Part IV

A SUMMARY OF REQUIRED AND PROPOSED IMPROVEMENTS (JEFF-3)

Introduction to Part IV

A number of errors and deficiencies have been found in the JEF-2.2 library. They are listed in Chapter 13, and it is recommended that library users take note of these. The errors are being corrected and other improvements are being made in a new nuclear data library, JEFF-3. This is designed to be suitable for both fission reactor technology and fusion reactor applications, and account is also being taken of the requirements for accelerator driven systems (intermediate energy data).

As examples of the errors and deficiencies in JEF-2.2, mention can be made of the ambiguity in the specification of the ^{239}Pu fission spectrum and a problem in the specification of parameters in the unresolved resonance region. There are inconsistencies in the time dependent delayed neutron parameters for both ^{235}U and ^{239}Pu (the six time group decay constants and relative abundances being inconsistent). In the decay data library gamma-ray data for $^{144}_{59}$Pr are missing (in particular, the 2.186 MeV line), an important component of the gamma emission from fuel following a long irradiation and several years cooling (in this case the data had been derived from ENSDF).

The validation studies have shown the need to re-evaluate the resonance capture in ^{235}U, and the resolved region data (to 2 keV) have been re-evaluated at ORNL, the new evaluation being incorporated in ENDF/B-IV.5. The validation studies which have been undertaken with new evaluations are discussed further in Chapter 15.

The fast reactor validation studies have shown the need for a new evaluation of sodium cross-sections above the inelastic scattering threshold and a new evaluation has been produced based on recent measurements made at ORNL and IRMM, Geel.

There are new measurements of important items of nuclear data, such as the fine structure in the iron total cross-section above the inelastic scattering threshold and the inelastic scattering below 2 MeV. A new JEFF-3 evaluation based on these measurements has been found to give improved agreement with measurements of the transmission through blocks of iron. Recent re-evaluations of the resonance parameters for ^{240}Pu and ^{241}Pu have been found to result in improved agreement with integral measurements. In JEF/DOC-800 [1], E. Fort has summarised the materials for which it has been concluded that re-evaluations of the cross-sections are required, based on the Cadarache analysis of fast reactor measurements and the cross-section adjustment studies. Re-evaluation work which is expected to provide the required improvements is also indicated. A summary of this information is presented Tables III.1-III.3.

It is also noted that more integral measurements are required to adequately validate the cross-sections for many of these materials, in particular the structural materials and ^{242}Pu.

A new fission yield data library, UKFY3, has been produced by R.W. Mills, the author of the JEF-2.2 fission yield library (Chapter 3), and the validation studies have given indications on discrepancies in the present library (see Chapter 5). This work provides the basis for updating the fission yield library. The evaluation methodology underlying the development of UKFY3 is described in Ref. [2].

Table III.1. Major actinides

Nucleus	Major observations	Re-evaluations required
^{239}Pu	Unresolved range; $\sigma_{n,f}$ + 2%, E > 1.5 MeV; σ (n,2n)	Partial re-evaluation (Cadarache)
^{240}Pu	Increase ν_p; reduce $\sigma_{n,\gamma}$ $\sigma_{n,f}$ (E < 2 MeV)	• Complete re-evaluation • Resonance region (Cadarache), continuum (Bologna, Bucharest)
^{241}Pu	Unresolved range; reduce $\sigma_{n,\gamma}$; $\sigma_{n,f}$ in first plateau (5%)	Partial re-evaluation (Cadarache)
^{242}Pu	Insufficient integral information; reduce $\sigma_{n,\gamma}$ by 20%	Re-evaluation (Bologna, Bucharest)
^{238}U	Increase ν_p 1.2% (E < 6 MeV), 0.7% (E > 6 MeV); sub-threshold fission? Increase σ (n,n′) 5% (E > 2 MeV)	Local corrections
^{235}U	$\sigma_{n,\gamma}$ in the resolved and unresolved resonance range	Re-evaluation at Oak Ridge

Table III.2. Coolants, absorbers and scatterers

Nucleus	Major observations	Re-evaluations required
^{23}Na	E < 2 MeV; reduce σ (n,n′) by 30%, increase σ (n,n) by 30%	Complete re-evaluation (Cadarache, Geel)
^{16}O	Increase $\sigma_{n,\gamma}$ 10%(E > 1 MeV), increase $\sigma_{n,\alpha}$ 20% (E > 3 MeV)	

Table III.3. Structural materials

Nucleus	Major observations	Re-evaluations required
Fe	Total cross-section; reduce σ (n,n′) 20% (E < 2 MeV); $\sigma_{n,\gamma}$ in the first resonance of ^{54}Fe?	Re-evaluation complete (JEFF Project re-evaluation)
^{58}Ni	Reduce $\sigma_{n,\gamma}$ 10%	Complete re-evaluation
^{52}Cr	Reduce σ (n,n′) 20% (25 keV < E < 1.3 MeV)	Complete re-evaluation?

