Present status of JEFF-3.1 validation for fast reactors Using the ERANOS-2.1 code system

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Abstract

The latest release (2.1) of the ERANOS code system, using JEF-2.2, JEFF-3.1 and ENDF/B-VI r8 multigroup cross-section libraries is currently being validated on fast reactor critical experiments at CEA-Cadarache (France). This paper briefly presents the library effect studies and the detailed best-estimate validation studies performed up to now as part of the validation process. The library effect studies are performed over a wide range of experimental configurations, using simple model and method options. They yield global trends about the shift from JEF-2.2 to JEFF-3.1 cross-section libraries, that can be related to individual sensitivities and cross-section changes. The more detailed, best-estimate, calculations have been performed up to now over three experimental configurations carried out in the MASURCA critical facility at CEA-Cadarache: two cores with a softened spectrum due to large amounts of graphite (MAS1A' and MAS1B), and a core representative of sodium-cooled fast reactors (CIRANO ZONA2A). Calculated values have been compared to measurements, and discrepancies analyzed in detail using perturbation theory. Values calculated with JEFF-3.1 were found to be within 3 standard deviations of the measured values, and at least of the same quality as the JEF-2.2 based results.

KEYWORDS: Fast reactors, validation, ERANOS-2.1, JEF-2.2, JEFF-3.1, ENDF/B-VI r8

1 Introduction

The ERANOS code system has been developed and validated to establish a suitable basis for reliable neutronic calculations of current, as well as advanced fast reactor cores of the GEN IV Forum. The ERANOS-2.1 code package contains several cross section libraries, all derived from the JEFF-3.1, JENDL3.3 and ENDF/B-VI r8 nuclear data evaluated files. In particular, the JEFF-3.1 Nuclear Data Library is the latest version of the Joint Evaluated Fission and Fusion Library. The complete sequence of data files was released in May 2005, and contains general purpose nuclear data evaluations (neutron reaction data, incident proton data and thermal neutron scattering law data in the ENDF-6 format) compiled at the NEA Data Bank, radioactive decay data, activation data and fission yields data. It combines the efforts of the JEFF and EFF Working Groups contributing to this combined fission and fusion file. The aim of this paper is to present the current status of the validation of this library using the ERANOS-2.1 code system.

Cell calculations are performed by the ECCO cell/lattice code, which prepares self-shielded cross sections and matrices by combining a slowing-down treatment in many groups with the subgroup method within each fine group. The sub-group method takes into account the resonance structure of heavy nuclides by means of probability tables and by assuming that the neutron source is uniform in lethargy within a given fine group. Core and shielding

calculation codes offer various options, such as: 1-D, 2-D or 3-D diffusion, 1-D or 2-D (X- Y, R-Z, R-θ) Sn transport, 2-D or 3-D (Cartesian and hexagonal) Variational Nodal transport.

Library effects have been checked over a set of critical mock-up experiments, computed with simple model and method options (section 2). More detailed, best-estimate, calculations have been performed up to now over a few experimental configurations carried out in the MASURCA critical facility at CEA-Cadarache (section 3).

2 Trends in fast spectrum integral experiments

Integral parameter calculations using the ERANOS-2.1 code system [1] and the associated JEF-2.2, JEFF-3.1 and ENDB/B-VI r8 libraries have been performed over an experimental database [2] containing 40 selected experimental values : 18 critical masses and 22 spectral indices (F28/F25, C28/F25 and F49/F25). These values are part of the larger database used at CEA in the previous adjustment of the ERALIB1 library [3,4]. The integral experiments selected here have been performed in mock-up configurations in the MASURCA or SNEAK facilities.

This section presents a brief analysis of the global library-dependent trends observed in critical mass predictions. The aim of such an analysis is to check the impact of new nuclear data evaluations or processed libraries in the fast spectrum reactor range. Simplified modeling with corrective factors are used for these calculations. Besides the usual calculation vs. experiment comparisons, a complete sensitivity analysis (not presented in this paper) of the integral results to the nuclear data allows to explain most of the differences observed between libraries in terms of differential nuclear data.

