjustment still hold, if proper redefinitions of the symbols is
made. For this purpose, we shall define, along with Eqns. (4/I) and (15/I), the new quantities

\[
\frac{q_{1} - q_{a,1}}{q_{a,1}} = \gamma_{j=1}, \quad (i = 1, \ldots, K) \quad (4,1)
\]

\[
\frac{q_{1}^{\text{ex}} - q_{a,1}}{q_{a,1}} = \gamma_{j=1}^{\text{ex}}, \quad (i = 1, \ldots, K) \quad (5,1)
\]

the dispersion matrix

\[
\begin{pmatrix}
\rho_{Q} & 0 \\
0 & \rho_{Q}
\end{pmatrix}, \quad (6,1)
\]

\(\rho_{Q}\) and \(\rho_{Q}\) being the dispersion matrices of the integral experiments and nuclear parameters, respectively, and the matrix

\[
\mathcal{S} = \mathcal{W} \times \mathcal{Y}, \quad (7,1)
\]

\(\mathcal{S}\) being the number of group cross-sections, \(\mathcal{W}\) representing a \((J \times J)\) unit matrix, i.e. of dimensions equal to the number of integral data \(Q_{j}\), and \(\mathcal{Y}\) the \((K \times K)\) matrix of the new coefficients \(Z_{ik}\) which multiplies that of the usual sensitivity coefficients \(\frac{\partial Q_{j}}{\partial q_{a,1}} \frac{\partial q_{a,1}}{\partial \sigma_{i}}\). If we suppose that the number
of nuclear parameters results, which is likely, greater than the number of integral experiments, the Lagrange multipliers method results preferable and the formulations derived in part 1 (namely, Eqns. (21/1), (34/1) and (35/1) in which \( \Delta \) is set zero) should be adopted. We obtain:

\[
\mathbf{\tilde{y}} = \left[ \mathbf{\theta} - \mathbf{\theta}_y \mathbf{S}_y^T \mathbf{G}^{-1} \mathbf{S}_y \right] \mathbf{x}^\infty
\]

(6.1)

where

\[
\mathbf{G} = \mathbf{S}_y \mathbf{S}_y^T.
\]

(9.1)

Similarly, the dispersion matrix of the resulting estimates is given, along with Eqn. (42/1), by the expression:

\[
\mathbf{\tilde{\sigma}_y} = \left( \mathbf{\sigma}_y - \mathbf{c} \mathbf{\theta}_y \right)
\]

(10.1)

where

\[
\mathbf{c} = \mathbf{\theta}_y \mathbf{S}_y^T \mathbf{G}^{-1} \mathbf{S}_y.
\]

(11.1)

\( \mathbf{\theta}_y, \mathbf{S}_y^T \) and \( \mathbf{G} \) being defined by Eqns. (6.1), (7.1) and (9.1) respectively.

Once an integral parameter \( \mathbf{\tilde{p}} \) has been evaluated using the cross-sections \( \tilde{\sigma} \), adjusted in accordance with parameters \( \tilde{\mathbf{a}} \), it is usually required to know the accuracy of this estimate. Since this integral quantity may be expressed by a linear expansion around a value \( P_0 \) calculated using given cross-sections \( \sigma_0 \) (sufficiently close to the expected ones), i.e.

\[
\mathbf{\tilde{p}} - P_0 = \mathcal{L} \mathbf{\tilde{\sigma}}
\]

(12.1)

\( \mathcal{L} \) representing a given one-row matrix, and since the dispersion matrix \( \mathbf{\tilde{\sigma}} \) of \( \mathbf{\tilde{\sigma}} \) is given, in accordance with Eqn. (3.1),
by the expression
\[ \Omega_{\varphi} = \mathcal{L} \Omega_{\varphi} \mathcal{L}^{-1} , \quad (13.1) \]
the variance \( \mathcal{D}(\widehat{\varphi}) \) of the given integral parameter results
\[ \mathcal{D}(\widehat{\varphi}) = \mathcal{L} \Omega_{\varphi} \mathcal{L}^{-1} . \quad (14.1) \]
3. ACCURACY OF THE SELF-SHIELING FACTORS

A few problems arise in presence of resonances of the various materials constituting the reactors. If the factorization formulation inherent with the self-shielding approach is used, the basic approximation which, for simplicity, has to be adopted consists in assuming that the inaccuracies of the self-shielding coefficients are second-order with respect to those of the infinite dilution cross-sections. We shall try to analyse this point. Since the self-shielding coefficients \( f_x \) are given, within a generic group of lethargy width \( \Delta u \) of limits \( u_1 \) and \( u_2 \), by the expression

\[
f_x = \frac{1}{\sigma_{x\infty}} \left( \frac{u_2}{u_1} \right) \int_{u_1}^{u_2} \frac{\sigma_x(u)}{\Sigma_T(u)} \, du \tag{1.2}
\]