New decay data evaluations have been produced for a list of isotopes which had been identified as either missing from JEF-2.2 or in need of revision (or updating to take account of new measurements). This work is described in Chapter 14.

The European Activation File (EAF) will be associated with JEFF-3. This includes reaction cross-section and decay data for a large number of isotopes.

There are measurement programmes and developments of nuclear theory in progress in a number of laboratories and research centres. The JEFF project evaluators will be taking these into account when developing JEFF-3 from the initial "Starter File" version. One can note, for example the

programmes of measurements of fission fragment properties at IRMM Geel and ILL Grenoble and of cross-sections at IRMM Geel.

A limitation of JEF-2.2 is that covariance data for cross-sections are given for only a few materials. Consideration is being given to providing data more generally. (Note that EAF includes uncertainty data.)

The development of JEFF-3 also provides the opportunity for consideration to be given to adopting some of the more recent evaluations from other nuclear data libraries, in particular when the materials concerned have not formed a significant part of the JEF-2.2 validation studies.

REFERENCES

[1] E. Fort, "JEF2 validation: Performances in the fast range (Unresolved Range -> 10 MeV) ", JEF/DOC-800.

[2] R.W. Mills, "Fission Product Yields", lecture notes from a presentation at the 1999 Frédéric Joliot/Otto Hahn Summer School on Neutron Measurements and Evaluation, Geel, Belgium, May 1999.

Chapter 13

A LIST OF KNOWN ERRORS IN JEF-2.2

Nuclide	From	Date	Comment	Status
$^{104}_{49}$In	F. Chukreev	18.10.93	15.4 s state missing.	
$^{126}_{49}$In	F. Chukreev	18.10.93	Isomer and ground states probably transposed. At present Q (isomer) < Q (g.s.). Comparing spin and T1/2 with nuclear wallet supports this assumption.	
$^{126}_{49}$In	F. Chukreev	11.11.93	^{129}Ba decay data contains gamma line 419.83 keV twice.	
Many	M. Konieczny	10.11.93	All data taken from ENSDF – error in translating ENSDF to ENDF format: error in RADLST (SIGFIG) causes uncertainties to reset to zero when in fact they are non-zero.	
$^{147}_{66}$Dy $^{149}_{68}$Er $^{160}_{67}$Ho $^{183}_{81}$Tl $^{185}_{81}$Tl $^{185}_{81}$Tl $^{191}_{81}$Tl $^{197}_{83}$Bi $^{248}_{97}$Bk	M. Konieczny	30.11.93	Ground state missing in decay file. In the case of: $^{147}_{66}$Dy , $^{149}_{68}$Er , $^{160}_{67}$Ho , $^{185}_{81}$Tl , $^{197}_{83}$Bi , $^{248}_{97}$Bk , the g.s. is known in ENSDF should be included in JEF.	
$^{235m}_{92}$U	A. Nichols	05.03.96	In JEF-2.2 the average gamma energy is given as 76 eV (equal to the Q-value). In the original evaluation, A. Nichols had the average gamma energy set to 0.0, since the internal conversion coefficient has been set to 10E17, indicating that nearly all the gammas are internally converted (i.e. only 76 eV/10E17 are emitted as gamma rays). However, it appears that the pre-processing of UKHEDD2_1 into JEF-2.2 using CORDECAY has reset the average gamma energy to be equal to the Q-value – which is clearly wrong. This looks like a problem with CORDECAY.	

