Fission Product Yields Covariance Generation Methodologies and Uncertainty Propagation Using the URANIE Platform

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ABSTRACT

In modern nuclear technology, integral reactor parameter uncertainty evaluation plays a crucial role for both economical and safety purposes. Recent safety-by-design standards require strict margins of uncertainty, then intense activities of verification and validation are therefore necessary to ensure the precision needed for safe and sustainable modern technologies exploitation. The uncertainty associated to nuclear data plays a relevant role in this sense and many efforts have been recently spent to improve the whole input chain we provide to reactor code design procedures. Since some of them are not sufficiently detailed or even do not exist in modern nuclear data libraries yet, in this work we propose a methodology to generate, test and propagate covariance matrices for fission product yields. The main goal is to reproduce the JEFF-3.1.1 fission yields library and find associated covariances to be propagated using Monte Carlo and deterministic techniques in burn-up test-case calculations. Some results on the reactivity and decay heat uncertainty are presented for simple cases. Finally, a whole reactor geometries such as the Jules Horowitz Reactor (JHR), a material testing reactor under construction at CEA-Cadarache, is treated.

Key Words: **Fission Yields, Covariance, Uncertainty Propagation**

1. INTRODUCTION

Nuclear data improvement gained an outstanding importance in the scientific community in the last decades, becoming a prior need in advanced nuclear system design. Future innovative nuclear facilities, to be safe, environmental sustainable and economically competitive, must satisfy strict safety-by-design standards, requiring highly accurate engineering parameter uncertainty estimation. Several efforts have been spent in this direction for cross section uncertainty reduction, to improve the basic nuclear data knowledge to be applied in nuclear design calculation tools. It was in fact quickly recognized that the value and the credibility of any uncertainty analysis was strictly dependent on the scientific quality of variances and correlations [1, 2] associated to basic input data. Supplying complete and consistent covariance information gives in fact the opportunity to estimate realistically the interval of confidence on integral reactor parameters, providing reliable indications of the most significant sources of uncertainty.

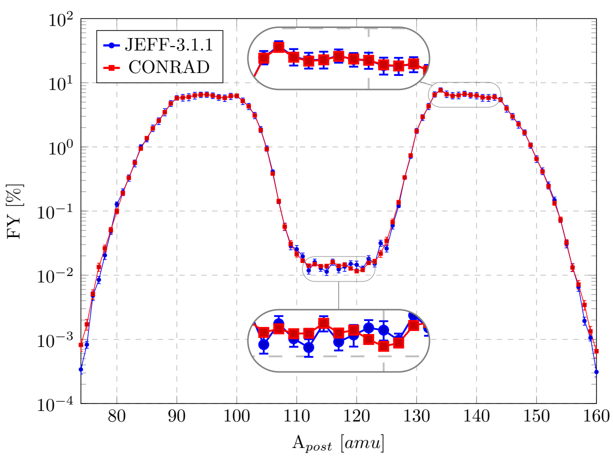
In modern nuclear data libraries such as JEFF-3.1.1 or ENDF/B-VII.1 no fission yield correlations are available. The main goal of the present work is to propose a methodology to evaluate and test covariance matrices for fission product yields, providing results on reactivity loss and decay heat uncertainty for simple reactor geometries. Covariance matrices are generated using the CONRAD code [3] (COde for Nuclear Reaction Analysis and Data assimilation) developed at CEA-Cadarache. Bayesian techniques are used to adjust the parameters of the semi-empirical models commonly used to evaluate fission yields in present libraries. The Generalized Least Square Method (GLSM), available in CONRAD, yields simultaneously best estimates and covariance matrices that can be provided to uncertainty propagation tools.
Since calculating exact sensitivity coefficients for the coupled Boltzmann-Bateman problem is not trivial, we decided to resort to two straightforward approaches. The former relies on a deterministic linearized calculation of FY sensitivity coefficients by simple direct perturbations. The latter consists in a Monte Carlo uncertainty propagation technique, which is quite straightforward to set up and which gives reliable results if the sample size is sufficiently large. To achieve that, we used the URANIE platform [4], a set of sensitivity and uncertainty estimation libraries written at CEA and based on ROOT, (a framework developed at CERN). The two methods have been compared for simple geometries, propagating covariances for the most important fissioning systems for practical purposes. The impact of FY covariances will be also discussed for a real case, such as the Jules Horowitz Reactor (JHR), under construction at CEA Cadarache.

