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The JEFF-3.1.1 Nuclear Data Library

JEFF Report 22

Validation Results from JEF-2.2 to JEFF-3.1.1

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Foreword

This report describes the incremental method used to improve JEFF evaluations since the release of the JEF-2.2 library in 1992. In order to be accepted as a JEFF-3 evaluation, new evaluations must be demonstrated to be more consistent with both differential and targeted integral measurements. The report first describes the validation of the JEF-2 library and the user feedback received by evaluators. The main improvements introduced in the JEFF-3.0 file, and in a second step in JEFF-3.1, are then presented. The report highlights the modifications that would be required for JEFF-3.1 evaluations to fit with integral experiments and to meet LWR target accuracy. The new evaluations (^{237}Np, ^{239}Pu, ^{16O,91,96}Zr and seven fission products) introduced in the recommended JEFF-3.1.1 file are also described.

The current validation of the JEFF-3.1.1 file is detailed. Fundamental targeted experiments, LWR mock-up experiments, PWR and BWR chemical assays and SNF reactivity worth measurements are analysed using both TRIPOLI4 and APOLLO2.8 reference calculations.

This report demonstrates that JEFF-3.1.1 is probably the best international library currently available. It is more accurate than ENDFB/VII for fuel inventory, MOX reactivity and plutonium ageing, and reactivity coefficients such as temperature coefficient and stainless tell reflectors. Moreover, JEFF-3.1.1 evaluations benefit from the feedback of validation studies for fast breeder reactors, the fuel cycle, criticality safety and burn-up credit.

JEFF-3.1.1 is used worldwide for PWR and BWR calculations, particularly in the new ARCADIA package of Areva-NP. It is also used in ERANOS2 for Generation IV designs.

Please note that while this report is printed in black and white, several of the graphics are best viewed in colour. A colour version may be viewed on the NEA website at *www.nea.fr/html/dbdata/nds_jefreports/*.

Acknowledgements

The authors and editors acknowledge the JEFF Working Group participants, particularly Drs. Sublet and van der Marck, for their contribution to the JEFF-3 experimental validation of ICSBEP benchmarks, as well as experts from Areva-NP for their contribution to the JEFF-3.1.1 library validation throughout the full light water reactor (LWR) cycle. The authors also wish to thank EDF for its financial support of *Commissariat à l'énergie atomique* (CEA) participation in this project.

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Chapter 1: Introduction

Since the release of the JEF-2 European File in 1992, incremental improvement of this library has been ongoing. Contrary to the global evaluation substitution employed when moving from ENDF/B-VI to B-VII, the incremental method sustained by the CEA allowed new evaluations only if JEF-2 nuclear data were found in disagreement with differential measurements and if calculation-measurement bias in targeted integral experiments was unacceptable. The proposed new evaluation must be demonstrated to be more consistent with both differential and integral measurements in order to be accepted as a JEFF-3 evaluation.

Chapter 2 of this report summarises the experimental validation of the JEF-2 library and the feedback provided to evaluators, which leads to improved JEFF-3 evaluations. Chapter 3 presents the main improvements introduced in a first step in the JEFF-3.0 file and in a second step in the JEFF-3.1.0 file. Chapter 4 highlights the modifications necessary for JEFF-3.1.0 evaluations to maintain compatibility with integral experiments and to meet LWR target accuracy. The new evaluations (^{237}Np, ^{239}Pu, ^{16}O, ^{91,96}Zr and seven FP) introduced in the recommended JEFF-3.1.1 file are described. Chapter 5 presents the CEA2005v4.1 multi-group library recommended for APOLLO2.8, processed from JEFF-3.1.1. Chapter 6 summarises the current validation of the JEFF-3.1.1 file and the CEA2005v4.1 library.

Chapter 2: JEF-2 validation. Feedback for improved evaluations

Over a ten-year period, an extensive validation of the JEF-2 evaluation was performed at the CEA. Both the JEF-2 and the CEA93 libraries of the APOLLO2.5 code (processed from JEF-2.2) were validated (Santamarina, 2002). Activities undertaken in this regard include:

- fundamental experiments and reactivity worth measurements in the MINERVE pool reactor;
- LWR mock-up experiments in the "zero-power" reactor EOLE;
- chemical assays on PWR spent fuel assemblies.

Sensitivity studies (Chabert, 2002) as well as nuclear data re-estimation using the RDN code were carried out (Courcelle, 2004).

Traditional nuclear data feedback is often based on reactivity experiments and central reaction rate ratio measurements of specific isotopes. The strength of the CEA study was that it considered not only k_{eff} measurements in UOX and MOX water-moderated lattices and highly-enriched uranium experiments, but also included isotopic ratios measured in PWR post-irradiation evaluations. These evaluations consist of measuring fuel rod cuts for the relative concentration N_i/N_{U238} of nuclides during irradiation. The samples to be analysed are extracted from the assembly at each end of cycle. After cooling and transportation, samples are dissolved in a hot acid solution and analysed by various techniques depending on the isotopic ratio to be measured (alpha, gamma or mass spectrometry). Each experimental value can be considered as an individual integral measurement: about 400 C/E values from UOX and MOX assemblies have been included in the RDN code. Measured actinides include ^{234,235,236}U, ^{237}Np, ^{238,239,240,241,242}Pu, ^{241,243}Am and ^{244,245}Cm. Table 1 summarises the PIE measurements included in the statistical adjustment.

APOLLO2.5 calculations follow the recommendations of the accurate reference scheme "CEA-97" (Santamarina, 2004), as defined specifically for MOX (Chabert, 2000) and taking into account thermo-mechanics and cycle irradiation history (Chabert, 2000a). The calculation/experiment biases obtained for major actinides and used in JEF-2 nuclear data re-evaluation are summarised in Table 2. These results point out the large underestimation of ^{238}Pu and ^{242}Pu build-ups (about -8% at 40 GWd/t).

Table 1: Spent fuel measurements used in the JEF-2 data re-estimation

Fuel UOX PWR name	U enrich^{t} ^{235}U wt.%	Number of samples	Burn-up range
Bugey-3	3.10%	7	20-38 GWd/t
Fessenheim-2	3.14%	8	49-58 GWd/t
Gravelines	4.50%	8	26-60 GWd/t

Fuel MOX PWR name	Pu enrich^{t} Pu wt.%	Number of samples	Burn-up range
Saint-Laurent B1	2.91%	3	10-38 GWd/t
	4.42%	4	13-42 GWd/t
	5.64%	2	28-45 GWd/t

Table 2: Calculation/experiment comparison (C/E – 1 in %) in PWR UOX assemblies

Isotope		20 GWd/t	40 GWd/t	60 GWd/t
^{234}U	e = 3.1%	3.5	2.3	
	e = 4.5%	0.5	1.0	0.7
	Uncertainty	±1.1	±1.4	±2.0
^{235}U	e = 3.1%	0.9	2.6	2.0
	e = 4.5%	1.4	2.5	3.1
	Uncertainty	±1.1	±2.0	±3.5
^{236}U	e = 3.1%	-3.7	-3.4	-3.8
	e = 4.5%	-4.8	-4.7	-4.5
	Uncertainty	±1.3	±0.9	±0.6
^{237}Np	e = 3.1%	-9.1	-2.0	-2.0
	e = 4.5%	-2.3	-3.7	-4.5
	Uncertainty	±3.0	±2.8	±2.7
^{238}Pu	e = 3.1%	-8.7	-5.3	-4.5
	e = 4.5%	-12.2	-10.6	-9.0
	Uncertainty	±4.0	±3.9	±3.7
^{239}Pu	e = 3.1%	0.6	2.1	2.0
	e = 4.5%	-0.7	0.4	2.5
	Uncertainty	±0.9	±1.1	±1.3
^{240}Pu	e = 3.1%	-0.3	-0.2	0.3
	e = 4.5%	-2.9	-2.1	-0.5
	Uncertainty	±1.9	±1.5	±1.1
^{241}Pu	e = 3.1%	-2.7	-1.0	-0.5
	e = 4.5%	-5.3	-4.2	-1.5
	Uncertainty	±2.3	±1.8	±1.6
^{242}Pu	e = 3.1%	-6.6	-6.9	-5.5
	e = 4.5%	-9.8	-9.3	-7.8
	Uncertainty	±4.0	±3.4	±2.8

The selected K_{eff} and buckling measurements in low-enriched UO_2 lattice experiments cover a wide range of moderation ratios. Most of them are LWR-type and have been carried out in the EOLE and MINERVE reactors. VVER and HCPWR critical experiments are taken from the International Criticality Safety Database ICSBEP handbook (Table 3).

Table 3: K_{eff} measurements in low-enriched LWR lattices included in the JEF-2 data re-estimation

Experiment	Lattice pitch (cm)	V_{H2O}/V_{UO2}	^{235}U wt.%	Number of C/E
CRISTO III	0.96	0.45	3.3%	1
EPICURE	1.26	1.25	3.7%	1
MISTRAL1	1.32	1.75	3.7%	1
CAMELEON	1.26	1.80	3.5%	2
CRISTO I, II	1.58-1.86	3.50-5.46	3.0%	3
VALDUC	1.26-2.10	1.82-7.58	4.8%	3
VVER Δpitch	1.10-1.90	0.89-5.51	3.6%	5
ZPR-HiC	1.17-1.35	0.43-1.37	3.0%	5

Experiments using highly-enriched uranium solution [UO_2F_2+H_2O or $UO_2(NO_3)_2$+HNO_2] are widely used in criticality safety to verify the accuracy of nuclear data, particularly η_{U235}. As summarised in Table 4, we investigated experiments from various international laboratories involving uranium concentrations ranging from 20 g/l (corresponding to softer neutron spectrum) up to 700 g/l (intermediate neutron spectrum).

Table 4: K_{eff} measurements in highly-enriched uranium solutions used in JEF-2 ND re-estimation

Laboratory	ICSBEP name	Solution	Conc. range g/l U	Number of C/E values
ORNL	Heu-Sol-Therm-009	UO_2F_2+H_2O	213-696	4
ORNL	Heu-Sol-Therm-010	UO_2F_2+H_2O	95	1
ORNL	Heu-Sol-Therm-011	UO_2F_2+H_2O	53	2
ORNL	Heu-Sol-Therm-012	UO_2F_2+H_2O	20	1
ORNL	Heu-Sol-Therm-032	$UO_2(NO_3)_2$	14.8	1
Rocky Flats	Heu-Sol-Therm-001	$UO_2(NO_3)_2$	55-358	8
IPPE Obninsk	Heu-Sol-Therm-018	$UO_2(NO_3)_2$	300	1
IPPE Obninsk	Heu-Sol-Therm-019	$UO_2(NO_3)_2$	447	1

In an effort to minimise errors in the K_{eff} calculation of UOX lattices and highly-enriched systems, the Monte Carlo code TRIPOLI-4 was used with a JEF-2 pointwise cross-section. Resonance self-shielding in the unresolved range was also accounted for using probability tables. The calculation/experiment comparison for UOX regular lattices is plotted in Figure 1.

C/E values for highly-enriched uranium solutions are displayed in Figure 2, which shows an overestimation of the JEF-2.2 eigenvalues for high ^{235}U content.

Figure 1: Calculation/experiment bias (in pcm) on the critical K_{eff} of UOX lattices

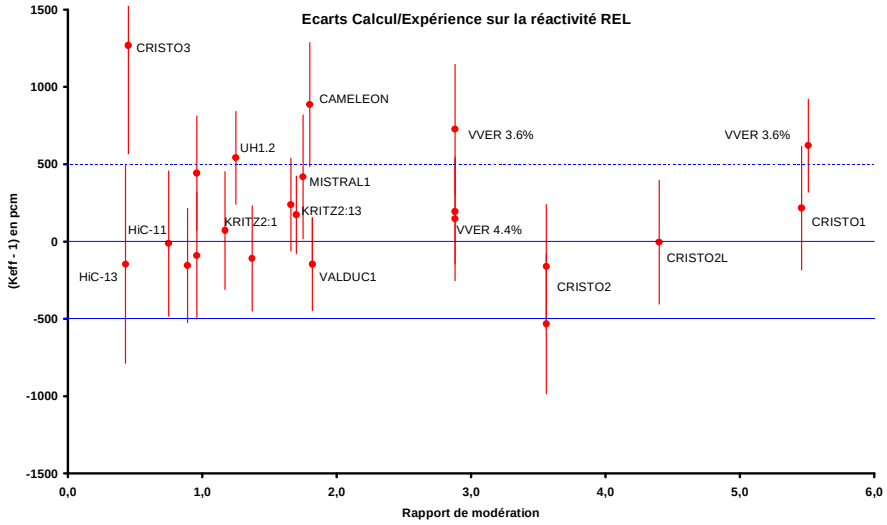
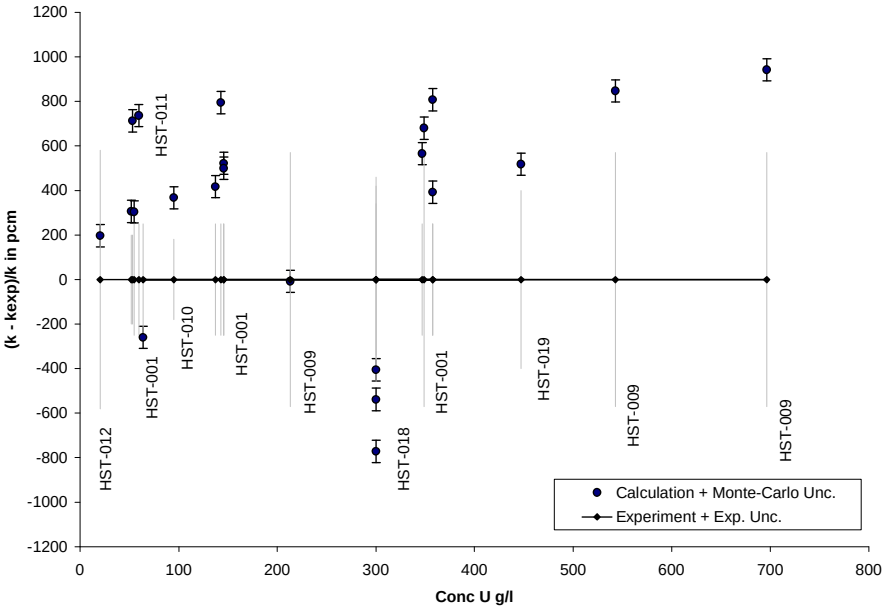


Figure 2: Calculation/experiment bias (in pcm) on the critical K_{eff} of uranium solutions



K_{eff} sensitivity profiles to nuclear data were easily obtained from the First Order Perturbation Theory implemented in APOLLO2. Sensitivity coefficients to the cross-sections and multiplicities of the main isotopes were derived from the European JEF 15-group structure. For isotopic ratios, sensitivity coefficients have to be assessed as a function of the burn-up; therefore direct APOLLO2 calculations were carried out.

