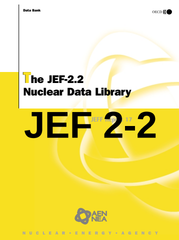

JEF/DOC-759

JEF2 validation
Part 1 - General purpose file

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I. Objective of data validation

The activity on nuclear Data evaluation, at least for the majority of them, is clearly justified by their use in the nuclear energy applications.

Once the nuclear data have been evaluated by using supposedly the whole Nuclear Physics information (experimental data, nuclear models...) ie an information totally independent from the application one has to demonstrate that they are appropriate for accurate predictions for a wide range of applications.

This demonstration is exactly the objective of the so called nuclear data validation.

Basically, it is made by using the evaluated nuclear data to calculate synthetic parameters for numerous media chosen for their representativity of the application.

But unambiguous conclusions about the quality of the nuclear data can be drawn only if some conditions are respected. These ones will be reviewed in the following.

II. Short description of the methodologies used for validation

At this point, two approaches can be envisaged :

- One approach, systematically used in the past, consists of judging on a global point of view, just by comparing the calculated values to the experimental ones for a reduced number of application types (for example Keff data and/or burned fuel analysis). If the benchmark results are judged non satisfactory tentative explanation are produced on a qualitative basis. Actually, it is very difficult, without sensitivity calculation to judge about possible compensations between nuclei or cross sections of a same nuclide.
  This approach, which gives quick results and can be efficient in some cases, is restricted to the simultaneous analysis of very few data.

- The second approach, we could call the modern approach, is possible only because of the continuous improvements in calculational methods in several application fields of neutronics. Using a statistical adjustment procedure it is now possible to identify the deficiencies and in numerous cases to quantify them. In what follows we will justify this assessment.
  This approach, more costly than the previous one has the advantage to limit the reevaluation work to the questionable energy ranges and nuclear processes, making possible significant savings in time and money.
  It can be applied to an unlimited number of integral parameters.

III. Description of the validation work

For the conclusions to be unquestionable several conditions have to be fulfilled. They are related to :

- *The calculational methods*

The methods we used are essentially deterministic methods. The calculations have been performed using the most recent cell codes : APOLLO 2 (thermal), ECCO (fast) and the ERANOS system of spatial neutronic codes. All these codes have been extensively validated on a long period of time. Some checks have been made with MONTE-CARLO methods using MCNP and TRIPOLI4 codes. These checks have shown reasonable agreement for simple systems, in any case of the same order of magnitude of the experimental error [from 50 to 200 pcm for critical masses). For complex systems greater differences have been sometimes found.

All these checks demonstrate that the biases due to the modelization have been minimized in the above mentioned codes.

The sensitivity coefficient calculations were based on perturbation theory (SPT (keff), GPT (reaction rate) EGPT ($\Delta\rho$). These coefficients have been carefully and sometimes checked by direct calculations.

- *The nuclear data treatment*

The aim is to treat the nuclear data without significant distortion or loss of information.

Infinite dilute cross sections have been calculated with a validated version of NOY (NJOY 89.69*) [1], with conditions imposed on NJOY parameters such that an error of less than 0,1 % is guaranteed. This is consistent with the recent observation of ~ 80 pcm differences for Keff data of thermal systems according to the JEF2 data treated either by NJOY 89.69* or NJOY 94.

Probability tables to calculate self shielding factors or collision probability in unhomogeneous situations have been produced with CALENDF [2]. Consistent libraries with the appropriate weighting function have been obtained in different energy schemes :

172 g (XMAS) for thermal reactor applications,
175 g (VITAMIN-J) for shielding applications,
1968 g (ECCO for fast reactor and more general calculations.

- *The reference integral data base*

There should be enough information to represent with a good statistical accuracy over the whole energy range the competition between the basic neutronic processes : production, absorption, slowing down and leakage which are represented by the following nuclear parameters : ν (total number of neutrons produced by fission), $\sigma_{n,f}$ (fission cross section), $\sigma_{n,\gamma}$ (capture cross section), $\sigma_{n,n}$ and $\sigma_{n,n'}$ (elastic and inelastic scattering cross sections).

This is the reason why there are in the data base different types of integral data : critical mass, buckling, spectral index, response function data for neutron transmission, sodium void reactivity and reactivity worths, sensitive to different energy ranges. In total 472 integral parameters from 71 different systems have been used.

We are convinced that most of these data are clean and able to be correctly modelled. It is worth mentioning that the energy range between thermal and a few MeV is entirely covered by experimental information except in the resonance range above the first few resonances in heavy nuclei (range of the hundreds of eV).

- *The theoretical tool to demonstrate the consistency of the nuclear data and the integral data*

The necessary qualities for such a tool are to be : self important, unique and the best.

Self important means that it should have the capabilities :

- to detect the insufficiencies of real situations ; in particular it should detect and identify the biases in integral data. This is the case for our tool as an identifier (statistical procedure) of inconsistent data has been implemented in the code AMERE [3],

- to identify erroneous uncertainties on the observable or the nuclear parameters.

A careful analysis of the values of the differents terms of the χ^2 estimator can provide the answer.

Unique and the best ?

It is known that the Bayesian approach is the exact one, while the maximum likelihood and/or KHI2 minimization methods (the one we used) are approximations giving close results under specific circunstances.