2. FISSION YIELDS COVARIANCES GENERATION

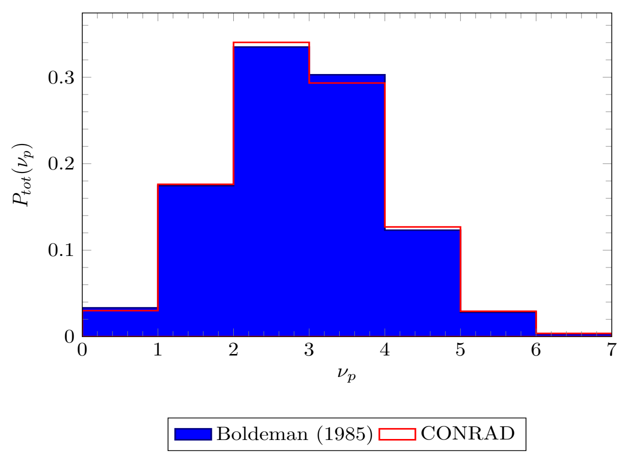
Fission product yields (FY) are fundamental nuclear data for burn-up calculations, but also to evaluate decay heat, shielding, dosimetry, fuel handling, waste disposal and safety [5]. Nowadays full uncertainty information are not available in the actual nuclear data repositories and the nuclear community expressed the need for full fission yield covariance matrices to be able to produce inventory calculation results, taking into account complete uncertainty data [6].
The main objective of the present work is not to perform a new FY evaluation, but, instead, to achieve a satisfactory representation of the existing evaluated fission product yield data collected in the JEFF-3.1.1 library (average values and variances), adopting the same nuclear models used in such evaluation [5].

2.1. Covariance Matrix Generation Procedure

To achieve JEFF-3.1.1 representation, we performed a Bayesian model parameters adjustment through the GLSM (Generalized Least Square Method) [3, 7, 8] available in CONRAD. FYs can be in fact represented by semi-empirical models based on physical assumptions for mass, isotopic and isomeric distributions (see Reference [5, 9, 10] for further details).
To calculate mass fission yields, we used a convolution of the Brosa fission modes [11] with a simplified model to describe prompt neutron distribution probabilities [9]. Isotopic fission yields are obtained using Wahl systematics [12] and the isomeric ratios are calculated resorting the Madland and England model [13]. JEFF fission yields average values have been reproduced adjusting model parameters on the evaluated FY library, which has been taken as a pseudo-experimental knowledge in the Bayesian learning process. In the GLS procedure completely independent experiments for miscellaneous quantities such as the total prompt neutron emission probability distribution and the average number of prompt neutrons emitted have been considered and well represented by the models.



