REALISATION AND PERFORMANCE OF THE ADJUSTED NUCLEAR DATA LIBRARY ERALIB1 FOR CALCULATING FAST REACTOR NEUTRONICS

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ABSTRACT

The adjusted nuclear data library ERALIB1 is described in this paper. It is the first step in the process towards a unique data set which will be valid for all applications (core neutronics, shielding, fuel cycle) and for all types of fission reactor (thermal, epithermal, fast). It has been derived from a 1968 group application library based on JEF2.2 and a large integral data base containing the ad hoc required data to validate the cross sections for the major nuclear processes. The consistency of the integral and microscopic information is demonstrated by using the rules of information theory and a simple recipe to identify the nonconsistent integral data. The energy scheme used for the statistical consistent adjustment procedure has been designed to optimize the decoupling of cross section effects.
The performance of ERALIB1 for fast reactor applications is considered to be satisfactory. Nevertheless the integral data base needs to be enlarged in order to widen the applicability of the library .

INTRODUCTION

In recent years the conceptual designs of fast reactors have been evolving towards better demonstrated safety, an improved economic performance, and enlarged capabilities such as waste incineration. Instead of multiplying the number of formulaires ,each dedicated to one specific application , it has been judged more judicious to produce one single formulaire with a wide range of applications.

This is the reason why , CEA and its European partners have decided to develop a new nuclear data set and calculational scheme to calculate the neutronic parameters for any type of fast reactor.

The new nuclear data set, ERALIB1 is based on a formal adjustment procedure which takes into account a very wide range of integral data. It is derived from JEF2.2 which performs sufficiently well ,as demonstrated by the validation calculations, to be of sufficient quality for the adjustment to be efficient .

BASIC CHARACTERISTICS OF ERALIB1

Accurate predictions for a wide range of new applications are made possible by using a cross-section library in which the adjustments to the individual cross-sections are uniquely determined and there are no "compensation" effects between errors in cross-sections. This is obtained if one can decouple the effects of each cross-section with respect to the other ones and also as a function of energy. This requires using different types of integral data sensitivity

to different parts of the energy range in an adjustment procedure. There is also the usual additional condition relative to the strict consensus of the integral and microscopic information that is obtained if :

- the reference integral data are clean and sufficiently informative,
- the calculational methods are with limited bias,
- the nuclear data are treated without any significant distortion or loss of information,
- there is an efficient theoretical tool to demonstrate the consistency of the microscopic and integral data.

REALISATION OF ERALIB1

The nuclear data have been taken from the JEF2.2 Library. A 1968 g scheme (1/120 in lethargy) has been chosen and an application Library, JECCOLIB2, has been obtained by processing the data with a validated version of NJOY (NJOY89.69*) in order to obtain the infinite dilute cross sections. The conditions imposed on the NJOY parameters used in the processing give the guarantee that all group constants represent exactly (within an error of less than 0.1%) the initial information contained in JEF2. JECCOLIB2 also contains probability tables (or subgroup data) obtained using CALENDF[1] to calculate self shielding and collision probabilities for homogeneous and heterogeneous media. Secondary data bases adapted to specific applications have been derived from this master scheme using appropriate weighting functions : 172 g (XMAS scheme) for thermal reactor applications, 175 g (VITAMIN-J) for shielding applications, the 1968 gr scheme being used for fast reactor and more general calculations.

Ideally in the integral data base there should be enough information to represent with a good statistical accuracy the competition between the basic neutronic processes : production, absorption, slowing down and leakage, over the whole energy range of interest. In the available data base there are different types of integral data such as critical masses, bucklings, spectral indices, response function data for neutron transmission, sodium void reactivity and more general reactivity worths (substitution or oscillation) sensitive to different energy ranges (thermal, epithermal, fast). In total, 355 integral parameters from 71 different systems have been used but the future developments will lead to a much larger figure. They have been chosen according to criteria of cleanness of the experimental environment that is the ability to model them accurately in calculations. Table 1 shows which kinds of information are included and what isotopes are concerned.

The neutronics calculations have been performed using the most recent cell codes APOLLO2 (thermal)[2], ECCO (fast)[3] and the ERANOS system of spatial neutronic codes[4]. All these codes are based on deterministic methods. Extensive validation has been performed as a result of a long period of development. As often as possible the results are checked using Monte Carlo methods in particular the MCNP or TRIPOLI4 codes[5] which use Libraries based on JEF2.2 .

The sensitivity coefficient calculations were based on perturbation theory (GPT or EGPT) . These coefficients have been carefully and systematically checked.