In this work, we had a permanent regard for such circunstances in order to justify the nuclear data adjustment as an improvement, improvement obtained by the inclusion of the integral information into the nuclear data.

The technic to do that is well known as a result of numerous and continuous theoretical developments starting with DUNNINGTON in 1939. Very few syntheses exist and it is worth mentioning the comprehensive studies by F. FROHNER [4], [5]. All the applications to nuclear data performed everywhere in the world accept the same theoretical basis which can be summarized in an approach in 3 steps.

1. The information theory is an useful tool to define a probability density when information is missing.

This is based on the maximum Eutropy principle, the Information Eutropy being defined by the so called "SHANNON" formula :

$$W = -\sum_{\nu} p_{\nu} \, \mathrm{Ln}\, p_{\nu} \text{, given probabilities } p_{\nu} \text{ for alternatives } \nu.$$

This formula has been transformed by JAYNES for continuous distributions with probability density p(x) into :

$$W = -\int p(x) \, \mathrm{Ln}\, p(x) \, dx$$

The maximum entropy Principle tells that one has to choose for p(x) the density probability which maximises W subject to the constraints of the available (a priori) but partial information of macroscopic nature.

This kind of problem is solved by the method of LAGRANGE's multipliers.

The following example, given by F. FROHNER is important by its repetitive use and consequences in applications.

If a probability density p(x) is only known by the 2 first moments (the average value <x> and the variance var x = $(\Delta x)^2$, a trivial situation in Physics), the Entropy maximisation assigns a Gaussian representation as the "most objective probability density for further inference" [5].

$$p(x|<x>, \Delta x)\, dx = \frac{1}{\sqrt{2\,(\Delta x)^2}} \exp\left[-\frac{1}{2}\left(\frac{x-<x>}{\Delta x}\right)^2\right] dx, \; -\infty < x < +\infty$$

When there are several quantities x_J with average values $<x_y>$ and a covariance matrix C relating Δx_i to Δx_J, the maximum entropy yields a multivariate Gaussian.

$$p(x|<x>, C)\, d(x) = \frac{1}{\sqrt{\det(2\pi C)^2}} \exp\left[-\frac{1}{2}(x-<x>)\, C^{-1}\,(x-<x>)\right] d(x)$$

This justifies the assumption, sometimes blindly made, of a normal distribution for the uncertainties for both the microscopic and the integral data.

2. The inclusion of the integral information

Let be the vector y for the "observables" (integral parameters) Y_i, i = 1, 2, ..., I.

Let be the vector x for the "parameters" (nuclear parameters) x_μ, μ = 1, ..., M and y(x) the relationship between y and x.

An a priori information exists :

a. For the vector x

They are represented by the vector ξ (evaluated data) and uncertainty covariance matrix C_ξ. Applying the Maximum Entropy principle and (taking into account the a priori information), the probability distribution p(x) is :

$$p(x|\, \xi, C_\xi)\, d^M(x) \cong \exp\left[-\frac{1}{2}(x-\xi)^+\, C_\xi^{-1}\,(x-\xi)\right] d^M(x)$$

b. For the vector y

They are represented by the vector η of the integral data and an associated uncertainty covariance matrix C_η.

The likelihood to obtain the η values from the true (unknown) x values is given by the following equation :

$$p\left(\eta \middle| \; y(x)\, C_{\eta}\right) d^{I}\eta \cong \exp\left[-\frac{1}{2}\left(\eta - y(x)\right)^{+} C_{\eta}^{-1} \left(n - y(x)\right)\right] d^{I}\eta$$

which is nothing else but the result of the application, again, of the principle of maximum Entropy. This equation is important since it represents the contribution of the integral information in the common set.

The probability density distribution resulting from taking into account both the a priori information ξ and the integral information η is obtained, in the Bayesian approach, as the product of the a priori distribution times the likelihood function.

$$p\left(x \middle| \; C_{x}, \xi, C_{\eta}, y(x)\right) dM \cong \exp -\frac{1}{2}\left[(x-\xi)^{+} C_{x}^{-I} (x-\xi) + \left(\eta - y(x)\right)^{+} C_{\eta}^{-I} \left(\eta - y(x)\right)\right]$$

We are looking for the "best estimate" of the , always unknown, true vector. It is the most probable vector $\tilde{x}$ of the a posteriori distribution, ie, the one which maximizes the right hand side term of the above equation. It is obtained by minimising the quantity :

$$(x-\xi)^{+} C_{x}^{-I} (x-\xi) + \left(\eta - y(x)\right)^{+} C_{\eta}^{-I} \left(\eta - y(x)\right)$$

This term is a quadratic form involving both the parameters and the observables. This is the so called generalized χ^2.

Thus, we have to consider the system :

$$\begin{cases} \chi^{2} = (x-\xi)^{+} C_{\xi}^{-1}(x-\xi) \; + \left(\left(\eta - y(x)\right)^{+} C_{\eta}^{-1}\left(\eta - y(x)\right)\right) \text{minimum} \\ y(x) \; - \; y(\xi) \; = \; S(x - \xi) \end{cases} \qquad (1)$$

S stands for the derivatives of y(x) for the a priori values ξ of x.