The main trends on JEF-2 data obtained from the RDN re-estimation are summarised in Table 5. In this table, nuclear data modifications in bold are considered to be significant, as the uncertainty (1σ) after adjustment is significantly reduced and lower than the data modification.

Table 5: JEF-2 data modifications (%) obtained from RDN re-estimation

Energy range	Change in %	Std. dev. after adj	Std. dev. before adj
^{235}U	*Capture*		
12.03 keV-454 eV	+6.3	8.8	10.0
454 eV-22.6 eV	**+12.9**	**3.1**	**10.0**
22.6 eV-4.0 eV	**+12.8**	**3.6**	**10.0**
4.0 eV-0.54 eV	**+12.4**	**3.7**	**10.0**
0.54 eV-0.1 eV	+0.7	1.6	2.0
< 0.1 eV	+0.4	0.8	1.0
^{235}U	ν_t		
22.6 eV-4.0 eV	+0.1	0.7	0.7
4.0 eV-0.54 eV	+0.2	0.7	0.7
0.54 eV-0.1 eV	+0.3	0.5	0.7
< 0.1 eV	**+0.1**	**0.2**	**0.4**
^{238}U	*Capture*		
12.03 keV-454 eV	-0.1	2.2	2.2
454 eV-22.6 eV	-0.5	1.6	2.0
22.6 eV-4.0 eV	-0.7	1.7	2.0
4.0 eV-0.54 eV	0.0	1.0	1.0
^{238}U	*n,2n*		
19.6 MeV-6.07 MeV	**+6.8**	**2.1**	**10.0**
^{241}Pu	*Capture*		
454 eV-22.6 eV	+4.9	10.0	10.0
22.6 eV-4.0 eV	+11.2	9.8	10.0
4.0 eV-0.54 eV	+0.8	7.0	7.0
0.54 eV-0.1 eV	**+7.4**	**2.6**	**5.0**
< 0.1 eV	+0.4	1.5	1.5

Concerning the ^{238}U evaluation, a slight reduction by 0.6% of the shielded capture cross-section in the resolved range is suggested. However, considering the importance of this data for K_{eff} and Pu build-up calculations, this result is worth mention. An increase by 7% ± 2%(1σ) of the (n,2n) cross-section is requested.

The need for increasing ^{235}U capture resonance integral in JEF-2 is quantified: +12% ± 3%. The thermal value of $\nu_t^{U235} = 2.437$ is confirmed within 0.2% accuracy.

An accurate trend is shown for the epithermal capture of ^{241}Pu. The capture integral of the 0.26 eV resonance in JEF-2 should be increased by 7.4% ± 2.6% (correction linked to the underestimation of the ^{242}Pu build-up).

Concerning the main fission products (FP), the validation of the capture cross-section was achieved through reactivity worth measurement in MINERVE of separated FP samples. The JEF-2 calculation/experiment bias (average value between R1-UO_2 and R2-UO_2 experiments, *i.e.* LWR and thermal spectrum respectively) is summarised in Table 6.

Table 6: Calculation/experiment bias on the reactivity worth of separated FP

FP isotope	(C-E)/E ± 1σ
^{95}Mo	-2% ± 3%
^{99}Tc	+3% ± 3%
^{103}Rh	+10% ± 3%
^{109}Ag	-3% ± 3%
^{133}Cs	+5% ± 3%
^{143}Nd	-5% ± 2%
^{145}Nd	0% ± 1%
^{147}Sm	+2% ± 3%
^{149}Sm	-5% ± 2%
^{152}Sm	-1% ± 2%
^{153}Eu	-3% ± 3%
^{155}Gd	-3% ± 3%

From these results on the 12 main poisoning FP (except decaying ^{135}Xe and ^{151}Sm, and gaseous ^{131}Xe), the following conclusions on the JEF-2 evaluations were drawn (Santamarina, 1999):

- ^{95}Mo, ^{99}Tc, ^{109}Ag, ^{145}Nd, ^{147}Sm, ^{152}Sm and ^{155}Gd are satisfactory.
- ^{153}Eu capture is acceptable, though the JENDL-3.2 evaluation improves the C/E agreement.
- A new evaluation of the ^{133}Cs is required in the resonance range, mainly for the large first resonance E_{Cs133} = 5.9 eV, the resonance integral of which should be decreased by 6%.
- The E_R = 1.3 eV resonance integral of the ^{103}Rh nuclide should be strongly decreased by 10%. Since ^{103}Rh evaluations in international data files are no longer suitable, differential measurements must be launched at the Geel European Center.
- New evaluations of ^{149}Sm and ^{143}Nd are necessary for JEFF-3, in order to increase the (n,γ) cross-section by 5% in the 0-0.2 eV energy range.

From FP chemical analyses in PWR spent fuels, it was pointed out (Santamarina, 2000) that the ^{154}Eu and ^{155}Eu evaluations in JEF-2 are inaccurate; furthermore, ^{144}Nd build-up at high burn-ups confirmed the need to increase ^{143}Nd capture by 5%.

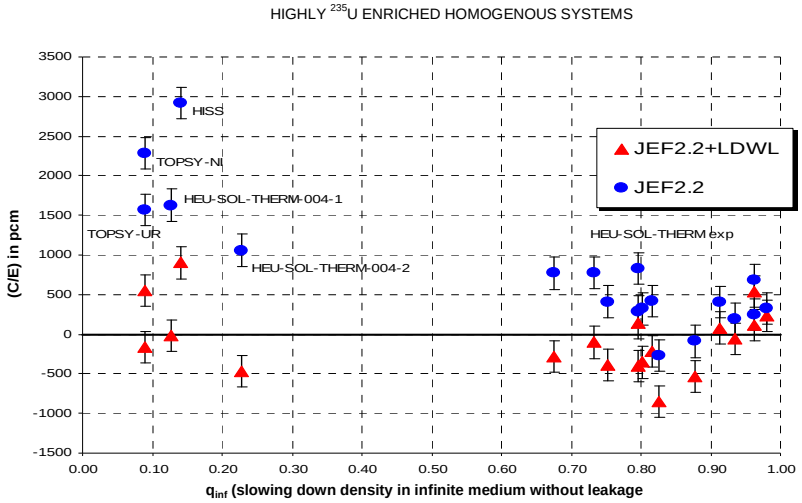
French PIE also contributed to suggestions for improvements in terms of FP yields, an example being that the ^{133}Cs yields of ^{235}U and ^{239}Pu thermal fissions must be increased by 2%. ^{148}Nd and ^{137}Cs are not absorbing FPs, but they are used as burn-up monitors and their calculated amounts must be predicted within 2% accuracy. Unfortunately, the JEF-2 ^{148}Nd yield from ^{239}Pu fission is elevated compared to the Meek and Rider values, leading to a -2% low burn-up estimation.

These suggestions were made to the JEFF Group (Santamarina, 2008a), and have greatly contributed to the content of the JEFF-3.1 file.

Chapter 3: Main improved evaluations in JEFF-3.1

The 7% increase of the LDWL capture resonance integral (Leal, 1999) (<Γγ> = 40 meV instead of 35 meV in JEF-2) in the new ^{235}U evaluation allowed to dispel the longstanding underestimation of ^{236}U-^{237}Np-^{238}Pu build-up in LWR spent fuel. Further, and as shown in Figure 3, this JEFF-3.0 evaluation enabled to halt the trend in K_{eff} overestimation of enriched uranium systems with hardened spectra (Courcelle, 2001).

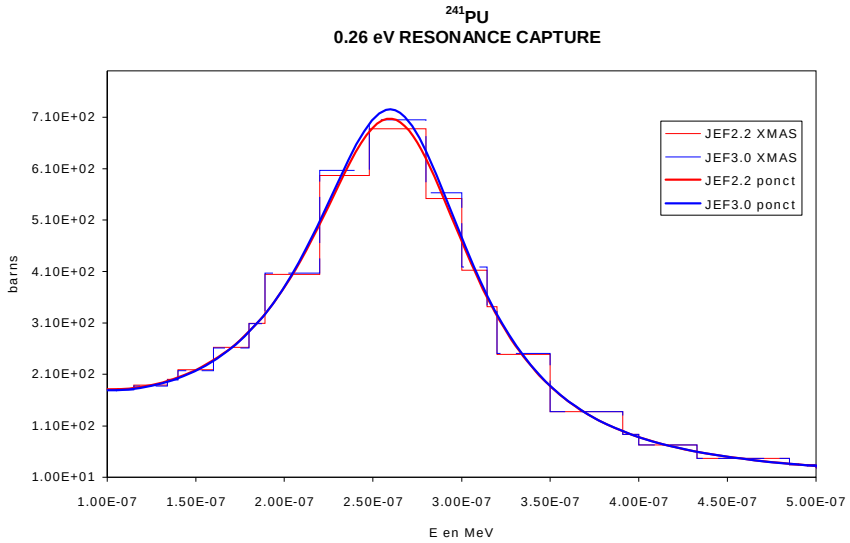
Figure 3: Calculation/experiment comparison for the K_{eff} of ^{235}U homogeneous systems



The ^{238}U evaluation was slightly improved with the (n,2n) cross-section increase of 10%. However, this JEFF-3.0 evaluation did not follow all our recommendations (Courcelle, 2001a). In particular the reduction of capture and the improvement of inelastic scattering were not performed.

The ^{241}Pu evaluation carried out in collaboration with ORNL (Derrien, 2005) allowed a correct prediction of ^{242}Pu and ^{243}Am build-up, thanks to the increase of the capture resonance integral (+6%) and $\Gamma\gamma^{E=0.3eV}$ = 33.3 meV (instead of 32.5 meV in JEF-2, as shown in Figure 4).

Figure 4: JEFF-3 and JEF-2 capture cross-section in the first ^{241}Pu resonance



The ^{239}Pu evaluation was mainly improved in the fast range.

Finally, as pertains to major actinides, the ^{240}Pu evaluation performed by the CEA (Bouland, 1997) was adopted. This evaluation corrected the erroneous JEF-2 capture cross-section between resonances.

New evaluations were performed for the main poisoning FP (Courcelle, 2002) on the basis of our recommendations (separated FP worth in MINERVE oscillations and PIE). These JEFF-3.0 evaluations of ^{149}Sm, ^{143}Nd, ^{133}Cs and Eu isotopes are consistent both with integral and differential measurements. Concerning ^{149}Sm, an increase by 3% of the Γ_n neutron width was introduced for the first resonance. The compilation of the ^{143}Nd measurements with the MINERVE trend led to a JEFF-3.0 thermal value σ_{2200} = 338 b. The new ^{133}Cs evaluation was based mainly on the recent Nakajima (1990) measurements, as shown in Table 7. ^{154}Eu and ^{155}Eu evaluations in JEFF-3 originate from the ENDF/B-VI.7 file, in agreement with PIE results and actual Anufriev differential measurements.

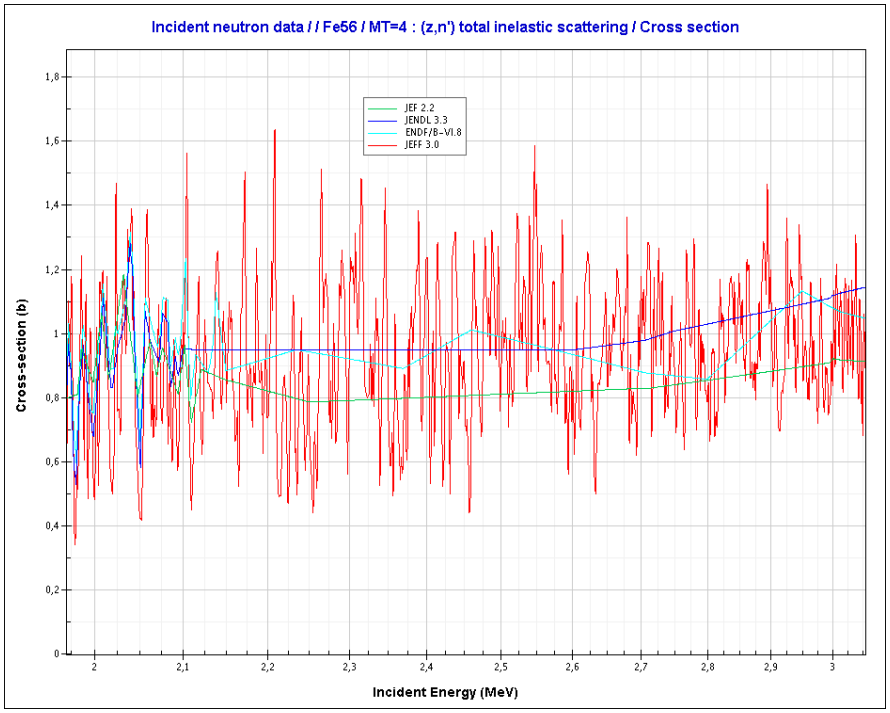
Table 7: Resonance parameters of the ^{133}Cs strong resonance

	Eres. (eV)	Spin	Γtot (meV)	Γn (meV)	Γγ (meV)
JEF-2.2	5.90	3	122.119	7.119	115
JENDL-3.2	5.88	3	130.103	6.103	124
JEFF-3.0	5.86	3	129.562	6.562	123
Nakajima	5.86	3	129.380	6.38 ± 0.26	123 ± 6

Furthermore, improved evaluations were introduced in JEFF-3.0 for important structural materials. The ^{56}Fe evaluation, derived from the previous

European Fusion File EFF-3, is recognised as the best world-wide evaluation because it involves the recent high-resolution Gelina measurements with refined fluctuations described up to 10 MeV; Figure 5 compares the various ^{56}Fe international evaluations, which demonstrates that inelastic cross-section fluctuations above 2 MeV are represented only in JEFF-3.0. This refined representation allows accounting for resonance self-shielding, which is a key point for accurate calculation of steel core reflector (EPR and GEN-IV reactors).