The shapes of the sensitivity curves are useful guides in deciding the most appropriate energy scheme for the adjustment procedure : the adjustment is most efficient if the nuclear parameters have different behaviour with energy in a macrogroup. This is feasible in the fast range, but difficult in the thermal range where fission and capture cross sections have identical shapes (for this particular energy range, irradiated fuel data are most appropriate). On the basis

of these considerations a 15 macrogroup scheme has been used for the adjustment.It is consistent with all above mentionned schemes .

CRITICALS	MEASURED QUANTITIES	INFORMATION ON NUCLEI FOR ERALIB1	INFORMATION ON NUCLEI FOR ENLARGED ERALIB1
LOS ALAMOS SPHERES	Mc, I_c	MAJOR ACTINIDES	MINOR ACTINIDES
MASURCA ZEBRA SNEAK MINERVE	Mc, B^2m, $K_\infty = 1$, I_S $\Delta\rho$	MAJOR ACTINIDES STRUCTURALS	MINOR ACTINIDES
PHENIX	I_c	MAJOR ACTINIDES	MINOR ACTINIDES FP
RB2	$\Delta\rho$	STRUCTURALS ^{10}B,^{5}U	
ASPIS	RESPONSE FUNCTIONS	Fe	
NESTDIP2 PCA-REPLICA BLOC GRAPHITE	RESPONSE FUNCTIONS	Fe,H2O C	
SEG (4,5,6,7)	$\Delta\rho$	Fe,Cr,Ni	FP
SOME THERMAL EXPERIMENTS	B^2m, I_c	MAJOR ACTINIDES	MINOR ACTINIDES

Table 1: Integral data base used to produce ERALIB1

The adjustment has to be considered as the improvement of the "a priori" (evaluated) data obtained by the inclusion of the integral information into the nuclear data. This is achieved by using the rules of INFORMATION Theory based on Entropy maximisation with constraints. Continuously developed by numerous (famous) contributors from the early studies in 1939 by DUNNINGTON this theory has received now its full developpment . Useful syntheses are now available ,among others, by F.FROEHNER[7] or D.SMITH[8] .

The problem of Entropy maximisation is solved by the use of LAGRANGE multipliers which leads to the maximisation of a likelihood function and consequently to the minimisation of a generalized χ^2.This is the direct consequence of the assumption that all the uncertainties have a normal distribution .This technique is known also as the "statistical consistent" adjustment method .

The following nomenclature is adopted :

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

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

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

The parameter r is a spectral hardness index defined as: $r = \frac{<\nu\Sigma_f>}{<\xi\Sigma_s>}$

The covariance matrices have been defined in the following way:

- By expert judgment and comparison with external information for what concerns M, since no convariance data are provided for JEF2 (except ^{238}U, ^{239}Pu).
- To generate the covariance matrix I estimated systematic errors and their correlations have been combined with the statistical uncertainties published in the literature.

In practice, for our consistent statistical adjustment procedure, we have used the code AMERE, a version of the AMARA code written by GANDINI and PETILLI[6].

The set of observables (integral data) and parameters (evaluated nuclear data) are put in a single vector F_{exp} with which is associated a global dispersion matrix D consisting of the covariance matrices I and M, assuming there are no a priori correlations between microscopic and integral data .

$$D = \begin{vmatrix} I & 0 \\ 0 & M \end{vmatrix}$$

If F stands for any adjusted vector, the likelihood function is written as :

$$L = \frac{1}{\sqrt{\det(2\pi D)}} \exp -\frac{1}{2}\left(F_{exp} - F\right)^T D^{-1}\left(F_{exp} - F\right)$$

The condition for a maximized likelihood function that is supposed to define an optimum "adjusted" vector $\tilde{F}$ or "best estimate" as close as possible to the always unknown, true vector is identical to the condition to obtain a minimized generalized χ^2.

$$\chi^2 = \left(F_{exp} - \tilde{F}\right)^T D^{-1}\left(F_{exp} - \tilde{F}\right), \text{ ie the system}$$

$$\begin{cases} (\tilde{\sigma} - \sigma_o)^T M^{-1}(\tilde{\sigma} - \sigma_o) + \left(E - \tilde{C}\right)^T I^{-1}\left(E - \tilde{C}\right) \text{ is.a.minimum} \\ \tilde{C} = f(\tilde{\sigma}) \end{cases}$$

where f is a linear relationship law relating the observables to the parameters though sensitivity coefficients S ($\tilde{C} = C(1 + S\frac{\delta\sigma}{\sigma_o})$).

