EPJ Web of Conferences **106**, 04015 (2016)
DOI: 10.1051/epjconf/201610604015

Generation of ^{238}U Covariance Matrices by Using the Integral Data Assimilation Technique of the CONRAD Code

E. Privas[1,a], P. Archier[1], D. Bernard[1], C. De Saint Jean[1], C. Destouche[1], P. Leconte[1], G. Noguère[1], Y. Peneliau[1], and R. Capote[2]

[1] CEA, DEN Cadarache, 13108 Saint Paul Les Durance, France
[2] NAPC-Nuclear Data Section, International Atomic Energy Agency, P.O. Box 100, Vienna A-1400, Austria

Abstract. A new IAEA Coordinated Research Project (CRP) aims to test, validate and improve the IRDF library. Among the isotopes of interest, the modelisation of the ^{238}U capture and fission cross sections represents a challenging task. A new description of the ^{238}U neutrons induced reactions in the fast energy range is within progress in the frame of an IAEA evaluation consortium. The Nuclear Data group of Cadarache participates in this effort utilizing the ^{238}U spectral indices measurements and Post Irradiated Experiments (PIE) carried out in the fast reactors MASURCA (CEA Cadarache) and PHENIX (CEA Marcoule). Such a collection of experimental results provides reliable integral information on the (n,γ) and (n,f) cross sections. This paper presents the Integral Data Assimilation (IDA) technique of the CONRAD code used to propagate the uncertainties of the integral data on the ^{238}U cross sections of interest for dosimetry applications.

1. Introduction

Covariance matrices for the neutron cross sections are produced via two types of information: microscopic experiments (such as transmission, capture and fission reaction yields measured in dedicated facilities) and integral experiments (such as ICSBEP benchmarks [1]). An Integral Data Assimilation (IDA) method was implemented in the nuclear data code CONRAD [2, 3] to account for a large kind of existing results provided by specific integral experiments. Performances of the IDA technique were demonstrated via pile-oscillation measurements carried out in the pool-type reactor MINERVE of the CEA Cadarache [4].

In the present work, two types of experiments are taken into account to generate covariance matrices for the ^{238}U capture and fission cross sections above $E > 1$ keV. For the capture reaction, we use the PROFIL and PROFIL-2 experiments carried out in the PHENIX reactor of CEA Marcoule. For the fission reaction, we use spectral indices measured in the SFR configuration ZONA2A of the MASURCA reactor located at the CEA Cadarache. Experimental analysis obtained with the ^{238}U evaluation of the

[a] Corresponding author: edwin.privas@cea.fr

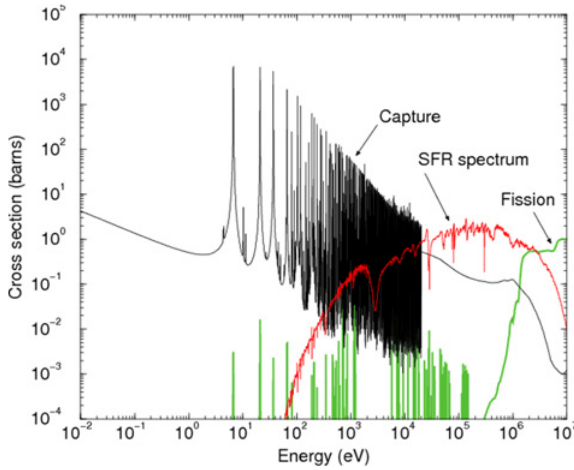

Figure 1. The ^{238}U capture and fission cross sections and a SFR lethargy neutron spectrum.

JEFF-31 and JEFF-311 libraries are reported in Refs. [5–7]. Preliminary results obtained with a new evaluation, produced in the frame of an IAEA consortium, were presented in the NEMEA-7 workshop [8, 9]. This evaluation is labeled "ib33". Figure 1 illustrates the fission and capture cross sections.

This paper is structured as follows. The second section presents the equations involved in the Integral Data Assimilation procedure of the CONRAD code. The integral benchmarks used in this work are described in the third section. The resulting variances and covariances on the capture and fission cross sections are given in Sect. 4.