Figure 5: Comparison of the ^{56}Fe inelastic scattering in major evaluations (JEFF-3 in red)



The ^{27}Al evaluation was improved (Leal, 2002) with a more realistic capture cross-section in the thermal range: σ_c^{2200} = 233 mb (to compare with the 231 ± 3 Mughabghab recommendation).

Isotopic evaluations were introduced for Zr isotopes.

The first Fission and Fusion File JEFF-3.0 was released in April 2002 (NEA, 2005) and the general-purpose library contains data for 340 materials from $_1$H^1 to $_{99}$Es^{255}.

JEFF-3.0 was immediately validated against experiments, and CEA feedback quickly suggested that this first version of JEFF-3 could not be used as a reference library for LWR calculations.

- Fuel inventory calculation was clearly improved using JEFF-3.0 as opposed to JEF-2, particularly for correct prediction of ^{235}U depletion, ^{236}U-^{237}Np-^{238}Pu build-up and ^{242}Pu-^{243}Am build-up. This result was demonstrated with SNF chemical analyses from French PWR (Bernard, 2004a) and Takahama (Courcelle, 2004a). Improvement of the fuel depletion calculation was also highlighted for MOX assemblies (Bernard, 2004). Predictions of ^{235}U and ^{237}Np from fuel cuts extracted after four and five irradiation cycles in Dampierre were improved.

  ^{239}Pu build-up, however, remained unsatisfactory (an overestimation by about 4%), as did ^{241}Am and ^{242m}Am build-ups, which respectively remained overpredicted (about +20% EOC) and underpredicted (-20%).

- The reactivity of CEA LWR cores was slightly underestimated (Courcelle, 2002), as were low-enriched uranium (LEU) benchmarks (Marck, 2003) from the ICSBEP International Database. Due to the fact that all major libraries underpredict LEU reactivity (-473, -475 and -338 pcm for JEFF-3.0, ENDF/B-VI.8 and JENDL-3.3 respectively, in average on LEU-COMP-THERM benchmarks) an OECD working group was set up to address this issue (WPEC Subgroup 22) (NEA, 2006a).

From all this integral information (including direct capture rate in EOLE experiments), it was concluded that the ^{238}U evaluation must be improved (Derrien, 2005). Such improvements should include a decrease in the integral resonance by 1.0% ± 0.6% (1σ), and a slight increase in inelastic scattering above 4 MeV. These modifications would correct the K_{eff} underestimation of small cores characterised by large neutron leakage.

The ^{238}U evaluation for JEFF-3.1 was performed in the framework of OECD WPEC Subgroup 22. The evaluation of resonance parameters from 0 to 20 keV (Courcelle, 2005), carried out in close co-operation by the CEA and ORNL, includes the most recent high resolution and transmission data. The effective resonance integral is reduced by 0.4% (mainly due to smaller neutron widths of the lowest s-wave resonances) and the thermal value was adjusted according to the recent Trkov recommendation σ_c^{2200} = 2.683 b. The CEA-BRC evaluation, based on coupled-channel calculations, was adopted for the unresolved resonance range and inelastic scattering (Lopez-Jimenez, 2005). This JEFF-3.1 evaluation enabled an improved prediction of ^{239}Pu formation in LWR spent fuels and an accurate prediction of K_{eff} for LWR-LEU cores (Sublet, 2004).

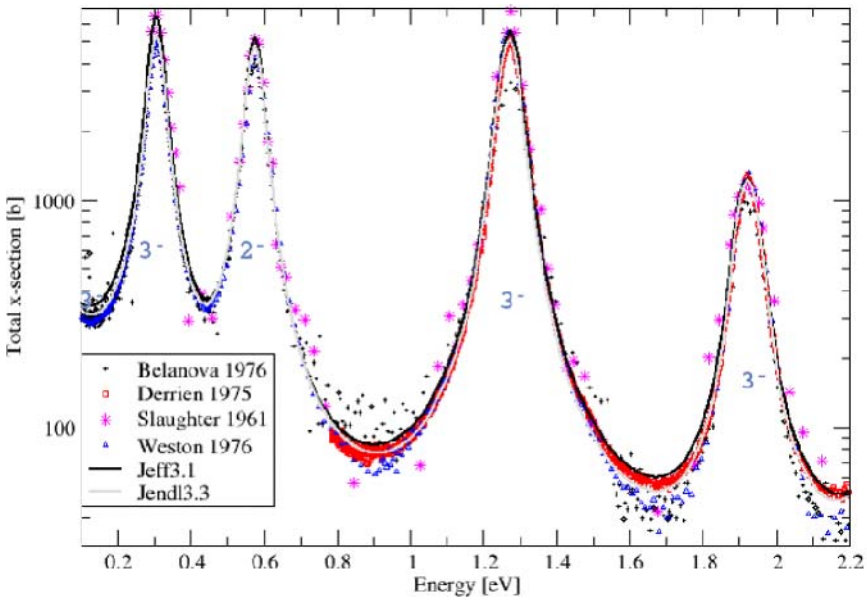
In order to improve Pu ageing calculation and minor actinide inventory prediction, a new ^{241}Am evaluation was proposed for JEFF-3.1 (Bernard, 2004a). From four types of integral information (^{241}Am/^{241}Pu chemical assays, ^{242}Cm and ^{243}Cm at low burn-up, Pu ageing reactivity worth in EOLE MOX cores, irradiation of separated ^{241}Am in the ICARE experiment), the following modifications to the previous evaluation were derived:

- ^{241}Am (n,γ) increased by +15% ± 3% (1σ) in the range 0.01-2 eV;
- branching ratio ^{241}Am → ^{242m}Am increased up to BR = 0.13 ± 0.01.

The new ^{241}Am evaluation (Bouland, 2005) has a thermal value increased by 5% (σ_c^{2200} = 647 b), more consistent with French measurements carried out by Fioni in 2001 (σ_c^{2200} = 696 ± 48 b). The JEFF-3.0 resonance evaluation was mainly

based on Belanova differential measurements. In the JEFF-3.1 evaluation, for the 0.3 eV thermal resonance the Slaughter measurement was also introduced in the SAMMY analysis (which gave a 22% increase in the resonance area), and the Derrien 1975 measurements were used for the next three resonances predominant for the ^{241}Am capture rate (Figure 6).

Figure 6: Comparison of JEFF-3.1 evaluation and measurements for the first resonances of ^{241}Am



Differential and integral experiments (^{242m}Am build-up) and theoretical assumptions (Bernard, 2006d) allowed establishing an accurate branching ratio of ^{242g}Am dependent on neutron energy, as shown in Figure 7.

In order to improve ^{245}Cm and ^{246}Cm build-up, the ^{245}Cm evaluation was changed in JEFF-3.1 with a 3.8% capture increase (σ_c^{2200} = 359 b), in agreement with our recommendation (Bernard, 2004a).

The improvement of two main FP, ^{103}Rh and ^{95}Mo, was introduced in JEFF-3.1. The ^{103}Rh evaluation was performed at the CEA (Dupont, 2005) using the transmission measurements from the IRMM European Centre: compared to JEFF-3.0, the thermal capture and the 1.3 eV resonance integral are respectively lowered by -1.7% and -6.4%, as shown in Figure 8 (in agreement with the reactivity worth of ^{103}Rh measured in MINERVE).

Reactivity worth measurements of Hf rods in EOLE and Hf plates in AZUR zero-power reactors at Cadarache led to the realisation that Hf poisoning worth was overestimated. New JEFF-3.1 evaluations for Hf isotopes were therefore performed (Noguère, 2005) using recent TOF measurements at RPI. These

Figure 7: ^{241}Am to ^{242g}Am branching ratio as a function of energy in JEFF-3.1

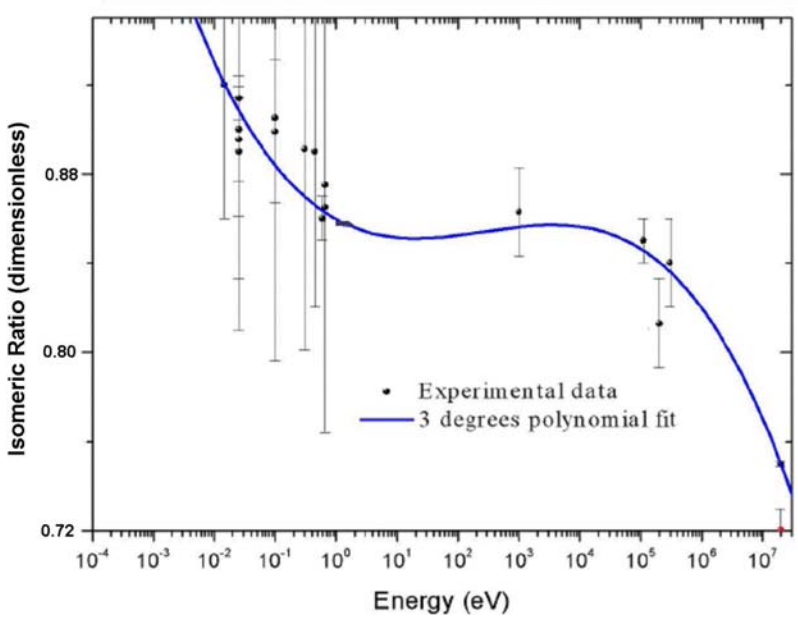
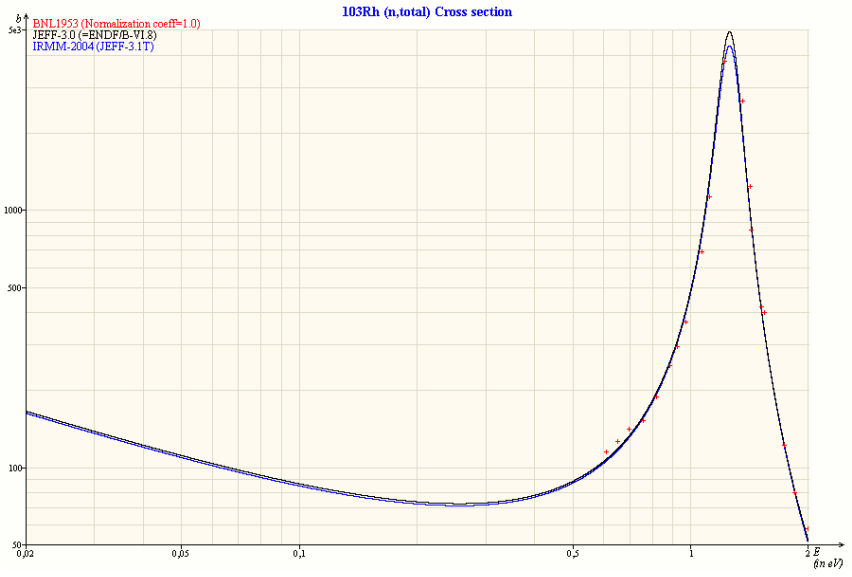


Figure 8: Comparison of ^{103}Rh measured cross-section with JEFF-3.0 and JEFF-3.1 evaluations



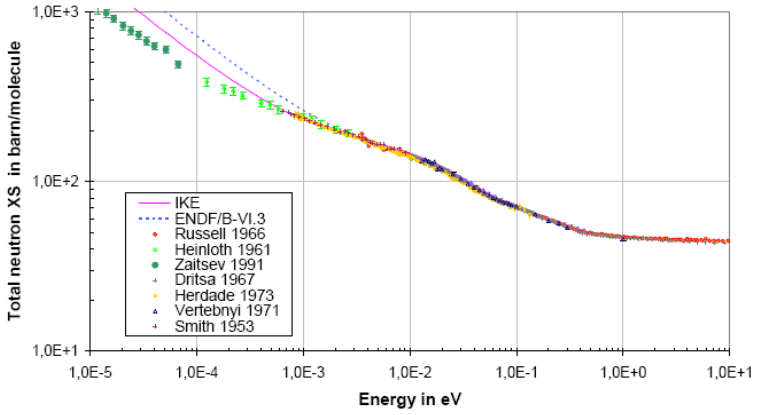
evaluations allow the reduction of the resonance integral of the natural Hf, as shown in Table 8, thanks to ^{178}Hf-^{179}Hf-^{180}Hf and not to the major poisoning isotope ^{177}Hf. The TRIPOLI-4 calculation of Hf absorber worth in EOLE and AZUR experiments is improved by 0.8% compared to the JEFF-3.0-based calculation.

Table 8: Comparison of Hf capture in JEF-2, JEFF-3.0-JENDL-3.3 and the new JEFF-3.1 evaluations

Hf evaluation	JEF-2.2	JEFF-3.0 (JENDL-3.3)	JEFF-3.1
σ_{2200} (barn)	102.7	104.9	104.2
Iγ (barn)	1 989.1	1 993.9	1 968.7

The thermal scattering law library contains nine evaluations. Except ^{9}Be and H in CH_2 (polyethylene) originating from JEFF-3.0, these files are new evaluations. In 2003, work started at IKE for the re-evaluation of S(α,β) for H in H_2O, D in D_2O and H in ZrH_x as a function of temperatures (Trkov, 2004). The improvement includes updating of models and a denser grid for both momentum transfer α and energy transfer β parameters. The evaluated thermal scattering law for water was checked against available experimental measurements of the total and the double differential cross-sections. The improvement due to JEFF-3.1 is observed, particularly at low energies as shown in Figure 9.

