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Validation of Iron and Structural Materials Data of JEF2

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E. FORT, K. DIETZE

Commissariat à l'Energie Atomique
Centre d'Etudes de CADARACHE
Service de Physique des Réacteurs et du Cycle
Département d'Etudes des Réacteurs
13108 St PAUL-LEZ-DURANCE Cedex FRANCE

14080176

The structural materials, especially Iron, implied in a power reactor, in the structures, claddings or shielding, by large quantities, play an important role in neutronics especially in the neutron balance in the core.

The major process is the neutron absorption by radiative capture or (n, charged particle) reactions. The angular distributions of the secondary particles are of negligible importance.

In shielding, when the protection of the humans against radiation is obtained by important thicknesses, the neutron deep penetration is dependent on the energy transfer per collision. This process is due to the inelastic (essentially) scattering involving the cross section and the angular distributions. From numerous studies performed in the past, it has been demonstrated that the neutron flux transmitted after large thicknesses is strongly dependent on the exact determination of the forwards anisotropy. In a similar and complementary way the so called "reflector effect" as it appears in complete core calculation (critical mass) is dependent on the backwards anisotropy of the neutron scattering. For the purpose of data validation it would be certainly interesting to systematize studies about the "reflector effect" in fast reactors to have information on the backwards anisotropy and to check its consistency with the forwards anisotropy.

To have a complete picture of the quality of the data, it is important to have both types of data (neutron balance in reactor core, transmission) in the integral data base.

The specific information about the structural materials is extracted from the global validation of JEF2 [1].

With respect to the previous report on that item [2], there are two important differences :

- 1) Most of the thermal and epithermal data (few B^2_m data have been kept) have been removed from the integral data base on the argument of non correct sensitivity coefficient calculation. Therefore the information in the thermal range is very scarce. In addition all data (but the B10/F25 data) of the RB2 program have been eliminated for numerous reasons (not clean data, probable mistakes in sensitivity calculation).

- About 60 additional integral data of the fast range have been recalculated.

- The SEG experiments, specially designed to check either the capture, or the inelastic cross section data by controlling the shape of $\Phi^+(E)$.

- New experimental data appeared.

- 2) A statistical method has been used to purify the integral data base from spurious information in the case of χ^2 values after adjustment lying outside the theoretical limits.

The χ^2 term is written as follows :

$$\chi^2 = (\sigma - \sigma_0)^T M^{-1} (\sigma - \sigma_0) + (E - C)^T I^{-1} (E - C)$$

where the nomenclature is as follows :

E : vector of measured integral data with covariance I
 σ_0 : vector of nuclear constants with covariance M
 C : vector of integral parameters calculated from σ_0 .

The term of $(E - C)^T I^{-1} (E - C)$ which are the contribution of integral data to the a posteriori χ^2 are ordered by increasing values. The largest terms which contribute to the quantity in excess in χ^2 correspond to integral data to be eliminated. This is done in the framework of an iterative procedure where the adjustment is repeated each time an integral datum is eliminated.

In that way, a small percentage of integral data have been subtracted from the integral data base (24 out of 157).

The quantity $(\sigma' - \sigma_0)^T M^{-1} (\sigma' - \sigma_0)$, which represents the contributions to χ^2 of the microscopic data, gives interesting information : one notes, in particular, an expected constant behaviour versus N as long as the condition $\frac{\chi^2}{N} = 1 \pm \sqrt{\frac{2}{N}}$ is respected.

Generally, the sensitivities of the Reactor integral parameters to the cross sections of structurals are small (10^{-3} per macrogroup, smaller by an order of magnitude than those of the heavy nuclei) but they are numerous. The exception concerns the spectral indices such as $\frac{F8}{F5}$ for which the sensitivity to $\sigma_{n,n'}$ or $\sigma_{n,n}$ is of the order of several percents per macrogroup.

On the contrary, transmission experiments, such as ASPIS, exhibit high sensitivities to the inelastic/elastic cross-sections. The results of the global JEF2 validation are as follows [2]:

^{56}Fe

- $\sigma_{n,n'}$: The requirements are clear :
 .increase by $6\% \pm 2\%$ for $E > 2,2 \text{ MeV}$,
 .decrease by $\sim 25\% \pm 7\%$ (threshold $< E < 1,35 \text{ MeV}$).
- $\sigma_{n,n}$: There is a trend for a decrease on the full energy range, but the magnitude is well inside the error bar ($\sim 6\%$).
- $\sigma_{n,\text{absorption}}$: No requirement .
- $\sigma_{n,T}$: Modest modification in the high energy range:
 . $\sim 3\%$ for $E > 6 \text{ MeV}$,
 . $\sim 2\%$ for $2,2 \text{ MeV} < E < 6 \text{ MeV}$.

