FAST REACTOR BENCHMARKS AND INTEGRAL DATA TESTING AND FEEDBACK INTO JEF2

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ABSTRACT

Studies relating to the validation of the JEF2.2 library in the KeV and MeV energy ranges are described. The processing of the file into group constants and probability tables has been made in a 1968 group scheme with the care required for Quality Assurance. The selection for inclusion in the Integral Data Base, limited for the moment to Reactor core data, has been made on the basis of experimental environment cleanness and suitability for accurate neutronic calculation. The uncertainty information is almost absent in JEF2. Covariance data have been elaborated on the basis of personal judgment and systematic studies have defined the condition for a statistical adjustment procedure to preserve the consistency of a maximum of useful integral data information with microscopic information. Although the results are not final since not all available integral data have been considered the conditions of the adjustment are such that the present conclusions are unlikely to be modified : ^{235}U, ^{238}U, ^{58}Ni, ^{16}O evaluations need revisions.

Introduction

In the past, when the information in the evaluation was of relatively poor quality the integral data were considered as absolute references to correct the nuclear data which were considered to be affected by significant systematic errors. The covariance matrices, when existing, played little role in the adjustments.

The somewhat recent improvements of the quality of the evaluations and the development of theories and tools for data adjustment have made it possible to consider now the microscopic and the integral data as two complementary sources of information about the same basic physical phenomenon. The validation of evaluated data becomes more and more the research into the extent of the consistency in the complementarity. In this operation the uncertainty information plays a key role, provided that some conditions are fulfilled.

General Conditions for Adjustments

Nuclear data adjustment is a long process involving several steps :

1. Processing the evaluated data into parameter or group constants in a way that preserves the quality and the integrity of the information. This requires that fully validated tools are used for the processing and that methods sophisticated enough exist to use the processed data.

2. A choice of integral data according to criteria of cleanness of the experimental environment. The integral data should be derived from the raw data by applying corrections of small amplitude so that the integral values are not

sensitive to uncertainties in the corrections (Doppler, heterogeneity, self-shielding, ...) nor to the methods used to calculate them. It has to be noted that in recent years these methods have received considerable improvements so that a number of additional experiments can be considered now as valuable benchmarks.

On the other side, in order to obtain the energy dependence of the nuclear data corrections the integral data should have differing energy dependent sensitivities.

This is the reason why the benchmark integral data set should contain as many experiments with different spectral indices as possible, and for a given integral experiment as many parameters (K_{eff}, B^2_m', reaction rate ratios) as possible in order to separate the effects of the different cross-section types.

3. Neutronics calculations which must be as <u>exact</u> as possible so that the calculated integral parameters are not dependent on the calculational method nor on the calculational scheme. If these conditions are satisfied the differences between experimental data and calculated data are the exact measures of the imperfect quality of the input data.

The sensitivity coefficient calculations are based on perturbation theory or variational methods. Both types of methods are equivalent provided that the amplitude of the nuclear data modification in the adjustment is small enough for the linearity principle to apply.

But here again the condition of exact calculations imposes an energy scheme that is adapted to the fine structure of the flux $\phi(E)$ as a function of energy. In fact, sensitivity calculations using perturbation theory imply the calculation of expressions like $<\phi^*.dx.\Phi>$ which are integrals over space, angle, energy of the product of the vector $dx.\Phi$ by the adjoint flux ϕ^*, dx being the variation of the Boltzman operator which acts on the vector flux. Keeping in mind that the components Φ_g (g stands for a given group number in the energy scheme) are average values, incorrect values of ϕ_g induce incorrect values for ϕ^*_g and the errors are "squared" in the integral.

This condition is easily satisfied with fast and very fast systems, but one has to be careful in analysing thermal and epithermal systems.

4. The main objective in nuclear data adjustment is to check the consistency of Integral and microscopic data so as to create data set able to calculate any <u>integral parameter with the best reliability</u> and with an <u>accuracy at least equal that of the measurements</u>.

Everything has already been said about adjustments, their general theoretical bases, the conditions and limitations in application.

