Part III

ADJUSTMENT STUDIES

Chapter 12

VALIDATION OF THE JEF-2.2 GENERAL PURPOSE FILE BY MEANS OF CROSS-SECTION ADJUSTMENT STUDIES

Objective of data validation

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

Once the nuclear data have been evaluated by using, supposedly, the whole of the available Nuclear Physics information (experimental data, nuclear models...), i.e., an information source totally independent from the proposed applications, one has to demonstrate that they are appropriate for making 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 representation of the application.

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

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, from a global point of view, just by comparing the calculated values to the experimental ones for a limited number of types of application (for example k_{eff} data and/or irradiated fuel compositions). If the benchmark results are judged unsatisfactory tentative explanations are produced on a qualitative basis. Actually, it is very difficult, without sensitivity calculations, to make judgements about possible compensations between nuclei or between the different cross-sections of a 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, which we could call the modern approach, is possible only because of the continuous improvements in calculation methods in several application fields of neutronics. Using a statistical adjustment procedure it is now possible to identify the deficiencies and, in many 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 re-evaluation 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.

Description of the validation work

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

The calculation methods

The methods we have 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 over a long period of time. Some checks have been made with Monte Carlo methods using MCNP and TRIPOLI-4 codes. These checks have shown reasonable agreement for simple systems, in any case, of the same order of magnitude as the experimental error (from 50 to 200 pcm for critical masses). For complex systems, greater differences have sometimes been found.

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

The sensitivity coefficient calculations have been based on perturbation theory (SPT (k_{eff}), GPT (reaction rate), EGPT ($\Delta\rho$) [1], [2]. These coefficients have been carefully made 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*), 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 ~50 pcm differences for k_{eff} data [3] of thermal systems according to the options in NJOY used to process the JEF-2 data.

Probability tables to calculate self-shielding factors or collision probabilities in non-homogeneous situations have been produced with CALENDF [4]. 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
1 968 g (ECCO) for fast reactor and more general calculations

The reference integral database

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 database, 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. An additional reason can be found in the objective to decouple the effects of the adjustment on the different group cross-sections.

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

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, which has been implemented in the code AMERE [5].

- To identify when erroneous uncertainties have been assigned to the observable or the nuclear parameters.

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

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

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

The technique to do this 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 [6,7]. All the applications to nuclear data performed everywhere in the world accept the same theoretical basis which can be summarised as an approach in three steps.

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

This is based on the maximum entropy principle, the information entropy being defined by the so-called “SHANNON” formula:

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

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

$$W = -\int p(x) Lnp(x) dx$$

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 can be 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 two 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" [7].

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

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

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

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

Step 2. The inclusion of the integral information

Let the vector y denote the "observables" (integral parameters):

$$Y_i,\ i = 1, 2, ..., I.$$

Let the vector x denote the "parameters" (nuclear parameters):

$$x_{\mu},\ \mu = 1, ..., M$$

Finally, let $y(x)$ denote the relationship between y and x.

A priori information exists:

- *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:

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

- *For the vector y*. They are represented by the vector η of the integral data and an associated uncertainty covariance matrix $C\eta$.

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

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

  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.

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

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, i.e. the one that maximises the right hand side term of the above equation. It is obtained by minimising the quantity:

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

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

Thus, we have to consider the system:

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

where *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 the (x - ξ) perturbation. This condition preserves the consistency with GPT and also with the Bayesian theory since the solution obtained by the χ^2 minimisation is exact in these conditions.

In the frame of Decision Theory the solution we are looking for is a vector which minimises the consequences of choosing a vector different from the always unknown true vector, i.e. which minimises 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 minimises 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 minimises both χ^2 and $(x - \xi)^+ (x - \xi)$ or the proportional quantity $(x - \xi)^+ \mathrm{C}^{-1} (x - \xi)$.

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

In the present case, when using the JEF-2.2 file and the 480 data of our integral database one obtains a value of 20 (${}^{\text{prior}}\chi_r^2 \simeq 20$). Since at this stage the JEF-2.2 file cannot be considered as a reference, the responsibility for this high value of χ_r^2 has to be attributed first to the nuclear data. This simply means that JEF-2.2 does not perfectly 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 make judgements about the consistency of additional integral data. We have made extensive use of this property.