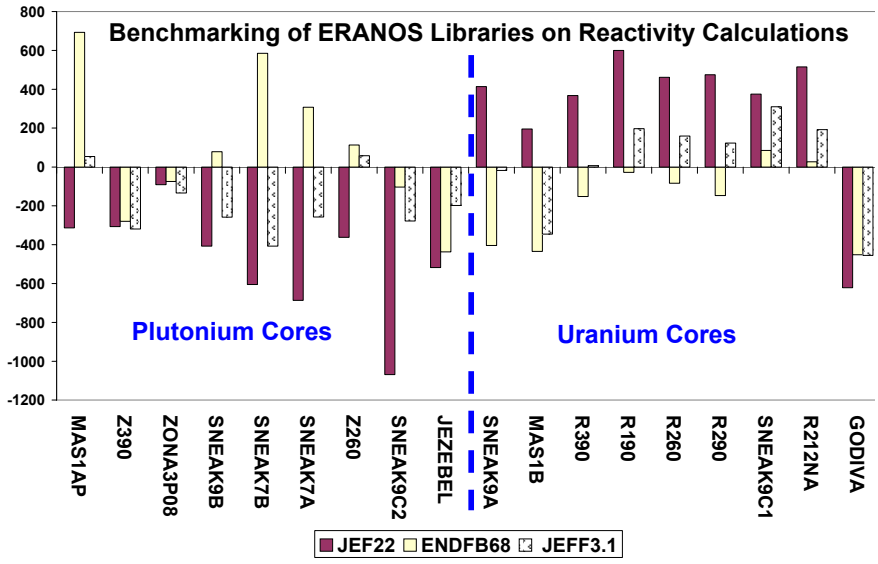

Figure 1 — Library effects of reactivity predictions (C-E in pcm[1])

Figure 1 shows the ERANOS2.1 results for criticality obtained with the JEF-2.2, JEFF-3.1 and ENDFB-6.8 libraries. Experiments are divided in two categories, i.e. plutonium fuelled

[1] 1 pcm = 10^{-5} Δk/kk'

cores (left hand side of the graph) and uranium fuelled cores (right hand side of the graphs). Inside each category, experiments are ranked from left to right by order of increasing spectrum hardness.

In this paper, only the results with JEFF3.1 are discussed. Generally, the use of the JEFF-3.1 (vs. JEF-2.2) library leads to higher k-effective values for plutonium cores and lower ones for uranium cores. These reactivity effects reduce significantly the dispersion on critical mass predictions. However, some singularities occur, like the results on the Z390 and ZONA3P08 experiments ("softer" spectrum) SNEAK9C2 (hard spectrum), and the GODIVA experiment (very hard spectrum). If we compare to experiment, MAS1B exhibits a peculiar behavior also.

If we compare to experiment, JEFF-3.1 critical mass calculations for "plutonium" cores (which may also contain uranium, although not in the *central part* of the core), corrective factors being applied, yield C-E values ranging between -200 and -300 pcm, except for SNEAK7B which is more sensitive (C-E ~ -410 pcm) and MAS1AP and Z260 which are in good agreement (C-E ~ +55 pcm). One can note that SNEAK7B contains about twice as many ^{238}U atoms as the other experiments.

JEFF-3.1 critical mass calculations for uranium cores, corrective factors being applied, show C-E values ranging between -20 and +310 pcm, except for MAS1B that is overestimated by ~235 pcm with JEF2.2 and underestimated by ~350 pcm with JEFF3.1. For GODIVA, the critical mass calculation remains underestimated by ~450 pcm.

The reliability of the above C-E value lies on the modeling and method options used to compute raw values and corrective coefficients. More accurate calculations, in order to decrease method and modeling errors, have been undertaken on several critical experiment configurations.

3 Detailed comparisons to experiment

		1A'	1B	ZONA2A
Pu/(U+Pu) (%)		25.2	—	27.6
U235/U (%)		—	30.0	—
Core height (cm)		61.0	61.0	61.0
Core diameter (cm)		35.4	33.1	47.5
Volume fractions (%) :	Fuel	16.6	17.6	32.4
	Steel	8.6	7.6	11.9
	Graphite	67.9	67.9	—
	Sodium	—	—	42.8

Table 1 — Geometry and composition parameters

Detailed ERANOS-2.1 validation studies using both JEF-2.2 and JEFF-3.1 nuclear data have been performed on three past configurations of MASURCA. The two first experiments analyzed, named MAS1A' and MAS1B, were performed in the late 1960's and involved small compact cores with large amounts of graphite (≈ 68% volume fraction in the core), resulting in a significantly softened spectrum with respect to standard Na-cooled fast reactors (see Figure 2). The MAS1A' core was loaded with UPuFe metal fuel, and the MAS1B core with enriched U metal fuel. Both were surrounded by fertile blankets (metallic depleted U). The third experiment was a specific configuration of the CIRANO experimental program named ZONA2A (loaded in 1994) [5]. It modeled a small $(U,Pu)O_2$-fuelled and Na-cooled

fast reactor core, surrounded by depleted UO_2 fertile blankets. Table 1 gives some geometric and composition parameters.