2. Governing Equations

For the evaluation of nuclear data, model parameters and multi-group cross-sections are routinely inferred from iterative maximum likelihood methods. An overview of the current knowledge for computing best-estimate predictive results using experimental information is given in Ref. [10].

By using the generalization of the Bayes' theorem to continuous variables, a fitting procedure can be seen as an estimation of the first two moments of the posterior probability density $P(\vec{x}|\vec{E}, U)$, where $\vec{x}$ denotes the parameters (model parameters or neutron cross-sections), $\vec{E}$ are the experimental integral results and U represents the "prior" information. To solve this problem, one has to make some assumptions on the prior probability distribution. According to the principle of maximum entropy, a multivariate joint normal distribution is chosen for the probability density $P(\vec{x}|U)$. Thanks to the Laplace approximation, the evaluation of the posterior expectation $\vec{x}_m$ and of the covariance M_x is achieved by finding the minimun of the following cost function (generalized least-square):

$$\chi^2_{GLS} = (\vec{x} - \vec{x}_m)^T M_x^{-1} (\vec{x} - \vec{x}_m) + \left(\vec{C} - \vec{E}\right)^T M_E^{-1} \left(\vec{E} - \vec{C}\right). \tag{1}$$

In the CONRAD code, a Gauss-Newton iterative scheme is used to solve Eq. (1). The latter leads to the system of equations:

$$M_x^{(n+1)} = \left[\left(M_x^{(0)}\right)^{-1} + G_x^{(n)^T} M_E^{-1} G_x^{(n)}\right]^{-1}, \tag{2}$$

and

$$\vec{x}^{(n+1)} = \vec{x}^{(0)} + M_x^{(n+1)} G_x^{(n)^T} M_E^{-1} \left[\vec{E} - \vec{C}^{(n)} - G_x^{(n)} \left(\vec{x}^{(0)} - \vec{x}^{(n)}\right)\right], \tag{3}$$

in which $\vec{x}^{(0)}$ contains the prior parameters and $M_x^{(0)}$ represents the associated covariance matrix. The matrix $G_x^{(n)}$ contains the partial derivatives at the n^{th} iteration:

$$G_{x_{i,j}}^{(n)} = \left(\frac{\partial C_i^{(n)}}{\partial x_j^{(n)}} \right), \tag{4}$$

where $C_i^{(n)}$ is the calculated theoretical result of the i^{th} experimental value. This adjustement procedure can be applied to differential cross section measurements and integral measurements. For the Integral Data Assimilation procedure, the vector $\vec{E}$ contains integral data and the vector $\vec{C}$ contains the corresponding theoretical results calculated via deterministic or Monte-Carlo transport codes. The derivative matrix G_x can be calculated by direct perturbations of $\vec{x}$ or via more elaborated perturbation formalisms, such as those implemented in the code PARIS [11].

In the present work, a so-called "retroactive" analysis is performed. This method permits one to generate realistic uncertainties for existing neutron cross section evaluations by taking into account all sources of experimental uncertainties. Such an easy-to-use analytic treatment was implemented within the SAMMY code. Its uncertainty propagation methodology was designed to "retroactively" generate a covariance matrix for already evaluated resonance parameters. A similar treatment was developed in the CONRAD code and generalized to the Integral Data Assimilation procedure [12]. Here, the procedure consists of calculating the matrix elements of the neutron cross sections covariance under the assumption $\vec{C} = \vec{E}$. Equation (2) becomes:

$$M_x = \left[\left(M_x^{(0)} \right)^{-1} + G_x^T M_E^{-1} G_x \right]^{-1}. \tag{5}$$

The marginalization procedure of the CONRAD code can be added to account for the uncertainties of the nuisance parameters θ. In the Integral Data Assimilation procedure, the nuisance parameters are mainly the normalization factors. The final covariance matrix between the model parameters or the neutron cross sections is given by [13]:

$$\Sigma = M_x + (G_x^T G_x)^{-1} G_x^T G_\theta M_\theta G_\theta^T G_x (G_x^T G_x)^{-1}, \tag{6}$$

where the matrix G_θ contains the partial derivatives:

$$G_{\theta_{i,j}} = \left(\frac{\partial C_i}{\partial \theta_j} \right). \tag{7}$$

3. Description of the Integral Benchmarks

The integral benchmarks selected for this work provide integral information on the ^{238}U capture and fission cross sections over a fast neutron spectrum. The integral results are also sensitive to the ^{235}U fission cross sections. Its contribution is introduced as a "latent" parameter. This term reflects the fact that such parameter is really there, but it cannot be observed directly.