Step 3. Precautions to be observed in the application of theoretical principles

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:

- Existence of non-linearities in the sensitivity coefficients.
- Underestimation of uncertainties, microscopic or integral.
- Presence in the integral database of some inconsistent values.

In validating the JEF-2.2 major nuclei with 480 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, then, can it be improved? 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 are obviously partly responsible for the high value of $^{\text{post}}\chi_r^2$. 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 was used because of limitations of time and the magnitude of the task.

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

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

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 analysed the published uncertainties when available and documented. We have reconsidered them by introducing estimated systematic uncertainties in the experimental procedure or calculation methods with the consequence of a significant increase, in some cases, of the error bars.

The importance of the departure from unity for $^{\text{post}}\chi_r^2$ gives some support to the hypothesis of the existence of non-consistent integral data. The great difficulty, however, is their identification. We suggest an approach in two parts:

1. Identification by means of statistical analysis.
2. Contradictory reanalysis of the identified experiments by using experimental techniques and reactor physics arguments.

Identification by means of statistical analysis

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

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

where χ_{mac}^2 is the sum of the squared terms of $\left(\eta - y(x)\right)^r C_\eta^{-1}\left(\eta - y(x)\right)$:

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

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

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

The residual E contains all the terms complementary to χ^2_{mic} and χ^2_{mac}, i.e. all the cross-terms related to the observables plus some squared terms additional to those of χ^2_{mac} 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, $\chi^2_{mac}, \chi^2_{mic}, E$ 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 (2).

The X_i^2 terms are ordered by increasing values.

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

where N_{max} is the maximum number of integral data in the database.

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. $X_{N\,max}^2$. This one identifies the experimental datum to be first discarded. The adjustment procedure is repeated with $N = N_{max} - 1$ 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 1.00003. Such a situation corresponds to $n = 58$ rejected integral data and defines an “effective” integral database 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 minimised as required by the theoretical conditions of the adjustment. With respect to the results obtained with a complete integral database, the adjustments obtained with the "effective" database 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.

Contradictory reanalysis of the "discarded" experiments by using experimental technique and reactor physics arguments

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

1. Buckling measurements in the thermal and fast ranges.
2. Spectral indices.
3. Large Na voids.

These data are being reanalysed at Cadarache. It is too early to report in detail on a work that will still go on for a long period but, nevertheless, some conclusions can be drawn.

Bucklings

The thermal range has not yet been reviewed, but it has been said that some refinements have to be made to the calculations.

For fast range, to distinguish one fast critical from another, we used the usual spectral index r defined by $r = \frac{\langle \nu\Sigma_f \rangle}{\langle \xi\Sigma_s \rangle}$; in this relationship, the notations are obvious while the brackets denote an averaging over a fundamental mode spectrum at the centre of the core. The greater is r the faster is the spectrum. All the discarded data belongs to the higher energy part ($r > 0.3$) of the range and concerns small size cores. In this range the buckling values are systematically overestimated. The biases calculated using JEF-2 are significant (-210 pcm on average) and increase using the adjusted values (-260 pcm), while they are reduced down to 0 for the bucklings measured in the softer spectrum systems ($r < 0.3$).

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

Spectral indices

There are no characteristics attached to the "removed" spectral indices. We do not see any reason related to the calculation methods, and the causes of deficiency are probably experimental, as 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 $\frac{F25(\bar{r})}{F25(0)}, \frac{F49(\bar{r})}{F49(0)}, \frac{F28(\bar{r})}{F28(0)}$, the 0 position referring to the centre of the core.

All the data for different positions $\bar{r}$ 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 the correction of the content values, the $\frac{F25(\bar{r})}{F25(0)}$ and $\frac{F28(\bar{r})}{F28(0)}$ have been kept, this providing significant information on the elastic cross-section of ^{52}Cr.

This demonstrates the necessity to have as much data as possible in a database as well as 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 understanding this problem [8].

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.

In 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 [9] 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.