We will incidentally recall some special features of relevance to the present topics and used in the work described here below as an illustration.

A set of measured integral quantities, combined in a vector E with covariance matrix V is considered. The nuclear data implied in these integral parameters are

combined also in a vector T with a covariance matrix M. The integral parameters calculated from T are denoted by the vector C.

If the sensitivity matrix S expresses the dependence of $\overline{R}$ on relative variations of T one has :

$$\frac{dC}{C} = S\frac{dT}{T} \tag{1}$$

The use of such logarithmic variates (with possibility of variation between $-\infty$ and $+\infty$) is the most appropriate to be used in the operation of entropy maximisation.

Actually, in the adjustment the objective is to minimise the quantity :

$$\frac{E-C}{C} = S\frac{dT}{T}, \tag{2}$$

that is obtained by maximising a likelihood function corresponding to the system ϵ+T.

A vector T' is obtained. This vector is recommended as the best estimate of the unknown true vector since it minimises the expected consequences of choosing a vector deviating from the true vector [1].

T' needs to be close to T in order to satisfy the linearity assumption. Statistical adjustments are meaningful only when the a priori evaluated data are of sufficient quality, i.e. when non excessive values are obtained for any component of :

$$\frac{E-C}{C} \tag{3}$$

(let say less than 4% - 5%).

The final vector C' for the integral data is :

$$C' = C + S\left(\frac{T'-T}{T'}\right) \tag{4}$$

with a new covariance matrix V', while the covariance matrix for T' is denoted by M'.

Simplifications are obtained if the assumption is made that the probability distributions for T and C are Gaussian. The Gaussian distributions are kept in the adjustment for T' and C' and it is supposed that the true unknown distributions are also Gaussian.

Significant deviations from this assumption (existence of systematic errors) are detected by large :

$\left(\frac{E-C'}{C'}\right)$ values, or/and by adjustments to cross-sections much greater than the assigned standard deviations. The existence of such deviations lead to a deviation of the χ^2 parameter from its expected normal value that should equal N, the number of integral data (whether they are correlated or not).

If $\chi^2 > N$ the consistency between integral and microscopic data is not good. It is well known that the solution is to correct the discrepant data when possible, or to increase by judgment the related uncertainties or to reject the data when justified.

Finally, to keep the goodness of the fit all the "a posteriori" standard deviations have to be enhanced by the factor :

$$\left(\frac{\chi^2}{N}\right)^{1/2} \tag{5}$$

that will be referred to, in the following as the enhancement factor.

It follows that, for a given integral observable i the standard deviation after adjustment is :

$$\left(V_{ii}\,\frac{\chi^2}{N}\right)^{1/2} = \left[S_i\,M'\,S_i^T\,.\,\frac{\chi^2}{N}\right]^{1/2} \quad \text{when} \quad \chi^2 > N. \tag{6}$$

Practical Conditions of JEF2 Validation

- *Data processing :*

The JEF2 file has been processed, for the purpose of benchmarking, in different group schemes : 33g for the analysis of the LOS ALAMOS criticals, 172g for thermal systems and minor constituents, 1968g for fast systems. All have common boundaries and are therefore consistent.

The processing work has been performed using the NJOY version 89.62* with agreed updates to specific modules (treatment of the unresolved region, fine flux calculation in GROUPR ...). As agreed by the JEF project the same parameter values were used by all the Laboratories participating in the data processing (CADARACHE, BOLOGNE, WINFRITH) : Control of the number of points for cross-section reconstruction (ERMAX=10^{-3}), the numerical accuracy (NDIGITS=8), accuracy on the resonance integral RI, ...

The 33g library, called FASTLIB [3], has been processed on an IBM machine, while the other Libraries have been processed on a CRAY. There is consistency between both procedures provided that the double length word version of NJOY is used on the IBM. The 33g library contains only infinite dilution cross-section since it has been demonstrated for the hard spectrum Los Alamos criticals [3] that the selfshielding effect is negligible. It has been developed in the P5 order although a P3 development was sufficient.