3.1 The PROFIL and PROFIL-2 Experiments

The PROFIL and PROFIL-2 experiments were performed four decades ago during the first cycles of the 250 MWe sodium-cooled fast reactor PHENIX. Figure 1 shows the typical fast neutron spectrum of PHENIX. The first program PROFIL consisted in an experimental pin placed in the middle of the PHENIX core with 46 isotopically enriched samples. The second program PROFIL-2 consisted in two experimental pins with 42 separate samples each. Those two pins were placed in a first ring assembly. Each irradiated pin contains three samples of ^{238}U. After irradiation, the neutron capture cross section can be deduced from the initial and final isotopic ratio (^{239}Pu/^{238}U). More details on the PROFIL experiments are given in Refs. [5, 6].

The interpretation is performed with the ERANOS code system. The main issue is the determination of the uncertainties. The experimental uncertainty on each isotopic ratio is very low (lower than 1%) because of the high accuracy achieved with the ICPMS measurements. The final uncertainties are dominated by the contribution of the normalization. The calculations are normalized via the ^{235}U fission cross section. In order to avoid a strong dependence of the normalization to the ^{235}U capture cross section, a new normalization procedure was performed by the marginalization technique implemented in the CONRAD code [14]. The isotopic ratio (^{235}U+^{236}U)/^{238}U characterizes the ^{235}U fission. It allows to determine a relative uncertainty of 2% on the calculated ratio (^{239}Pu/^{238}U).

3.2 Spectral Indices Measured in the SFR Configuration ZONA2A

A selected set of results for integral experiments performed in the MASURCA Mock-up (CEA Cadarache) was reported in Ref. [7]. The interpretation was performed with the ERANOS code. Results for ^{238}U(n,f)/^{235}U(n,f) spectral indices measured in the reference cores of several configurations (MASURCA-1A', MASURCA-1B, CIRANO-ZONA2A, CIRANO-ZONA2B and MUSE4) are given with a relative uncertainty ranging from 2.0% to 2.8%. All these indices were calculated by using the ^{235}U fission cross section as reference.

In the present work, we use the C/E value reported for the ZONA2A configuration carried out in the frame of the CIRANO program (1994–1997). The latter was designed to investigate Pu-burning fast reactors via the progressive substitution of fertile blankets by steel reflectors. The shape of the neutron spectrum in the PROFIL and CIRANO experiments are nearly similar. The experimental uncertainty quoted in Ref. [7] is 2.4%. By taking into account the uncertainty of the ^{235}U fission cross section, the global uncertainty reaches 3%.

4. Results and Discussions

4.1 Prior Covariance Matrices

The generation of neutron cross sections covariance matrices with the IDA technique requires prior information on the variances and covariances. We have used the covariance matrices compiled in the COMAC data base developed at the CEA of Cadarache. The methodology used to estimate multi-group covariances for some major isotopes used in reactor physics is presented in Ref. [15]. The latter relies on the description of the neutron induced reactions with nuclear reaction models. The Reich-Moore or Multi-Level Breit-Wigner approximations of the R-Matrix theory are used in the Resolved Resonance Range. The high energy part of the neutron cross sections are calculated with the TALYS code. The optimization of the model parameters and the propagation of the experimental uncertainties is performed with the CONRAD code. The last step consists of producing covariance matrices for the neutron cross sections by using the Model Parameter Covariance Matrix established with CONRAD.