Results and provisional conclusions relative to the evaluated data

Thanks to the statistical adjustment procedure, enhanced 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 JEF-2.2. Keeping in mind the unavoidable imperfections of the data treatment, whose consequences on thermal reactor calculations have been recently quantified by the intercomparison of results obtained with different versions of the APOLLO-2 code and its cross-section library, we reached the conclusion, at the end of a lengthy study, that the evaluations of most of the main isotopes 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 section, we will briefly report on the results and will emphasise only the negative points.

^{239}Pu

The JEF-2.2 evaluation is a genuine European evaluation based on model calculations: deformed optical model with coupled channel calculations (ECiS), statistical-plus pre-equilibrium models (FISINGA + Si4N).

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) bucklings.

Fifty-eight 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 does not reveal any major problem and confirms all the major options of the evaluation. It suggests that the most recent semi-phenomenological parametrisation of the deformed optical model obtained in the framework of Subgroup 5 of WPEC [10] could still improve the calculation of the (n,n′) cross-section.

Fission neutron yield

ν_p

The adjustment suggests an upwards renormalisation 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} measurements 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-sections and energy groups, the suggested corrections are of the order of 1%. However, for the radiative capture cross-section in the range (2-60 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 [11] exhibit a surprising behaviour (quasi-null values) on a 2 MeV range above the threshold. The theoretical calculations using the FISINGA and SI4N codes were unable to reproduce the experimental data. At the time of the evaluation. Frehaut’s data was not suspected of systematic errors. In the evaluation, preference has been given to the measured data. It appears now, from recent (still unpublished) experiments, that the original theoretical calculations were correct.

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 in the irradiated ^{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 JEF-2.2 evaluation is the old (1979) JENDL-2 evaluation, with parts taken from ENDF/B-IV.

The validation reveals several defective important points suggesting the need for a complete re-evaluation.

In the fast range the integral information is given by:

- 30 critical mass data; 29 of them correspond to media with normal (poor) content in ^{240}Pu and one (ZONA4K) to a Pu vector enriched in ^{240}Pu.
- 25 buckling 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 buckling 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 ENDF/B-IV based on Frehaut's data (1974) with renormalisation. 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 region of the 1st resonance at 1 eV. 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 JEF-2 is most likely due to the available experimental data on which the evaluation is based.

This is obvious in the resonance range since an important background is superimposed on the cross-section calculated with the resonance parameters. At higher energies, model calculations would have given better results since the radiative strength function extracted from JEF-2 resonance parameters is 2.34 10^{-3}, which is lower than the one (2.65 10^{-3}) used to produce the evaluation whose primary aim was to fit 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 [12].

The (n,2n) cross-section is correctly estimated according to information from the PROFIL experiment.

^{241}Pu

For energies below 162 keV the JEF-2.2 evaluation is the result of a collaboration between ORNL, CEA (Cadarache) and KFK Laboratories. For higher energies the data have been taken from the JENDL-2 evaluation, revised in 1983.

The validation identifies the capture cross-section over 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 JEFF-3 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 three spectral indices F41/F49 obtained in the EOLE facility and some buckling data.

Fission neutron yield

ν_p and ν_p

The validation confirms over 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 exhibits 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 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 to those in the unresolved range but less pronounced. They are confirmed by the recent evaluation by H. Derrien included in JENDL-3.

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

^{242}Pu

As for ^{240}Pu, the JEF-2 evaluation is taken from JENDL-2. Modifications have been proposed 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 a 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 the PHENIX power reactor (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), and one in the thermal range (SHERWOOD system).

The criticals use fuel having a very small content of ^{242}Pu so that poor information is obtained for the neutron balance and consequently on the fission neutron 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 two integral data, although they concern two 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, confirmed by 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 recognises 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) bucklings.

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 renormalisation 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 2nd chance fission exists.

ν_d

It confirms the high value of ν_d in JEF-2.2 (compared to ENDBF-VI). The following ν_d values are recommended:

- Thermal range: 4 846 (10^{-5}) ± 3.8%.
- Fast range: 4 864 (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 from 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 is no experimental data.

Inelastic

This is an important cross-section because of its role in the neutron slowing down process. 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 optical model calculations. Subgroup 4 of WPEC has been set up to solve this problem. The present validation does confirm the JEF-2.2 evaluation for energies below 2 MeV. Above this limit an increase by (5% ± 5%) is required. This statement does not 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 the conclusion of this validation work at very high energies.