The 1968g multitemperature library JECCOLIB2 [4] has been established with systematic controls for quality assurance. It contains infinite dilute cross-sections and probability tables. These probability tables were produced by using CALENDF [5] and are used in selfshielding calculation for heterogeneous media. They have been established by using the so-called "Moments" method whose basis is the following relationship which defines Mn as the n^{th} order moment of the total cross-section and Mx_n as the moments of the partial cross-section [σ_{xi}]:

$$Mn = \frac{1}{\Delta E}\int \sigma_t^n(E)dE = \sum_{i=1}^{I} p_i\,\sigma_{t_i}^n \tag{7}$$

$$Mx_n = \frac{1}{\Delta E}\int \sigma_x(E)\,\sigma_t^n(E)\,dE = \sum p_i\,\sigma_{xi}\,\sigma_{t_i}^n \qquad (8)$$

The set of values $\{p_i, \sigma_{ti}, [\sigma_{xi}]\}$ is the probability table or the subgroup parameters for the energy group of reference. For a given i^{th} subgroup p_i represents the probability, σ_{ti} the i^{th} subgroup value for the total cross-section and $[\sigma_{xi}]$ stands for every partial cross-section. The cross-sections are recalculated in CALENDF with the same basic formalism as NJOY (with a few exception, e.g. ^{58}Ni) but in different conditions for the energy grid and the numerical approach (ladders of resonances being used in the unresolved region ...).

BONDARENKO (NJOY) and subgroup parameter (CALENDF) formalisms can be related so that one has for any energy group, for a given grid of dilution values σ_d :

$$\sigma_{x,eff}^{(\sigma_d)} = \frac{\int \frac{\sigma_x(E)dE}{\sigma_t(E)+\sigma_d}}{\int \frac{dE}{\sigma_t(E)+\sigma_d}} = \frac{\sum_i \frac{p_i\,\sigma_{x_i}}{\sigma_{t_i}+\sigma_d}}{\sum_i \frac{p_i}{\sigma_{t_i}+\sigma_d}} \qquad (9)$$

($\sigma_{x,eff}^{(\sigma_d)}$ is the effective value of the cross-section σ_x corresponding to the "dilution" σ_d value).

This intercomparison provided a good opportunity to check the quality of NJOY production. Isolated differences of the order of 2% per group were tolerated because of differences in the numerical treatment. Systematic differences were examined and explanations found.

Very many errors have been detected in the evaluations, in NJOY and in CALENDF. But such rigorous and systematic controls are a guarantee that the information in the evaluated data has been group averaged without any distortion.

In addition, checks have been performed at each step of the transformation of the group constants into formatted data for use by the cell code.

- *Choice of integral experiments :*

It is reasonable to think that all the experiments considered for the JEF2 benchmarking a priori fulfil the conditions of cleanness of the experimental environment.

Most of them were extensively used in the past for this purpose of validation, mainly with the objective to produce data sets for specific applications (Fast BREEDER CORE Formulaire, as an example) and were (and still are) proprietary. With the few exceptions of the experiments in the very fast range (LOS ALAMOS spheres) the chosen experiments have been performed on the MASURCA (FRANCE) or RB2 (ITALY) critical facilities, or the power Reactor PHENIX (FRANCE). These

experimental programs were part of the EUROPEAN FAST REACTOR project and were designed to check the data involved in specific applications : major actinides for clean cores or start up cores (^{235}U, ^{238}U, ^{239}Pu : Program RZ on MASURCA, importance of higher Pu isotopes in reprocessed fuels (^{240}Pu, ^{241}Pu, ^{242}Pu : Program PLUTO on MASURCA), contribution of the structural material (Fe, Cr, Ni) to the neutron balance measured relative to ^{235}U fission or ^{10}B capture program on RB2. Data from other programs (ZEBRA, SNEAK) will be included in future adjustments.