(a) ^{235}U mass FY distribution



(b) ^{235}U total $P(\nu_P)$ distribution

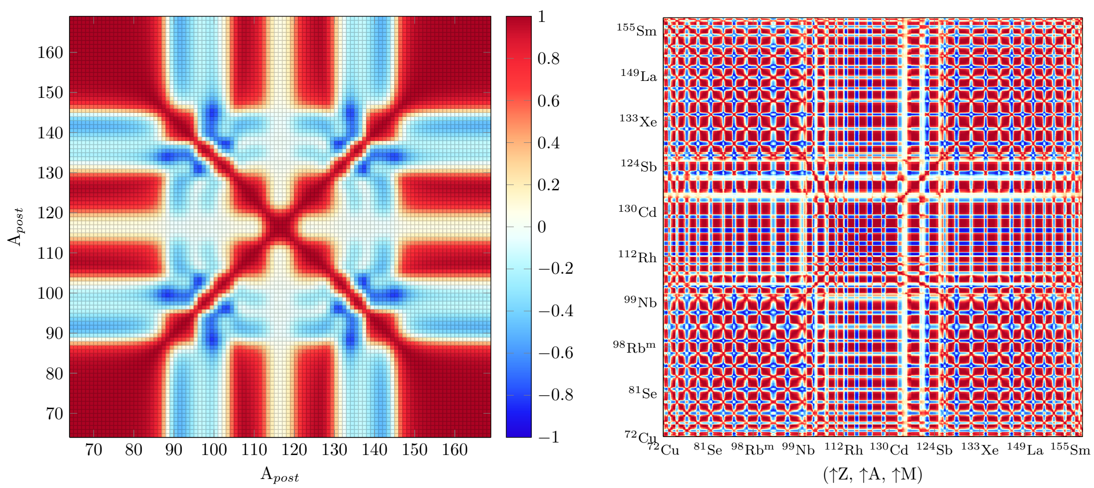
Figure 1. Comparison between JEFF-3.1.1 and CONRAD mass FY distribution for ^{235}U(n_{th}, f) (left). FY model parameters adjusted by CONRAD can also represent quite well experimental data on the total prompt neutron emission probability (right).

In Figure 1(a) the mass FY distribution for the thermal fission of ^{235}U is presented. JEFF-3.1.1 average values are nicely reproduced by CONRAD, which provides also a satisfactory comparison to experimental data on the total prompt neutron emission probability distribution, shown in Figure 1(b).
To be close also to JEFF-3.1.1 FY uncertainties, providing covariances truly representative of the existing evaluation, analytical marginalization techniques [14] have been employed to introduce systematic errors on model parameters. Evaluated JEFF-3.1.1 data and independent experiments were simultaneously and consistently represented by CONRAD for several fissioning systems such as ^{235}U(n_{th}, f), ^{239}Pu(n_{th}, f), ^{241}Pu(n_{th}, f), ^{238}U(n_{fs}, f) (see Reference [9, 10] for further details). This induced us to consider the covariance information coming from the GLS adjustment process suitable to be pre-

liminarily associated to the JEFF-3.1.1 FY library as additional uncertainty information. In the next section some results on FY covariance matrices generated by CONRAD will be briefly presented.

2.2. Covariance Matrix Results

The procedure presented so far allowed us to have model parameters best estimates and covariances which generates FY quite representative of JEFF-3.1.1 library. They showed furthermore a satisfactory consistency with totally independent experimental values on fission miscellaneous quantities, such as the total prompt neutron emission probability. Hereinafter we provide some results limited to only some fissioning systems.



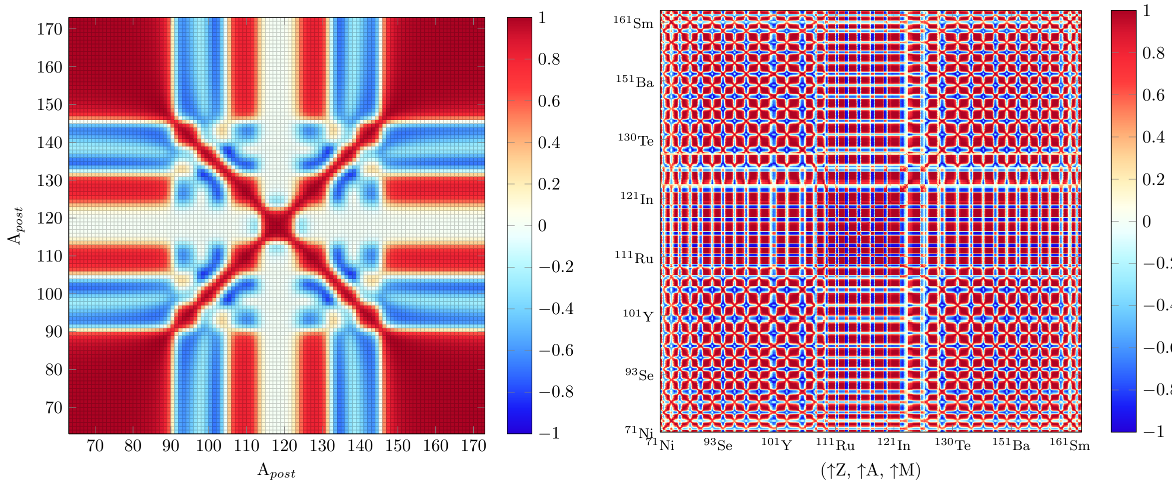
(a) Mass FY Correlation Matrix ^{235}U(n$_{th}$, f) (b) Isomeric FY Correlation Matrix ^{235}U(n$_{th}$, f)

