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Re-estimation of Nuclear Data and JEFF3.1.1 Uncertainty Calculations

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ABSTRACT

This paper describes the method to define relevant targeted integral measurements that allow the improvement of nuclear data evaluations and the determination of corresponding reliable covariances. ^{235}U and ^{56}Fe examples are pointed out for the improvement of JEFF3 data. Utilizations of these covariances are shown for Sensitivity and Representativity studies, Uncertainty calculations, and Transposition of experimental results to industrial applications.

Key Words: Integral experiments, Re-estimation, JEFF3.1.1, Sensitivity, Covariance, Uncertainty.

1. INTRODUCTION

Sensitivity and Uncertainty analyses are more and more used in Reactor Physics [1] and Nuclear Criticality-Safety [2] [3]. However, these kinds of studies require realistic covariance matrices corresponding to the Nuclear Data evaluation implemented in the ND library. The main components of LWR calculation uncertainty is linked to actinides (^{235}U, ^{238}U, ^{239}Pu) and H_2O, with a contribution of Fe cross-sections in GEN-3 reactors due to the Stainless Steel reflector.

New ^{56}Fe ND Covariances associated with JEFF3.1.1 evaluation have been obtained, mainly from the GEN3 SS-reflected mockup experiment PERLE [4]. Furthermore, realistic ^{235}U covariance matrices have been established from the feedback of targeted integral experiments.

This paper presents the RDN method used to derive realistic ^{235}U and ^{56}Fe covariances associated with JEFF3.1.1 evaluations [5]. Utilizations of these covariances in JEFF3.1.1-based calculations are shown, particularly for Sensitivity and Representativity studies, Uncertainty calculations, and Transposition of experimental results to industrial applications.

2. NUCLEAR DATA RE-ESTIMATION

q integral measurements are described by the random vector Y_i $(i=1,\ldots q)$ of experimental values.

Formally $Y=n+\epsilon_Y$, with n a vector containing the "true" integral and ϵ_Y a random vector assumed centered and normally distributed, representing the experimental errors. The covariance matrix Σ_Y is associated to ϵ_Y .

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The p microscopic data m_j $(j=1,\ldots p)$ are the unknown parameters of the problem, described by $X=m+\epsilon_X$, where the random vector ϵ_X is also centered, normally distributed and associated to ND covariance matrix Σ_X.

The formal relationship between n and m is: $n = f(m)$. The f function relates integral values to the microscopic nuclear data and mathematically describes the physical processes (Boltzmann and Bateman equations).

The mathematical expression can be written as :

$$Z = \eta(m) + \epsilon \tag{1}$$

with :

$$Z = \begin{pmatrix} X \\ Y \end{pmatrix}, \quad \eta(m) = \begin{pmatrix} m \\ n = f(m) \end{pmatrix}, \quad \varepsilon = \begin{pmatrix} \varepsilon_X \\ \varepsilon_Y \end{pmatrix}, \quad \Sigma = \begin{pmatrix} \Sigma_X & 0 \\ 0 & \Sigma_Y \end{pmatrix} \tag{2}$$

This problem is viewed in our RDN method as a non-linear regression problem with known covariance matrix [6].

In order to maximize the Likelihood function, we use the Gauss-Newton method for the minimization of the non-linear square sum. It is an iterative technique that needs a good m_0 initial estimation for m parameter. Each iteration consists in replacing the η function by the approximate formula near the m_k current estimated value:

$$\eta(m) = \eta(m_k) + D\eta(m_k)(m - m_k) \tag{3}$$

$D\eta(m_k)$ is the Jacobian matrix, also called “generalized sensitivity matrix”.

At every step k, the new estimation m_{k+1} is given by :

$$m_{k+1} = m_k + \left\{ D\eta(m_k)^t \Sigma^{-1} D\eta(m_k) \right\}^{-1} D\eta(m_k)^t \Sigma^{-1} (Z - \eta(m_k)) \tag{4}$$

The posterior covariance matrix of the re-estimated m is:

$$\Sigma_{\hat{m}} = \left\{ \Sigma_X^{-1} + Df(m_k)^t \Sigma_Y^{-1} Df(m_k) \right\}^{-1} \tag{5}$$

3. RDN EXPERIMENTAL DATABASE

We selected targeted Integral Experiments that supply accurate information on ^{235}U nuclear data [7]:

- Post-Irradiation Experiments on French PWR assemblies were used. UOX fuels, with various initial enrichments (3.1%, 3.2%, 4.5%) and irradiation from 20 up to 61 GWd/t, give an information within 1% accuracy on (n,γ) capture through measured ^{236}U concentration. ^{236}U/^{238}U isotopic ratio in MOX fuel with hardened spectrum gives specific information on capture Resonance Integral.
- Highly Enriched Uranium Solutions (from HEU-SOL-THERM benchmarks of the ICSBEP Handbook) supply accurate information on η^{U235}. This $\eta = \nu/(1+\alpha)$ value allows to determine the multiplicity ν in the thermal range within 0.2% accuracy (1σ).