S is the matrix of Sensitivity Coefficients.

The second equation of system (1) contains the implicit so called linearity condition which limits the amplitude of $(x - \xi)$ perturbation. This condition preserves the consistency with GPT and also with the Bayesian theory since the solution obtained by the χ^2 minimization is exact in these conditions.

In the frame of the Decision Theory the solution we are looking for is a vector which minimizes the consequences of choosing a vector different from the always unknown true vector, i.e which minimizes a "loss function". By definition of this "loss function", $\tilde{x}$ appears as a vector of minimum variance.

In others words, the solution of the above system is a vector which minimizes χ^2 for minimal deviations with respect to the a priori vector ξ considered as an approximation of the truth. It is equivalent to say that we have to find a vector which minimizes both χ^2 and $(x-\xi)^+ (x - \xi)$ or the proportional quantity $(x - \xi)^+ C^{-1} (x - \xi)$.

$$\left\{ \begin{array}{l} \chi^2 = (x-\xi)^+ \, C_\xi^{-1}(x-\xi) \; + \; \Big((\eta - y(x))^+ \, C_\eta^{-1}(\eta - y(x)) \Big) \text{ minimum} \\ \\ (x-\xi)^+ \, C^{-1}(x-\xi) \text{ minimum} \end{array} \right. \qquad (2)$$

In the present case, when using JEF2.2 file and the 472 data of our integral data base one obtains a value of 20 (${}^{\text{prior}}\chi_r^2 \simeq 20$). Since at this stage JEF2.2 file cannot be considered as a reference, this high value of χ_r^2 simply means that JEF2.2 doesn't meet the Reactor Physics requirements and the same conclusion probably applies to any evaluated data library. On the contrary a file modified by inclusion of the integral information is made consistent with the integral data and consequently becomes a reference for this type of data : by using a (correctly) adjusted file it is possible to judge about the consistency of additional integral data.

If after an adjustment considering all the data of the base the χ_r^2 value (a posteriori value, noted ${}^{\text{post}}\chi_r^2$) lies outside the confidence limits the reasons have to be found in one or several of the following items :

<u>a</u> existence of non linearities in the sensitivity coefficients,
<u>b</u> underestimation of uncertainties, microscopic or integral,
<u>c</u> presence in the integral data base of some inconsistent values.

In validating the JEF2.2 major nuclei with 472 integral data we obtained the following value for the a posteriori reduced χ_r^2 : ${}^{\text{post}}\chi_r^2$ = 6.96, far outside the confidence range which is [0.8047, 1.195].

Obviously such a situation is not acceptable.

How to improve it ?

a : First, we note that large corrections are indicated by the adjustment :

~ 15 % for the capture cross section of ^{58}Ni
~ 55 % for the (n,2n) cross section of ^{239}Pu
~ - 30 % for the (n,n') cross section of ^{23}Na
~ + 30 % for the (n,n) cross section of ^{23}Na.

Non linearities in the sensitivity coefficients of these nuclei have obviously a part of responsibility in the high value of ${}^{post}\chi_r^2$. The solution for such cases is to calculate higher order terms for the sensitivity coefficients, or to use an iterative adjustment procedure. Neither of these options were used due to limitation of time.

In addition we suspect that this adjustment doesn't fulfil the condition of minimal variation of a priori initial parameter values ($(x-\xi)$ minimal).

But, the contribution of the mentioned nuclear data is minor and we have to complete by other arguments.

b : The argument of the underestimation of the uncertainties cannot be used. As a matter of fact, prior to any calculation of integral experiments we have carefully analyzed the published uncertainties when available and documented. We have reconsidered them by introducing estimated systematic uncertainties in the experimental procedure or calculationnal methods with the consequence of a significant increase, in some cases, of the error bars.

c : The importance of the departure from unity for ${}^{post}\chi_r^2$ gives some support to the hypothesis of the existence of non consistent integral data.

The great difficulty is to identify them.

We suggest an approach in two parts :

1 Identification by means of statistical analysis.
2 Contradictory reanalysis of the identified experiments by using experimental technic and Reactor Physics arguments.

1 Identification by means of statistical analysis

The a posteriori χ_r^2 value, namely ${}^{post}\chi_r^2$, can be written as the sum of three terms :

$$ {}^{post}\chi_r^2 = \chi_{mac}^2 + \chi_{mic}^2 + E $$

χ_{mac}^2 is the sum of the squared terms of $(\eta - y(x))^r \, C_\eta^{-1} \, (\eta - y(x))$.

$$ \chi_{mac}^2 = \frac{1}{N} \sum_i X_i^2 $$

The i[th] element can be written in a more usual form : $X_i^2 = \left(\frac{E - C}{\varepsilon}\right)_i^2$ where E_i and C_i stand respectively for the experimental and the calculated value of the i[th] observable, while ε. is the associated uncertainty.

χ_{mic}^2 is proportional to the quadratic term related to nuclear data only in χ^2 :

$$ \chi_{mic}^2 = \frac{1}{N} (x - \xi)^+ \, C_\xi^{-1} \, (x - \xi) $$

The residual E contains all the terms complementary to χ_{mic}^2 and χ_{mac}^2, i.e., all the cross terms related to the observables plus some additional squared terms additional to those of χ_{mac}^2 and which result from the inversion of the C_η matrix that is not diagonal.