The integral data of reference are : bücklings, critical masses, K^+ for $K_\infty = 1$ experiments, reaction rate ratios. If the parameter :

$$r = \frac{<\nu \Sigma_f>}{<\xi \Sigma_s>} \qquad (10)$$

(where the numerator stands for the total number of neutrons produced by fission and the denominator for the integral of the slowing down density) is used as the spectral index, one notes a very large spread of the values ($0.2 < r <$), a situation that satisfies the condition of energy dependent sensitivities in the integral experiments.

- *Neutronics calculations :*

The integral data in the very fast range (GODIVA, ...) need a very accurate spatial and angular treatment. This has been performed in the P^3 S^{32} approximations with S^N corrections made to Keff calculations, corrections obtained from the following relationship :

$$\left(K_{4n} = \frac{4.K_{2n} - K_n}{3}\right) \qquad (11)$$

Mesh and energy grid effects were investigated in order to specify the optimal calculational conditions.

The integral data of the fast reactor range were assumed to have been obtained in the conditions of the asymptotic flux. Therefore, the calculations have been limited to cell calculations, using the recent European cell code ECCO [6].

The essential approximations [7] are related to the anisotropy treatment :

a. By using a transport cross-section, in particular for collision probability calculations and the treatment of leakage, defined as :

   $\sigma_{tr} = \sigma_t - \bar{\mu}\, \sigma_s$

   In this relationship σ_t refers to the total cross-section, $\bar{\mu}$ to the average cosine, σ_s to the scattering cross-section. The correct anisotropy is replaced by a forward scattering anisotropy without energy change.

b. The so called P_1 inconsistent approximation is used for flux calculation. It is not clear whether the B1 approximation which is better in principle, would be more appropriate.

c. The leakage is assumed to be isotropic

In addition one has to mention that no correlation is represented between the probability tables, even in the fine group Library. This is an approximation in the resonance structure, of very small importance for fast and very fast systems.

All the approximations here above mentioned have impacts which have not yet been estimated, but assumed to be small.

The uncertainties on the integral parameters should ideally be increased to allow for these approximations.

The sensitivity coefficients have been calculated using the ERANOS code system.

The Standard Perturbation theory has been applied for the K_{eff} sensitivity calculations. For a given energy group g the sensitivity coefficient to a nuclear constant variation inducing variations δF and δA on the neutron production and removal operators respectively is expressed as :

$$\left(S^{K_{eff}}\right) = \frac{< \varnothing^*, \delta F \varnothing > - < \varnothing^*, \delta A \varnothing >}{< \varnothing^*, F' \varnothing' >} \qquad (12)$$

($\varnothing$ is the scalar flux, $\varnothing^*$ the adjoint flux and $\varnothing'$ is the perturbated flux). In this expression the denominator represents the fission normalization integral.

For a spectral Index I the sensitivity coefficient to the cross-section Σ_x has two components :

- the "direct effect" component whose expression is obvious,
- the component corresponding to the modification of the neutron energy spectrum. It is easy to demonstrate, in the frame of the Generalized Perturbation Theory, that the expression for the "spectral effect" is :

$$\left(S_x^I\right) = \frac{\frac{dI}{I}}{\frac{d\Sigma_x}{\Sigma_x}} = - < \varnothing^*, \Sigma_x \varnothing > \qquad (13)$$

- *Adjustments :*

The adjustments have been performed using the code AMERE [8].

The a posteriori χ^2 parameter value has been used as a test of goodness of the fit, and consequently as a test of reliability of integral parameter prediction, by the adjusted data set.

The "a posteriori" average uncertainty on integral parameters served as a criterion of accuracy of prediction.

In practice a sequential procedure has been adopted to implement the system of integral data so as to detect the introduction of any inconsistent integral datum by a sharp increase of the χ^2 value.

The different experimental programs have been considered first separately (i.e., the "LOS ALAMOS spheres" data only, or the "MASURCA" data only, ...) in order to test their internal consistency. Some experiments have been rejected on a statistical criterion, but the elimination has been found justified by arguments of experimental technics. Finally a system of N=50 integral data has been selected.

