JEF2 VALIDATION
METHODOLOGY - PRESENT RESULTS - FUTURE PLANS

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ABSTRACT

The JEF2.2 file is being validated on a large integral data base including thermal and fast critical data, transmission data, and irradiation data obtained in power plants. A microscopic data statistical adjustment technique is used to identify the nuclei subject to revision. Attention is paid to the non-avoidable approximations which could be at the origin of non linearities. Future plans concern the extension of the integral data base to integral data involving structural materials, Minor Actinides, F.P's and also the methodology to adjust basic model parameters.

I. INTRODUCTION

The JEF project is a Cooperation on the evaluation and validation of nuclear data libraries carried out within the framework of the OECD NEA data Bank (Paris). The current version is JEF2.2. Many people have contributed to the development of the library and are participating in its validation.

The basic approach to a validation consists of using the complementarity of the integral and microscopic information. Obviously in each class there are spurious data which have to be adequately corrected or eliminated. Validation is a lengthy process involving various data treatments, neutronics calculation, covariance assessment, data adjustment procedure.

Each step is essential and great care has to be taken to prevent from modification of the initial information.

The fundamental strategy for this work is to investigate simultaneously all energy ranges of interest to take benefit of all physical correlations. This unitary concept has led to the definition of a single multigroup data base (1968 gr). Secondary data bases adapted to specific applications have been derived from this master scheme using adequate weighting functions : 172 g (XMAS Scheme) for thermal data, 175 g (VITAMIN-J) for shieldings, the 1968 gr scheme being used for calculations in the fast range.

The neutronics calculations have been performed with state-of-the-art deterministic methods, regardless of computational cost : Diffusion theory when asymptotic flux conditions are established, S_N-transport theory otherwise, using the most recent cell codes APOLLO 2 (thermal), ECCO (fast) and the ERANOS system of codes.

The integral data base was made of the cleanest experimental data available. The integral data are of different types : critical mass M_c, Buckling B^2_m, K+ (for $K\infty = 1$ experiments), Spectral Index Is, response function at different thicknesses in the case of neutron penetration.

Covariances for these data were established by considering the uncertainties given by the experimentalists and assuming correlations of fixed magnitude for a type of parameters (for example, correlations of 2 % were assumed for the spectral indices involving the same nuclei).

For the JEF2 evaluated data, the information uncertainty is lacking, except for ^{238}U and ^{239}Pu. The covariances matrices have been generated on the basis of personal judgement, sometimes guided by information in the open literature (BNL 325, ENDF documentation, ...) for standard deviations and by adopting "medium" range correlations.

II. METHODOLOGY

The following nomenclature is adopted :

E is the vector matrix of measured integral quantities with covariance I.

σ_0 is the vector of nuclear constants with covariance matrix M.

The integral parameters calculated from σ_0 are denoted by the vector C.

If the calculationnal methods are perfect, quantities such as $\left(\frac{E-C}{E}\right)_k$ or $(E\text{-}C)_k$ measure the imperfect quality of the input nuclear data. Very often a nuclear data file validation is limited to the exhibition of the spread of the $\frac{E-C}{E}$ or E-C values. Restricted to this aspect, the performances of the JEF2 file are as follows :

	Average $\frac{E-C}{C}$	Standard deviation	Maximum deviation
M_c	- 257 pcm	536 pcm	± 1600 pcm
B^2_m	- 125 pcm	600 pcm	± 1600 pcm
K+	- 143 pcm	1060 pcm	± 1500 pcm
Spectral Indices :			
F9 / F5	2.4 %	1.25 %	- 3.8 % , + 2.8 %
F40 / F5	- 5.3 %	4 %	- 4.6 % , + 8 %
F41 / F5	- 0.3 %	3.4 %	- 4 % , + 5 %
F8 / F5	- 1.5 %	2.4 %	- 4.6 % , + 4.6 %
C8 / F5	1.7 %	1.5 %	- 2.25% , + 2.25%
B10 / F5	- 2 %	0.4 %	- 2.7 % , - 1.3 %

This approach gives only a general picture of the value of JEF2 that is globally satisfactory.

Nevertheless it is of prime interest for a complete validation purpose to identify the nuclei, the cross sections, the energy ranges which need improvements.