where

\[
\sigma_{x\infty} - \langle \sigma_x \rangle = \frac{1}{\Delta u} \int_{u_1}^{u_2} \sigma_x(u) \, du \tag{2.2}
\]

and
\[ \frac{1}{\Sigma_T} = \frac{1}{\Delta u} \int_{u_1}^{u_2} \frac{1}{\Sigma_T(u)} \, du, \quad (3.2) \]

deriving it with respect to a generic nuclear parameter \( q_k \), gives
\[
\frac{\partial f_x}{\partial q_k} = \frac{1}{\Delta u} \int_{u_1}^{u_2} \frac{1}{\Sigma_T(u)} \frac{\partial \Sigma_T(u)}{\partial q_k} \left( f_x - \frac{\sigma_x(u)}{\sigma_{x,\infty}} \right) \, du + \\
+ \frac{1}{\Delta u} \frac{1}{\sigma_{x,\infty}} \int_{u_1}^{u_2} \frac{\partial \sigma_x(u)}{\partial q_k} \left( \frac{1}{\Sigma_T(u)} \sigma_{x,\infty} \right) \, du. \quad (4.2)
\]

In order that the factorization formulation of the cross-sections be acceptable, it should result that this derivative is small as compared to \( \frac{f_x}{\sigma_{x,\infty}} \). We see first that the quantity
\[
\frac{1}{\Sigma_T^2} \left( f_x - \frac{\sigma_x}{\sigma_{x,\infty}} \right) \quad (5.2)
\]
clearly oscillates around zero and in those cases where the deviation from zero is high the coefficient \( 1/\Sigma_T^2 \) makes the contribution again small (at least for those situations in which the density of the resonant material is significant so that the infinite dilution approximation does not result automatic). The major difficulties arise from the second term at the right hand side of Eqn. (4.2). However, since this term
may also be written

\[
\frac{1}{\sigma_{x_{\infty}}} \left( g_{x, k} - f_{x} \right) \left\langle \frac{\partial \sigma_{x}}{\partial q_{k}} \right\rangle \tag{6.2}
\]

where \( g_{x, k} \) represents the self-shielding coefficient of the derivative \( \partial \sigma_{x}/\partial q_{k} \), i.e.

\[
g_{x, k} = \int_{u_{l}}^{u_{u}} u \frac{\partial \sigma_{x}(u)}{\partial q_{k}} \frac{1}{E_{T}(u)} \, du \\
\Delta u \left\langle \frac{1}{E_{T}} \right\rangle \left\langle \frac{\partial \sigma_{x}}{\partial q_{k}} \right\rangle \tag{7.2}
\]

and assuming that the difference \( (g_{x, k} - f_{x}) \) is small, the self-shielding effect presumably influencing in a similar fashion the cross-section and its derivative, we see that it should result second order as compared to the average value \( 1/\sigma_{x_{\infty}} \left\langle \frac{\partial \sigma_{x}}{\partial q_{k}} \right\rangle \) (and therefore, to \( \frac{f_{x}}{\sigma_{x_{\infty}}} \frac{\partial \sigma_{x_{\infty}}}{\partial q_{k}} \)).

In order to derive the formulations giving the coefficients \( z_{1k} \), we will consider separately the unresolved and resolved resonance regions. Within the first region we will examine the parameters relevant to absorption and fission processes. Within the second region we will consider the elastic scattering and the absorption cross-section of the fertile and structural materials.
4. UNRESOLVED RESONANCES REGION PARAMETERS

Let us consider the infinite dilution capture (radiative absorption and fission) cross-sections in the unresolved region. This region extends from about 1 KeV (4 KeV for U-238, 0.5 KeV for Pu-239 and U-235) to about 50 KeV and is of major interest for fast reactors as far as the sensitivity of the relevant integral parameters to differential data is concerned. Let us then assume that the sensitivity \( a_x^g \) of the integral parameters is calculated in a relatively small number (\( \sim 30 \)) of groups. Since the change \( \delta Q \) of a given integral parameter is given by the expression

\[
\delta Q = \sum_{\kappa, g, k} a_x^g f_x^g \frac{\partial \sigma_{\infty}^g}{\partial q_k} \delta q_k
\]

(1.3)

\( f_x^g \) being the self-shielding coefficient while \( \kappa, g, k \) reaction, group, nuclear parameter indexes, respectively, the problem consists in the evaluation of the derivatives \( \frac{\partial \sigma_{\infty}^g}{\partial q_k} \). At this point a discussion on the relevant nuclear parameters and on the assumptions made about them in the reference nuclear data files is necessary. The arguments may be synthetized in the following points.

1. The average resonance widths \( \Gamma, \Gamma_n, \Gamma_y, \Gamma_f \) and the level spacing \( \Delta \) are evaluated by fitting experimental values of
infinite dilution cross-sections $\sigma_{\infty}$ by means of more or less sophisticated nuclear models. Since these models result often inadequate to reproduce the experimental data, "smooth" corrections $\sigma_{\text{smooth}}$ are implemented into the nuclear data file by the evaluator.

