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Validation of Iron and Structural Materials Data of JEF2

Status

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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 % ± 2 % for E > 2,2 MeV,
.decrease by ~ 25 % ± 7 % (threshold < E < 1,35 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 (~ 6 %).

$\sigma_{n,absorption}$: No requirement .

$\sigma_{n,T}$: Modest modification in the high energy range:
. ~ 3 % for E > 6 MeV,
.~ 2 % for 2,2 MeV < E < 6 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.

$\sigma_{n,absorption}$: Clear requirement for a decrease on the full energy range by ~ 15 % ± 10 % (in the 100 KeV region).

$\sigma_{n,T}$: no requirement .

^{52}Cr

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

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

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

$\sigma_{n,T}$: Increase by ~ 5 % for E > 6 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 :

$$\rho = \frac{1}{F}\left\{-\iint_{V,E}\Phi\Sigma_{abs}\Phi^{+} + \iiint_{V,E,E'}\Phi\Sigma_{s}(\Phi_{E'}^{+} - \Phi_{E}^{+}) + \iiint_{V,E,E'}\Phi\nu\Sigma_{F}\chi\Phi^{+} - \iint_{V,E} Dgrad\Phi.grad\Phi^{+}\right\}$$

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:	SEG-5		SEG-7A	SEG-6/EK10		SEG-6/EK45	
Main sens. to:	capture		capture	scattering		scattering	
	C/E rel.B-10		C/E rel.B-10	C/E rel.C		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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Validation of Iron and Structural materials data of JEF2

Provisional conclusions on the 14/6/1993

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The structural materials, especially Iron,by the large quantities implied in a power reactor, in the structures, cladings or shieldings, play an important role in neutronics.

They play an important role in the neutron balance in the core and the major process is the neutron absorption by radiative capture or (n, charged particle) reactions. The angular distributions of the secondary particules are of negligible importance.

In shieldings, when the protection of the humans against radiations is obtained by important thicknesses the neutron deep penetration is dependent on the energy transfert 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 transmited 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" 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.

The integral data considered so far to get information are:

1) Core data obtained in fast mock-ups designed (**RB2** program, **ON10** experiment in **MASURCA**) or not (**MASURCA**, **ERMINE**) with the specific purpose to test the structural material data.

These experiments bring information on the capture or the absorption cross section essentially.

2) Transmission data obtained in source reactors which are extremely sensitive to the inelastic and elastic scattering as already said.

This is the case of the **ASPIS** experiment analyzed by **ZHENG**, **KODELI** and coworkers (1)

The core data have been analysed in **CADARACHE** (**MASURCA**,**MINERVE**..)(2), or **BOLOGNA** (**RB2** program) (3) with the same tools: **ECCO** cell code and ERANOS system of codes for neutronics and sensitivity calculations.

The transmission data have been treated in **SACLAY** (1) with different calculationnal methods to check their adequacy with the problems involved in deep - penetration:

different weigthing functions and different energy schemes for the data processing, use of probability tables, use of deterministic or **MONTE-CARLO** calculationnal methods.

The information about the nuclear data quality is obtained through a group data adjustment. This one minimizes the set of $(^{(E-C)}/_{C})^2$ values where E and C stand respectively to the experimental and calculated values of the integral parameter of interest : Keff, Spectral indices, response functions.

The method chosen for the adjustment is the one of the statistical adjustment based on the minimization of a maximum likelihood estimator using the technique of **LAGRANGE multipliers**. The code used is the code **AMERE** that is the french version of the **AMARA** code (4)

The covariances matrices on nuclear data have been generated, except for ^{239}Pu and ^{238}U on the basis of personnal judgment assuming medium range correlations

For the integral data the covariance matrices are reduced, in a first step, to variances.

The sensitivity profiles of the integral parameters to the nuclear data have been calculated on the basis of the perturbation theory.

The nuclear parameters concerned by the adjustments are:

(the notation are obvious) $\nu, \sigma_f, \sigma^{removal}_{n,n}, \sigma^{removal}_{n,n'}, \sigma_c$

The data adjustment has been performed in a 15 macrogroup scheme consistent with the 1968g (fast systems), 172g (thermal systems), 175g (VITAMIN-J) group schemes used to calculate the C values.

This means a collapsing of the primary sensitivity and covariance data . The integral data of each experimental program have been analyzed separately in order to check their internal consistency (**RB2** data or **ASPIS** data at once...) and eventually to modify the quoted a priori accuracies by an enhancement factor $EF = (X^2/_N)^{1/2}$ that is the square root of the XHI2 per degree of freedom.