3.1 Calculation scheme

The fine and broad group libraries (1968 and 33 energy groups respectively) processed for the ERANOS code system from the JEF-2.2 and JEFF-3.1 evaluated nuclear data files are used.

Lattice calculations are performed with the ECCO module. The geometrical description of fuel subassemblies (S/A) can be homogeneous, heterogeneous 1D cylindrical (2 zones: fuel pellet + mixture of clad, coolant/graphite and steel), or heterogeneous 2D geometry (S/A cross-cut). Fertile blankets are processed either in homogeneous or in 1D cylindrical geometry. ECCO flux calculations are performed in 1968 energy groups with subsequent condensation and homogenization, providing 33-group data for whole core calculations.

In heterogeneous geometry, ECCO computes collision probabilities, either exactly, e.g. in 1D cylindrical geometries, or approximately, e.g. in 2D S/A geometry with Roth-like methods, and solves fully coupled flux-current equations [1]. An approximation to those "consistent" equations are the decoupled "inconsistent" equations, approximating leakage by a non-leakage factor and current by a Fick-like law [1]. In standard fast reactor spectra, the inconsistent approximation is quite accurate, but looses validity in case of important anisotropic scattering by light nuclides.

An ECCO run is made of several chained "steps". The "reference" calculation route involves a fine-group step in heterogeneous geometry, which may require a large running time. In fast spectra, we can compute slowing down in fine groups and homogenized geometry, then condense to broad groups and perform self shielding calculations in heterogeneous geometry. This is called the "design" calculation route. Once again, this approximation proves quite accurate in standard fast reactor spectra, but it becomes questionable in softened spectra.

The BISTRO 2D Sn transport module is used for whole core calculations, in a RZ geometry (specific checks in XY and R geometries are performed to assess the cylindrization effects). S4, S8 and S16 angular discretizations are available. A fine spatial mesh size is retained (1 cm in R and in Z). Scattering anisotropy is P1 Legendre order.

Finally, the whole core model may or may not include the fine geometrical description of the end caps of the rodlets used to build the core, and of the air mixing devices placed directly above and below the fuel zone in order to enhance the cooling efficiency.

3.2 Core criticality prediction

Method and modeling effects are given in Table 2. The cores being close to cylinders, the cylindrization correction is small. The angular mesh effect is less than 0.12% on the multiplication factor, and the spatial mesh effect has been checked as negligible with 1 cm meshes. Whole core geometrical corrections (end caps and air mixing devices) compensate each other, and the resulting correction never exceeds 0.15% on the multiplication factor.

Taking into account fuel heterogeneity yields a significant effect in the 1A' and 1B cores, softened with graphite, where the main effect is due to the geometrical separation of fuel and

graphite (the 0D → 1D effect in table 2). To the contrary, heterogeneity effects are small in ZONA2A, mock-up of a "classical" sodium-cooled fast reactor core.

	1A'	1B	ZONA2A
Cylindrization	-0.00110	-0.00212	-0.00069
Fuel S/A geometry : 0D → 1D	+0.02576	+0.01531	+0.00093
1D → 2D	+0.00356	+0.00231	+0.00002
Fertile S/A geometry : 0D → 1D	-0.00064	-0.00080	-0.00177
Angular discretization : S4 → S8	-0.00088	-0.00096	-0.00094
S8 → S16	-0.00021	-0.00024	-0.00020
Calculation methods : inconsistent → consistent	+0.00206	+0.00172	+0.00097
design → reference	+0.01375	+0.00815	+0.00173
Corrections to geometry : end caps	+0.00259	—	+0.00251
air mixing devices	-0.00110	-0.00137	-0.00223

Table 2 — Method and modeling effects on multiplication factor

The consistent/inconsistent treatment of the flux and current equations in heterogeneous geometry has an effect of no more than 0.2% on the multiplication factor, while the choice of the design route, involving slowing-down calculations in a homogeneous geometry has a very important effect of the multiplication factor (≈1%) in case of softened spectrum.