The JEF2 evaluations are not provided with covariance matrices, with the exception of ^{239}Pu [9] and ^{238}U [10]. Covariances have been generated on the basis of personal judgement for what concerns both the standard deviations and the range of correlations (medium range). (A covariance matrix can be written as $B=\Sigma P\Sigma$ in a way that displays explicitly the standard deviations (diagonal matrix Σ) and their correlations (matrix P)).

As a compromise between constraints relevant to physics and to have common boundaries with the 3 above mentioned schemes a 15 group scheme has been established to perform the sensitivity calculations and the cross-section adjustments (see the table 1). The covariance matrices have been collapsed into this 15 group scheme.

Table 1 - 15 groups scheme used for adjustment calculations

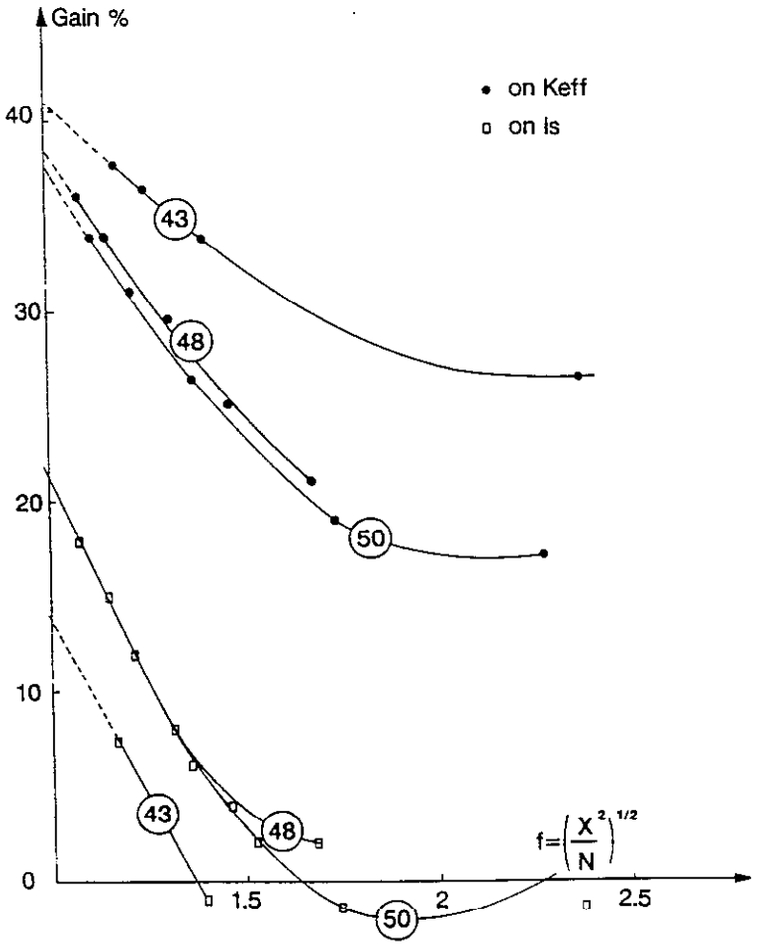
Group boundaries upper limit (eV)	Group	Scheme 1968 g	Scheme 172 g	Scheme 33 g	Lethargy
19.64033 + 6	1	1	1	1	-0.675
6.06531 + 6	2	142	9	3	0.500
2.231302 + 6	3	262	15	5	1.500
1.353353 + 6	4	322	18	6	2.000
4.978707 + 5	5	442	26	8	3.000
1.831564 + 5	6	664	32	10	4.000
6.737947 + 4	7	686	36	12	5.000
2.478752 + 4	8	808	42	14	6.000
9.118820 + 3	9	928	46	16	7.000
2.034684 + 3	10	1108	53	19	8.500
4.539993 + 2	11	1268	61	22	10.000
2.260329 + 1	12	1648	80	28	13.000
4. + 0	13	1837	93		14.731
5.3158 - 1	14	1920	137	33	16.75
1. - 1	15	1952	156		18.42068
1.1 - 4		1968	172		

This system was well adapted for systematic studies so as to define the optimal conditions for the JEF2 validation.