Nuclide	From	Date	Comment	Status
$^{206}_{90}$Th	A. Nichols		In JEF-2.2 the spin/parity is given as +0.0. However, A. Nichols maintains that he had evaluated it as -0.0. Upon investigation, it appears that it was set as -0.0 in UKHEDD1 but changed to +0.0 in UKHEDD2. 6/3/96 – A. Nichols has determined that the +0 and -0 problem is caused by computer dependancy. Some machine will see -0 and reset this to +0.	
$^{79}_{34}$Se		12.03.96	^{79}Se decays by beta emission (150 keV) to Br (g.s.). No internal bremsstrahlung, no annihilation radiation, no x-rays, no gamma-rays. Thus, mean electromagnetic energy (or mean gamma energy in ENDF terminology) is zero. However, in JEF-2.2, then mean gamma energy is reset to 0.0496662 MeV! N.B. Mean beta energy is not all the energy of the decay because the neutrino energy is not included.	
$^{93}_{40}$Zr	A. Nichols		^{93}Zr decays to Nb (g.s) (Q-value = 91 keV) and to Nb (m.s) (Q-val = 62 keV). From Blachot's evaluation (JEF-2.2) we only have the m.s. decay. A. Nichols thinks that this decay should be clearly labelled as a branching to the two states of Nb.	
$^{88}_{35}$Br $^{89}_{35}$Br $^{90}_{35}$Br *Possibly* $^{87}_{35}$Br $^{93}_{37}$Rb $^{94}_{37}$Rb $^{94}_{37}$Rb $^{95}_{37}$Rb $^{98}_{39}$Y $^{99}_{39}$Y $^{135}_{51}$Y $^{137}_{53}$I $^{139}_{53}$I $_{85}$At	A. Nichols	15.03.96	In the JEF-2.2 file, for both modes 1.0 (beta – decay) and 1.5 (beta – followed by neutron emission), LCON = 2 indicating that both discrete and continuous spectra are given. In each case FD (the discrete spectrum normalisation factor is set, but FC (the continuum spectra normalisation factor) is given as zero (INCORRECT) ==> multiply the continuum spectravalues by this number.	

Nuclide	From	Date	Comment	Status
$^{144}_{59}$Pr	R.W. Mills	24.01.97	Two major gamma lines at 1 489 and 2 186 keV missing.	

Feedback on JEF-2.2 General Purpose File

Nuclide	From	Date	Comment	Status
$^{16}_{8}$O	C. Nordborg	26.01.94	(n,α) reaction MT = 107, 800s. At one of the first energies these reactions have cross-sections of 10e-38 which may cause problems on short word machines.	
$^{27}_{13}$Al	C. Dean	22.10.94	MT = 102 SIGMA is recorded as having been changed from 232 mb to 213 mb (upon recommendation from Bologna?). However, c.f. with Mughabgabab which quotes 231±3 and this change looks suspicious.	
$^{16}_{6}$O	C. Dean	6.10.94	Atomic weights on the 1994 WIMS library. The atomic mass values on the 1994 WIMS library are listed in Table 10 of AEA-RS 5690. They are taken from the relevant JEF-2.2 evaluation. These are given relative to a neutron. The NJOY code converts them to the C12 scale by multiplying by the neutron mass. Values on JEF-2.2 are often dated because "current" values were included when the evaluation was first produced. Many parts of JEF and ENDF libraries are converted from older issues without updating the mass values. Values from the latest mass evaluations should be included in later WIMS libraries. 6/10/94 – M. Halsall noted Table 10 contained a value of 15.9905 for ^{16}O. He expected a value of ~15.995. The JEF-2.2 evaluation is taken from ENDF/B-VI. Both contain a mass of 15.85316 relative to a neutron giving 15.9905 on the C12 scale. JENDL-3 contains 15.8575 and JEF-1.1 15.858. ENDF/B-VI hydrogen in H_2O contains an oxygen mass of 15.858. Checks against the latest mass evaluation indicate the JEF-2.2/ENDFB-VI evaluations may be wrong! Currently JEF and ENDF/B-VI will not be changed – neither will the WIMS 1994 library. However the US evaluators should be asked to examine the value.	