- Keff and Bucklings Bm^2, measured for various moderation ratios in LWR critical experiments at EOLE reactor, were also included in the RDN re-estimation.
The analysis of these Keff and P. I. Experiments is carried out by reference calculations: continuous-energy Monte Carlo TRIPOLI4 [8] for Keff benchmarks and APOLLO2.8 exact-2D MOC [9] for P.I.Es. The JEFF3.1.1 Calc-Exp comparison is very satisfactory [10], with C/E biases consistent with experimental uncertainty margins.

4. ^{235}U COVARIANCE LINKED TO JEFF3.1.1 EVALUATION

The prior covariance matrix Σ_X is obtained from the retroactive method [11]. In the CONRAD code, retroactive Covariance of Nuclear Model Parameters is derived from a Marginalization Technique [12]. Therefore, Resonance Parameter Covariance processing by CONRAD supplies reliable multigroup correlation matrices.

Finally, the JEFF3.1.1 posterior covariance matrix is obtained from the RDN re-estimation. Prior and posterior ND Uncertainties (diagonal term of covariance matrices) are compared in Table I. The strength of the re-estimation method based on targeted integral experiments is to obtain 'calibrated' ND standard deviations. The correlation matrix is plotted in Figure 1. Inter-group correlations are consistent with the ENDF/B-VIIp ones.

Table I. ^{235}U Prior and Posterior uncertainty (%)

Energy	$(n,\gamma)^{prior}$	$(n,\gamma)^{post}$	$(n,f)^{prior}$	$(n,f)^{post}$	ν^{prior}	ν^{post}
23 – 4 eV	10	3.6	3.0	2.3	0.8	0.7
4 – 0.5 eV	10	3.7	3.0	2.4	0.8	0.7
0.5 – 1 eV	2	1.6	1.0	0.8	0.8	0.5
E < 0.1 eV	1	0.8	0.4	0.3	0.4	0.2

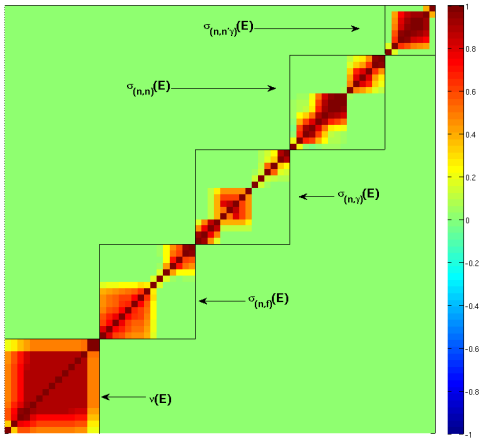

Figure 1. Correlation matrix of ^{235}U Nuclear Data.

5. ^{56}Fe COVARIANCE LINKED TO JEFF3.1.1 EVALUATION

In order to validate ^{56}Fe nuclear data in JEFF3.1.1 evaluation and to derive reliable covariances, CEA has conceived the PERLE targeted experiment. The core is composed of standard PWR 3.7% ^{235}U enriched UO_2 fuel pins, with zircaloy4 clads. The 1.32 cm lattice pitch allows a representative PWR spectrum. To pattern an analytical 1D fuel/reflector interface, the PERLE configuration is constituted by a regular 27x27 square core (Fig. 2a). This core is surrounded by a 22cm-thick Stainless Steel block, which mockups the EPR reflector. Three blocks are hollowed on the main median plane, down to the core mid-plane to enable the insertion of measurement items such as fission chambers or activation foils (Fig. 2b). These holes are filled with SS rods of proper diameter when no measurement is foreseen, to allow uniformity of the SS material.