The gains (expressed in percent) on the accuracy of K_{eff} and the spectral indices I_S resulting from adjustments are defined as : $\left(1-\frac{<\Delta K_{eff}>^*}{<\Delta K_{eff}>}\right)$ x 100 and $\left(1-\frac{<\Delta I_s>^*}{<\Delta I_s>}\right)$ x 100 respectively. The brackets denote the average value and the star * distinguishes the "a posteriori" value from the "a priori" value. The variations in the gains have been investigated as functions of the enhancement factor for different standard deviations obtained from this nominal a priori values by a multiplication by factors 0.3, 0.6, 1.3, 1.5, and for different values of the range of the "a priori" correlations labelled by R = 1, 2, ..., 15.

Figure 1 shows that the gains are generally improved by an increase of the standard deviations in the case of no energy correlation (R=0). This situation is practically unchanged by introducing correlations of any range (R = 1, 2, ..., 12).

Figure 1- Gains (%) in accuracy on K_{eff} and I_S as functions of enhancement factor variations resulting from changes in a priori standard deviations



Two experiments have been rejected from the N = 50 system because of adjustment $\left(\left|\frac{E-C'}{C'}\right| > 3\sigma\right)$.

With this new system of N=48 experiments the situation is globally improved : better consistency with integral experiments is obtained with the nominal a priori standard deviations $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.314$, against $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.37$ in the case of N=50). Both gains in Keff and Is are increased but the importance of "a priori" correlations remains small (effect of ~ 5% on $<\Delta Keff>$ * for example).

If one reduces the system to the N = 43 integral data such that $\left|\frac{E-C'}{C'}\right| < 1.5\,\sigma$, one notes (see fig. 1) when using the nominal a priori standard deviations :

- a less good consistency :

$$\left(\left(\frac{\chi^2}{N}\right)^{1/2} = 1.9\right) \qquad (14)$$

- a large improvement in accuracy of K_{eff} and a worsening in accuracy of I_S.

In addition, the cross-section adjustments are different in sign and amplitude if one compares them to the adjustments with N = 48 or N = 50. This suggests some inconsistency between K_{eff} and Is data. This is confirmed if one considers the systems of K_{eff} data (N=28) or spectral index Is data (N=20) separately. One observes a good consistency between microscopic and integral data since good $\left(\frac{\chi^2}{N}\right)^{1/2}$ values are obtained with "a priori" nominal uncertainties [$\left(\frac{\chi^2}{N}\right)^{1/2} = 1.11$ in the case of the Keff data system ; $\left(\frac{\chi^2}{N}\right)^{1/2} = 1.043$ in the case of Is data]. For these configurations the importance of the off diagonal terms is more significant (14% on K_{eff} calculation, 10% on spectral index calculation).

Finally some general conclusions can be drawn :

1. The optimum system for data validation is the one which simultaneously exhibits :
   - Good consistency between integral and microscopic data (enhancement factor $\left(\frac{\chi^2}{N}\right)^{1/2}$ as close to 1 as possible).
   - Most accurate prediction for each integral parameter.

2. Concerning the microscopic data, the very sophisticated covariance matrices with very small standard deviations are not of practical use, at present, because of the existence of some degree of inconsistency between integral and microscopic data, which limits the importance of the "a priori" off diagonal terms.
   In inconsistent situations the weight of the integral data is dominant in the "a posteriori" microscopic correlations. This is visible since the accuracies on the integral parameters are improved when the "a posteriori" standard deviations are increased.

This suggests :

- The correlations existing between integral data of the same type (I_s essentially), in a given experimental program should be taken into account in the adjustment. In the present study their effects have not been investigated.
- Uncertainty calculations for practical configurations should be performed only with adjusted data sets.

- *Results :*

According to the conclusions of the systematic studies the system of N = 48 experiments is the more adapted, for the moment, to validate JEF2. For what concerns the microscopic data the range of the correlations has been fixed to 3 groups, unless it has been differently assigned in the evaluated covariances (^{238}U, ^{239}Pu).

We have considered as valuable adjustments only those which are greater than the a posteriori standard deviations. As demonstrated in the systematic study, the sign and the energy range of these adjustments are independent of the input standard deviations, so that they can be considered as significant.