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/B-VI evaluation when a neutron standard is concerned, the JEF-2 evaluation is the one produced by De Saussure and Leal. It has been modified as follows:

- JEF-2 evaluations have been adopted for ν_p and ν_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) bucklings

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

Fission neutron yield

ν_p

The validation does not reveal any major problem.

In particular, the epithermal data confirms 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

Twenty 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: 1 643 (10^{-5}) ± 1.3%.
- Fast range: 1 662 (10^{-5}) ± 1.8%.

Cross-sections

Fission

The validation confirms the evaluated data over 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 limits of validity of the method.

In this context, it is worth mentioning a very recent (1997) evaluation (named SBB97) of this cross-section [13] by R.M. White (LLNL) for energies between 200 keV and 20 MeV. The consistency between the trends of the adjustment and the differences $\frac{SBB97 - BVI}{BVI}$ 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 database $\left(\chi_n^2 = 2.435\right)$, 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%.

Radiative capture

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

- 10-15% in the resonance range.
- 5-7% in the fast range.

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

The adjustment indications are fully confirmed by the recent resonance range evaluation ENDF/B-VI release 4 by Leal, Derrien and Larson.

n, 2n

The integral information is brought by the irradiation experiment PROFIL in the PHENIX core as a spectral index value N2N/F25. A very slight underestimation is revealed: 1.5% ± 5%.

^{23}Na

The JEF-2.2 evaluation has been taken from JENDL3, which actually results from an evaluation 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 contain 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 experimental data, such as the measurement 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.

In the present state of the art [8], the total Na effect can be split into two 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 realised in MASURCA [16] to check both data and calculation methods.

By changing the volume and the location of the voided zone, going from the centre 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 analysing 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 the JEF-2.2 values above 700 keV.

To overcome this insufficiency (of the adjustment procedure), several arguments can be invoked which are related to the method used 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 made in GEEL [9]. This produced a curve that exhibits huge differences from JEF-2.2 for what concerns both the level and the shape. Several additional resonances have been observed and may raise the question of the correctness of 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 region, i.e., the range of a few MeV.

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

For the JEF-2.2 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 descriptions 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 JEF-2.2 data:

- Systematic greater values in the GEEL 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 really exist, they can have an impact on integral parameter calculations and the question is: are the conclusions of the validation meaningful for this nucleus.

Iron is present everywhere in 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, such 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 calculation methods need more refinements.

Cross-sections

Inelastic 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 [14].

- 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 has been used 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 1-10 keV. The required correction could concern, in fact, the broad “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/B-VI.

This is an experimental data fitting using DWBA statistical and pre-equilibrium formalisms. Consistency between cross-sections and energy balance is 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 [15].

^{52}Cr

This evaluation is a genuine JEF production.

The resonance parameters, to be used with the R matrix formalism, are defined up to 637 keV.

Spherical optical model (PRINCE parametrisation), statistical and pre-equilibrium models are used at higher energies.

The integral information is limited to a few spectral indices (actually deduced from neutron balance analysis) obtained in RB2. The main information has been obtained in the analysis of radial traverses in the steel reflector of the CIRANO experiment [16].

As a matter of fact, the validation results have to be considered as trend indications.

Cross-sections

Elastic and inelastic scattering

This elastic cross-section should be decreased by about -20% in the range 25 keV-1.3 MeV. There is no indication relative to the inelastic cross-section.

Capture

There is an indication that the capture cross-section could be underestimated in JEF-2.2.

^{16}O

The JEF-2 evaluation is ENDF/B-VI accepted without any modification.

The evaluation has been realised by considering all the reaction channels, which lead to the same compound nucleus:

$$^{13}C(\alpha,\alpha)^{13}C,\ ^{16}O(n,n)^{16}O,\ ^{16}O(n,n')^{16}O,\ ^{16}O(n,\alpha)^{13}C$$

Calculations were performed with the R matrix formalism in the resonance range and the statistical formalism to treat compound nucleus processes completed by the DWBA formalism for direct interaction processes at higher energies.

The integral information is significant since all the experiments have oxygen in the material composition excepting the transmission experiments.