According to the theory, the "best estimate" is obtained only when $\chi^2 = N \pm \sqrt{2N}$, N being the degree of freedom of the system. The degree of freedom is the number of input values (microscopic "priors" + integral observables) minus the number of solution parameters (adjusted microscopic data). It equals, in the present case, the number of integral data.

The χ^2 value has to be regarded as a test of consistency of the nuclear data with the experimental integral data and the internal consistency of the integral data .

Prior to any adjustment the "reduced" χ^2 (χ^2/N) can reache sometimes high values ; 6 or even more. This means that an evaluated data library, whatever its quality, cannot meet the

Reactor Physics requirements and that adjustment of the nuclear constants is a necessary procedure in any case.

If the a posteriori reduced χ^2 value lies outside the limits $1-\sqrt{2/N}$ and $1+\sqrt{2/N}$, this is mainly due to the following reasons :

- existence of nonlinearities in the sensitivity coefficients,
- presence in the integral data base of some inconsistent values due to systematic biases in the experiment or in the analysis .

The linearity condition is important since it preserves the consistency with GPT but also since it is needed to obtain an "exact" solution. Non linearities are observed when the magnitude of the adjustment goes beyond some limit (~ 10 % ?) depending on the integral parameter and the cross section type. The solution for such situations is to calculate the sensitivity coefficients to include higher order terms .

Although the notion of inconsistent integral information is perfectly justified on a statistic point of view one has to be careful before deciding that a particular item of integral information (experimental and/or analytical) is of insufficient quality :

a. A part of the excess value in χ^2/N can be due to particularly unrealistic uncertainties affecting the nuclear data and/or the integral data, these latter ones making the largest contribution. Such a situation can be improved by reanalysing (in particular, by inclusion of some systematic errors) or renormalizing the standard deviations (by $\left(\chi^2/N\right)^{1/2}$ for each type of parameter, for instance).

b. When there is some evidence of the existence of non consistent integral values the (great) difficulty is to identify them. Actually, one is facing the problem of selecting the greatest consistent subset among the set of the N integral data. To do this a recipe has been used.

It is based on the observation that the "a posteriori" χ^2 is the sum of three terms, one related to the microscopic data, one related to the integral data, the third resulting from correlations between microscopic and integral terms introduced by the adjustment :

$$\chi^2 = \chi^2_{mic} + \chi^2_{int} + \chi^2_{mic-int}$$

It happens that the $\chi^2_{mic-int}$ term can be often neglected.

The recipe consists of ordering the χ^2_{int} terms ,ie the terms of $(E-C)^T I^{-1}(E-C)(E-C)^T I^{-1}(E-C)$, in increasing order. The largest term designates the integral datum to be discarded.This operation is made stepwise, the adjustment being repeated each time, until an acceptable value for χ^2 is obtained.

This works correctly as is shown in figure 1, where it is interesting to note that the χ^2_{mic} term ,ie $(\sigma-\sigma_0)^T M^{-1}(\sigma-\sigma_0)$ remains constant as long as χ^2 lies between the consistency limits $(1\pm\sqrt{2/N})$. This constant behaviour indicates in statistical terms that the exact adjustment is obtained.

It is interesting to note that there is a subgroup of the integral measurements which have been eliminated which have a value of χ^2 which remains unchanged .If the uncertainties on these were to be increased by a small factor they could be reintroduced and consistency would be maintained .