It is worth mentioning that each of the above defined quantities, χ_{mac}^2, χ_{mic}^2, E is dependent on the degree of freedom.

The methodology we propose is actually based on the objective to verify the condition of a correct solution of the system (1).

The X_i^2 terms are ordered by increasing values.

$$ N_{max} \, \chi_{mac}^2 = X_1^2 + X_2^2 + - \ldots X_i^2 + \ldots X_N^2 + X_{N+1}^2 + \ldots + X_{Nmax}^2 $$

N_{max} being the maximum number of integral data in the data base.

If ${}^{post}\chi_r^2$ is greater than $1+3\sqrt{\frac{2}{N_{max}}}$ (general situation) it is because of abnormally large terms X^2, but in particular of the largest one, i.e. X^2_{Nmax}.

This one identifies the experimental datum to be first discarded.

The adjustment procedure is repeated with N = Nmax - 1 data and so on.

One observes that the $\chi_r^2(N)$ value is continuously decreasing when N decreases.

The process of discarding integral data is stopped when a minimum, different from 0, is obtained for χ^2_{mic}. A real difficulty is related to the guarantee to be given that the discarded integral data are not the unique sources of information for given nuclear data.

A minimum value for χ^2_{mic} was obtained for a χ_r^2 value equal to 0.99991. Such a situation corresponds to n = 58 rejected integral data and defines an "effective" integral data base made of $N = N_{max}-n$ data. These rejected data have to be considered as non informative for the purpose of nuclear data validation.

The identification of "non informative" integral data is a key point in the method and the consequences on both the microscopic data adjustment and the integral parameter calculation are significant :

The amplitude of nuclear data corrections is minimized as required by the theoretical conditions of the adjustment. With respect to the results obtained with a complete integral data base the adjustments obtained with the "effective" data base are sometimes of different signs demonstrating the importance of the selection of integral data.

As expected, the calculations of integral parameters are strongly improved even for those which have been discarded.

2 Contradictory reanalysis of the "discarded" experiments by using experimental technic and Reactor Physics arguments.

The integral experiments which have been discarded are essentially of 3 types :

- Bücklings in the thermal and fast ranges
- Spectral indices
- Large Na voids

These data are being reanalyzed at Cadarache.

It is too early to report in the detail one work that will still go on for a long period but, nevertheless, some conclusions can be drawn.

- **Bücklings**

Thermal range : this area has not been yet reviewed but it has been told that some refinements have to be added in the calculations.

Fast range : All the discarded data belong to the higher energy part (r > 0.3) of the range and concern small size cores. In this range the Bückling values are systematically overestimated. The biases are significant with JEF2 values (- 210 pcm on average) and still increased with adjusted values (- 260 pcm) while they are set down to 0 for the Bücklings of the low energy part (r < 0.3).

The primary experimental data have been reanalysed. Improvements have been obtained but not really significant suggesting a more basic reason : exact delimitation of the core zone where there is a fundamental mode, possible energy dependence in B_m^2 .... .

- **Spectral Indices**

There is no characteristics attached to the "removed" spectral indices. We do not see any reason related to the calculational methods and the causes of deficiency are probably experimental as it will be shown in the following example :

In the ZONA2B experiment to test the reflector effect in a fast core spectral index radial traverses were measured, such as $\frac{F25(\vec{r})}{F25(0)}, \frac{F49(\vec{r})}{F49(0)}, \frac{F28(\vec{r})}{F28(0)}$, the 0 position referring to the center of the core.

All the data for different positions $\vec{r}$ have been removed by the adjustment procedure. After examination it appeared that the composition given by the manufacturer concerning the Steel of the Reflector was erroneous. As a consequence of correction of the content values the $\frac{F25(\vec{r})}{F25(0)}$ and $\frac{F28(\vec{r})}{F28(0)}$ have been kept inducing a significant information on the elastic cross section of ^{52}Cr.

This demonstrates the necessity to have as many data as possible in a Data base and also the efficiency of our method.

- **Large Na voids**

The validation of ^{23}Na data has been the major problem in this validation work due to the extremely bad quality of the evaluated data and to the difficulty to properly calculate the integral Na void effect. A big effort has been devoted to understand this problem [ ].

The conclusions are :

The Na void configurations are correctly calculated with the recent methods but the extreme sensitivity of the reactivity change $\Delta\rho$ to the nuclear data of ^{23}Na makes difficult any correct adjustment of prior data very far from the truth.

As a fact, the first indications of the adjustment and the analysis of transmission data obtained at OAK-RIDGE and recent inelastic cross-section measurement performed at GEEL [ ] suggest that elastic and inelastic cross-sections could be erroneous by - 30 % and + 30 % respectively.

This bad situation explains why all the large Na voids are presently rejected by the procedure depriving the validation work of an important source of information.

IV. Results and provisional conclusions relative to the evaluated data

Thanks to be statistical adjustment procedure valorized by the methodology we propose to discard spurious integral information we have been able to, hopefully, accurately identify the most important deficiencies in the nuclear data of the general purpose file of JEF2.2. Keeping in mind the unavoidable imperfections of the data treatment, whose consequences on thermal Reactor calculation have been recently quantified by an intercomparison of results obtained with NJOY89.69 and NJOY94. We reached the conclusion, at the end of a lengthy work, that the evaluations of most of the main isotopes (for application) are of acceptable or even of good quality. There are a few important deficiencies which justify a complete revaluation work.