2. The width $\Gamma_{y}$ is generally kept constant. The other parameters considered above result energy-dependent. The width $\Gamma$ and $\Gamma_{n}$ exhibit sometimes remarkable fluctuations while the $\Gamma_{f}$ width behaviour may often be represented by a parametric expression.

3. The average values of the parameters are given for couples of values $(I, J)$ (neutron angular momentum and compound nucleus spin, respectively) at a limited number ($\sim 30$) of energy points.

In order to select the parameters to be adjusted, it seems appropriate to keep unchanged the given values $(I, J)$ and the energies at which they are estimated, together with the number of degrees of freedom of the $\chi^{2}$ Porter-Thomas distribution for the resonance widths, since assessment of these quantities should be of pertinence of the cross-section evaluator. The variable parameters are then represented by $\Gamma$.

\begin{equation}
\Gamma = \Gamma_{n} + \Gamma_{y} + \Gamma_{f}.
\end{equation}

We see that the number of parameters to be adjusted for this case results limited enough. For instance, in the case of the fertile U-238 the following coupled values $(I, J)$ would be considered: $(0, \frac{1}{2})$, $(1, \frac{1}{2})$, $(1, \frac{3}{2})$, corresponding to sequence indexes $s = 1, 2, 3$. Within each sequence the spacing $D$ would
be set constant together with $\Gamma_e$ and $\Gamma$. As mentioned above, 
$\Gamma_{\gamma}$ would be set constant for all the sequences. Besides, the 
following relationships are assumed:

$$D_{(s=1)} = D_{(s=2)} = \frac{1}{2} D_{(s=3)} \quad (3.3)$$

$$\Gamma_e(s=1) = \Gamma_e(s=2) \quad (4.3)$$

As a conclusion, there result only four parameters at each 
given energy point to be considered for the correlation, 
namely:

$$D_{(s=1)}, \Gamma_{\gamma}, \Gamma_e(s=1), \Gamma_e(s=2) \quad (5.3)$$

The expression which gives the fine group average infinite dilution cross-section $\sigma_{x,1\omega}$ around a given energy point $E^x_i$, 
considering the levels not fluctuating for the moment, results:

$$\sigma_{x,1\omega} = \frac{1}{E_{i,H} - E_{i,L}} \sum_s \int_{E_{i,L}}^{E_{i,H}} \sum_r \sigma_{x,s,r}^s(E) dE \quad (6.3)$$

where the sums are over sequences and resonances for a given 
sequence in the group energy width $(E_{i,H} - E_{i,L})$. If the Porter-
Thomas distribution is introduced and the interval $(E_{i,H} - E_{i,L})$
is replaced by $D_s N_s$ where $N_s$ is the number of the sequence 
s resonances within the interval, Eqn. (5.3), recalling the 
usual Breit-Wigner formulation and after some algebra, results:

$$\sigma_{x,1\omega} = \left< \sigma_x (E^x) \right>_P = 2 \pi^2 \lambda^2 \sum_s \frac{1}{D_s} g_j \left< \frac{\Gamma_{e,s}^{(s)}(E^x)}{\Gamma_s} \right>_P \quad (7.3)$$

where $\left< \right>_P$ stands for averaging over the Porter-Thomas distri-
bution. In the algorithms as used by the MC$^2$ code the averages $\langle \rangle_p$ are evaluated by expressions of the type:

$$\langle \frac{\Gamma_c \Gamma_x (E^*)}{\Gamma^s} \rangle_p = \frac{\Gamma_c \Gamma_x}{\Gamma^s} \sum_{n=1}^{N} \chi_n. \quad (8.3)$$

Since $\Gamma_c^s$, $\Gamma_x^s$, and $\Gamma^s$ represent the average values given at energy points $E^*$ and the coefficients $\chi_n$ result from the $N$-point integration over the Porter-Thomas distribution. Eqn. (7.3), with the term $\langle \rangle_p$ at the right hand side replaced by expression (8.3), may be used directly for the evaluation of the derivatives:

$$\frac{\partial \sigma_{x, \omega}}{\partial D_s} = -2\pi^2 \lambda^2 g_j \frac{1}{D_s^2} \frac{\Gamma_c \Gamma_x}{\Gamma^s} \sum_{n=1}^{N} \chi_n \quad (9.3)$$

$$\frac{\partial \sigma_{x, \omega}}{\partial \Gamma^s} = -2\pi^2 \lambda^2 g_j \frac{1}{D_s} \frac{\Gamma_c \Gamma_x}{(\Gamma^s)^2} \sum_{n=1}^{N} \chi_n \quad (10.3)$$

$$\frac{\partial \sigma_{x, \omega}}{\partial \Gamma_x} = 2\pi \lambda^2 g_j \frac{1}{D_s} \frac{\Gamma_c}{\Gamma^s} \sum_{n=1}^{N} \chi_n \quad (11.3)$$

$$\frac{\partial \sigma_{\omega}}{\partial \Gamma_c} = 2\pi \lambda^2 g_j \frac{1}{D_s} \frac{\Gamma_x}{\Gamma^s} \quad (12.3)$$
For what concerns the presence of the smooth corrections implemented into the data file (see point 1 at beginning of chapter), as far as the adjustment philosophy is concerned, three possibilities are envisaged (apart from the possibility of correcting only $\sigma_{\text{smooth}}$).