(a) (b)

Figure 2. (a) PERLE core in EOLE vessel. (b) SS reflector blocks with measurement holes

Critical soluble boron concentration was measured, as well as radial Buckling that gives the neutron reflector saving. Flux attenuation across the core and the SS reflector was measured using various response functions , from fast neutrons (^{56}Fe(n,p), ^{27}Al(n,α), ^{238}U(n,f)) down to thermal neutrons (^{55}Mn(n,γ), ^{235}U(n,f), ^{197}Au(n,γ), ^{115}In(n,γ)). ^{237}Np fission chambers and ^{115}In(n,n') foils were used to measure intermediate fluxes that are very sensitive to scattering cross sections [4].

The comparison between TRIPOLI4/JEFF3.1.1 calculation and Experiment highlights a good agreement both for Keff, core buckling and flux attenuation in reflector [13]. The C/E values that were taken into account in the RDN re-estimation process is summarized in Table II.

Sensitivity coefficients of response functions to ^{56}Fe nuclear data were calculated at each position by APOLLO2.8 in the JEF 15-group energy structure [14]. The results of the nuclear data re-estimation confirm that ^{56}Fe evaluation is satisfactory: the modifications of cross sections provided by the RDN code are within the posterior 2σ uncertainties (Fig. 3).

Prior and posterior standard deviations for ^{56}Fe main cross sections are compared in Table III. Uncertainty on inelastic scattering is drastically reduced by a factor 3.

Table II. Calculation / Experiment comparison for the PERLE experiment

Response function	Penetration in SS reflector (cm)	C/E (%)	Uncertainty (1σ in %)
^{197}Au(n,γ)^{198}Au	3.3	-4.9	2.4
	11.22	-2.1	2.7
	19.14	1.3	2.8
^{115}In(n,γ)^{116}In	3.3	-1.8	2.3
	11.22	1.6	2.3
	19.14	1.4	2.4
^{235}U(n,f)	3.3	-1.8	2.2
	11.22	0.9	2.2
	19.14	2.9	2.2
^{237}Np(n,f)	3.3	-1.4	2.2
	11.22	-0.3	2.2
	19.14	-0.5	2.2
^{115}In(n,n')^{115m}In	3.3	-1.8	2.4
	11.22	1.4	2.7
	19.14	-0.4	2.8
^{238}U(n,f)	3.3	1.2	2.2
	11.22	3.6	2.2
	13.86	4.3	2.2
^{58}Ni(n,p)^{58}Co	6.56	0.9	2.5
	14.03	4.5	2.6
	21.50	7.2	3.0
^{56}Fe(n,p)^{56}Mn	3.3	-2.7	2.4
	11.22	-2.1	2.8
	19.14	-1.3	3.6
^{27}Al(n,α)^{24}Na	3.3	-4.4	2.6
	11.22	1.9	3.0
	19.14	0.8	4.7

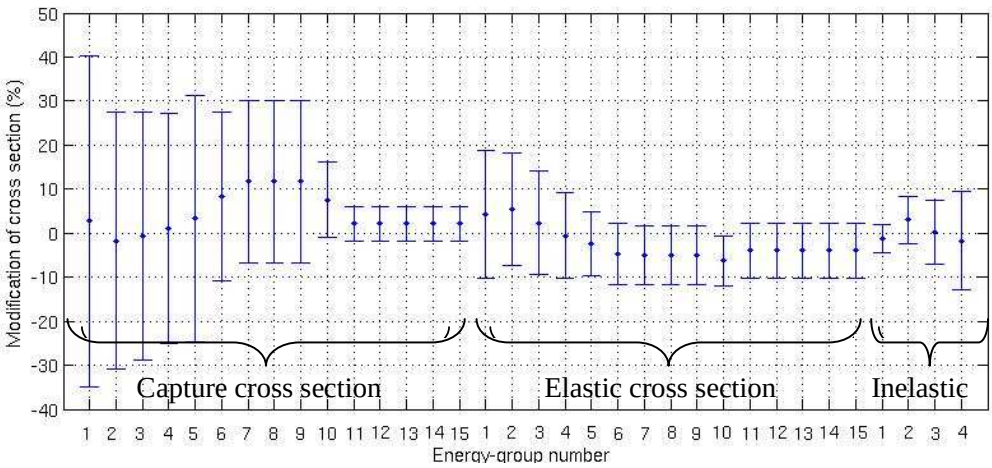

Figure 3. (a) PERLE core in EOLE vessel. (b) SS reflector blocks with measurement holes