Figure 9: Comparison of H_2O measured total cross-section with IKE (JEFF-3.1) and ENDF/B-VI



A strong improvement for delayed neutron data was implemented in JEFF-3.1. Eight groups of precursors are represented (instead of six in previous libraries), allowing the explicit description of the longest-lived precursors, and a unique set of mean lifetimes $\tau_i = 1/\lambda_i$ for any fissile isotope (Spriggs, 2002). Moreover, the delayed neutron fractions β_i were improved, particularly for ^{235}U fissions that give a lower β_{eff}^{UOX} value [in agreement with our JEF-2 analysis of MISTRAL1 measurements which suggested a reduction by -2.4% ± 1.6% (Litaize, 2002)].

The JEFF-3.1 Fission Yields library JEFF-3.1/NFY includes independent and cumulative yields for neutron-induced fission of Th, U, Np, Pu, Am and Cm isotopes. This library is mainly based on the UKFY-3.6 file (Mills, 2004), though some improvements were introduced as a result of CEA feedback on integral experiments (Sérot, 2004). Therefore, the ^{148}Nd yields were improved with a reduction in ^{239}Pu fission yields (^{148}Nd, which should be the reference burn-up indicator, is systematically overestimated in French LWR PIE by 1-2% using JEF-2 yields).

The JEFF-3.1 library was released in May 2005 (NEA, 2006). The library CEA2005-version0 of the new product APOLLO2.8 (Loubière, 1999) was immediately processed from the JEFF-3.1 file. Accurate APOLLO2.8 calculations were performed to validate LWR fuel inventory prediction. The analysis of Gravelines3 chemical assays indicated that actinide concentrations were predicted within experimental uncertainty (except ^{238}Pu and the unimportant ^{246}Cm minor actinide), as shown in Table 9 (Koning, 2008). Compared to JEFF-3.0, new improvements are obtained on ^{235}U depletion, ^{239}Pu formation and ^{241}Am-^{242m}Am build-up.

Table 9: Calculation/experiment comparison of actinide concentration in Gravelines PWR SNF

Gravelines 3 rods: 60 GWd/t ^{235}U 4.5% (w/o)	C/E – 1 (%) JEF-2.2	C/E – 1 (%) JEFF-3.1	Experimental uncertainty (1σ)
^{234}U/^{238}U	1.8	4.3	3.0
^{235}U/^{238}U	4.6	2.1	3.5
^{236}U/^{238}U	-4.2	-0.7	0.6
^{237}Np/^{238}U	-6.5	-1.3	3.2
^{238}Pu/^{238}U	-10.2	-9.0	3.7
^{239}Pu/^{238}U	1.4	0.4	1.3
^{240}Pu/^{238}U	-0.7	0.4	1.1
^{241}Pu/^{238}U	-2.3	-3.0	1.6
^{242}Pu/^{238}U	-8.6	-3.1	2.8
^{241}Am/^{238}U (EOC)	5.8	0.1	5.0
^{242M}Am/^{238}U	-21.6	2.3	7.1
^{243}Am/^{238}U	-8.7	-2.4	4.4
^{244}Cm/^{238}U	-11.7	-5.8	5.9
^{245}Cm/^{238}U	-17.8	-17.9	7.0
^{246}Cm/^{238}U	-29.2	-32.2	9.6
^{247}Cm/^{238}U	-16.0	-1.3	11.7
^{143}Nd/^{238}U	1.4	-0.7	1.0
^{144}Nd/^{238}U	-2.1	-0.5	2.3
^{145}Nd/^{238}U	-0.4	-0.4	1.1
^{146}Nd/^{238}U	0.9	1.3	1.8
^{148}Nd/^{238}U	1.5	1.4	1.5
^{150}Nd/^{238}U	0.7	0.7	1.8

The validation of critical systems was carried out with Monte Carlo continuous-energy calculations [TRIPOLI-4 (Hugot, 2008) and MCNP]. The homogeneous cores with regular LWR lattices in EOLE experiments were calculated with both APOLLO2 2D (Bernard, 2005) and TRIPOLI-4 (Litaize, 2006). Both buckling B_m^2 and critical K_{eff} measurements enhanced the following conclusions:

- For UOX cores the reactivity is perfectly predicted $\Delta K_{eff} = +120 \pm 150$ pcm (it was overestimated by +300 pcm using JEF-2 and underestimated by -150 pcm using JEFF-3.0).
- For MOX cores (MISTRAL2, MISTRAL3), K_{eff} overestimation is still observed. Compared to JEF-2 the reactivity is slightly increased using JEFF-3.1 due to positive components (^{238}U = 200 pcm, ^{239}Pu = 140 pcm, ^{240}Pu = 160 pcm, H_2O = 150 pcm), which are not exactly compensated by negative components (^{241}Pu = -180 pcm, ^{241}Am = -300 pcm, Zr = -80pcm). Concerning mixed-loading cores, MH1.2 is reasonably predicted using JEFF-3.1: $\Delta K_{eff} = +280 \pm 200$ pcm.
- These K_{eff} results were confirmed by the TRIPOLI-4/JEFF-3.1 analysis of some ICSBEP benchmarks data (Sublet, 2005). The MCNP-4C3 calculation by the NRG team of the main ICSBEP benchmarks gave consistent results and enhanced the correct K_{eff} value obtained for LEU-COMP-THERM LWR-type benchmarks (Marck, 2005): Figures 10 and 11 show that the criticality of CEA Valduc experiments (LCT 07 and 39) are more accurately predicted using JEFF-3.1.
- MCNP-JEFF-3.1 calculations of highly-enriched uranium also highlighted satisfactory results for fast and intermediate spectra, with a slight improvement compared to JEFF-3.0 (Figure 12).

Figure 10: JEFF-3 calculation results of LEU-COMP-THERM benchmarks

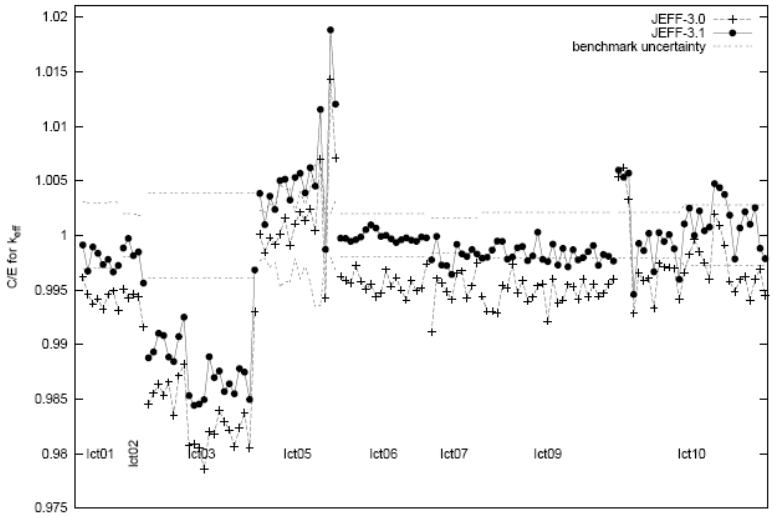


Figure 11: JEFF-3 calculation results of LEU-COMP-THERM benchmarks

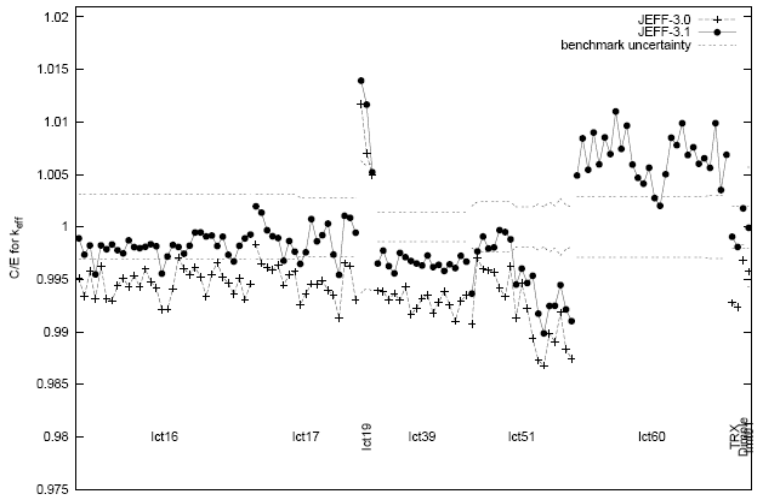
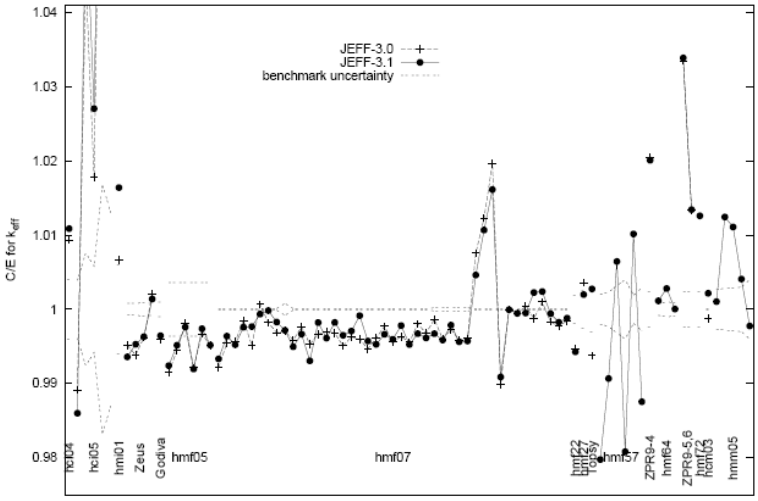


Figure 12: JEFF-3 calculation of HEU benchmarks with a fast or intermediate spectrum



The K_{eff} validation for FBR was performed using MASURCA critical experiments (Tommasi, 2006). The calculation/experiment comparison using either JEF-2 or JEFF-3.1 is summarised in Table 10. The MASURCA 1B result confirmed the improvement in uranium fast systems linked to JEFF-3.1, with a reactivity which is no longer overestimated. Concerning MOX cores ZONA2 and MUSE, the reactivity is reasonably predicted.

Table 10: C/E bias (in pcm) on various MASURCA FBR cores

Core	1B	1A′	ZONA 2A	ZONA 2B	MUSE-4
Fuel Mod/coolant Reflector	U Graphite U_{app} metal	Pu Graphite U_{app} metal	UO_2-PuO_2 Sodium Fertile blanket	UO_2-PuO_2 Sodium Na/SS	UO_2-PuO_2 Sodium Na/SS
JEF-2.2	+512	+165	-384	-104	-200
JEFF-3.0	-407	+107	-41		
JEFF-3.1	-80	+478	+387	-167	-182

The ERANOS2 (Ruggiéri, 2006) analysis of PROFIL and PROFIL-2, which are irradiation experiments of separated isotopes in the PHENIX FBR reactor (Tommasi, 2008), has demonstrated that JEFF-3.1 (n,γ) cross-sections are satisfactory for major actinides, except for ^{241}Pu capture which is overestimated by 8%.

Chapter 4: New evaluations for JEFF-3.1.1

The validation results of JEFF-3.1, summarised previously, have shown that ^{238}Pu build-up was inaccurately predicted, as was LWR-MOX reactivity. Improved evaluations were thus recommended for ^{237}Np (Bernard, 2006b) and ^{239}Pu (Bernard, 2006c). The JEFF Group approved this recommendation, and these evaluations were processed and implemented in Version 2 of the CEA2005 library.

However, the K_{eff} calculation of the fresh core of large French PWRs pointed out that K_{∞} of actual LWR-UO_2 lattices was slightly underestimated. Improved evaluations of ^{16}O and ^{91,96}Zr were therefore carried out in agreement with recent differential measurements (Bernard, 2007). These evaluations were included in the new version CEA2005v3 of the APOLLO2.8 library.

Furthermore, PWR and BWR cycle follow-up performed by CEA (Douce, 2008) and Areva-NP (German, French and US calculations of domestic LWRs) highlighted a slight overestimation trend for reactivity loss with fuel burn-up, which is consistent with SNF oscillation results in MINERVE (Bernard, 2006a). To correct this trend, seven improved FP evaluations were proposed for inclusion in the new file: JEFF-3.1.1. The full list of updates is provided in Table 11, and Table 12 displays an additional list of corrected evaluations which include smaller modifications.

Table 11. Updated isotopes in JEFF-3.1.1

Isotope	Documentation	Modifications
^{237}Np	JEFDOC1144/1174	JEFF-3.0
^{239}Pu	JEFDOC1158	New MF1(MT456) & MF2(MT18,102)
^{16}O	JEFDOC1207/1226	New (MT800)
^{91}Zr	JEFDOC1208/1226	New (MT102)
^{96}Zr	JEFDOC1208/1226	New (MT102)
^{93}Zr	JEFDOC1238	New (MT102)
^{99}Tc	JEFDOC1238	New (MT102)
^{103}Ru	JEFDOC1238	New (MT102)
^{135}Cs	JEFDOC1238	New (MT102)
^{147}Pm	JEFDOC1238	New (MT102)
^{148g}Pm	JEFDOC1238	New (MT102)
^{154}Eu	JEFDOC1238	New (MT102)

Table 12. Corrected evaluations in JEFF-3.1.1

Isotope	Modifications
^{52}Cr	MF4(MT2)
^{35}Cl	NK(MF12)=NK(MF13)
^{191,193}Ir	NK(MF14)=NK(MF12&13)
^{127,129}I	Modif MF6(MT5)
^{103}Rh	Modif MF6(MT5)
^{233}U	$\lambda_{i=4}$*10
^{46}Ca	MF3(MT1)=0<1keV
^{56}Fe	Neut. Inelastic thresh. MF12
^{95}Mo	$P_{Legendre}$ description

4.1 ^{237}Np evaluation

The recent JENDL-3.3 evaluation has been introduced with a new ^{237}Np evaluation in JEFF-3.1. However, this evaluation was based on a recent Japanese thermal cross-section measurement carried out using a challenging activation technique. To the contrary of the previous JEFF-3.0 evaluation, this JEFF-3.1 evaluation led to inaccurate prediction of ^{238}Pu build-up in LWR spent fuel:

^{236}U/^{238}U: (C-E)/E = -1% ± 1%
^{237}Np/^{238}U: (C-E)/E = -1% ± 3%
^{238}Pu/^{238}U: (C-E)/E = -8% ± 3%

Since ^{237}Np content is well predicted, these chemical analysis results demonstrated that ^{238}Pu underestimation at low burn-ups is due to ^{237}Np capture cross-section.