Nuclide	From	Date	Comment	Status
$^{90}_{38}$Sr	M. Sowerby	6.2.95	Problem in ^{90}Sr capture cross-section – thermal capture is x60 to high in JEF-2.2	
Many	P. Ribon		All energy points in the partial sections should be present in the total sections. Examples: ^{174}Hf, ^{176}Hf, ^{235}U.	
$^{9}_{4}$Be $^{10}_{5}$B $^{14}_{7}$N $^{16}_{8}$O	G.C. Panini		Missing angular distributions for the following light isotopes: ^{9}Be (MT = 700-701), ^{10}B (600-603, 800-801), ^{14}N (600-604, 650-653, 700-701, 800-810), ^{16}O (800-803).	
$^{11}_{5}$B $^{19}_{9}$F $^{23}_{11}$Na $^{nat}_{19}$K $^{182}_{74}$W $^{183}_{74}$W $^{184}_{74}$W $^{186}_{74}$W $^{209}_{83}$Bi	G.C. Panini		Kerma calculation problems for some isotopes.	
Many	C. Dean		Checking of the unresolved resonance parameters needed. Processing problems, especially with parameters taken from KEDAK formatted evaluations, have been encountered.	
$^{55}_{25}$Mn	P. Ribon		Modification of the capture resonance region background cross-section needed.	
$^{100}_{42}$Mo	C. Gragg		(n,2n) – tabulated subsection must be last.	
$^{122}_{50}$Sn	T. Nakagawa		Upper limit of the resolved resonance region should be 8.603905 + 3 eV.	
$^{154}_{63}$Eu	T. Nakagawa C. Gragg		Contains artificial resonance parameters from ENDF/B-V.	
$^{155}_{63}$Eu	T. Nakagawa C. Gragg		Needs updating.	
$^{166}_{68}$Er	C. Gragg		Resonance integral and 2 200 m/s values much larger than ENDF/B-VI.	
$^{233}_{92}$U	H. Tellier		Needs updating.	
$^{235}_{92}$U	P. Ribon		There are two resonances with the same energy and same spin at 2.2 keV.	
$^{235}_{92}$U	C. Dean		Verify the consistency between the JEF-2.2 and ENDF/B-VI rev. 1 evaluations.	
$^{239}_{94}$Pu	P. Ribon		Neutron widths for L = 1, J = 1 unresolved resonance parameters should be divided by 2, following an earlier correction to the value of parameter AMUN.	

Nuclide	From	Date	Comment	Status
$^{239}_{94}$Pu	H. Derrien		New resonance parameters up to 2 keV from H. Derrien available.	
$^{241}_{95}$Am	J.L. Rowlands	25.08.95	Resonance widths, for capture and fission need x7/6 adjustment. Resonance width for neutron needs x2 adjustment.	
$^{nat}_{82}$Pb	A. Hogenbirk	08.04.97	Format problem; for threshold energies in the MF6 data the distribution is not normalised. It occurs for MT numbers for which MF6 data are given (not only MT16 and MT91).	
$^{239}_{94}$Pu	M. Mattes	21.02.96	Redundancy in fission spectra (MF = 5) leads to processing problems with NJOY. JEF-2.2 evaluation contains both MT = 18 and also the partials – MT = 19,20,21 and 38.	
$^{235}_{92}$U	P. Ribon	13.05.97	Resolved resonance region: J = 4 – two resonances with the same energy (744.2 eV).	
$^{235}_{92}$U	P. Ribon	13.05.97	Resolved resonance region: 300-500 eV: six pairs of resonances with spacings of < 0.04 eV, i.e. statistically impossible.	
$^{nat}_{48}$Cd	P. Ribon	13.05.97	Pointwise cross-sections: the resonance at 58.7 eV is a phantom (i.e. does not exist in JENDL and has not been observed in GEEL experiments).	
$^{103}_{45}$Rh	P. Ribon	13.05.97	Spin of resonance at 154 eV is J = 0. This gives a poor fit to with predictions from GEEL, and older experiments.	
$^{166}_{68}$Er	P. Ribon	13.05.97	Resolved resonance region: missing resonance at 170 eV.	
$^{166}_{68}$Er	P. Ribon	13.05.97	Pointwise cross-section: interpolation of a background capture cross-section between 0.025 eV (33.3b) and 2 000 eV (0.118b); this is an absurd interpolation.	
$^{105}_{45}$Rh	P. Ribon	13.05.97	Pointwise cross-section: lack of data between 0.5 and 2.0 eV.	
$^{56}_{26}$Fe	P. Ribon	13.05.97	Pointwise cross-section: inelastic cross-section too low between 1.5 and 4.5 MeV.	

Feedback on JEF-2.2 Fission Yield Data

Nuclide	From	Date	Comment	Status
$^{235}_{92}$U $^{241}_{94}$Pu	P. de Leege	08.10.97	Values of NN and NNP incorrect (at E = 4.0E+5, mt = 454,459).	