Table III. ^{56}Fe Prior and Posterior uncertainty (%)

Energy (eV)	$(n,\gamma)^{prior}$	$(n,\gamma)^{post}$	$(n,n)^{prior}$	$(n,n)^{post}$	$(n,n')^{prior}$	$(n,n')^{post}$
1.9640E+07	20.0	18.8	8.0	7.3	10.0	1.6
6.0653E+06	14.6	14.6	8.0	6.4	10.0	2.7
2.2313E+06	14.1	14.1	7.0	5.9	10.0	3.6
1.3534E+06	13.1	13.0	6.0	4.9	10.0	5.6
4.9787E+05	14.1	14.0	4.0	3.6	-	-
1.8316E+05	10.0	9.6	4.0	3.5	-	-
6.7379E+04	10.0	9.2	4.0	3.4	-	-
2.4788E+04	10.0	9.2	4.0	3.4	-	-
9.1188E+03	10.0	9.2	4.0	3.4	-	-
2.0347E+03	7.3	4.3	4.0	2.8	-	-
4.5400E+02	6.0	2.0	4.0	3.1	-	-
2.2603E+01	6.0	2.0	4.0	3.1	-	-
4.0000E+00	6.0	2.0	4.0	3.1	-	-
5.4000E-01	6.0	2.0	4.0	3.1	-	-
1.0000E-01	6.0	2.0	4.0	3.1	-	-

Furthermore, Table IV points out that correlation between energy groups is strongly reduced (compared to prior correlation matrix and to BOLNA proposal [15]), thanks to PERLE integral measurements using various threshold reactions.

Table IV. Correlation matrix for ^{56}Fe inelastic scattering

Energy Group	JEFF3.1.1-p				BOLNA [15]			
	1	**2**	**3**	**4**	**1**	**2**	**3**	**4**
1	1.000	0.190	0.105	0.046	1.000	0.573	-0.498	-0.523
2	0.190	1.000	0.222	0.139	0.573	1.000	-0.721	-0.779
3	0.105	0.222	1.000	0.399	-0.498	-0.721	1.000	0.996
4	0.046	0.139	0.399	1.000	-0.523	-0.779	0.996	1.000

6. PROPAGATION OF NUCLEAR DATA UNCERTAINTIES

The proposed covariances JEFF3.1.1-p were used for Uncertainty propagation.

The uncertainty $\epsilon=\Delta R_k/R_k$ on a neutronics parameter R_k due to nuclear data is given at the first order by the "sandwich" rule [16]:

$$\frac{\Delta R_k}{R_k} = \left(S_k D S_k^t\right)^{1/2} \tag{6}$$

D: nuclear data multigroup covariance matrix
S_k: sensitivity vector of the parameter R_k to ND

The results of nuclear data uncertainty propagation on the multiplication factor Keff of commercial PWRs are summarized in Table V. Compared to JEFF3.1.1-p calculation, the BOLNA uncertainty is underestimated for ^{235}U fission and overestimated at thermal energies for $^{235}\nu$ component. Table V points out that Keff prior uncertainty is reduced using JEFF3.1.1, from 760 pcm to 570 pcm, thanks to the use of targeted integral experiments in ^{235}U ND evaluation.

Table V. Uncertainty (pcm) on calculated Keff of a PWR

Isotope	Reaction	BOLNA	JEFF3.1.1
^{235}U	(n,f)	120	290
	ν	600	310
	(n,γ)	140	130
	(n,f)-(n,γ)	120	-
^{238}U	(n,f)	30	
	ν	90	
	(n,γ)	290	
	(n,n')	140	
^{16}O	(n,α)	240	110
H_2O	(n,γ) + (n,n)	44	
Total		760	570

7. SENSITIVITY STUDIES AND REPRESENTATIVITY FACTOR

Sensitivity studies were performed to optimize the 'representativity' of LWR mock-up experiments in EOLE :
- BASALA experiment to simulate BWR cores [17],
- EPICURE experiments to mock-up PWR cores.

The Representativity r_{AE} of an experiment E, whose measurement value is $I_E \pm \delta$ with respect to the application A, is given by the following expression [18]:

$$r_{AE} = \frac{\left(S_A^+ \, DS_E\right)}{\varepsilon_A \cdot \varepsilon_E} \qquad (7)$$

This correlation coefficient, r_{AE} represents the contribution of information provided by the Experiment common with the Application for a given design parameter I_A. In the state of the art, a satisfactory value of representativity is greater than 0.9. This value allows a significant reduction in the prior calculation uncertainty ϵ_A due to nuclear data.