a) Initial $\sigma_{\text{smooth}}$ kept fixed. This choice is consistent with the fact that the ratio $\sigma_{\text{smooth}}/\sigma$ is generally small, although the presence of these corrections introduces a rather subjective (although necessary in other circumstances) factor into the correlation.

b) $\sigma_{\text{smooth}}$ set zero and adjustment made only on resonance parameters.

c) Adjustment made on both resonance parameters and $\sigma_{\text{smooth}}$.

Choice b) results more consistent with the idea of basing the correlation on the theoretical model assumed with as little subjective intervention as possible. The correction on the group cross-sections resulting from the correlation would be in this case of the type:

$$\delta\sigma = \sum_{k} \frac{\partial \sigma}{\partial q_k} \delta q_k - \sigma_{\text{smooth}}$$  \hspace{1cm} (13.3)

Of course this choice implies, for consistency, that the integral calculations be made with $\sigma_{\text{smooth}}$ set equal to zero. If choice c) is assumed, the corrections would be of the type:

$$\delta\sigma = \sum_{k} \frac{\partial \sigma}{\partial q_k} \delta q_k + \delta\sigma_{\text{smooth}}$$  \hspace{1cm} (14.3)
where \( \delta \sigma_{\text{smooth}} \) corresponds to an adjusted value resulting from the correlation procedure together with the corrections \( \delta q_k \) of the nuclear parameters. If choice a) is made, the corrections would be of the type

\[
\delta \sigma = \sum_k \frac{2 \sigma}{\partial q_k} \delta q_k .
\]  

(15.3)

In this last instance, it may happen that the evaluator is not satisfied with the cross-section curve resulting from the adjusted parameters. Therefore he might impose again new smooth corrections. If this operation is iterated, it may be interpreted as a way of assigning progressively more weight to given cross-section curve shapes or values. Asymptotically, since the weighting becomes infinite, these shapes or values may result exactly reproduced. Since this weighting results independent from the errors assigned at the beginning to the experimental parameters, a strong subjective factor results introduced by this procedure.
5. **RESOLVED RESONANCES REGION PARAMETERS**

Within this region the following cross-sections result of main interest:

a) The elastic cross-sections of structural elements of interest to the fast reactors, i.e., as significant examples:

- Ni resonance at 60 KeV
- Fe " 27 "
- Mn " 20 "
- Na " 2.85 "

These mentioned represent isolated broad resonances where the Doppler broadening has a small influence.

b) Fission and capture cross sections of

- U-238 below 4 KeV
- Pu-239 " \sim 0.5 "
- U-235 " \sim 0.5 "

These resonances result rather narrow and therefore highly temperature dependent.

For what concerns the importance of these parameters within the resolved region, it results that integral quantities such as those, for example, measured (and so far usable for adjustments, in particular central reaction rate ratios) on the critical facilities SNEAK and ZPR VI, do not seem to result significantly sensitive to them, with the exception of a few
\( \sim 10 \) U-238 resonances between 1 and 4 KeV. In order to increase the sensitivity of the integral parameters, ad hoc reliable transport (leakage) and Doppler clean experiments should be adopted.

The generation of these cross-sections is made within an ultrafine group structure and adopting the infinite dilution cross-section approximation. Therefore, within each interval \( (E_{n,1} - E_{n,L}) \) of the ultrafine groups (in number \( N_i \) for each gross group \( i \)) the following average is evaluated:

\[
\langle \sigma \rangle_n = \int_{E_{n,L}}^{E_{n,H}} \frac{\sigma(E) \frac{dE}{E}}{E} \quad \text{(n=1, \ldots, N)}
\]

(where the prime is written to remind that the average is not normalized to unit flux) while the average gross group cross-section, again assuming a \( 1/E \) spectrum, is given by the expression

\[
\langle \sigma \rangle_i = \frac{\sum_{n=1}^{N_i} \langle \sigma \rangle_n}{\ln \frac{E_{I,H}}{E_{I,L}}}
\]