Cross-sections

Inelastic scattering

The validation suggests significant corrections from threshold to 20 MeV. This is not surprising given the assumption made relative to the (isotropic) distribution of emitted gammas.

Elastic scattering

The evaluated data are fully confirmed by the integral measurements.

Absorption

This cross-section includes the radiative capture plus those which have charged particles in outgoing channels, namely (n,p) and (n,α) reactions.

The adjustment, as a consequence of the method used to calculate the sensitivity coefficients, does not discriminate between the various cross-sections. Nevertheless, it is possible to conclude by observing the reaction thresholds, which are quite different:

$$Q = -2.215 \text{ MeV for } (n,\alpha) \text{ reaction}$$
$$Q = -9.6 \text{ MeV for } (n,p) \text{ reaction}$$

The (n,γ) cross-section should be increased by 10% but only above 1 MeV. Because the Q value for the (n,p) reaction is very high, it is assumed that the present integral data do not bring any information. In these conditions, it appears that the (n,α) cross-section should be increased by ~15%.

^{10}B

^{10}B (n,α) reaction is a neutron standard in the energy range thermal -100 keV where it has a 1/v behaviour.

Pointwise data has been obtained in the framework of a simultaneous evaluation of all the neutron standards associated with a covariance method for what concerns the total cross-section.

The proposed evaluated data results from an R matrix fit that produced consistent data for the inelastic cross-section, which has been obtained by different experimental techniques, based on neutron or γ detection.

The integral information is sufficient and is found in almost all types of integral data, but essentially in neutron balances or parameters such as the indices $\frac{B10}{F25}$ obtained in RB2.

Cross-sections

Elastic and inelastic scattering

No correction is required.

Absorption

This cross-section is dominated by the total (n,α) cross-section, that is the sum of two components corresponding to the fundamental and first excited states of the residual nucleus ^{7}Li. There is no need for correction and this contradicts some comments made in the past.

^{12}C

The angular distribution of the elastic scattering is a standard up to 1.8 MeV. This standard was taken from ENDF/B-V which, in fact, had adopted a French evaluation. Not all experiments have C in their composition but the integral information for this nucleus is distributed over all parameter types: critical mass (MASURCA), K^+ (ZEBRA), reactivity worth (RB2) and spectral indices.

Cross-sections

The proposed corrections are very small, of the order of 1% for the elastic cross-section, less for the inelastic cross-section, slightly superior (2-3%) for the absorption cross-section. This last conclusion suggests the need to re-examine the (n,p), (n,d), (n,t) reactions.

General conclusion

The validation of the general purpose file of JEF-2.2 is the result of a joint and constant effort developed over a large period of time. It has been made possible for the following reasons, each of them representing one recent progress:

- Improvement of the calculation methods. In particular in the European system of codes ERANOS used to calculate fast systems are included the formalism to calculate the sensitivity coefficient of any kind of integral parameter. In order to confirm the deterministic results and to estimate the biases some probabilistic calculations have been performed.

- Improvement of the adjustment technique. From the theoretical condition to be strictly respected, a methodology has been derived to identify spurious integral data with several important consequences. Now, one has a statistical tool:

  - To inform the reactor physicists about the improvements which are still to be made. The indications of this tool are, at least, a signal to initiate renewed checking or reanalyses with improved methods.

  - To introduce, reliably, the integral information so as to correct the evaluated nuclear data in a way that respects the physics laws.

Thanks to this work we have obtained clear information about most of the investigated nuclei, but essentially for the major actinides and the major coolant, absorber or scattering nuclei (with the exception of ^{242}Pu). Concerning the structural materials more integral information is required implying additional consideration for specific experiments such as transmission, deep penetration or reflector experiments. This may have the consequence to introduce in the adjustment procedure more nuclear parameters, in particular those related to the description of the angular distributions.

The validation of the general purpose file is the first but necessary step in the process to validate the total JEF-2.2 file.

The special data files, the minor actinides and FP files, require that adjusted libraries be used for all neutronics calculations.

Since all the new evaluations or measurements do confirm the conclusions of the validation it is reasonable to expect from JEFF-3 significantly improved performances with respect to those of JEF-2.2, if the conclusions of the validation are used as guidelines for the re-evaluation or selection work.

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