This conclusion was confirmed by the ^{237}Np reactivity worth measurement in the OSMOSE experiment (Bernard, 2006): compared to the JEFF-3.0 calculation, the ^{237}Np reactivity worth was degraded by -5% using the new JEFF-3.1 evaluation. It was concluded that this ^{237}Np worth underestimation was due to an inadequate capture value:

JEFF-3.1: σ_{2200} = 162 b
JEF-2.2: σ_{2200} = 181 b
Mughabghab: σ_{2200} = 176 b ± 3 b
Mini-Inca: σ_{2200} = 180 b ± 5 b

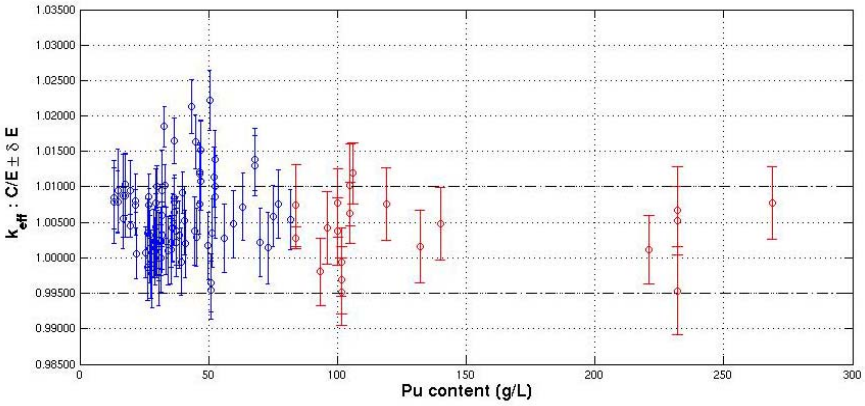
The 10% underestimation of JEFF-3.1 ^{237}Np(n,γ) cross-section seems to be due to incorrect values of gamma peak intensities inferred by the pandemonium effect of the ^{238}Np nucleus. Indeed, this underestimation was confirmed by the 2003 measurement in the Mini-Inca experiment at the Institute Laue-Langevin (Dupont, 2006). Hence, adoption of the Derrien evaluation was recommended for the final JEFF-3.1.1 file.

4.2 ^{239}Pu evaluation

The analysis of the K_{eff} multiplication factor of 100% MOX cores and plutonium solutions showed a systematic discrepancy between JEFF-3.1 calculation and experiment (Marck, 2005). A systematic overestimation of K_{eff} values, using Monte Carlo reference calculations, was observed in the analysis of critical experiments.

Plutonium-solution-thermal (PST) benchmarks of the ICSBEP database showed a systematic overestimation from +200 to +1 200 pcm as a function of the ^{239}Pu concentration (see Figure 13). As ^{239}Pu concentration infers a strong neutron spectrum hardening, the average overestimation by about +700 pcm ± 200 pcm in the low ^{239}Pu concentration range (C_{Pu} < 80 g/L) indicates that the $\eta = \nu.\sigma_f/\sigma_a$ value should be revised in the subthermal neutron range.

Figure 13: MCNP-JEFF-3.1 analysis of critical Pu solutions



Critical LWR-MOX lattices in the EOLE facility were investigated during the MISTRAL and BASALA experimental programmes (Vaglio-Gaudard, 2006, 2007). In addition to the poorly predicted plutonium ageing, TRIPOLI-4-JEFF-3.1 calculations indicated a K_{eff} overestimation of about +300 pcm for various moderation ratios or void fractions (Table 13).

Table 13: TRIPOLI-4-JEFF-3.1 analysis of EOLE 100% MOX cores

EOLE mock-up	Pu ageing	Mod ratio or void	(C-E) ± δE (pcm)
MH1.2 (PWR-MOX mixed core)	4 years	V_{H2O}/V_{MOX}=1.2	280 ± 250
MISTRAL-2 (PWR-MOX)	8 years	V_{H2O}/V_{MOX} =1.7	630 ± 250
MISTRAL-3 (PWR-MOX)	10 years	V_{H2O}/V_{MOX} =2.1	710 ± 250
BASALA-Hot (BWR-MOX)	12 years	42% void	610 ± 250
BASALA-Cold (BWR-MOX)	13 years	0% void	700 ± 250
FUBILA-Hot (BWR-MOX)	1 year	0% void	250 ± 250

Moreover, EOLE measurements of the isothermal temperature coefficient for MOX lattices were performed at room temperature (20-80°C in MISTRAL2 and MISTRAL3) and under hot operation conditions (from 20°C up to 300°C in the CREOLE experiment). The calculation of these experiments using both JEF-2.2 and JEFF-3.1 libraries pointed out (Erradi, 2003):

- a systematic underestimation of the MTC under cold conditions by (-2.0 ± 0.3) pcm/°C;
- a well-assessed MTC under hot conditions (+1.0 ± 2.0)pcm/°C.

Sensitivity analysis of physical phenomena has shown that the negative error in the low temperature range is linked to the thermal spectrum shift effect, which is strongly dependent on the subthermal and thermal shapes of ^{239}Pu capture and fission cross-sections.

Therefore, an improved ^{239}Pu evaluation was undertaken (Bernard, 2008a), which accounts for the observed integral experiment trends. The comparison of this evaluation to previous JEFF-3.1 and to experimental data is plotted in Figures 14 and 15 respectively for (n,γ) and (n,f) cross-sections in the thermal range.

These cross-section modifications were not sufficient to explain the K_{eff} overestimation of Pu system calculation. Indeed, ν_p needed to be revised, and a phenomenological formalism was applied up to 20 eV. The comparison of measured prompt multiplicity both to JEFF-3.1 and to our evaluation (plotted in red) in Figure 16 demonstrates that our proposal adopted in JEFF-3.1.1 is more consistent with Gwin differential measurements, particularly on the thermal wing of the large E_R = 0.3 eV resonance.

Figure 14: Experimental, JEFF-3.1 and JEFF-3.1.1 ^{239}Pu capture cross-section

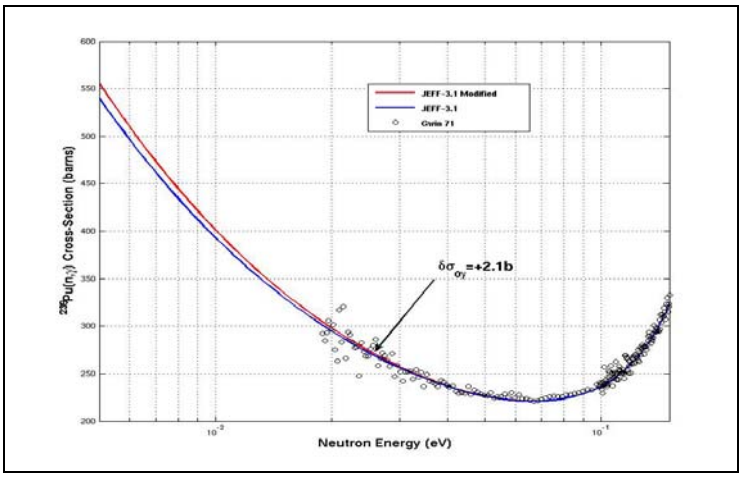


Figure 15: Experimental, JEFF-3.1 and JEFF-3.1.1 ^{239}Pu fission cross-section

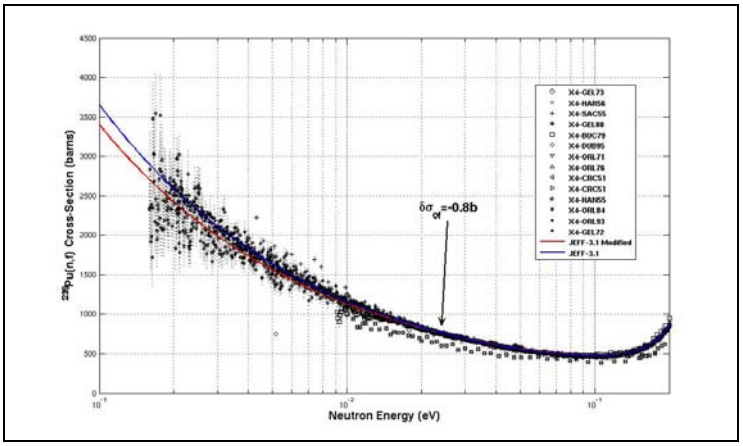
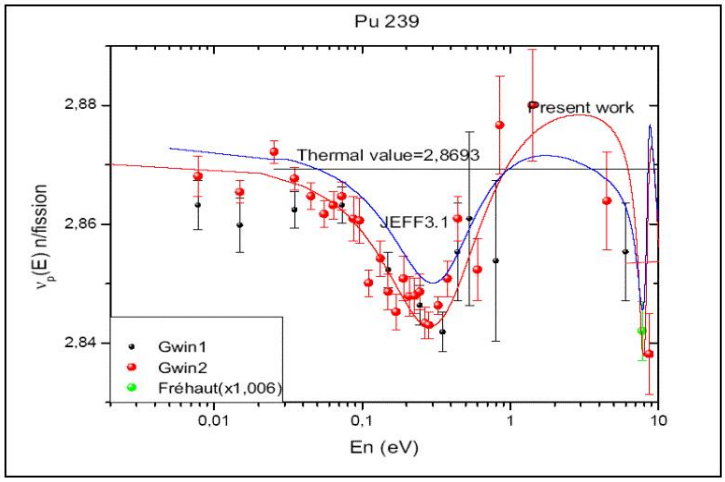


Figure 16: Comparison of measured ν_p multiplicity with JEFF-3.1 and JEFF-3.1.1 evaluations



This new ^{239}Pu evaluation allowed the following improvements:

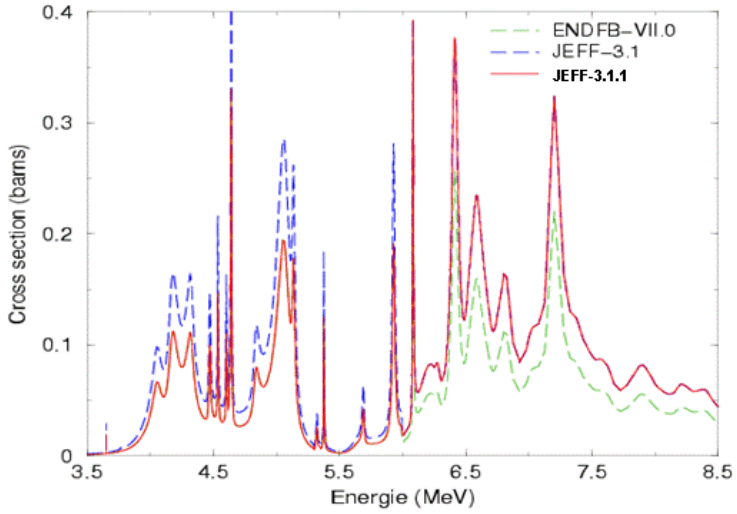
- K_{eff} MOX decreased by -150 pcm;
- K_{eff} of Pu solutions decreased by about -400 pcm;
- the MOX reactivity temperature coefficient prediction improved by 0.3 pcm/°C.

4.3 ^{16}O evaluation

In 2005, Harrisopoulos, *et al.* performed new measurements on $^{13}C(\alpha,n)^{16}O$. The velocity of the incident α particle increased from 0.8 MeV to 8.0 MeV due to the analysis of the inverse reaction $^{16}O(n,\alpha)$. In 2007, Giorginnis performed a direct measurement of $^{16}O(n,\alpha_0)$ at GELINA (IRMM) and confirmed the Harrisopoulous values below 6 MeV. These two differential measurements underline the need to decrease the JEFF-3.1 cross-section by about 30% (see Figure 17) (Noguère, 2007). Moreover, the validation of helium release in Al_2O_3 pins loaded in PWR seems to highlight the great improvement linked to this new JEFF-3.1.1 evaluation.

The K_∞ calculated value then increases by 100 pcm for LWR up to 120 pcm for FBR composed with UO_2 or MOX fuels (Bernard, 2007).

Figure 17: ^{16}O(n,α) cross-section in JEFF-3.1.1

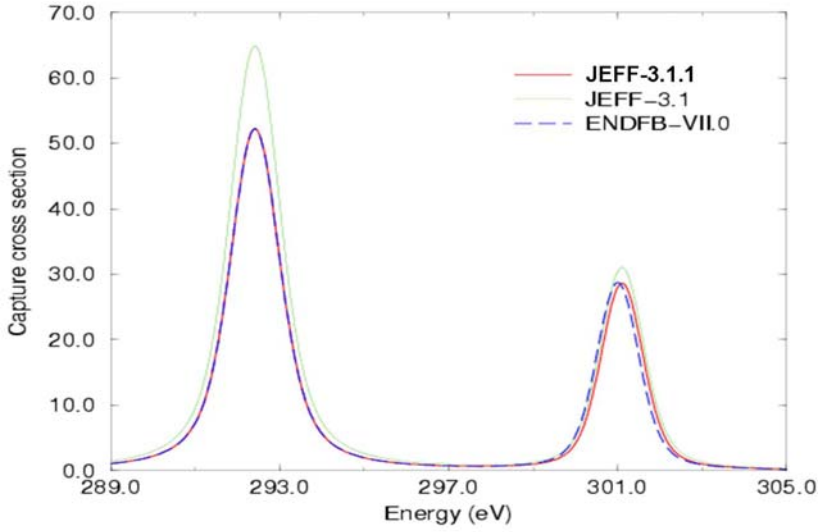


4.4 Zr evaluations

In the Segrè diagram, zirconium isotopes are located near the neutron magic line N=50. Thus, the complete neutron shell of such nuclides implies very small neutron capture cross-sections: 141 mb (^{90}Zr, abundance 51.45%), 6.9 b (^{91}Zr, ab. 11.22%), 621 mb (^{92}Zr, ab. 17.15%), 260 mb (^{94}Zr, ab. 17.38%) and 5.8 b (^{96}Zr, ab. 2.80%) for natural zirconia in the thermal range. The JEFF-3.1 thermal and resonance integral values for natural Zr are out of uncertainty bands as pertains to the BNL recommended values. This capture overestimation is mainly due to the huge increase in the 292.41 eV resonance capture of ^{91}Zr from JEF-2.2 ($J = 2$; $\Gamma_\gamma = 0.1$ meV) to JEFF-3.1 ($J = 3$, $\Gamma_\gamma = 0.17$ meV) (Bernard, 2007). Due to the large amount of Zr in LWRs (zircaloy fuel cladding) the absorption of Zr isotopes amounts to 600 pcm in a typical PWR K_{eff} neutron balance.