A retroactive analysis in association with the marginalization procedure of the CONRAD code was applied to produce the covariance matrices for ^{238}U. Covariances obtained in the resonance range are mainly based on the transmission data measured by Olsen [16]. A relative uncertainty of 5% was taken to generate prior uncertainties for the radiation and neutron widths. For the fission widths, a relative uncertainty of 10% was applied to calculate prior information on the fission widths. The normalization and a "pseudo" background were included in the marginalization procedure. For the high energy range, optical and statistical model parameters were adjusted on the neutron cross sections of JEFF-311 by marginalizing the normalization of the total and partial cross sections.

Table 1. C/E results obtained for the PROFIL experiements and for the spectral indices measured in the ZONA2A configuration of MASURCA.

Benchmarks	Reaction	Uncertainty	JEFF-311	JEFF-311 with "ib33"
PROFIL, PROFIL-2	^{238}U(n,γ)	$\pm 2\%$	0.991	1.016
ZONA2A	^{238}U(n,f)	$\pm 3\%$	1.010	1.017

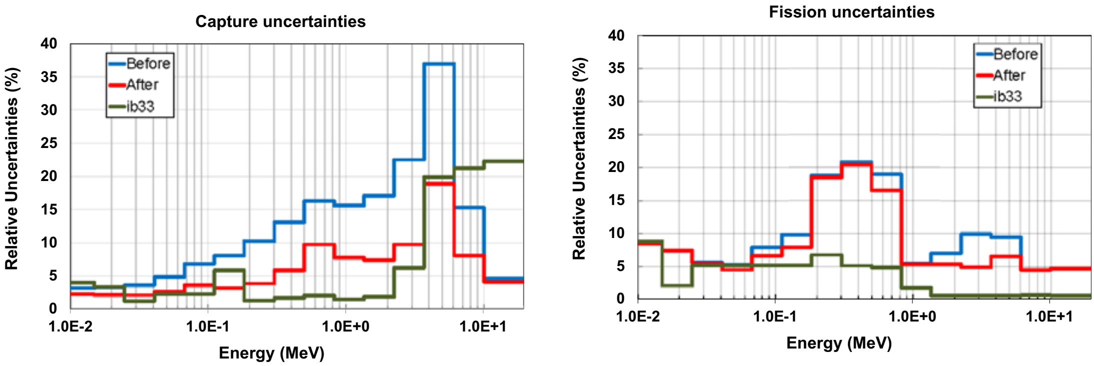

Figure 2. Prior and posterior relative uncertainties for the ^{238}U capture and fission cross sections above 1 keV.

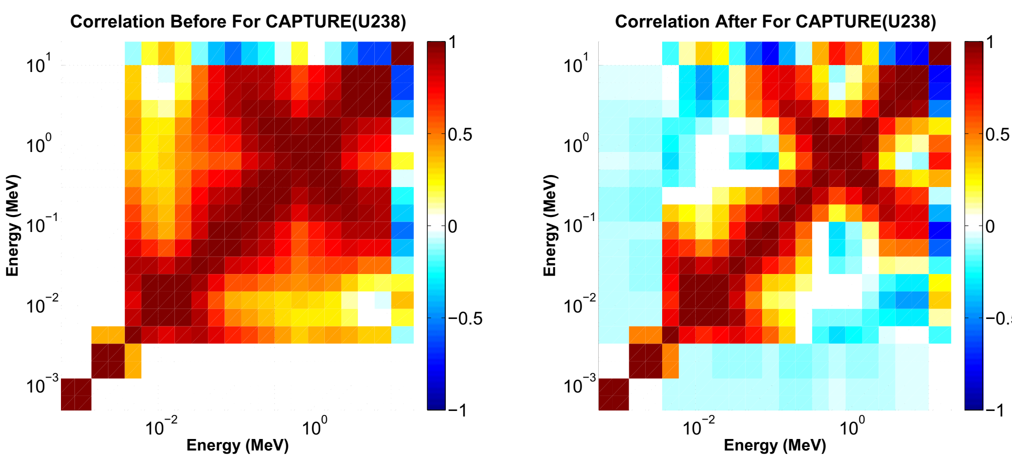

Figure 3. Prior and posterior correlation matrices for the ^{238}U capture cross sections above 1 keV.