All the corrections suggested by the adjustment are statistical and have to be considered with their error bars.

In this chapter we will briefly report on the results and will emphasize only the negative points.

^{239}Pu

The JEF2 evaluation is a genuine European evaluation.

For this nucleus, the direct integral information is abundant but mostly in the fast range (figures between parentheses) and represented by :

- 30 (30) critical masses, all with significant content in ^{239}Pu,
- 16 (16) K^+,
- 40 (25) Bücklings.

58 Spectral Indices distributed amongst :

35 (32) F49/F25, 3 (0) F42/F49, 3 (0) F41/F49, 3 (0) F40/F49, 3 (3) F28/F49, 1 (1) F25/F49, 1 (0) C49/F49, 2 (1) C49/F25, 6 (6) C28/F49, 1 (1) N2N49/F25.

Except for the (n,2n) cross section, the adjustment do not reveal any major problem and confirms all the major options of the evaluation. It suggests that the most recent semi phenomenological parametrization of the deformed optical model obtained in the framework of the subgroup 5 of WPEC [ ] could still improve the calculation of the (n,n') cross section.

- **Fission neutron yield**

ν_p

The adjustment suggests an upwards renormalization by 0.5 % above 50 KeV, with a special mention to the range 20 KeV - 50 to reinstall the « bump » observed by GWIN and neglected in the evaluation.

ν_d

The validation on 20 β_{eff} data confirms the evaluation based on the LENDEL formalism and proposes the recommended values :

thermal range : 653 (10^{-5}) ± 1.9 %
fast range : 654 (10^{-5}) ± 1.6 %

- **Cross sections**

For most of the cross section and energy groups the suggested corrections are of the order of the percent. However, for the radiative capture cross section in the range (2 KeV - 60 KeV) the corrections are between 2 % and 4 %.

n,2n

The (n,2n) cross section is a real problem and is a good example of a severe conflict between the microscopic and the integral data.

The microscopic data produced by J. FREHAUT [ ] exhibit a strange behaviour (quasi null values) on a 2 MeV range above the threshold. The theoretical calculations using FISINGA and SI4N codes were unable to reproduce the experimental data. But in the evaluation the preference has been given to the measured data.

The integral datum has been obtained in PHENIX in the framework of the PROFIL1 and PROFIL2 irradiation experiments by measuring the quantity of ^{238}Pu produced by ^{239}Pu samples.

The corrective factor (1.55) resulting from the adjustment supports the integral experiment and the initial model calculation.

^{240}Pu

For this nucleus the JEF2 evaluation is an old (1979) Japanese evaluation with parts taken from ENDF B-IV.

The validation reveals several defective important points suggesting a complete reevaluation work.

In the fast range the integral information is given by :

- 30 critical mass data ; 29 correspond to media with normal (poor) content in ^{240}Pu and one (ZONA4K) to a Pu vector enriched in ^{240}Pu,
- 25 Bückling data for media with poor content,
- 19 spectral indices, related to ^{240}Pu fission (18 values) or to the capture (1 value).

In the thermal range, we have used only one capture spectral index obtained in the so called SHERWOOD experiment and a few tens of Bückling data. In this energy range there is a deficit of data but it should be stressed that there is in the epithermal range (resonance range) an overlap of information from the fast and thermal data.

- **Fission neutron yields**

ν_p

The original evaluation is ENDFB IV based on FREHAUT's data (1974) with renormalization. The validation indicates a systematic underestimation of this parameter, the correction being energy dependent with an average value turning around 1.4 %.

- **Cross sections**

With the provided integral information it is not possible to judge about the elastic and inelastic cross sections but only about the fission and capture cross sections.

Both appear incorrect, the fission cross section from below the threshold up to 2.2 MeV, the capture cross section on the whole energy range except in the thermal and the 1 eV region of the 1st resonance. Both are significantly overestimated by energy dependent quantities which can reach high values, especially for the capture cross section (~ 20 % in the range 200 KeV - 2.2 MeV).

The bad quality of JEF2 is likely due to the available experimental data on which is based the evaluation.

This is obvious in the resonance range since an important background is superimposed to the cross section calculated with the resonance parameters. At higher energy model calculation would have given better results since the radiative Strength function extracted from JEF2 resonance parameters is 2.34 10^{-3}, lower than the one used to produce the evaluation (2.65 10^{-3}) whose primary aim was to fit into the experimental data.

For both fission and capture in the resonance range the trends of the adjustment are confirmed by the recent evaluation by O. BOULAND and H. DERRIEN [ ].

The (n,2n) cross section is correctly estimated as a result of an information from the PROFIL experiment.

^{241}Pu

The JEF2.2 evaluation is the result of a collaboration between ORNL, CEA (Cadarache) and KFK Laboratories for the energies lower than 162 keV. For higher energy the data have been taken from the JENDL2 evaluation revised in 1983.

The validation identifies the capture cross section on the whole energy range and the fission cross section in the unresolved range as the only defective items. An updating procedure taking into account the numerical results of the validation (with minor correlative modifications on the total cross section) would lead to a set of nuclear data of good quality, possibly suggested for inclusion in the JEFF3 starter file.