This is obtained by the "general least squares method".

The system to be considered is :

$$\begin{cases} (\sigma-\sigma_0)^T M^{-1}(\sigma-\sigma_0)+(E-C)^T I^{-1}(E-C) \min & (1a) \\ & (1) \\ C=f(\sigma) & (1b) \end{cases}$$

In system (1) the relationship (1a) expresses the χ^2 while the constraint $C=f(\sigma)$ which relates the "observables" to the parameters σ generally belongs to the linear regression model.

It is adopted $\frac{E-C}{E}=S\frac{\partial\sigma}{\sigma_0}$ (1b) where S stands for the matrix of sensitivity coefficients of the integral parameters to the nuclear data.

The sensitivity coefficients S^k defined as logarithmic derivatives are calculated by using the General Perturbation Theory (GPT) [1].

Linearity condition (1b) is needed to preserve the consistency with GPT but also to obtain an "exact" solution [2].

Practically system (1) is solved using the Lagrange multipliers method. The technique was suggested by GANDINI [3] : the set of observables (integral data) and parameters (evaluated nuclear data) are put in a single vector F_{exp} to which is associated a global dispersion matrix D made of the covariance matrices I and M.

$$D=\left|\begin{array}{c|c} I & \\ \hline & M \end{array}\right|$$

One notes that χ^2 takes now the form :

$$\chi^2=\left(F_{exp}-F\right)^T D^{-1}\left(F_{exp}-F\right) \qquad (2)$$

The condition for χ^2 to be minimized is also the condition for the likelihood function L defined as :

$$L=\frac{1}{\sqrt{2\pi}\,D^{1/2}}\,e^{-\frac{1}{2}\left(F_{exp}-F\right)^T D^{-1}\left(F_{exp}-F\right)} \qquad (3)$$

to be maximized.

A vector $\tilde{F}$ is obtained. It is the "best estimate" that minimizes the consequences of choosing a vector different from the true (unknown) vector.

The quality of the data adjustment is measured by the χ^2 value after adjustment that, according to the theory should equal $N\pm\sqrt{2N}$, N being the number of degree of freedom.

$$\chi^2=N\pm\sqrt{2N} \quad \text{or} \quad \frac{\chi^2}{N}=1\pm\sqrt{\frac{2}{N}} \qquad (4)$$

The number of degrees of freedom, that is the number of input values (microscopic "priors" + integral observables) minus the number of solution parameters (adjusted microscopic data), equals in the present case the number N of integral data.

If the χ^2 value lie outside the theoretical limits this is due either to inconsistent integral values or to non linearities, if one assumes again that the calculational methods are perfect.

To purify the integral data base from spurious information one compares the practical χ^2 distribution to the theoretical expected distribution.

The terms of $(E-C')^T \; I^{-1} \; (E-C')$, are the contributions of integral data to the χ^2 (according to 1a) after adjustment. They are ordered by increasing values. The largest terms which contribute to the quantity in excess in χ^2 are eliminated ("reserved for further analysis") one by one, the adjustment being repeated at each time. (This iterative procedure is used because the adjustment results also depend on the rejected data).

Using this procedure, a small percentage of integral data have been subtracted from the integral data base, (24 out of 157, i.e 15 %).

All these provisionally eliminated data are to be further analyzed before being definitively rejected.

Some qualitative arguments can already be proposed to explain the inconsistencies :

- Some critical mass data strongly contribute to the χ^2 value.

This is due, seemingly, to the abnormally small experimental error bars (< 100 pcm). This is a general comment that the error bars on integral data are very often too optimistic. The quoted uncertainties take into account only the statistical components, the systematic (or correlated) errors being systematically ignored, in particular those of "Technical origin" which may be of non negligible size as demonstrated by Z. SZATMARY [4].

- The Buckling data show a systematic trend in the $\frac{E-C}{C}$ values before adjustment. This trend is not totally corrected by the adjustment at least for $r \geq 0.45$. (The parameter $r = \frac{\langle \nu \, \Sigma_f \rangle}{\langle \xi \, \Sigma_s \rangle}$ is a spectral hardness indicator). This could be due to the contamination by harmonics of the flux which is assumed to be "asymptotic" in the full range of measurement.