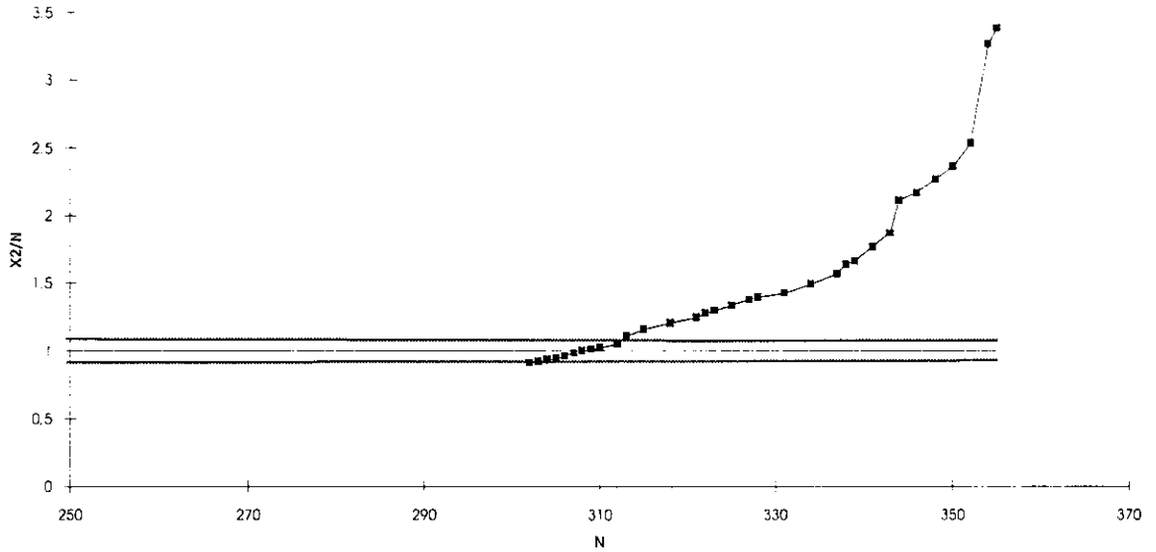

Fig 1 : Evolution of reduced χ^2 when inconsistent data are removed

c. It is wise to justify the eliminated integral measurements by arguments based on Reactor Physics even if these results are confirmed by simple statistical criteria such as (E-C) > 3.exp.st.dev.

PERFORMANCE OF ERALIB1

ERALIB1 is directly derived from JECCOLIB2 by distributing into the 1968 fine groups the adjustment results obtained in 15 macrogroups. The transformation may introduce specific biases due to nonlinearity or unfolding effects. These biases have been estimated by comparing the performances predicted by the adjustment to results obtained with the 1968 group ERALIB1 on one side, and to calculation based on the nuclear parameter perturbations indicated by the 15 group adjustment with respect to JECCOLIB2 on the other side. The non linearity effect is negligible while the deconvolution effect (~ 70 pcm on average) suggests that the deconvolution technique could be improved.

In this first stage ERALIB1 includes adjustments for the 17 main (major actinides, structural materials, absorbants, scatterers), ie nuclei of the General Purpose file.

The adjustments, which are strongly dependent on the covariance data , have been carefully checked:

This has been done by comparing the cross section modifications suggested by the adjustment procedure to the indications from new measurements, new evaluations not included in JEF2, and more generally to what is well known in terms of basic nuclear physics or model calculations. For each significant adjustment of each nucleus the checking has been very satisfactory.

This confirms the value of ERALIB1 in terms of nuclear physics.

The ERALIB1 data base, in association with the neutronic code system ERANOS has been produced to predict in a confident and accurate way the parameters required for reactor design.

JECCOLIB2 (JEF 2) ; ERALIB1

	before adjustment		after adjustment	
	Standard deviation	Bias	Standard deviation	Bias
Critical core Keff	1460 pcm	323 pcm	100 pcm	83 pcm
B_m^2	1200 pcm	-210 pcm	150 pcm	-260 pcm
K^+	2200 pcm	-50 pcm	240 pcm	123 pcm
F49/F25	2.6%	1.1%	0.5%	+0.3%
F28/F25	3.7%	-1. %	0.8%	-1%
C28/F25	2.2%	1.4%	0.5%	1%
F40/F25	8.6%	-4%	1.5%	-1.3%
F41/F25	5%	-1.4%	1.2%	0.5%
F42/F25	8%	-5.2%	1.3%	-1.6%
B10/F25	2.3%	-2%	0.8%	-1.3%

Table 2: Comparison of the performance of JEF2 and ERALIB1

Table 2 summarizes the main characteristics of the present performance (uncertainties and biases) of ERALIB1 with respect to the reduction of uncertainties or the improved quality of prediction.

The reduction of the uncertainties is substantial for most parameters. This is ,in particular, the case for the critical masses : the statistical uncertainty is decreased by a factor greater than 10, the final average value being significantly smaller than the experimental one .It is worthwhile noting that the systematic underprediction by JEF2 is almost totally removed over the whole range of r values (figure 2).