In the fast range the integral information is given by :

- 29 critical mass data,
- 15 K^+ data,
- 19 spectral indices related to fission and 1 to the capture.

In the thermal or epithermal range, the integral information is limited to 3 spectral indices F41/F49 obtained in EOLE facility and some Bückling data.

- **Fission neutron yield**

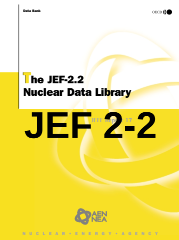
ν_p and ν_p

The validation confirms on the whole energy range the excellent quality of the evaluated data based on FREHAUT's and GWIN's experimental data. The integral information is too scarce to comment on the ν_d data.

- **Cross sections**

No correction is needed for the cross section of the neutron channel, even in the unresolved range where this evaluation exhibit some weaknesses for the cross sections of the non neutron channels. In this unresolved range (10 keV - 70 keV) both fission and capture are overestimated respectively by 4.5 % and 10 % respectively. A correction should consider the consistency of the cross sections at the boundary between the continuum and the unresolved ranges.

In addition the fission cross section seems to be overestimated by 5 % in the 1st chance plateau.



In the resonance range the trends are similar as in the unresolved one but less pronounced. They are confirmed by the recent evaluation [ ] by H. DERRIEN included in JENDL3.

There is no information for the (n,2n) cross section.

^{242}Pu

As for ^{240}Pu, the JEF2 evaluation is taken from JENDL2. Modifications have been brought to :

- the thermal range,
- the resonance range by increasing the scattering radius to correct the cross section between resonances.

This is an old evaluation which carries an heavy heritage.

The integral information concerns essentially the fission in the fast range with 15 spectral indices (F42/F25, F42/F28, F42/F49) obtained in PHENIX power plant (PROFIL experiment) or in MASURCA (ZOCO, ZONA experiments) or MINERVE (OP and OU experiments) criticals.

Two spectral indices related to capture (irradiation method) C42/F25 have been considered, one in the fast range (PROFIL), one in the thermal range (SHERWOOD system).

The criticals use fuel with weak load in ^{242}Pu so that poor information is obtained for the neutron balance and consequently on the neutron fission yield.

- **Cross sections**

Fission

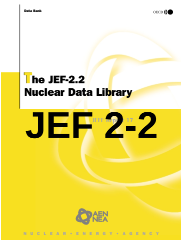
The integral information suggests a moderate overestimation (~ 4 %) in the first and the second chance plateau. This conclusion has to be considered as reliable, in spite of the small statistics, since the information is obtained from consistent values of spectral indices referring to different nuclei (^{235}U, ^{238}U, ^{239}Pu).

Capture

The 2 integral data, although they concern 2 different energy ranges appear inconsistent. The ratio C42/F25 obtained in SHERWOOD has been discarded as a result of the rejection criterion of the method and of a technical analysis based on a posteriori control of the Pu content of the sample.

n,2n

There is no information for this cross section.



^{238}U

This is a production by the JEF project which includes the results of a collaboration with Pr KANDA (Kyoto University) concerning especially, the well known problem of the inelastic cross section.

The validation recognizes for this evaluation a quality that would justify its inclusion in a JEFF 3 starter file, after very minor corrections.

Direct integral information is given by the following data :

- 29 (29) critical masses,
- 15 (15) K^{+},
- 99 spectral indices distributed amongst : 5 (5) F42/F28, 8 (7) F40/F28, 41 (32) F28/F25, 35 (25) C28/F25, 8 (6) C28/F49, 1 (1) F28/F28,
- 93 (20) Bücklings

This is a rather complete data set, especially in the fast range (figures between parentheses) which allows definite conclusions to be drawn.

- **Fission Neutron Yield**

ν_p

The statistical adjustment indicates a need for an upwards renormalization by 0-8 % below 6 MeV and by 0.3 % above, suggesting a change in $\frac{\partial \upsilon p}{\partial E}$ in the energy range where the 2^{sd} chance fission exists.

ν_d

It confirms the high value of ν_d in JEF2 (compared to ENDBF VI). The following ν_d values are recommended :

Thermal range	:	4846 (10^{-5}) ± 3.8 %
Fast range	:	4864 (10^{-5}) ± 3.5 %

- **Cross sections**

Fission :

The only correction (~ + 10 %) proposed by the validation concerns the subthreshold range where the fission cross section is very weak.

Capture :

This cross section that is a neutron standard for the ENDF-B project is confirmed in the whole energy range. The statistical corrections (± 1 %) non significant on a Physics point of view, are well inside the error bars (± 2 %) given by the evaluation.

Elastic :

Surprisingly for a "modern" evaluation, the cross section is obtained as the difference between the total cross section and the sum of partial cross section. Nevertheless, it seems to be correctly estimated since a small correction (+ 4 %) is proposed in the fast range below 1 MeV, where there are no experimental data.

Inelastic :

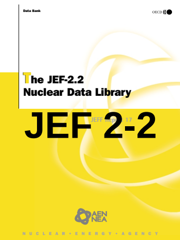
This is an important cross section because of its role in the neutron slowing down. There has been in the past a long standing problem concerning the part of the cross section for energies below 2 MeV illustrated by systematic discrepancies between the rare experimental data and the evaluations based on the optical model calculations. The subgroup number 4 of WPEC has been set up to solve this problem.