Natural zirconium differential measurements were performed at the RPI laboratory (see Figure 18). The results of this experiment are the basis for the new JEFF-3.1.1 evaluations for ^{91}Zr and ^{96}Zr (Noguère, 2007a). The reduction of capture integral values by about 10% leads to an increase in the multiplication factor by 50 pcm for PWR up to 100 pcm for BWR.

Figure 18: ^{Nat}Zr(n,γ) cross-section in JEFF-3.1.1



4.5 FP evaluations

Seven fission product cross-sections were revisited (Bernard, 2008) to account for feedback from SNF oscillations (Douce, 2008; Leconte, 2007) and recent OECD/WPEC Subgroup23 work (NEA, 2009). Thus, ^{93}Zr, ^{103}Ru (Figure 19), ^{135}Cs, ^{148g}Pm and ^{154}Eu (Figure 20) evaluations were adopted from WPEC SG23. The JEFF-3.1 evaluation of the poisoning isotope ^{147}Pm was found satisfactory in the FBR spectrum, but was slightly modified in the thermal range.

The ^{99}Tc evaluation was improved in agreement with its reactivity worth measurement in MINERVE and the new thermal capture value of 21 b proposed by Weil (2008). Moreover, the neutron width of the first 5.58 eV resonance was reduced within its 1σ uncertainty margin (see Figure 21).

The bulk poisoning worth of a fission product is sensitive first to its fission yield, lifetime and neutron capture cross-section, and secondly to its mother by activation or radioactive decay. Then, each fission product induces different reactivity worth components at beginning of cycle and during reactor cycle length. The contribution of each new FP evaluation in the JEFF-3.1.1 file on the modification of K_{eff} ($\delta Keff_{BOC}$) and reactivity swing ($\delta\Delta\rho_{cycle}$) is summarised in the table below (PWR Bu_{BOC} = 20 GWd/t, Bu_{EOC} = 35 GWd/t):

FP evaluation	$\delta Keff_{BOC}$	$\delta\Delta\rho_{cycle}$
^{103}Ru	15 pcm	15 pcm
^{99}Tc	6 pcm	3 pcm
^{148g}Pm	90 pcm	85 pcm
^{93}Zr	21 pcm	11 pcm
^{147}Pm	4 pcm	2 pcm
^{154}Eu	18 pcm	11 pcm
^{135}Cs	6 pcm	3 pcm
Total	+160 pcm	+130 pcm

Therefore, new FP evaluations in the JEFF-3.1.1 library increase the BOC activity by about 160 pcm and the reactivity swing for LWR equilibrium cycle by about 130 pcm, in agreement with the experimental information from PWR and BWR cycle follow-up.

Figure 19: ^{103}Ru(n,γ) ($T_{1/2}$ = 39 d) cross-section in JEF(F)-2.2/3.1.0 and WPEC23

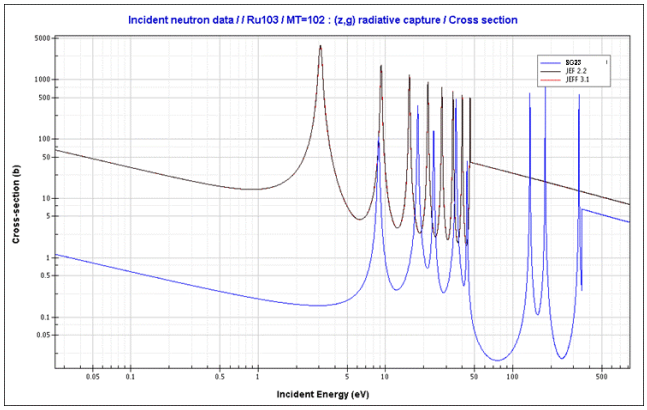


Figure 20: ^{154}Eu(n,γ) ($T_{1/2}$ = 8.6 y) cross-section in JEF(F)-2.2/3.1.0 and WPEC23

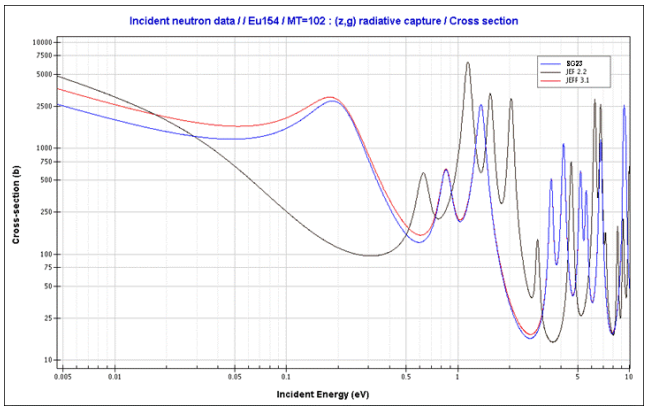
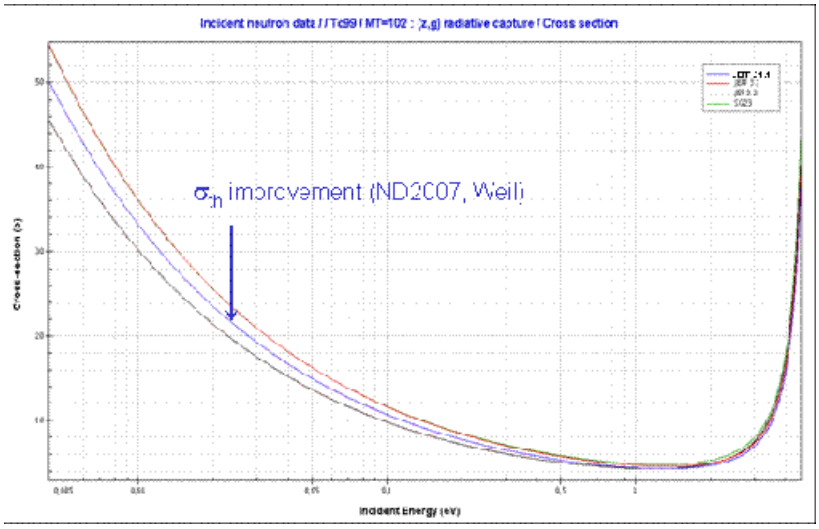
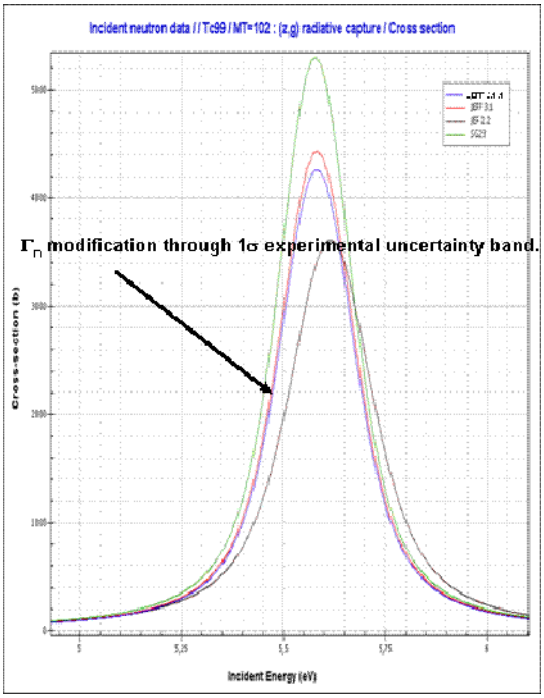


Figure 21: ^{99}Tc(n,γ) ($T_{1/2}$ = 2.1^{E5} y) cross-section in JEF(F)-2.2/3.1.0/3.1.1





Chapter 5: The recommended CEA2005v4 library for APOLLO2.8

The processing of these JEFF-3.1.1 evaluations, added to JEFF-3.1 evaluations for other isotopes, results in the recommended library CEA2005V4.1.1 for APOLLO2.8.

A slight modification has been undertaken on the ^{235}U and ^{239}Pu incident neutron fission yields files in order to account for the PIE interpretation (^{103}Rh and ^{109}Ag build-up overestimations with JEFF-3.1 files). Thus, four independent fission yields are modified within their 1σ uncertainty:

$^{235}U \rightarrow {}^{103}Nb$	From 1.7781E-2 to 1.7021E-2 (back to JEF-2.2 value)
$^{235}U \rightarrow {}^{88}Kr$	From 1.6512E-2 to 1.7272E-2 (to keep fission yields normalised)
$^{239}Pu \rightarrow {}^{109}Rh$	From 2.3799E-3 to 0.3339E-3 (back to JEF-2.2 value)
$^{239}Pu \rightarrow {}^{142}Ba$	From 3.0401E-2 to 3.2447E-2 (to keep fission yields normalised)

The processing tool GALILEE.V0 (Coste-Delclaux, 2008) includes the NJOY-259 (Macfarlane, 2000) code for the resolved resonance range (RRR) and the CALENDF-2005 (Sublet, 2006) code for the unresolved resonance region (URR). It allows performing "natural isotopes" such as ZRNAT using a validated mutual shielding approach with an isotopic probability table formalism. Energies released by fission are taken directly from ENDF files. The CEA2005.G281.V4.1.DIRECT binary file (Mengelle, 2008) includes 427 isotopes, mainly from JEFF-3.1 evaluations as shown in Table 14. Probability tables for mutual shielding are included in a second binary file CEA2005.V4.1.UNIVSH.TP.

The recommended depletion chain, using the JEFF-3.1.1 Decay Data (File 8) (Kellet, 2007), involves 160 nuclides (Mengelle, 2008a). The adoption of such a detailed FP chain enables avoiding the utilisation of the approximate collapsed pseudo-FP method. The validation of this FP chain against a full 683 depletion chain (up to 60 GWj/t for LWR and FBR) allowed establishing that 99.9% of the total FP poisoning is accounted for by this CEA2005v4 chain. Furthermore, this chain accounts for poisoning kinetics (^{135}I for instance) and long cooling time (^{151}Eu build-up).

Moreover, the JEFF-3.1.1/DD library improves the previous JEFF-3.1 file mainly based on NUBASE (Audi, 2003) by taking into account the total absorption gamma-ray spectrometry measurements (Greenwood, 1997) of several fission products. Therefore, β and γ decay heat are now consistently predicted with measured values for ^{235}U and ^{239}Pu fission pulse (Huynh, 2007), as well as ^{238}U and ^{241}Pu fission pulse (Mills, 2007). For longer cooling times (two to six years in PWR assembly calorimetric measurements), the decay heat is calculated to within 5% accuracy (Mills, 2007).

The JEFF-3.1.1/GP/^{241}Am neutron file proposes a smoothed energy-dependent isomeric ratio: ^{241}Am(n,γ)$^{242g/m}$Am. In order to account for the incident neutron energy dependence, a new "procedure" called FACTEUR_BRANCHEMENT_S was achieved in APOLLO2. Figure 22 shows the optimised americium chain (the ^{242g}Am isotope is not described).