^{58}Ni

In general, the sensitivities are modest (fraction of percent per macrogroup), except when considering the ON 10 experiment.

- $\sigma_{n,n'}$: No requirement.
- $\sigma_{n,n}$: No requirement.
- $\sigma_{n,\text{absorption}}$: Clear requirement for a decrease on the full energy range by $\sim 15\% \pm 10\%$ (in the 100 KeV region).
- $\sigma_{n,T}$: no requirement .

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^{52}Cr

The conclusions are less significant because the sensitivities are modest (fraction of percent per macrogroup), especially for the $\sigma_{n,\text{absorption}}$ (less than 10^{-3} , except for the macrogroup 10 (resonance $E_r = 1.626 \text{ KeV}$, $l = 1$, $J = 3/2$)).

$\sigma_{n,n}$: Trend for lower values in the 100 KeV region : $-7\% \pm 14\%$.

$\sigma_{n,\text{absorption}}$: no indication

$\sigma_{n,T}$: Increase by $\sim 5\%$ for $E > 6 \text{ MeV}$.

With respect to the results obtained by a statistical adjustment, two sources of data have recently brought additional information.

① The analysis of the ROSSENDORF SEG experiments .

These experiments are sample reactivity measurements . The technical arrangement is described in references [3, 4].

The sample reactivity can be written in a very simple way as :

$$\rho = \frac{1}{F} \left\{ - \iint_{V,E} \Phi \Sigma_{abs} \Phi^+ + \iiint_{V,E,E'} \Phi \Sigma_s (\Phi_E^+ - \Phi_{E'}^+) + \iiint_{V,E,E'} \Phi v \Sigma_F \chi \Phi^+ - \iint_{V,E} D \text{grad} \Phi . \text{grad} \Phi^+ \right\}$$

The capture and scattering terms of the sample reactivity have been separated by means of specially designed adjoint spectra in different configurations .

In the case of an energy-independent adjoint spectrum (SEG-4 , SEG-5), the slowing-down effect disappears and the sample reactivity is only due to capture .

On the other hand , the scattering effect is dominant in the SEG-6 configurations characterized by a strong dependence of the adjoint spectra on energy .

A mixed situation exists in both SEG-7 configurations.

Concerning the structural materials the results obtained by K. DIETZE [5] are as follows :

Configuration: Main sens. to:	SEG-5 capture C/E rel.B-10	SEG-7A capture C/E rel.B-10	SEG-6/EK10 scattering C/E rel.C	SEG-6/EK45 scattering C/E rel.C
Fe	1.084 11%		0.890 5%	0.916 5%
Cr	1.032 10%			0.915 5%
Ni	1.073 10%		1.121 7%	1.133 7%

They globally agree with the indication of the adjustment.

The SEG integral data will be integrated in the Data base in a next future.

② Recently, Corvi, Moxon and Athanassopoulos measured the neutron resonance capture of ^{58}Ni for energy lower than 264 KeV. The experimental set-up is described in reference [6]. Analysed with the R matrix code, REFIT, the experimental data indicate a decrease of the radiative capture by 16.6 % relative to the ORELA measurement by C.M. PEREY [7, 8] which was the basis for the ENDF B6 evaluation (for ^{58}Ni , JEF2 = ENDFB6).

These experimental data strongly support the adjustment suggested by the JEF2 global analysis.

Conclusion - Trends for the future

Due to an improved adjustment method and the adjunction of more integral data (additional information on the capture cross section) the indications from the global analysis concerning Iron are now becoming trustworthy.

There are more restrictions concerning Ni and Cr due to the scarcity of integral information, although there is a strong support from experimental data concerning ^{58}Ni . That's why a lot is expected from the inclusion of SEG information in the data base, keeping in mind the difficulty of sensitivity calculations for that type of data.

To have a validation on the full energy range, it would be extremely valuable to include in the data base the high energy benchmarks used for EFF validation.

That would be an excellent occasion for both projects to cooperate so as to produce a common file.

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