As an example, the representativity theory was used to optimize various EPICURE-type experiments (UO_2 Zy4-clad pins, 3.7%^{235}U enrichment) to mock-up PWR fresh cores at Hot Zero Power conditions.
Sensitivity profiles were calculated by APOLLO2 transport calculations in SHEM-281group. Sensitivity of the multiplication factor to ^{238}U capture cross section is plotted in Fig. 4 : comparison in EPICURE-UH1.2 and PWR cores points out the similarity of profiles, except in

thermal energy range due to spectral shift with temperature in PWR. Fig. 5 shows the sensitivity profiles to ^{235}U fission cross section.

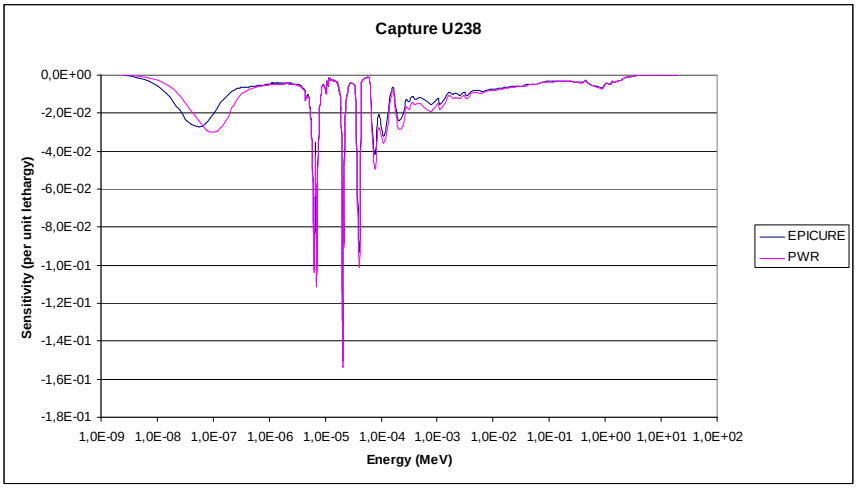

Figure 4. Keff Sensitivity profile to ^{238}U capture cross section.

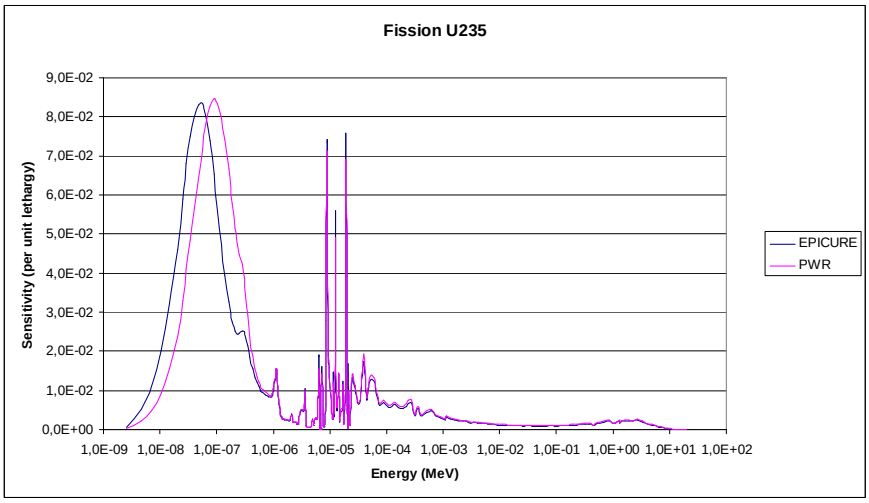

Figure 5. Keff Sensitivity profile to ^{235}U fission cross section.

Considering the Keff integral parameter and using formula (7), the representativity factor of EPICURE UH1.4 configuration to various PWR concepts is:

r = 0.984 for current PWR enrichment (e^{U235} = 4.0%)

r = 0.945 for Advanced PWRs (e^{U235} = 8.6%)

8. TRANSPOSITION OF EXPERIMENT RESULTS TO APPLICATION

The transposition of integral measurements results to Safety-Criticality applications is a major topic because it enables the determination of reliable posterior C/E Bias and bias Uncertainty. The automated transposition from representative ICSBEP Benchmarks to a specified Application (characterized by its sensitivity vector S_A) was recently implemented in the RIB tool [19].