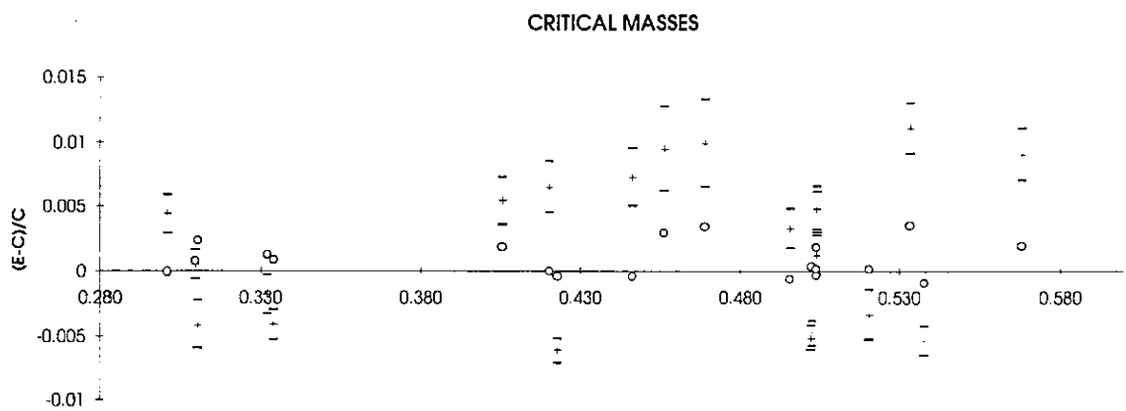

Fig 2 : Distribution of (E-C)/C values before(+) and after adjustment (o)

Concerning the biases the situation is similar except for some notable cases.

For the fundamental mode K_{eff} data (B^2_m, K^+ ...) there is no improvement of the biases. It is interesting to note that both B^2_m and K^+ data exhibit a similar trend: the slope of $\frac{E-C}{C}$ values (figure3) as a function of r is negative. This trend is not totally corrected by the adjustment. A satisfactory explanation for such a situation has still to be found.

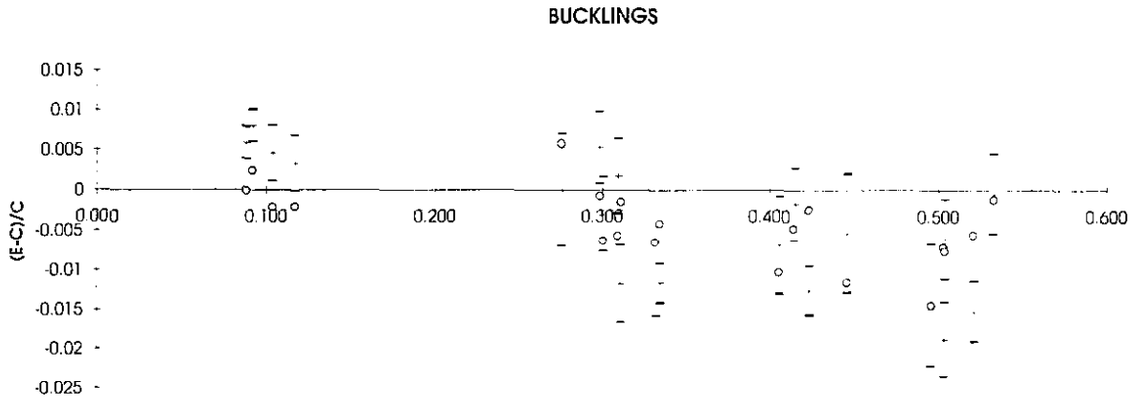

Fig 3 : Distribution of (E-C)/C values before (+) and after adjustment (o)

The spectral indices play a modest role in parameter adjustment because of their limited accuracy (roughly of the same order as the a priori calculated values), unless they are very numerous and consistent as is the case for F49/F25 (figure 4) and F28/F25 .

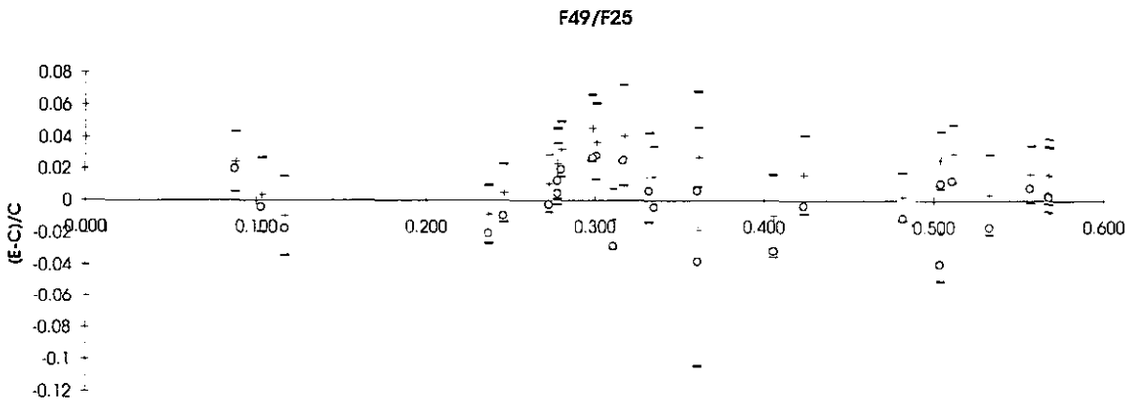

Fig. 4 : Distribution of (E-C)/C values before (+) and after adjustment (o)