The present validation does confirm the JEF2 evaluation for energies below 2 MeV. Above this limit an increase by (5 % ± 5 %) is required. This statement doesn't support the recent calculations of MASLOV and Parodzinskij [ ] which go in the opposite direction.

Additional experimental data are required such as for example deep penetration data in a ^{238}U block using a 14 MeV neutron source, to confirm for very high energies the conclusion of this validation work.

n, 2n :

There is no specific integral information for this cross section.



^{235}U

According to the general policy of the JEF project to systematically adopt the ENDF BVI evaluation when a neutron standard is concerned, the JEF2 evaluation is the one produced by De SAUSSURE and LEAL. It has been modified as follows :

- JEF2 evaluations have been adopted for γ_p and γ_d.
- In the subthermal range the fission and capture cross section have been modified so as to reproduce the data measured by GEEL for the η parameter. These data indicate a positive value for $\frac{\partial \eta}{\partial E}$ that is necessary to properly calculate the temperature coefficient for the thermal reactors.

Direct integral information is given by the following data :

- 30 (30) critical mass
- 15 (15) K+
- 126 (103) spectral indices distributed amongst :
  3(3) CFE6/F25, 1(0)CCR2/F25, 7(7)F42/F25, 16(15) F41/F25, 7(7)F40/F25
  3(3) F25($\vec{r}$)/F25(0), 41(32) F28/F25, 1(1) F25/F49, 2(1) C49/F25,
  2(2) C42/F25, 1(1) C41/F25, 2(1) C40/F25, 25 (18) C28/F25,
  3(1) C25/F25, 1(1) N2N25/F25, 1(1) N2N240/F25,
  1(1) N2N49/F25, 9(8) B10/F25,
  93 (20) Bücklings

This data set may be considered as sufficiently informative for all the nuclear constants of interest.

- **Fission Neutron Yield**

ν_p :

The validation doesn't reveal any major problem.

In particular, the epithermal data confirm the existence of fluctuations in the resonance domain. These fluctuations result in an average value that is lower than the thermal value. Above 60 KeV a constant increase by 0.6 % is required.

ν_d

20 β_{eff} data covering the full energy range support the JEF evaluation based on calculations using the LENDEL model.

After adjustment the recommend values are :

Thermal range : 1643 (10^{-5}) ± 1.3 %
Fast range : 1662 (10^{-5}) ± 1.8 %

- **Cross sections**

Fission :

The validation confirms the evaluated data on the whole energy range with proposed corrections alternatively positive and negative but whose amplitude is always lower than 1 % (except in the range 67 KeV < E < 183 KeV) for which the correction is : - 1.4 % ± 1.3 %).

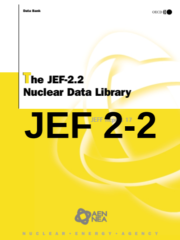
It is clear, considering the amplitude of the corrections, that they represent the validity limits of the method.

In this context it is worth mentioning a very recent (1977) evaluation (named SBB97) of this cross section [ ] by R.M. WHITE (LLNL) for energies between 200 KeV and 20 MeV. The consistency between the trends of the adjustment and the differences $\frac{SBB97 - BVI}{BVI}$ (see attached the fissure) is perfect, in particular, regarding the energy ranges where modifications are required.

Inelastic scattering :

The very fast experiment GODIVA and FLATTOP25 indicate a need not really significant (+ 5 % ± 8 %), for an increase between 200 KeV and 1.3 MeV. As indicated by perturbation calculations this correction is without any real practical consequence for power Reactors.

This cross section illustrates the effectiveness of the "rejection" criterion of our method since with a complete integral data base $\left(\chi_n^2 = 2.435\right)$ the correction required by the adjustment procedure is exactly the opposite.



Elastic scattering

There is a good agreement between the integral and the microscopic information. The corrections are less than 2.8 % ± 6.5 %.

This is really the weak point of the evaluation on the whole energy range as indicated by all the integral data, thermal or fast, of any type (critical mass, K^+ Bückling, Spectral index). This cross section is significantly underestimated :

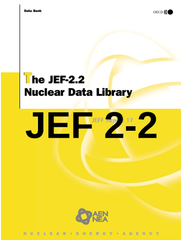
10 to 15 % in the resonance range,
5 to 7 % in the fast range.

The amplitude of the correction is systematically greater than the associated uncertainty, a configuration which undoubtedly indicates the presence of an error of systematic type.

n, 2n :

The integral information is brought by the irradiation experiment PROFIL in PHENIX core as a spectral index value N2N/F25.

A very slight underestimation is revealed : 1.5 % ± 5 %.



^{23}Na

The JEF2 evaluation has been taken from JENDL3 which actually results from a work performed in 1975 for ENDF B-V which, in turn, was based on earlier experimental data.

It is clearly demonstrated by the validation that this evaluation is of very bad quality. The consequences on Sodium void calculations are important.

Obviously, a completely new evaluation is urgently required. All the fast experiments are loaded with Na.