4.2 Posterior Results

Results obtained for the integral benchmarks of interest for this work are reported in Table 1. For the PROFIL experiments, the C/E values for the different samples are lumped in a single average value.

The comparison of the C/E values shows the good performances of the "ib33" evaluation produced in the frame of an IAEA consortium. The C/E results remains within the limit of the quoted uncertainties. The good agreement with the spectral indices measured in the MASURCA facility is of great importance because the ^{238}U fission cross section of "ib33" follows the recommendation of the standard group of IAEA.

Owing to these results, a retroactive analysis can be safely applied to establish covariance matrices for the ^{238}U capture and fission cross sections. The IDA results are shown in Figs. 2 and 3 and are compared to ib33. As expected, the relative uncertainties on the capture and fission cross sections are significantly decreased within the energy range of interest for fast reactor applications. For the fission reaction, the large relative uncertainty close to 10% over the first-chance plateau reaches a more realistic uncertainty of 5%. The structures observed on the prior and posterior covariance matrices are also strongly modified. For the capture reaction, anti-correlations near 30 keV are created.

5. Conclusions

The present work shows the performances of the IDA technique implemented in the CONRAD code. Integral benchmarks, which were designed to investigate specific nuclear data, lead to significant reductions of the uncertainties on the neutron cross sections. Improved variances and covariances can be achieved thanks to the retroactive analysis in association with the marginalization procedure. In this work, we obtain an uncertainty of 5% for the ^{238}U fission cross section in the first-chance plateau and an uncertainty lower than 5% below 300 keV for the capture cross section. These techniques will provide valuable integral feedbacks in order to improve the future ^{238}U evaluation of IAEA.

References

[1] J. Blair Briggs, International Handbook of Evaluated Criticality Safety Benchmark Experiments, OECD/Nucl. Sci. (2011)
[2] C. De Saint Jean et al., Status of CONRAD, a nuclear reaction analysis tool, in: Proc. of the International Conference on Nuclear Data for Science and Technology, ND2007, France (2007)
[3] P. Archier et al., CONRAD Evaluation Code: Development Status and Perspectives, in: Proc. of the International Conference on Nuclear Data for Science and Technology, ND2013, New-York, USA 2(013)
[4] G. Noguere et al. Nucl. Inst. Meth. A **629**, 288 (2011)
[5] J. Tommasi et al., Nucl. Sci. Eng. **154**, 119 (2006)
[6] J. Tommasi et al., Nucl. Sci. Eng. **160**, 232 (2008)
[7] J-M. Ruggieri et al., JEFF-31 nuclear data validation for fast reactor physics, in: Proc. of the International Conference on Physics and Technology of Reactors and Applications, PHYTRA, Marakech, Morocco (2007)
[8] R. Capote et al., Evaluation of neutron induced reactions on ^{238}U nucleus, in: Proc. of the NEMEA-7 workshop, Geel, Belgium (2013)
[9] R. Capote et al., EPJ Web of Conferences, **69**, 00008 (2014)
[10] D.G. Cacuci and M. Ionescu-Bujor, Nucl. Sci. Eng. **165**, 18 (2010)
[11] R. Le Tellier et al.., Nucl. Sci. Eng. **167**, 209 (2011)
[12] B. Habert et al., Nucl. Sci. Eng. **166**, 276 (2010)
[13] G. Noguere et al., Nucl. Sci. Eng. **172**, 164 (2012)
[14] E. Privas et al., Experimental uncertainty estimation in PROFIL and PROFIL-2 sample irradiation experiments in PHENIX, in: Proc. of the PHYSOR-2014 International Conference, Kyoto, Japan (2014)
[15] C. De Saint Jean, Estimation of multi-group cross section covariances for ^{235,238}U, ^{239}Pu, ^{241}Am, ^{56}Fe, ^{23}Na and ^{27}Al, in: Proc. of the PHYSOR-2012 International Conference, Knoxville, USA (2012)
[16] D.K. Olsen *et al*. Nucl. Sci. Eng. **62**, 479 (1977)