In order to obtain the expressions of the derivatives of \( \langle \sigma \rangle_i \) with respect to the nuclear parameters, it is necessary to know the corresponding derivatives of \( \langle \sigma \rangle_n \) which in turn require to know in detail function \( \sigma(E) \) vs. nuclear parameters. For the case of elastic scattering and absorption or fission capture, it results:
\[
\sigma_x(E) = \sum_{s=1}^{N} \sum_{r=1}^{N_s} \sigma_{x,s,r}(E) \quad \text{(capture or fission)} \quad (3.4)
\]

\[
\sigma_e(E) = \sum_{s=1}^{N} \sum_{r=1}^{N_s} \sigma_{e,s,r}(E) + \sigma_p \quad (4.4)
\]

where, as in the previous chapter, index \( s \) represents a sequence of \( N \) coupled values \((i, j)\), while \( N^s \) the number of resonances for that sequence. Functions \( \sigma_{x,s,r}(E) \) and \( \sigma_{e,s,r}(E) \) are given by the expressions:

\[
\sigma_{x,s,r}(E) = \sigma_{x,s,r}^e \sum \psi(\bar{E}, s, r, x) + \sigma_{x,s,r}^p \chi(\bar{E}, s, r, x) \quad (5.4)
\]

\[
\sigma_{e,s,r}(E) = \sum \psi(\bar{E}, s, r, x) + \sigma_{e,s,r}^p \chi(\bar{E}, s, r, x) \quad (6.4)
\]

where \( \psi \) and \( \chi \) represent the usual Doppler Broadening functions and where:
\[ \sigma_p = 4 \pi \frac{\lambda^2}{\Delta} \sum_{l} (2l + 1) \sin \varphi_l \]

\[ \sigma_o^{s,r} = 4 \pi g_j \frac{k^2}{\Gamma^{s,r}} \frac{\Gamma_e^{s,r}}{\Gamma^{s,r} \left( \frac{A+1}{A} \right)^2} \]

\[ \xi^{s,r} = \frac{r^{s,r}}{\Delta} \]

\[ \Delta = \left( \frac{4 E K T}{A} \right)^{\frac{1}{2}} \]

\[ \chi^{s,r} = \frac{2(E-E_f)}{\Gamma^{s,r}} \]

\[ \varphi \] being the phase shift.

### 5.1 Elastic Scattering Resonance

Since for these resolved resonances, as mentioned above, the Doppler broadening is not significant, the natural line of the resonance given by function \( \left[ 1 + (\chi^{s,r})^2 \right]^{-1} \) in place of function \( \psi^{s,r} \) is assumed. Consequently, function \( \chi^{s,r} \) becomes \( 2 \chi^{s,r} \left[ 1 + (\chi^{s,r})^2 \right]^{-1} \). The only parameter to be considered for the correlation appears to be \( r^{s,r} \) since the other parameters which enter into the group cross section generation result relatively well known and
since $\Gamma_{e}^{s,r}/\Gamma_{e}^{s,r} \ll 1$. Therefore, since the cross-section for resonance $r$ of sequence $s$ has the form:

$$\sigma_{e}^{s,r} = 4\pi \lambda^2 g_{J} \left( \frac{\Delta + 1}{A} \right)^2 \left[ 1 + (x^{s,r})^2 \right]^{-1} +$$

$$+ \left[ 4\pi g_{J}^2 \lambda^2 \left( \frac{\Delta+1}{A} \right)^2 \sigma_{p} \right]^\frac{1}{2} 2x^{s,r} \left[ 1 + (x^{s,r})^2 \right]^{-1},$$

the derivative with respect to the parameter $\Gamma_{e}^{s,r}$ results:

$$\frac{\partial \sigma_{e}^{s,r}}{\partial \Gamma_{e}^{s,r}} = 4\pi \lambda^2 g_{J} \left( \frac{\Delta + 1}{A} \right)^2 \frac{4(x^{s,r})^2}{\left[ 1 + (x^{s,r})^2 \right]^2} +$$

$$+ \left[ 4\pi g_{J}^2 \lambda^2 \left( \frac{\Delta+1}{A} \right)^2 \sigma_{p} \right]^\frac{1}{2} \begin{vmatrix} \frac{8(x^{s,r})^3}{\left[ 1 + (x^{s,r})^2 \right]^2} - \frac{2x^{s,r}}{\Gamma_{e}^{s,r}} \frac{1}{1 + (x^{s,r})^2} \end{vmatrix}.$$  \hspace{1cm} (5.4)

5.2 Capture Resonances

Since, as mentioned before, among the resolved
resonances those pertinent to capture of U-238 are of some significance with respect to the integral experiments available from the fact critical facilities, we will limit the present analysis to these ones. The resulting formulations and conclusions, however, may be easily extended to other materials, such as the structural Fe, Cr, Ni, etc., if ad hoc integral experiments had to be interpreted.