For this first approach in the general process of JEF2 validation, 5 nuclear constants have been considered :

- the average number of neutrons emitted per fission : ν,
- the fission cross-section : σ_f,
- the neutron absorption cross-section : $\sigma_a = \sigma_c + \sigma_{n,p} + \sigma_{n,\alpha} + \ldots$,
- the elastic and the inelastic scattering cross-sections : $\sigma_{n,n}$ and $\sigma_{n,n'}$.

For these 2 last nuclear constants the sensitivity coefficients correspond to the global energy transfer so that both the cross-sections and the secondary angular and energy distributions are concerned by the adjustments.

The significant adjustments involve very few nuclei :

$^{235}U : \sigma_f$; 67 KeV < E < 497 KeV
decrease by about -1.5 %

σ_c ; 450 eV < E < 2 KeV
increase by ~ 12 %

$^{238}U : \sigma_{n,n}$; 180 KeV < E < 1.35 MeV
decrease by ~ - 7 %

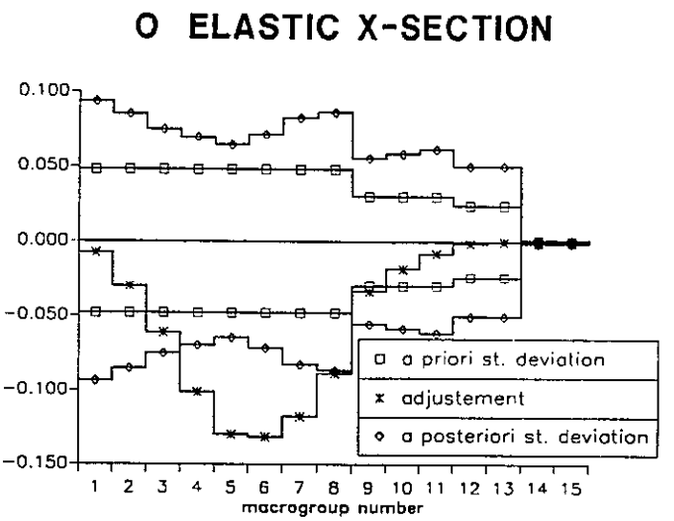
$^{58}Ni : \sigma_a$; 25 KeV < E < 2.23 MeV
decrease by ~ - 28 %

The capture and probably the (n,p) cross-section are affected by adjustments. Further studies are needed to separate the effects on both cross-sections.

^{16}O : $\sigma_{n,n}$; 25 KeV < E < 500 KeV
decrease by ~ 10 %

This is a surprising conclusion of the present benchmarking considering the quality of the evaluation. Essentially the concerned energy range is the one below the first resonance at ~ 450 KeV (see figure 2). It is worthwhile noting that the transport cross-section is higher than the total cross-section below the resonance energy and lower above because of the sign of $\bar{\mu}$ that changes at the resonance energy.

Figure 2 - Adjustment of the elastic cross-section of ^{16}O as requested by the benchmarking



Conclusions

The validation of nuclear constants on selected integral data is a difficult exercise of compromise resulting from the need to have simultaneously complete and consistent information. The methodology for cross-section adjustment is based on a strong theoretical support but some limitation results from the relative inconsistency between the integral and the microscopic data. A part of the responsibility in this situation belongs to the integral data (too optimistic uncertainties, in particular for some types of spectral index ?) and to the calculational methods.

In this situation, the constraints on the quality of uncertainty information on the nuclear data are less stringent and it seems, for the time being, that for valuable data adjustments relatively simple covariance are sufficient : standard deviations on large energy bands which can match the current multigroup energy structures of applications libraries and correlation coefficients both in energy and between nuclei.

In addition to limited revisions to cross-sections of some nuclei such as ^{235}U, ^{238}U, ^{58}Ni, the present JEF2 benchmarking has revealed a severe conflict between the integral and the microscopic data concerning the elastic cross-section and/or the related angular distributions of ^{16}O.

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