It is probably because of the insufficiently accurate integral information that the C28/F25 index keeps an important bias after adjustment and this would affect the accuracy of the prediction of the breeding gain (figure 5).

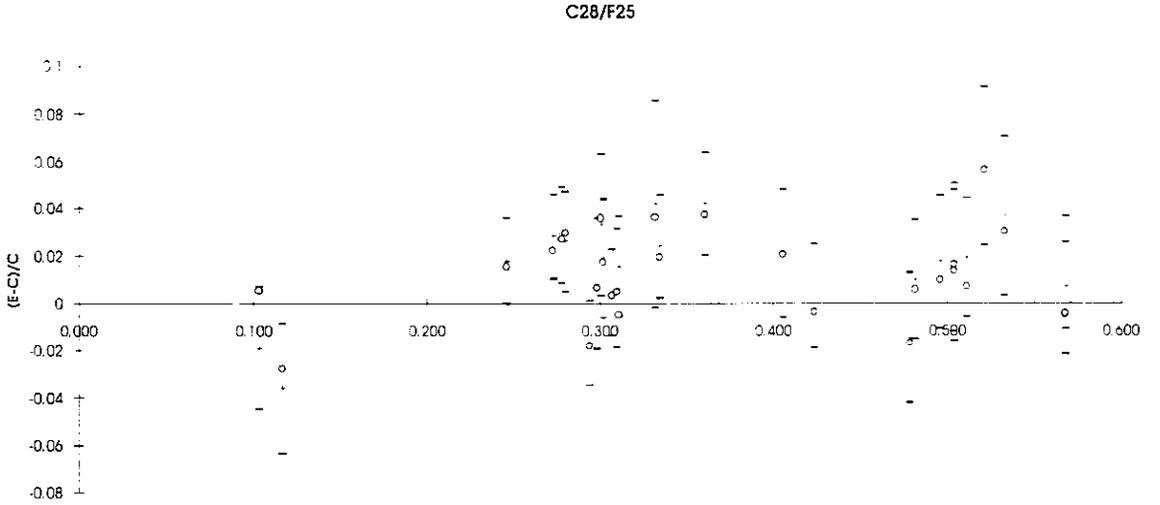

Fig. 5 : Distribution of (E-C)/C values before (+) and after adjustment (o)

Concerning the indices relating to the higher Pu isotopes an additional explanation has to be invoked : the deficiency in some evaluated cross sections. As examples , the capture cross sections of all higher Pu isotopes should be decreased by significant amounts (10% or more)

Material worths, in general, proved inconsistent. For this kind of parameter the difficulty of obtaining correct calculations must be emphasized.

There are too few data related to Na void configurations to draw reliable conclusions. Neither control rod worth nor power distributions are mentioned because of a lack of data in the present data base. Nevertheless the adjustment confirms the good quality of the $^{10}B(n,\alpha)$ cross section data in JEF2.2

CONCLUSIONS

The adjustments based on Generalized Least Squares methods have proved efficient in data uncertainty and bias reduction provided that techniques to identify inconsistent data are introduced.

The quality of the covariance data, especially those of the Integral observables is of crucial importance for an adjusted data set consistent with Nuclear Physics to be obtained .In these conditions a statistical consistent adjustment procedure should be considered as a powerful tool to demonstrate the quality of an experimental program .

The present ERALIB1 application Library, which has been developed with the aim of creating a multi-application multi-system Library, has demonstrated high capabilities to calculate most of the important parameters of a classical fast reactor core over a wide range of spectral hardnesses.

In the future its application area will be enlarged to include the Plutonium and Actinide burner cores and also to fuel cycle applications.

ACKNOWLEDGMENTS

Acknowledgments are due to R.JACQMIN for his contribution to the general checking , to P.LONG for his maintenance of the AMERE code ,and to Mrs M.TOUPIN for data preparation .We gratefully acknowledge the technical interest and financial support from E.D.F. and FRAMATOME .

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