The integral information is distributed between :

- Neutron balance type data, whose sensitivities are small.
- Spectral index data for nuclei other than Na, with significant sensitivities.
- Very specific experiments data, such as the measure of reactivity worth of more or less large voided volumes in cores. These data are very sensitive to the ^{23}Na cross sections, in particular the elastic and inelastic cross-sections. To understand properly the relationship between this integral parameter and the above mentioned cross sections one must know :

In the present « State of the Arte » [ ], the total Na effect can be split into 2 components :

- One central component essentially sensitive to the neutron slowing down by a predominant contribution from inelastic scattering.
- One leakage component sensitive to the total cross section which is dominated by the elastic scattering.

A specific experimental program has been realized in MASURCA [ ] to check data and calculational methods.

By changing the volume and the location of the voided zone going from the center to the periphery one obtains reactivity changes that are more sensitive to the « central » or to the « leakage » component.

Cross Sections

- Elastic scattering

This is the major component in the total cross section and this characteristic has to be kept in mind when analyzing integral data.

The adjustment doesn't indicate any significant correction. However there are good reasons to consider as correct the experimental data obtained at OAK-RIDGE and which are (25 % - 30 %) higher than JEF2 values above 700 keV.

To overcome this insufficiency (of the adjustment procedure), several arguments can be invoked which are related to the method to calculate the sensitivity coefficients :

- use of a finer energy scheme (172 g instead of 33 g), so as to better express the « removal » component in the elastic cross section,

- use of non linear formalisms because of the narrow range of linearity of the sensitivity coefficients to the cross section values.

- Inelastic scattering

The indication of the adjustment, namely a very slight increase just above the threshold and a strong decrease (- 25 %) everywhere else, is totally confirmed by a recent measurement in GEEL [ ]. This one produced a curve that exhibits hedge differences with JEF2 for what concerns both the level and the shape. Several additional resonances have been observed and may raise the question of correct self shielding calculations so that the perfect agreement between adjustment and measurement indications could be simply fortuitous.

^{56}Fe

This evaluation is a JEF production.

For this nucleus of medium mass the resolved resonances are located in the energy range of main interest for Reactor Core Calculations.

For transmission or deep penetration problems, the energy range of interest concerns also the unresolved resonance resonance region, ie, the range of a few MeV.

This means that the resolved and unresolved parameters are of prime importance in the evaluation.

For the JEF2 file the resonance parameters have been derived from a simultaneous analysis of transmission data obtained with ORELA and capture data obtained in OAK-RIDGE KARLSRUHE and GEEL.

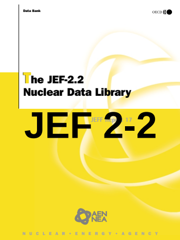
Recently, measurements have been performed at GEEL with an upgraded GELINA machine with considerably improved energy resolution characteristics. Very fine description of the total cross section up to 20 MeV and of the inelastic cross section up to 2 MeV have been obtained.

Differences are observed with respect to JEF2 data :

- systematic greater values in GEEL's data for the total cross section,
- new structures in the inelastic cross section above about 1 MeV and in the total cross section in the unresolved range.

Investigations to explain these differences are still going on. If these ones really exist, they can have an impact on integral parameter calculation and the question is : are the conclusions of the validation meaningful for this nucleus.

Iron is present everywhere in the reactor structures. A contribution from ^{56}Fe is present in all neutron balance data but with a modest sensitivity. More sensitive data have been obtained in specific experiments, such as substitution experiments in RB2. The integral data set is completed by some simple penetration data, as ASPIS. More complicated penetration systems like JANUS, JASON (Sandwiches Fe-Na), although they are very informative have been discarded on the conviction that present calculational methods need more refinements.



Cross sections

- Inelastic scattering scattering

  The validation indicates :

  - a strong decrease (> 20 %) below 2 MeV.
    This indication is consistent with the new measurement in GEEL not yet fully finalised.

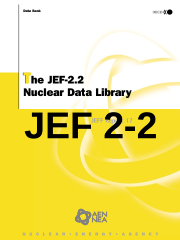
  - a slight increase for energies above 2 MeV. There are no new measurements in this range. Nevertheless an explanation could be found in the fact that a spherical optical model for this « deformed » nucleus. The required correction (~ 6 ± 3 %) may represent the omitted direct component.

- Elastic scattering

  There is no clear indication that this cross section should be corrected.

- Radiative capture

This cross section appears to be correct except for the range 1 keV - 10 keV. The required correction could concern, in fact, the large « s » resonance at 7,6 keV of ^{54}Fe whose sensitivity has been neglected.



^{58}Ni

The evaluation for this nucleus has been taken from ENDF BVI.

This is an experimental data fitting using DWBA statistical and preequilibrium formalisms. Consistency between cross sections and energy balance are preserved.

Small sensitivities are found in several experiments, but the main information is given by the K^+ parameter of the ON10 experiment performed in MASURCA.

- **Cross sections**

Elastic and inelastic scattering

The K^+ parameter has a small sensitivity to these cross sections, and the proposed cross sections are very small.

Capture

The validation indicates a strong overestimation (~ - 10 % ± 7 %) over the whole energy range. This indication is given by all the integral data with small sensitivities and confirmed by ON10. It is also confirmed by a recent measurement performed in GEEL.