The value \( J \) (and therefore \( g_j \)) and the resonance energy levels should be held fixed, especially in consideration of the relevant error associated with the \( \Gamma \) width values. The main problem here is connected with the presence of function \( \Psi_s, r \) in expression (5.4) if this is not substituted by the natural line shape \( (1 + x^2)^{-1} \) in consideration of the significant temperature dependence. If for each resonance we explicitate the dependence of the absorption capture cross-section from the parameters \( \Gamma^s, r \) and \( \Gamma^y, r \), we obtain:

\[
\sigma_y^{s, r}(E) = 4\pi \lambda^2 g_j \left( \frac{\Gamma^s, r - \Gamma^y, r}{\Gamma^y, r} \right)^2 \frac{A + 1}{A} \left( \frac{E}{E_r} \right)^3 \Psi_s, r \left( \xi^s, r, x^s, r \right).
\]

(10.4)

The derivatives with respect to the various parameters result:

\[
\frac{\partial \sigma_y^{s, r}}{\partial \Gamma^y, r} = 4\pi \lambda^2 g_j \left( \frac{A + 1}{A} \right)^2 \left( \frac{E}{E_r} \right)^3 \Psi_s, r \left( \xi^s, r, x^s, r \right) \frac{\Gamma^s, r - 2 \Gamma^y, r}{(\Gamma^y, r)^2}.
\]

(11.4)
\[
\frac{\sigma_s^c,r}{\sigma_s^s,r} = 4\pi \lambda^2 \sum_j \frac{(A+1)_j}{A} \left( \frac{E_j}{E} \right)^{1/2} \psi_s^s,r (x_s^s,r, x^s,r).
\]

\[
\left[ \frac{\Gamma_s^s,r}{(x_s^s,r)^2} - \frac{\Gamma_s^s,r (\Gamma_s^s,r - \Gamma_{s,0}^s,r)}{(x_s^s,r)^3} \right] + 
\]

\[
+ 4\pi \lambda^2 \sum_j \frac{(A+1)_j}{A} \left( \frac{E_j}{E} \right)^{1/2} \frac{\Gamma_s^s,r (\Gamma_s^s,r - \Gamma_{s,0}^s,r)}{(x_s^s,r)^2} \frac{x_s^s,r}{\Delta} \frac{1}{\partial x_s^s,r} \frac{\partial \psi_s^s,r}{\partial \Gamma_s^s,r}.
\]

\[
- 4\pi \lambda^2 \sum_j \frac{(A+1)_j}{A} \left( \frac{E_j}{E} \right)^{1/2} \frac{\Gamma_s^s,r (\Gamma_s^s,r - \Gamma_{s,0}^s,r)}{(x_s^s,r)^2} \frac{\partial \psi_s^s,r}{\partial x_s^s,r} \frac{x_s^s,r}{\Gamma_s^s,r}.
\]

\[(12.4)\]

In this last expression the derivatives \(\partial \psi_s^s,r/\partial x_s^s,r\) and \(\partial \psi_s^s,r/\partial \Gamma_s^s,r\) have to be evaluated. The first one is given (see Ref. [57]) by the expression:
\[
\frac{\partial \psi^{s,r}}{\partial x^{s,r}} = \frac{1}{4} (\ell^{s,r})^2 \left[ \chi^{s,r} \eta^{s,r} \chi^{s,r} \eta^{s,r} - 2 \chi^{s,r} \eta^{s,r} \psi^{s,r} (\ell^{s,r} - \chi^{s,r}) \right]
\]

while the second one satisfies the relation (see Ref. [47]):

\[
\frac{\partial \psi^{s,r}}{\partial \chi^{s,r}} = -2 (\ell^{s,r})^{-3} \frac{\psi^{s,r} \chi^{s,r}}{\chi^{s,r}}
\]

which, by using Eqn. (13.4), becomes:

\[
\frac{\partial \psi^{s,r}}{\partial \chi^{s,r}} = -\frac{1}{2} (\ell^{s,r})^{-1} \left[ -\frac{(\ell^{s,r})^2}{2} \chi^{s,r} \chi^{s,r} + \right.
\]

\[
+ (\ell^{s,r})^2 \int_{-\infty}^{+\infty} \frac{\chi^2}{1+y^2} \exp \left[ -\frac{(\ell^{s,r})^2}{4} (\chi^{s,r} - y)^2 \right] dy - \left. -\frac{1}{4} \chi^{s,r} (\ell^{s,r})^2 (\chi^{s,r} \psi^{s,r} - 2 \chi^{s,r} \eta^{s,r}) - 2 \chi^{s,r} \eta^{s,r} \right] .
\]

The main difficulty therefore results in the evaluation of the integral:
\[
\int_{-\infty}^{+\infty} \frac{y^2}{1+y^2} \exp \left[ - \frac{(1+sr)^2}{4} (x^2 + r^2 - y^2)^2 \right] \, dy
\] (16.4)

which has to be performed and tabulated separately.