The **ASPIS** program gives the response function of **In**,**S**,**Rh** detectors at different thicknesses. In the analysis of this program one obtains:

for **In** detector (N=5), $x^2/_N = 2.3$ EF = 1.5
S detector (N=5), $x^2/_N = 0.65$ EF = 0.8
Rh detector (N=7), $x^2/_N = 5$ EF = 2.25

The Rh data exhibit some inconsistency in particular at small thicknesses and it seems that the incertainties are underestimated. (they will be multiplied by a factor 2)

The **RB2** program provides data for Keff and spectral indices related to the capture of the structural material or the $^{10}B(n,\alpha)$ cross section relatively to the ^{235}U fission cross section. One obtains:

$$(N=31),\ x^2/_N = 3 \qquad EF = 1.74$$

When looking more attentively one observes some inconsistency between the Keff data and the structural material Spectral Indices.(On the contrary the set of indices of $^{10}B(n,\alpha)/^{235}U(n,f)$ is quite perfect.).

This inconsistency is partly due to the experimental data of the structural material indices which are not obtained in a direct way.

Systematic studies performed elsewhere (5) showed the strict obligation to have a XHI2 per degree of freedom after adjustment as close to 1 as possible.

In the final adjustment, when the integral data are considered together (Fast, Thermal, Transmission...) , this conclusion led to the rejection of 42 integral data out of 169. In particular all the spectral indices relative to the structural material capture had to be eliminated.

For the 127 experiments retained the XHI2 per degree of freedom is:

$x^2/_N = 1.073.$

The result obtained for the major structural materials ^{56}Fe, ^{58}Ni, ^{57}Cr are summarized in the table 1.

CONCLUSION

Although it has not been possible to include the information contained in the capture data of the the **RB2** program it is possible to draw the following conclusions which will be hardly modified in the future course of the **JEF2** validation process:

About ^{56}Fe:

The inelastic cross section should be decreased by an important amount (20%) from the threshold to 1.3 Mev. The firt inelastic level cross section is essentially concerned. Above 2 Mev a 5 % increase is required.But the modifications concernig the capture (general decrease) and the elastic cross sections (decrease above 10 Kev, increase below) are well inside the quoted uncertainties.The general trend for the total cross section is a moderate decrease from the Kev region to 2 Mev.

About ^{58}Ni.

The main indication is relative to the absorption cross section: An important decrease is needed on the full energy range involving the radiative capture cross section and probably the (n,p) cross section. The conclusion about the (n,α) cross section is more hazardous since the adjustment is getting smaller just above its threshold.

About the ^{52}Cr:

All the indications are well inside the error bars, except for the elastic cross section for which a decrease of about 6-8 % is required in the range 60 Kev - 300 Kev.

It is worthwile noting that the amplitude of the required cross-section modifications are large or even very large suggesting that the adjustments have not been performed in the linearity conditions.

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table 1

NUCLEAR DATA CALCULATED CORRECTIONS

1 E+6 19.64	2 E+6 6.06	3 E+6 2.231	4 E+6 1.353	5 E+5 4.978	6 E+5 1.831	7 E+4 6.737	8 E+4 2.478	9 E+3 9.118	10 E+3 2.034	11 E+2 4.539	12 E+1 2.26	13 E+0 4	14 E-1 5.31	15 E-1 1.	GROUP UPPER LIMIT
															Fe 56
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NU
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	FISSION
0.0603	0.0557	-0.0163	-0.2712	-0.0159	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	INELASTIC
-0.0044	-0.0018	-0.0083	-0.0098	-0.0251	-0.0435	-0.0329	-0.0097	0.0233	0.0550	0.0541	0.0389	0.0167	0.0019	0.0003	ELASTIC
-0.0064	-0.0086	-0.0133	-0.0260	-0.0400	-0.0516	-0.0628	-0.0574	-0.0484	-0.0458	-0.0337	-0.0444	-0.0567	-0.0438	-0.0495	CAPTURE
															Ni 58
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NU
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	FISSION
-0.0080	-0.0125	-0.0298	-0.0235	-0.0153	-0.0089	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	INELASTIC
0.0005	-0.0033	-0.0132	-0.0135	-0.0072	-0.0069	-0.0036	-0.0009	0.0022	0.0034	0.0021	0.0014	0.0002	-0.0003	0.0000	ELASTIC
-0.0832	-0.0727	-0.1264	-0.2099	-0.2885	-0.2902	-0.2957	-0.3219	-0.2220	-0.1464	-0.0826	-0.0541	-0.0622	-0.0165	-0.0162	CAPTURE
															Cr 52
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	NU
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	FISSION
0.0004	0.0001	-0.0008	-0.0009	-0.0005	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	INELASTIC
-0.0031	-0.0060	-0.0078	-0.0564	-0.0815	-0.0736	-0.0482	-0.0243	-0.0063	0.0026	0.0008	0.0003	-0.0002	-0.0002	0.0000	ELASTIC
0.0000	-0.0045	-0.0144	-0.0245	-0.0217	-0.0238	-0.0301	-0.0314	-0.0326	-0.0378	-0.0311	-0.0363	-0.0416	-0.0349	-0.0391	CAPTURE

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