The best estimate results obtained with ERANOS for the multiplication factor are given in the following table 3. These best estimate results involve the most sophisticated calculation options above, i.e. 2D fuel S/A geometry, 1D fertile S/A geometry, S16 angular discretization, consistent flux/current equations, reference route, and take into account end caps, air mixing devices and cylindrization corrections. A plot of average fluxes in the fuel region is given in Figure 2, showing the different shapes in the slowing-down tail below 10 keV.

	JEF-2.2	JEFF-3.1
MASURCA 1A'	+0.00165	+0.00479
MASURCA 1B	+0.00515	-0.00080
CIRANO ZONA2A	-0.00328	+0.00444

Table 3 — k_{eff}^{cal} (best estimate) - k_{eff}^{exp}

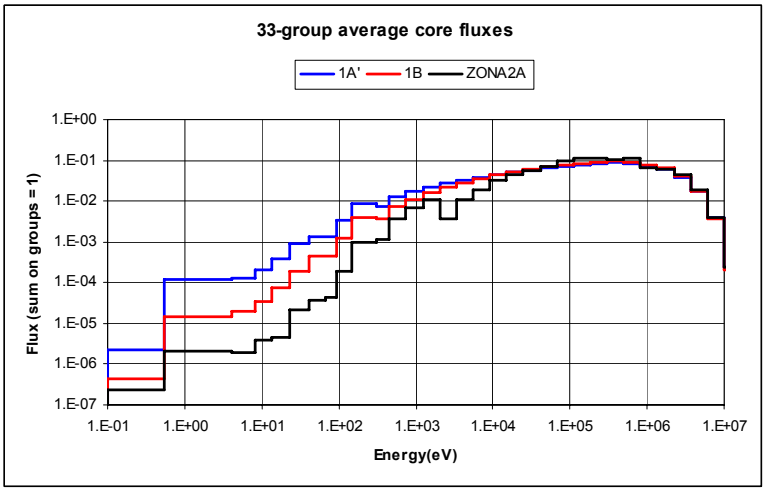

Figure 2 — Average core fluxes for the 1A', 1B and ZONA2A MASURCA cores

The reactivity difference $\delta\rho = \delta k/kk'$ between criticality predictions using either JEF-2.2 or JEFF-3.1 nuclear data, expressed in pcm (10^{-5}), has been computed using the perturbation and sensitivity analysis tools of the ERANOS-2.1 code system. Tables 4 and 5 give the global reaction-wise and nuclide-wise breakdowns of the reactivity effects.

	1A'	1B	ZONA2A
capture	+230	-515	+467
fission	+137	-119	+112
fission spectrum	-308	-230	-236
elastic	+361	+418	+266
inelastic	-121	-158	+148
n,xn	+16	+17	+19
total	+314	-588	+774

Table 4 — Reaction-wise breakdown of ($\rho_{JEFF-3.1}$ - $\rho_{JEF-2.2}$) in pcm (10^{-5})

	1A'	1B	ZONA2A
U235	-36	-908	-21
U238	+240	+356	+201
Pu239	-80	—	+10
Pu240	+178	—	+294
Pu241	—	—	+19
Am241	—	—	+46
Fe56	-34	-61	-57
Cr52	-16	-26	-88
Mn55	+35	+15	+29
O16	—	—	-26
Na23	—	—	+366
C	-2	+18	—
Total	+314	-587	+774

Table 5 — Nuclide-wise breakdown of ($\rho_{JEFF-3.1}$ - $\rho_{JEF-2.2}$) in pcm (10^{-5}) : main contributions

The improvement in criticality prediction for the 1B uranium core results from the correction of a well-known deficiency of the JEF-2.2 data for U235. According to perturbation analysis, the main impact lies on U235 capture (-0.6%, in the energy range from 100 eV to 3 keV) and fission (-0.3%). In all three experiments a large positive contribution (+0.33 to +0.50%) results from the change in the elastic scattering law for U238 in the 100 keV-1MeV energy range (the JEF-2.2 scattering law being slightly more anisotropic than the JEFF-3.1 law).