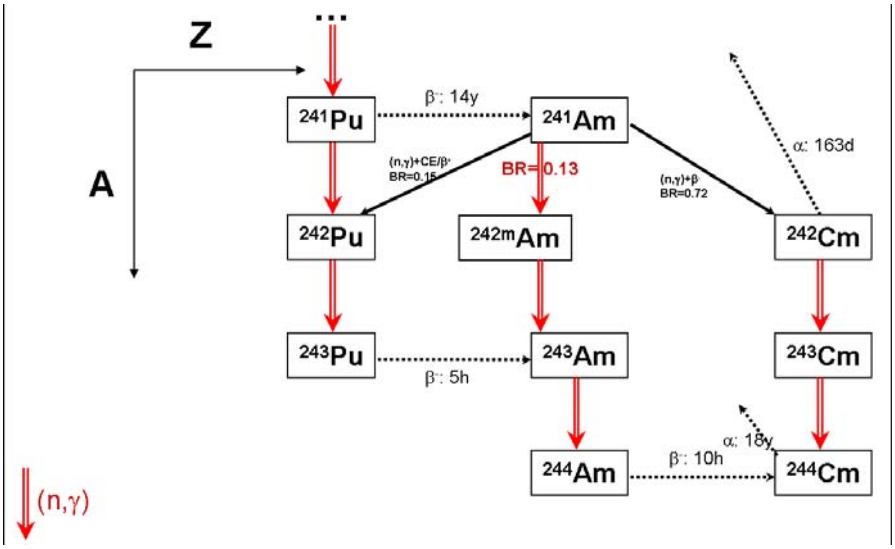
Table 14: CEA2005.V4.1 library content

ABS1SV	Ca40_CaH2	***CM244***	ES253	H2_D2O	**KR84**	*NI58*	***PU236***	SB126	**SR88**	***U234***
AC225	*CA42*	***CM245***	ES254	H2O	**KR85**	NI59	PU237	SC45	SR89	***U235***
AC226	Ca42_CaH2	***CM246***	ES255	**H3**	**KR86**	*NI60*	***PU238***	SE74	**SR90**	***U236***
AC227	*CA43*	***CM247***	***EU151***	**HE3**	LA138	*NI61*	***PU239***	SE76	*TA181*	***U237***
AG107	Ca43_CaH2	***CM248***	*EU152*	HE4	***LA139***	*NI62*	***PU240***	SE77	TA182	***U238***
AG109	*CA44*	CM249	EU152M	*HF174*	**LA140**	*NI64*	***PU241***	SE78	***TB159***	VNAT
AG110M	Ca44_CaH2	CM250	***EU153***	*HF176*	**LI6**	NP235	***PU242***	**SE79**	**TB160**	*W182*
AG111	*CA48*	CNAT	***EU154***	*HF177*	LI7	NP236	PU243	SE80	***TC99***	*W183*
AL27	Ca48_CaH2	CO58	***EU155***	*HF178*	*LU175*	***NP237***	PU244	SE82	TE120	*W184*
AM241	CAH2	CO59	**EU156**	*HF179*	*LU176*	***NP238***	PU246	*SI28*	TE122	*W186*
AM242	*CANAT*	CO60	**EU157**	*HF180*	*MG24*	***NP239***	RA223	*SI29*	TE123	XE124
AM242M	*CD106*	*CR50*	*F19*	*HFNAT*	*MG25*	***O16***	RA224	*SI30*	TE124	XE126
AM243	CD108	*CR52*	*FE54*	HG196	*MG26*	O16_TH2O	RA225	*SINAT*	**TE125**	*XE128*
AM244	***CD110***	*CR53*	*FE56*	HG198	*MGNAT*	**O17**	RA226	SM144	TE126	*XE129*
AM244M	***CD111***	*CR54*	*FE57*	HG199	*MN55*	OSNAT	**RB85**	***SM147***	**TE127M**	***XE130***
AR36	***CD112***	**CS133**	*FE58*	HG200	***MO100***	*P31*	RB86	**SM148**	**TE128**	***XE131***
AR38	***CD113***	***CS134***	*FENAT*	HG201	*MO92*	*PA231*	**RB87**	***SM149***	**TE129M**	***XE132***
AR40	***CD114***	***CS135***	FM255	HG202	*MO94*	PA232	*RE185*	***SM150***	**TE130**	**XE133**
AS75	CD115M	***CS136***	GANAT	HG204	***MO95***	*PA233*	*RE187*	***SM151***	**TE131M**	**XE134**
AU197	*CD116*	***CS137***	*GD152*	***HO165***	***MO96***	*PB204*	***RH103***	***SM152***	TE132	**XE135**
B10	***CE140***	*CU63*	GD153	***I127***	***MO97***	*PB206*	**RH105**	**SM153**	TH227	**XE136**
B11	***CE141***	*CU65*	***GD154***	I128	***MO98***	*PB207*	**RU100**	***SM154***	TH228	**YB9**
BA130	***CE142***	D2O	***GD155***	***I129***	***MO99***	*PB208*	***RU101***	*SN112*	TH229	Y90
BA132	CE143	DIF	***GD156***	I130	*MONAT*	PD102	***RU102***	*SN114*	*TH230*	Y91
BA134	***CE144***	***DY160***	***GD157***	**I131**	N14	**PD104**	***RU103***	*SN115*	*TH232*	YB170
BA135	*CF249*	***DY161***	***GD158***	**I135**	N15	***PD105***	***RU104***	*SN116*	TH233	YB171
BA136	*CF250*	***DY162***	***GD160***	IN113	NA22	***PD106***	**RU105**	*SN117*	TH234	*ZN64*
BA137	*CF251*	***DY163***	GE70	***IN115***	*NA23*	***PD107***	**RU106**	*SN118*	*TI46*	ZR_ZRH
BA138	*CF252*	***DY164***	GE72	*IR191*	*NB93*	***PD108***	RU96	*SN119*	*TI47*	*ZR90*
BA140	CF253	**DY165**	GE73	*IR193*	NB94	**PD110**	RU98	*SN120*	*TI48*	***ZR91***
BE9	CF254	*ER162*	GE74	*IRNAT*	***NB95***	***PM147***	RU99	*SN122*	*TI49*	***ZR92***
BI209	CH2	*ER164*	GE76	*K39*	**ND142**	**PM148**	*S32*	SN123	*TI50*	***ZR93***
BK247	*CL35*	***ER166***	GRAPH	*K40*	***ND143***	***PM148M***	*S33*	*SN124*	*TINAT*	***ZR94***
BK249	*CL37*	*ER167*	H_ZrH	*K41*	**ND144**	**PM149**	*S34*	SN125	TLNAT	***ZR95***
BK250	*CLNAT*	*ER168*	H1	*KNAT*	***ND145***	**PM151**	*S36*	SN126	TM169	***ZR96***
BR79	CM240	ER169	H1_CAH2	KR78	***ND146***	**PR141**	**SB121**	SNAT	TM170	ZRH
BR81	CM241	*ER170*	H1_CH2	KR80	***ND147***	PR142	**SB123**	SR84	TM171	*ZRNAT*
C_TCH2	***CM242***	ER171	H1_H2O	KR82	***ND148***	**PR143**	SB124	SR86	***U232***	
CA40	***CM243***	ER172	H2	***KR83***	***ND150***	PTNAT	**SB125**	SR87	***U233***	

JEF-2.2	EAF-03	JEFF-3.0	ENDF/B-VI.r4	JEFF-3.1	JEFF-3.1 corrected errors	JEFF-3.1.1 new evaluations

ISOTope with self-shielding data
ISOTope NOT present in the standard depletion chain
ISOTope present in the standard depletion chain

Figure 22: Americium standard depletion chain



Chapter 6: Validation of JEFF-3.1.1 and CEA2005v4

The precise validation of JEFF-3.1.1 was carried out using reference calculations:

- TRIPOLI-4 continuous-energy Monte Carlo for fissile solutions, LWR mock-up experiments and fresh PWR cores;
- APOLLO2.8 accurate calculations (Santamarina, 2008) [2-D heterogeneous MOC (Santandrea, 2005) and SHEM refined mesh (Hfaiedh, 2005)] for PIE and SNF reactivity worth.

6.1 K_{eff} of fresh UO_2 core

In order to validate the JEFF-3.1.1 calculation of UO_2 lattice reactivity, the LWR-type regular cores investigated in EOLE were analysed: EPICURE-UH1.2 and MISTRAL1 cores. These experiments utilise PWR-type fuel pins (3.7% ^{235}U-enriched) arranged respectively in 1.26 and 1.32 cm square pitch. The criticality of these cores is obtained through critical soluble boron concentration. The TRIPOLI-4/ experiment comparison is shown in Table 15. The slight overestimation of the K_{eff} in these EOLE cores is not confirmed by the average C/E obtained in the analysis of about 100 LEU cores from the Handbook of International Criticality Safety Benchmark Experiments (ICSBEP). Moreover, Table 15 indicates that the K_{eff} is also well predicted for the first core of the French N4 PWR reactor under hot conditions.

Table 15: Calculation/experiment comparison on the K_{eff} of EOLE UO_2 regular cores

Experiment	Square pitch	V_{H2O}/V_{UOX}	$K_{eff}^{AP2} - K_{eff}^{exp}$	1σ*
UH1.2	1.26 cm	1.3	+250 pcm	180 pcm
MISTRAL1	1.32 cm	1.7	+180 pcm	150 pcm
LEU-Comp-Therm	100 critical configurations		-60 pcm	100 pcm
N4: PWR-1450MWe	1.26 cm	2.0 (Hot)	+160 pcm	300 pcm

* Experimental uncertainty including residual core reactivity, boron concentration and technological uncertainties.

6.2 K_{eff} of Pu solutions and MOX cores

We analysed the various 100% MOX experiments performed in EOLE since 1993, using the same MOX 7%Pu fuel pins: these successive MH1.2, MISTRAL2 and MISTRAL3 experiments were carried out respectively in 1993, 1997 and 1999.

The material buckling B_m^2 of the regular lattice was measured in each core. The APOLLO2.8/experiment comparison presented in Table 16 points out a slight K_{eff} overprediction, which increases with Pu ageing.

Table 16: Calculation/experiment comparison of MOX lattice reactivity (B_m^2 measurement)

Experiment	Square pitch	V_{H2O}/V_{MOX}	$K_{eff}^{AP2} - 1$	1σ*
MH1.2	1.26 cm	1.3	-102 pcm	350 pcm
MISTRAL2	1.32 cm	1.7	+302 pcm	330 pcm
MISTRAL3	1.39 cm	2.1	+536 pcm	300 pcm

* Experimental uncertainty including buckling measurement uncertainty and technological uncertainties.

The TRIPOLI-4/JEFF-3.1.1 calculation of the regular core MISTRAL2, as well as the BWR mock-up BASALA, confirmed the slight K_{eff} overestimation for 100% MOX cores.

The K_{eff} calculation of Pu solutions encountered in criticality safety was validated against critical experiments from the ICSBEP database. Compared to previous results obtained with JEFF-3.1, the calculations based on JEFF-3.1.1 are quite satisfactory. The calculation/experiment is summarised in Table 17, where ENDF/B-VII calculation results are also reported. The reactivity of LWR-MOX lattices used in Pu recycling, as well as in Pu solutions, is strongly overestimated by ENDF/B-VII calculations (more than 1 000 pcm under the BWR cold conditions of BASALA-C). The C/E discrepancy is more acceptable using JEFF-3.1.1.

Table 17: C/E bias (pcm) on multiplication factor of Pu systems

	ICSBEP Pu-Sol-Therm C_{Pu} < 80 g/l	ICSBEP Pu-Sol-Therm C_{Pu} > 80 g/l	EOLE MISTRAL2 PWR core	EOLE BASALA-C BWR core
JEFF-3.1.1	+250 ± 200	+50 ± 200	+650 ± 220*	+690 ± 220*
ENDF/B-VII	+700 ± 200	+340 ± 200	+950 ± 220*	+1 180 ± 220*

* 1σ experimental uncertainty (technological uncertainties are the main components).

6.3 Depletion calculation and spent fuel inventory

APOLLO2.8 depletion calculations of PWR and BWR assemblies were carried out, using a precise reactor history follow-up (Chabert, 2000a). Actinide and FP isotopic concentrations are compared to chemical analyses, using a $^{i}Nd/^{238}U$ isotopics ratio as local burn-up indicators. The comparison between JEFF-3.1.1 calculation and experiment is summarised in Table 18 for the PWR-900 Gravelines5 case.

Table 18: (C-E)/E bias (%) for PWR spent fuel inventory (burn-up: 64 GWd/t)

	ENDF/B-VII	JEFF-3.1.1	ΔE/E (%)
$^{234}U/^{238}U$	1.2	1.7	± 2.0
$^{235}U/^{238}U$	9.9	8.0	± 6.1
$^{236}U/^{238}U$	-0.1	-0.9	± 1.1
$^{237}Np/^{238}U$	1.0	1.4	± 2.7
$^{238}Pu/^{238}U$	-9.9	-3.9	± 4.1
$^{239}Pu/^{238}U$	6.5	5.7	± 1.6
$^{240}Pu/^{238}U$	2.5	4.2	± 1.3
$^{241}Pu/^{238}U$	2.1	1.7	± 1.7
$^{242}Pu/^{238}U$	-6.4	-2.5	± 3.9
$^{241}Am/^{238}U$	4.8	2.4	± 5
$^{241}Am/^{238}U$ EOC	28.2	8.7	± 9
$^{242m}Am/^{238}U$	6.9	7.2	± 7.0
$^{243}Am/^{238}U$	4.5	-0.2	± 5.5
$^{243}Cm/^{238}U$	-20.9	-19.9	± 12
$^{244}Cm/^{238}U$	-4.4	-8.4	± 10
$^{245}Cm/^{238}U$	10.8	-5.4	± 11
$^{246}Cm/^{238}U$	-8.4	-21.5	± 14
$^{247}Cm/^{238}U$	-10.7	-17.4	± 16
$^{143}Nd/^{238}U$	3.1	2.1	± 1.1
$^{144}Nd/^{238}U$	-3.7	-2.4	± 2.9
$^{145}Nd/^{238}U$	-3.4	-0.7	± 1.5
$^{146}Nd/^{238}U$	0.4	-0.4	± 2.4
$^{148}Nd/^{238}U$	-1.0	0.2	± 2.1
$^{150}Nd/^{238}U$	-1.0	-0.5	± 2.3

This calculation/experiment comparison enhances important improvements:

- ^{238}Pu is no longer underestimated (improvement by +5% compared to JEF-2, JEFF-3.1 and B-VII);
- ^{239}Pu is less overestimated (improvement by -1%);
- ^{242}Pu is no longer overestimated (improvement by +4%);
- ^{241}Am is accurately predict (the strong overestimation by 28% of ^{241}Am at end of cycle in B-VII and JEF-2 calculations is drastically reduced using the JEFF-3.1.1 library).

The comparison of the JEFF-3.1.1 calculation and measured isotopics ratio in the Gundremmingen BWR assembly is presented for actinide concentrations in Table 19 (Leconte, 2008). This table summarises the results in the lower sample (H = 200 mm) where the void fraction is small (about 1%). Therefore, the C/E comparison is reliable, because not dependent on the estimated value of the void operating parameter. These BWR results confirm the improvements stressed in PWR spent fuels. Furthermore, Table 19 emphasises the satisfactory prediction of ^{242m}Am build-up (on the contrary, JEF-2 and B-VII calculations show an underestimation by -20% and -12%, respectively).

Table 19: (C-E)/E bias (%) for BWR actinide concentrations (burn-up: 33 GWd/t)

Isotopic ratio	(C-E)/E ± 1σ (%)
$^{235}U/^{238}U$	5.1 ± 4.1
$^{236}U/^{238}U$	0.1 ± 1.6
$^{237}Np/^{238}U$	-4.5 ± 3.1
$^{238}Pu/^{238}U$	-2.6 ± 4.4
$^{239}Pu/^{238}U$	3.0 ± 0.9
$^{240}Pu/^{238}U$	2.3 ± 1.7
$^{241}Pu/^{238}U$	1.1 ± 1.6
$^{242}Pu/^{238}U$	-1.4 ± 4.4
$^{241}Am/^{238}U$	-0.4 ± 2.1
$^{242m}Am/^{238}U$	-4.7 ± 2.3
$^{243}Am/^{238}U$	-1.4 ± 6.1
$^{243}Cm/^{238}U$	-13.0 ± 5.9
$^{244}Cm/^{238}U$	0.9 ± 8.2
$^{245}Cm/^{238}U$	-4.6 ± 9.3
$^{246}Cm/^{238}U$	-19.5 ± 12.6
$^{247}Cm/^{238}U$	-9.8 ± 15.2
$^{143}Nd/^{238}U$	0.6 ± 1.4
$^{144}Nd/^{238}U$	-2.0 ± 2.3
$^{145}Nd/^{238}U$	-0.2 ± 1.5
$^{146}Nd/^{238}U$	-0.5 ± 1.8
$^{148}Nd/^{238}U$	0.2 ± 1.8
$^{150}Nd/^{238}U$	-0.4 ± 1.8

C/E comparison for fission product concentrations is summarised in Table 20. The results correspond to two samples with increasing void fractions 50% and 80%, with respective axial heights H = 815 and 3 420 mm. A satisfactory prediction within 5% accuracy is obtained for the concentration of important poisoning FP (included in top 20): ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{153}Eu, ^{154}Eu, ^{153}Eu, ^{155}Eu, ^{155}Gd. The improvement is particularly significant for ^{154}Eu, ^{154}Gd, ^{155}Eu and ^{155}Gd concentrations, compared with previous C/E results based on JEF-2.2 [respectively +80%, +73%, +16% and +8% biases at 50 GWd/t (Courcelle, 2003)], thanks to the new ^{154}Eu and ^{155}Eu evaluations introduced in JEFF-3. Moreover, ^{150}Sm-^{151}Sm-^{152}Sm calculated concentrations are improved by 4% compared to B-VII underpredicted concentrations, due to our improved ^{149}Sm evaluation (Courcelle, 2003).