The posterior uncertainty, accounting for selected representative integral experiments, is obtained as :

$$\varepsilon_A^{*\,2} = S_A^T \cdot D_\sigma^* \cdot S_A = S_A^T \cdot D_\sigma \cdot S_A - S_A^T \cdot D_\sigma \cdot S_E \cdot \left[S_E^T \cdot D_\sigma \cdot S_E + D_E\right]^{-1} \cdot S_E^T \cdot D_\sigma \cdot S_A \qquad (8)$$

This method was used in the challenging criticality problem of MOX damp powders encountered in the MELOX fuel fabrication plant [2]. We selected two representative experiments, the ERASME/S experiment in EOLE (HCPWR-type 11%Pu V_{H2O}/V_{MOX}=0.5) and the 1A' experiment in MASURCA (U-Pu metallic fuel, 25%Pu).

Each experiment i affects the best estimate value $I_A^* = I_A\,(1 + \Delta I_A)$ and the associated uncertainty ε_A^* by its weight w_i (depending on experimental uncertainty δ_i: δ_{ERASME}=400 and $\delta_{1A'}$=500pcm) :

$$w_i = \frac{1}{1+\delta_i^2/\varepsilon_{E_i}^2} \qquad (9)$$

The calculation error ΔI_A is derived, from the C/E bias $\Delta I_E = \frac{I_E^m - I_E}{I_E}$, as follows :

$$\frac{\Delta I_A}{\varepsilon_A} = \frac{1}{1-\hat{r}_{1,2}^2 \cdot w_1 \cdot w_2}\left[r_{A,1} \cdot w_1 \cdot \frac{\Delta I_{E_1}}{\varepsilon_{E_1}} + r_{A,2} \cdot w_2 \cdot \frac{\Delta I_{E_2}}{\varepsilon_{E_2}} - r_{A,1} \cdot w_1 \cdot w_2 \left(r_{A,2} \cdot \frac{\Delta I_{E_1}}{\varepsilon_{E_1}} + r_{A,1} \cdot \frac{\Delta I_{E_2}}{\varepsilon_{E_2}}\right)\right] \qquad (10)$$

When using two experiments, general formula (8) gives the following posterior uncertainty ε^*_A :

$$\frac{\varepsilon_A^{*2}}{\varepsilon_A^2} = 1 - \frac{1}{1-\hat{r}_{1,2}^2 \cdot w_1 \cdot w_2}\left(r_{A,1} \cdot \sqrt{w_1} - r_{A,2} \cdot \sqrt{w_2}\right)^2 - \frac{2}{1+\hat{r}_{1,2} \cdot \sqrt{w_1 \cdot w_2}} \cdot r_{A,1} \cdot r_{A,2} \cdot \sqrt{w_1 \cdot w_2} \qquad (11)$$

The representativity factors and the transposition of the two selected experiments to the MOX powder applications are summarized in Table VI.

Table VI. Representativity and calculation uncertainty for damp MOX powders

Application	12.5% PuO_2 powder	30% PuO_2 powder	100% PuO_2 powder
ERASME/S Representativity	0.987	0.907	0.711
1A' Representativity	0.882	0.964	0.929
Prior uncertainty ε_A (pcm)	1310	1340	1585
Post uncertainty ε^*_A (pcm)	397	450	737

This transposition method, based on realistic ND covariances such as our JEFF3.1.1-p proposals, is also currently used to assess the uncertainty on the challenging calculations of the RJH new irradiation reactor [20], characterized by 20% enrichment (U_3Si_2 fuel plates). Using the targeted VALMONT oscillation experiment in MINERVE reactor [21], the posterior Keff uncertainty associated with JEFF-3.1.1 calculation is reduced to an acceptable value : ± 610 pcm (1σ).

9. CONCLUSION

S/U studies are more and more used in Reactor Physics and Safety-Criticality. However, the reliability of study results relies strongly on the ND covariance relevancy. Our method derives the real uncertainty associated with each evaluation from calibration on targeted integral measurements. These realistic covariance matrices allow reliable JEFF3.1.1 calculation of prior uncertainty due to nuclear data, as well as uncertainty reduction based on representative integral experiments, in challenging design calculations such as GEN3 and RJH reactors.

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