In the case the natural line is chosen, which might be justified by the relatively low sensitivity of integral quantities to cross-sections in this low energy region, the expressions would become greatly simplified and of the type of those derived in paragraph 5.1.
6. ELASTIC REMOVAL CROSS SECTION

If in gross group $i$ the derivative of the elastic removal cross-section $\sigma_{er,i}$ with respect to nuclear parameters is required, reference has to be made to the way by which it is obtained in the group cross-section generation code. If, for instance, it results:

$$
\sigma_{er,i} = \frac{\sum_{n \in \{E_{i,L}\}} <\sigma_e> n \psi_n}{\sum_{n=1}^{N_i} \psi_n},
$$

where $\psi_n$ represents the fine group structure and $\{E_{i,L}\}$ the energy interval of limits $E_{i,L}$, $F_{i,L}(1 + \xi)$, $\xi$ being the average lethargy increment, the partial derivatives with respect to the generic parameter $q_k$ would result:

$$
\frac{\partial \sigma_{er,i}}{\partial q_k} = \frac{1}{N_i} \sum_{n=1}^{\psi_n} \sum_{n \in \{E_{i,L}\}} <\sigma_e> n \frac{\partial \psi_n}{\partial q_k}
$$

and therefore the problem may be referred to that pertinent to the elastic scattering cross-sections.
7. INELASTIC SCATTERING PARAMETERS

Also for this case we have to distinguish between the discrete level region \(< 1+2\ MeV\) and the continuous level region.

In the case of the discrete level region the total inelastic cross-section \(\sigma'_\text{in}(E)\) at energy \(E\) results a sum of contributions \(\sigma'^k_{\text{in}}(E)\) of partial cross-sections starting from levels below \(E\), i.e.:

\[
\sigma'_\text{in}(E) = \sum_{k=1}^{N} \sigma'^k_{\text{in}}(E) .
\]  

The number of these levels results of the order of 10\(+20\) in the case of U-238 and should not exceed the number of 10 in the generality of cases. Their general expression has the form:

\[
\sigma'^k_{\text{in}}(E \rightarrow E') = \sigma'_\text{in}(E) p_k(E) \tau_k(E \rightarrow E')
\]  

where \(\sigma'_\text{in}(E)\) represents the total inelastic cross-section, \(p_k(E)\) the fraction of scattered neutron related to the \(k\)-th partial cross-section and \(\tau_k(E \rightarrow E')\) represents the distribution:
\[ f_k(E \rightarrow E') = \delta \left[ E' - \frac{A^2 + 1}{(A+1)^2} E + \frac{A}{A+1} \Theta_k \right] \]  \hspace{1cm} (3.6)

\( \delta \) being the Dirac's function and \( \Theta_k \) representing the excitation energy. Therefore the parameters which may be considered for adjustment are the percentage variations of the fractions \( p_k \) (or, better, their corresponding group averaged values\(^\text{x} \)) and the excitation energies \( \Theta_k \). In the case of continuous level region the inelastic cross-section is given by the expression:

\[ \sigma_{in}(E \rightarrow E') = E' \sigma_{in}(E) \exp \left( -E'/T(E) \right) \]  \hspace{1cm} (4.6)

\( T(E) \) representing the neutron temperature. In this case the parameters which may be considered for adjustment are the total cross-sections \( \sigma_{in}(E) \) and the neutron temperature \( T(E) \) for the parameter which enters into its energy dependence, according to the model chosen (Bethe, Weisskopf, etc.)\(^\text{y} \).

### 7.1 Discrete Level Region

The expression used in the generation of the inelastic group cross-section of gross group \( g \), with energy limits \( E_g, L' \) \( E_g, H' \), is the following:

\( \text{(x)} \)

In this specific case the parameters to be adjusted depend on the energy group structure chosen. Since they do not exhibit a resonance behaviour, their redefinition within a different group structure, in case this is required, does not pose any serious problem.
\[
\sigma_{\text{in}}^{g \rightarrow g'} = \sum_k \int_{E_g, L}^{E_g', L} \int_{E_g', L}^{E_g, H} dE' dE' \sigma_{\text{in}}^k (E \rightarrow E')
\]

\[
= \sum_k \int_{E_{k, 1}}^{E_{k, 2}} \sigma_{\text{in}}^k (E) dE,
\]

(5, 6)

where a constant flux weighting has been assumed and where the energy limits are given by the expressions:

\[
E_{k, 1} = \max \left[ E_{g, L}, E_{g', L} \right]
\]

(6, 6)

\[
E_{k, 2} = \min \left[ E_{g', H}, E_{g, H} \right]
\]

(7, 6)

\[
E_{g, L}, E_{g', H}
\]

representing the energy values:

\[
E_{g, L} = \frac{(A+1)^2}{A^2+1} \left( E_{g', L} + \Theta_k \frac{A}{A+1} \right)
\]