6.4 Fuel reactivity loss versus burn-up

The reactivity worth of three SNF-UO_2 samples (extracted at mid-height from fuel pins irradiated five or six cycles in Cruas2 PWR) was measured by oscillation at the centre of the MINERVE LWR-UO2 block. Furthermore, three rod cuts were extracted from the Gundremmingen BWR assembly at increasing

Table 20: (C-E)/E bias (%) for BWR fission product concentrations

Isotopic ratio	H = 815 cm	H = 3 420 cm
	Bu = 45 GWd/t	Bu = 30 GWd/t
$^{143}Nd/^{238}U$	1.2 ± 1.3	0.2 ± 1.4
$^{144}Nd/^{238}U$	-2.5 ± 2.6	-2.8 ± 2.7
$^{145}Nd/^{238}U$	-0.4 ± 1.5	-0.9 ± 1.7
$^{146}Nd/^{238}U$	-0.5 ± 1.9	-0.5 ± 1.8
$^{148}Nd/^{238}U$	0.2 ± 1.8	0.2 ± 1.8
$^{150}Nd/^{238}U$	-1.3 ± 1.3	-0.2 ± 1.8
$^{133}Cs/^{238}U$	-1.2 ± 1.6	0.5 ± 1.7
$^{134}Cs/^{238}U$	-3.0 ± 4.4	-5.9 ± 3.9
$^{135}Cs/^{238}U$	2.1 ± 2.6	7.5 ± 2.7
$^{137}Cs/^{238}U$	-3.1 ± 1.7	-1.2 ± 1.8
$^{147}Sm/^{238}U$	-4.6 ± 2.6	-5.3 ± 3.3
$^{149}Sm/^{238}U$	4.5 ± 6.2	-0.5 ± 6.9
$^{150}Sm/^{238}U$	-0.8 ± 1.8	-3.0 ± 1.8
$^{151}Sm/^{238}U$	-1.6 ± 4.1	0.1 ± 5.4
$^{152}Sm/^{238}U$	-3.1 ± 1.8	-4.0 ± 2.4
$^{153}Eu/^{238}U$	4.8 ± 1.8	3.8 ± 2.1
$^{154}Eu/^{238}U$	-4.3 ± 3.5	-2.4 ± 4.9
$^{155}Eu/^{238}U$	3.9 ± 2.2	3.4 ± 2.6
$^{154}Gd/^{238}U$	-7.1 ± 4.4	-11.4 ± 6.4
$^{155}Gd/^{238}U$	0.7 ± 8.4	

heights (H = 750, 1 750, 3 355 mm) and oscillated at the centre of the LWR-UO2 block (Leconte, 2008). The APOLLO2.8/CEA2005v4 analysis provides a satisfactory prediction of the reactivity loss due to fuel burn-up. The C/E comparison, summarised in Table 21, points out the improvement linked to JEFF-3.1.1 data, compared to previous JEF-2.2 file.

Table 21: (C-E)/E ± δE/E on reactivity loss with burn-up (MINERVE oscillation of LWR rod cuts)

	PWR Cruas2 UOX 4.5% 3 rod cuts 5- & 6-cycle	BWR Gundremmin. UOX 4.5% 3 rod cuts 4-cycle
JEFF-3.1.1	+0.2 ± 1.3%	+1.1 ± 2.0%
JEF-2.2	+2.3 ± 1.3%	+2.1 ± 2.0%

Concerning the critical boron follow-up within PWR cycles, both JEFF-3.1.1 and B-VII calculations are satisfactory. However, experimental data from PIE and isotopic reactivity worth indicate that error compensation occurs in the B-VII calculation.

MINERVE oscillations of MOX spent fuels were also performed at the centre of the R1-MOX lattice (Pu 4%). After assembly irradiation in Dampierre2 PWR-900 MWe, two rod cuts were extracted after four cycles, and two rod cuts

after five cycles (52 and 60 GWd/t respectively); these pins are located both in the MOX central zone e_{Pu} = 6.7% w/o and the intermediate zone e_{Pu} = 5.3% w/o. C/E biases on the reactivity loss with burn-up are consistent amongst the four samples (Bernard, 2006a). Table 22 shows that the target accuracy is met using JEFF-3.1.1 data, with a reactivity loss predicted within 3% accuracy.

Table 22: (C-E)/E ± δE/E on reactivity loss with burn-up (MINERVE oscillation of MOX rod cuts)

	PWR Dampierre2 MOX 5.3%, 6.7% Pu 4 rod cuts, 4- & 5-cycle
JEFF-3.1.1	+0.9 ± 1.5%
JEF-2.2	-1.0 ± 1.5%

6.5 Reactivity temperature coefficient

As with the previous K_{eff} neutronics parameter, this LWR reactivity coefficient is also very sensitive to nuclear data. Concerning UOX lattices, the isothermal temperature coefficient was already well predicted using JEF-2.2 (Erradi, 2003), and remains calculated within the 1 pcm/°C target accuracy using JEFF-3.1.1.

The temperature coefficient calculation using JEF-2.2, however, was too negative for MOX lattices at room temperatures. The isothermal temperature coefficient was accurately measured between 10°C and 80°C for 100% MOX cores in EOLE (MISTRAL2 and three PWR regular cores, and BASALA BWR mock-up). The calculation-experiment comparison is summarised in Table 23. C/E bias is reduced by 0.3 pcm/°C using JEFF-3.1.1 as compared to JEF-2 or B-VII calculation results.

Table 23: (C-E) ± δE on MOX temperature coefficient (pcm/°C)

	PWR MOX core MISTRAL2	PWR MOX core MISTRAL3	BWR MOX core BASALA
JEFF-3.1.1	-1.2 ± 0.3	-1.3 ± 0.3	-1.6 ± 0.3
JEF-2.2 or ENDF/B-VII	-1.5 ± 0.3	-1.6 ± 0.3	-2.0 ± 0.3

6.6 Stainless steel reflectors

JEFF-3.1.1 calculation of water reflector has been validated in EOLE experiments, such as MISTRAL1 characterised by a regular core lattice fuelled by standard PWR UO_2-3.7% ^{235}U rods; the reflector saving is estimated within 3 mm. A specific experiment FLUOLE has been performed in the EOLE facility, in order to validate the calculation of the Gen. II baffle-water reflector; the JEFF-3.1.1 calculation is also satisfactory (Vidal, 2008).

Heavy neutron reflectors are used in advanced PWRs, such as VVER1000 and EPR (Gen. III reactors) and will be probably utilised in Gen. IV FBR. The heavy reflector is a most challenging problem due to the nuclear data of SS components (mostly Fe, but also Cr and Ni) with their resonant behaviour and their strong inelastic scattering.

In order to provide representative experimental data, CEA performed the PERLE experiment (Santamarina, 2008b) (Figure 23). The reactivity worth of this 22-cm thick heavy reflector was measured and compared to the efficiency of a water reflector. JEFF-3.1.1 results are summarised in Table 24. Assuming the C/E bias in the water-reflected experiment MISTRAL1 as a reference, Table 24 shows a slight trend toward K_{eff} underestimation when implementing the SS reflector. However, compared to the 20 000 pcm radial leakage, this slight C/E shift (-155 ± 130 pcm) between MISTRAL1 and PERLE means that the heavy reflector worth is well predicted. It should be noted that the TRIPOLI-4/B-VII calculation increases the C/E shift between MISTRAL1 and PERLE up to -201 ± 130 pcm.

Figure 23: The PERLE core with SS reflector in the EOLE facility

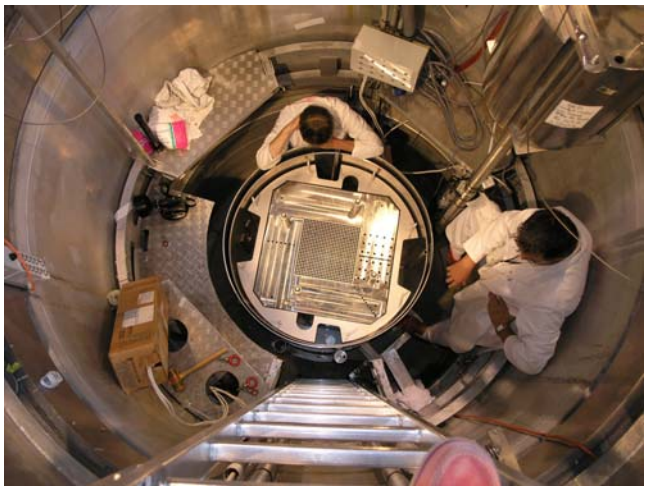


Table 24: Residual reactivity (pcm) in EOLE UO_2-3.7% ^{235}U regular cores

Experiment	MISTRAL1 H_2O reflector	PERLE SS reflector
Measurement	109 ± 24*	121 ± 22*
TRIPOLI-4/JEFF-3.1.1	205 (6)	62 (4)
C-E	+96 ± 95**	- 59 ± 98**

* Measurement uncertainty including soluble boron concentration, doubling time and β_{eff} components.

** Total uncertainty including measurement and technological components (enrichment, clad diameter, lattice pitch).

A reflector savings of $\delta_{SS} \approx 10$ cm was obtained from radial buckling measurements. JEFF-3.1.1 allows an accurate prediction of this neutronics parameter: C/E = -5 ± 2 mm, meeting the target accuracy required for radial power map calculation in Gen. III reactors.

These satisfactory JEFF-3.1.1 results for δ_{SS} and K_{eff} synthetic parameters were confirmed by measurements of the flux attenuation across the SS reflector. Both miniature fission chambers and foils activation detectors were used. These traverse measurements in the bulk SS are normalised to measurements performed at the centre of the core lattice, where the cosine flux is calculated with accuracy. The use of fission chambers with different deposits (^{235}U, ^{237}Np and ^{238}U for the thermal, epithermal and fast flux investigation respectively) enables an online cartography of the neutrons throughout the increasing stainless steel thickness, at the core mid-plane.

The calculation/experiment comparison (Table 25) displays an accurate prediction, versus SS penetration, of fast flux decrease and intermediate flux build-up. Based on C/E versus penetration, the sensitivity study has demonstrated that the ^{56}Fe inelastic scattering level in the JEFF-3.1.1 evaluation is satisfactory.

Table 25: C/E bias (%) on flux attenuation throughout the core and the SS reflector

FC position (cm)	SS penetration	FC ^{238}U	FC ^{237}Np	FC ^{235}U
0.0	Core centre	-0.2	-0.9	-1.2
2.64	Core		0.2	0.9
9.24	Core	0.2	0.8	0.5
19.80	1.98		-0.2	
21.12	3.30	0.4	-0.9	-1.5
22.44	4.62		2.7	
23.76	5.94	1.4	2.9	-0.5
25.08	7.26		2.2	
26.40	8.58	3.5	2.9	0.9
27.72	9.90		3.4	
29.04	11.22	3.4	4.1	0.9
30.36	12.54		2.8	
31.68	13.86	4.7	5.1	0.8
33.00	15.18		8.0	
34.32	16.50		8.0	1.7
35.64	17.82		4.9	
36.96	19.14		4.5	3.0

These satisfactory results for propagation calculations in steel are confirmed by the TRIPOLI-4/JEFF-3.1.1 analysis (Jouanne, 2008) of the ASPIS experiment with both Fe and SS. Fast and intermediate response functions [^{32}S(n,p), ^{115}In(n,n′) and ^{103}Rh(n,n′)] are predicted within 20% accuracy up to 70 cm deep penetration. The analysis results of the REPLICA experiment, with successive steel shielding and water blades, is also satisfactory. Finally, the current CEA recommendation for shielding (Poinot, 2008) is the same as that for reactor physics and fuel cycle calculations: JEFF-3.1.1 must be used.

Chapter 7: Conclusion

The JEFF-3.1.1 library is the result of 15 years of extensive validation against fundamental targeted experiments, LWR mock-up experiments, PWR and BWR chemical assays and SNF reactivity worth measurements. Moreover, JEFF-3 evaluations benefit from the feedback of experimental validation studies in FBR, fuel cycle, criticality safety and burn-up credit.

The corresponding CEA2005v4 library recommended for APOLLO2.8 is particularly qualified for accurate calculations of LWR neutronics parameters. This report has demonstrated that it is more accurate than ENDFB/VII-based calculations for fuel inventory, MOX reactivity and Pu ageing, and reactivity coefficients such as temperature coefficient, stainless steel reflectors.

JEFF-3.1.1 is used world wide for PWR and BWR calculations; CEA20005v4 is used inside the new ARCADIA package of Areva-NP (Curca-Tivig, 2008). It is also used in ERANOS2 for Gen. IV design.

Future JEFF-3 and APOLLO-3 libraries will continue to benefit from current fundamental experiments, such as OSMOSE and OCEAN devoted to nuclear data of actinides and absorber isotopes, as well as FBR experiments performed in MASURCA mock-ups and PHENIX irradiations.

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