Changes in Pu239 data have a limited global impact on reactivity (less than 0.1%) despite the large contribution of this nuclide to the reactivity balance of the 1A' and ZONA2A cores, and result from compensations between positive and negative contributions over the whole energy range. Data for Pu240 has also been changed, resulting in reactivity effects of +0.2 to +0.3% from JEF-2.2 to JEFF-3.1 data.

In the ZONA2A core, a large reactivity effect (+0.37%) is due to the change in sodium nuclear scattering data from JEF-2.2 to JEFF-3.1. The ZONA2A experiments involved four sodium voided configurations at core center playing on different amplitudes for the scattering and leakage contributions to the sodium void reactivity effect. The use of JEFF-3.1 nuclear

data for sodium improves dramatically the sodium void reactivity prediction. A least square analysis yields corrective coefficients to be applied to the scattering (S) and leakage (L) components of the sodium void reactivity obtained by a perturbation analysis: 0.96 (S) and 1.08 (L) with JEF-2.2 sodium data, but 1.00 (S) and 1.02 (L) with JEFF-3.1 data.

The following table 6 gives the ERANOS results for spectrum index prediction at the center of all three cores, and shows possible trends for nuclear data improvement.

1A'	JEF-2.2	JEFF-3.1	Exp. Unc. (%)
^{238}U(n,f) / ^{235}U(n,f)	1.016	0.980	± 2.4
^{239}Pu(n,f) / ^{235}U(n,f)	0.961	0.962	± 2.0
^{238}U(n,γ) / ^{235}U(n,f)	0.955	0.955	± 2.6

1B	JEF-2.2	JEFF-3.1	Exp. Unc. (%)
^{238}U(n,f) / ^{235}U(n,f)	1.041	1.011	± 2.0
^{239}Pu(n,f) / ^{235}U(n,f)	0.990	0.985	± 2.4
^{238}U(n,γ) / ^{235}U(n,f)	0.952	0.951	± 4.1

ZONA2A	JEF-2.2	JEFF-3.1	Exp. Unc. (%)
^{237}Np(n,f) / ^{235}U(n,f)	0.962	1.013	± 2.1
^{238}U(n,f) / ^{235}U(n,f)	1.024	1.006	± 2.4
^{238}Pu(n,f) / ^{235}U(n,f)	1.059	1.139	± 5.0
^{239}Pu(n,f) / ^{235}U(n,f)	0.986	0.989	± 1.4
^{240}Pu(n,f) / ^{235}U(n,f)	1.068	1.078	± 4.5
^{241}Pu(n,f) / ^{235}U(n,f)	1.003	1.005	± 3.8
^{242}Pu(n,f) / ^{235}U(n,f)	1.042	1.080	± 4.5
^{241}Am(n,f) / ^{235}U(n,f)	1.072	1.103	± 4.4
^{243}Am(n,f) / ^{235}U(n,f)	1.050	1.008	± 4.6
^{238}U(n,γ) / ^{235}U(n,f)	0.949	0.942	± 3.0
^{197}Au(n,γ) / ^{235}U(n,f)	1.062	1.062	± 3.2
^{55}Mn(n,γ) / ^{235}U(n,f)	1.400	1.014	± 4.8
^{10}B(n,α) / ^{235}U(n,f)	1.015	1.005	± 3.3

Table 6 — C/E for spectrum indices at the center of 1A', 1B and ZONA2A cores

4 Conclusion

Library effects between JEF-2.2, JEFF-3.1 and ENDF/B-VI r8 have been checked over a wide range of experimental configurations, using simple model and method options. They yield global trends about the shift from one cross-section library to another, that can be linked to individual contributions using perturbation theory.

The MASURCA 1A', 1B and CIRANO ZONA2A fast spectrum experiments have been analyzed with ERANOS-2.1 and JEF-2.2 / JEFF-3.1 data. The calculated values of reactivity, spectral index and sodium void were compared with the corresponding measurements, and the C/E were analysed in detail using perturbation theory. Values calculated with JEFF-3.1 were found to be within 3 standard deviations of measured values, better than, or of the same

quality as, the JEF-2.2 based results, and consistent with respect to the nuclear data changes between JEF-2.2 and JEFF-3.1 files.

The validation of ERANOS + JEFF-3.1 data is planned to be extended to other experiments in critical zero-power assemblies and power reactors, in order to cover a wide range of fast reactor applications.

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