(8, 6)

\[
E_{g', H} = \frac{(A+1)^2}{A^2+1} \left( E_{g, H} + \Theta_k \frac{A}{A+1} \right).
\]

(9, 6)
Recalling Eqn. (2.6) and that

\[ \sigma_k^{g \rightarrow g'} = \frac{E_{k,2} - E_{k,1}}{E_{g,H} - E_{g,L}} \]  \hspace{1cm} (10.6)\]

Eqn. (5.6) may be written, without significant loss of precision:

\[ \sigma_{in}^{g \rightarrow g'} = \sum_k \frac{E_{k,2} - E_{k,1}}{E_{g,H} - E_{g,L}} \sigma_{in,\kappa} \]  \hspace{1cm} (11.6)\]

where \( \sigma_{in,\kappa} \) is defined by the expression:

\[ \sigma_{in,\kappa} = \int_{E_{g,L}}^{E_{g,H}} \sigma_{in}(E) \rho_k(E) dE \]  \hspace{1cm} (12.6)\]

The derivative of \( \sigma_{in}^{g \rightarrow g'} \) with respect to the parameter \( \sigma_{in,\kappa} \) thereafter results:

\[ \frac{\partial \sigma_{in}^{g \rightarrow g'}}{\partial \sigma_{in,\kappa}} = \sum_k \frac{E_{k,2} - E_{k,1}}{E_{g,H} - E_{g,L}} \]  \hspace{1cm} (13.6)\]

while the derivatives with respect to the excitation energy \( \Theta_k \) result:
Clearly, if \( \sigma_{\text{in}}^k \) keeps constant within the group also the second value from top of the derivative goes to zero. Since the number of partial cross-sections is of the order of 10 and the number of broad groups (in the case of a 30 group scheme) is of the order of 5, the maximum number of parameters to be corrected results of the order of 100 or 50, depending on the inclusion or not into the adjustment of the excitation energies.
7.2 Continuous Level Region

In the multigroup formalism Eqn. (4.5) reduces to

\[ \sigma_{in}^{g \rightarrow g'} = \sigma_{in, g} \frac{p^{g \rightarrow g'}}{g_{max}} \sum_{g' = g} p^{g \rightarrow g'} \]  \hspace{1cm} (15.6)

where \( \sigma_{in, g} \) represents the total inelastic cross-section and where

\[ p^{g \rightarrow g'} = \int_{E_{g', L}}^{E_{g', H}} E \exp \left( -\frac{E}{T_g} \right) dE \]

\[ = T_g^2 \left[ \left( \frac{E_{g', L}}{T_g} + 1 \right) \exp \left( -\frac{E_{g', L}}{T_g} \right) - \left( \frac{E_{g', H}}{T_g} + 1 \right) \exp \left( -\frac{E_{g', H}}{T_g} \right) \right], \]  \hspace{1cm} (16.6)

\( T_g \) representing the average neutron temperature for group \( g \).

The derivatives with respect to the parameters \( \sigma_{in, g} \) and \( T_g \) are straightforward, i.e.:
\[
\frac{\partial \sigma_{\text{in}}^{g\rightarrow g'}}{\partial \sigma_{\text{in}, g}} = \frac{p^{g\rightarrow g'}}{\sum_{g' = g}^{g_{\text{max}}}} \frac{E^2}{E_{g', L} \exp(-E_{g', L}/T_g)} - \frac{E^2}{E_{g', H} \exp(-E_{g', H}/T_g)}
\]

\[
\frac{\partial \sigma_{\text{in}}^{g\rightarrow g'}}{\partial T_g} = \sigma_{\text{in}, g} \left\{ \frac{\sum_{g' = g}^{g_{\text{max}}}}{T_g} \left[ \frac{E^2}{E_{g', L} \exp(-E_{g', L}/T_g)} - \frac{E^2}{E_{g', H} \exp(-E_{g', H}/T_g)} \right] \right\}
\]

\[
= \frac{1}{T_g} \left( \sum_{g' = g}^{g_{\text{max}}} \frac{E^2}{E_{g', L} \exp(-E_{g', L}/T_g)} - \frac{E^2}{E_{g', H} \exp(-E_{g', H}/T_g)} \right)
\]

(17.6)

(19.6)

If an energy dependence, symbolically represented by the expression

\[
T_g = f(E_g | q)
\]

(19.6)

q being a parameter to be estimated, is assumed, Eqn. (18.6) should be replaced by a new one obtained by multiplying both terms by \(\frac{\partial T_g}{\partial q}\) in order to obtain the derivative with respect to q.
CONCLUSIONS

Looking into the cross-section generation formulations, it seems that the number of the nuclear parameters which should be adjusted by the correlation does not result in realistic cases significantly higher than the number of group cross-section to be considered in a 20+30 cross-section group scheme. However, the added difficulties inherent within this consistent correlation method appear well compensated by the independence of the adjustment from any group schematization.

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REFERENCES