The JEF2 validation has been limited so far to the most important nuclei of the General Purpose file. The hypothesis has been made that the adjustment would not affect the self-shielding correction when limited in magnitude. This hypothesis is valid for the fast and the thermal ranges but not for the resonance range. For this range the adjustments have to be considered as trend indicators only.

III. RESULTS

The modifications required by the adjustment procedure are as follows :

Major Actinides :

^{239}Pu :

ν : Indication to decrease by 1.3% (±1.8%) the "bump" observed by GWIN between 20 keV and 50 keV.

$\sigma_{n,f}$: Increase from 2 keV to 1.3 MeV. In the unresolved range (2 keV - 30 keV) there could be a problem of data treatment. At higher energy the trend for greater values (1.8% ± 1.5%) doesn't contradict significantly the conclusions of the subgroup 5 of the International Cooperation.

$\sigma_{n,n'}$: Decrease by 10% ± 13% up to 1 MeV. This is perfectly consistent with model calculations [5] based on recent high resolution measurement of σ_t at ORELA.

^{240}Pu :

$\sigma_{n,f}$: Decrease in the full range, but significantly in the threshold region.

$\sigma_{n,\gamma}$: Decrease significantly in the full range.

^{241}Pu :

$\sigma_{n,f}$: Increase by 8% ± 12% above 2 MeV.

$\sigma_{n,\gamma}$: Decrease significantly in the full range . but this results from one single experiment (PROFIL in PHENIX) .

^{242}Pu :

$\sigma_{n,\gamma}$: Decrease by 15% ± 7% for E > 0.5 keV.

^{238}U :

$\sigma_{n,n'}$: Increase by 10% ± 6% for E >2.2 keV.

^{235}U :

$\sigma_{n,n}$: Decrease by ~4% ± 5% for 25 keV < E < 2 MeV.

$\sigma_{n,\gamma}$: Increase by 3% ± 8% in the resolved range.

This trend is consistent with a renormalization for $<\Gamma_\gamma>$ value adopted in ENDF-B6 which seems to be too small (33 eV).

Structural Materials :

The integral data base is rather poor in data related to structural materials. Nevertheless, some clear trends can be observed.

^{56}Fe :

$\sigma_{n,n'}$: Increase above 2.2 MeV ; slightly decrease below.

$\sigma_{n,\gamma}$: Decrease slightly.

^{58}Ni :

$\sigma_{n,absorption}$: Decrease significantly on the full energy range by ~ 15% ± 8%.

Recently, F. CORVI [9] observed a similar trend in measuring the radiative capture cross section between thermal energy and 300 KeV.

^{52}Cr :

$\sigma_{n,n}$: Decrease by 8% ± 10%.

All the trends observed for the structural materials are consistent with those indicated by K. DIETZE in analysing SEG experiments [6].

Oxygen :

^{16}O :

$\sigma_{n,absorption}$: Decrease by ~ 15% ± 20%.

$\sigma_{n,n}$: It is not clear whether the required modification (increase ~ 10 % around 2.3 MeV, i.e., in the region of an important dip with minimum value ~ 100 mb) is due to the data or to approximations (slowing down treatment) in the calculational methods indicating "compensations" with other nuclei such as ^{239}Pu. The slight decrease ~ 3 % around 450 KeV can be explained by an absence of self-shielding treatment for the first resonance.

Decay Data and Fission Yields :

These data have been validated by means of decay heat calculations compared to best fits to values obtained by measurement [10].

IV. CONCLUSIONS - TRENDS FOR THE FUTURE

In the fast range, most of the required cross section modifications are within the assigned error bars, so that the present version JEF2.2 is an appropriate data base to derive adjusted data sets for applications. In particular, such application libraries will be used to analyse integral data related to nuclei of the special purpose files, such as MINAC's and FP's.

The value of JEF2 in the thermal range has been already stressed by TELLIER [7] and CATHALAU [8].

But in the thermal range, due to the self shielding effect and the unfolding from macrogroup (adjustment) to microgroup (application) it is difficult to derive from the adjustment clear information on the cross sections. It looks, a priori, more profitable to directly "adjust" the resonance parameters despite the problems arising from intrinsic non linearities.

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