Figure 2. Correlation matrices for mass (left) and isomeric (right) fission product yields for the thermal fission of ^{235}U. Only FY greater than 10^{-7} have been considered and ordered in ascending charge, mass and isomeric state.

In Figure 2 and 3 correlation matrices for mass and isomeric FY are shown respectively for the thermal fission of ^{235}U and for the fast fission of ^{238}U. Other fissioning systems have been considered [9] and decay heat uncertainty calculations have been performed using CYRUS [15] to test their effects on elementary fission [16].

3. UNCERTAINTY PROPAGATION FOR REACTOR PARAMETERS

Uncertainty propagation techniques allow us to evaluate fission yields effects on integral parameters of practical interest such as reactivity and decay heat. Since in a depletion calculation Boltzmann and Bateman equations are coupled, estimating reliable sensitivities is not trivial. We used essentially two



(a) Mass FY Correlation Matrix ^{238}U(n$_{fs}$, f) (b) Isomeric FY Correlation Matrix ^{238}U(n$_{fs}$, f)

Figure 3. Correlation matrices for mass (left) and isomeric (right) fission product yields for the fast fission of ^{238}U. Only FY greater than 10^{-7} have been considered and ordered in ascending charge, mass and isomeric state.

methods: the former is a straightforward direct perturbation deterministic technique, which calculates sensitivities by simple finite difference and finds reactor covariance matrices by the following well known equation [2]

$$\boldsymbol{C}_\pi = \boldsymbol{S}^t \boldsymbol{C}_{\boldsymbol{fy}} \boldsymbol{S} \tag{1}$$

where $\boldsymbol{C}_\pi$ is the covariance matrix for the reactor parameters of interest, $\boldsymbol{S}$ is the associated sensitivity matrix to fission yields and $\boldsymbol{C}_{\boldsymbol{fy}}$ is the FY covariance matrix generated by CONRAD. We decide to propose also a Monte Carlo uncertainty propagation method, which is better described in the following section.

3.1. Monte Carlo Uncertainty Propagation: the URANIE Platform

Monte Carlo uncertainty techniques consider nuclear data as random variables with a given distribution. We assumed fission yields distributed as Gaussian distributions, with only positive values. According to a sampling procedure based on a Cholesky decomposition of the CONRAD-generated covariance matrix $\mathbf{C}$ (see Reference [10] for further details), we can preserve correlations between fission yields and generate N sets of data that can be employed in an equal number of reactor calculations, where N is the sample size.

In Figure 4 we summarized the procedure we adopted to estimate uncertainties on neutronic parameters and on decay heat. Monte Carlo random samplings are made on independent fission yields, which give the probability for fission products having already emitted prompt neutrons, but before any radioactive decay. Cumulative fission yields, which are independent yields summations concerning fission products belonging to the same decay chain of the isotope we are considering, are successively obtained using the formalism of the Q-matrix [5]. The Q-matrix takes into account all the branching ratios between different isotopes. Once N sets of independent fission yields (IFY) are sampled using URANIE tools, an equal number of input files are generated for APOLLO2 [17] and MENDEL, the new depletion code under development at CEA.

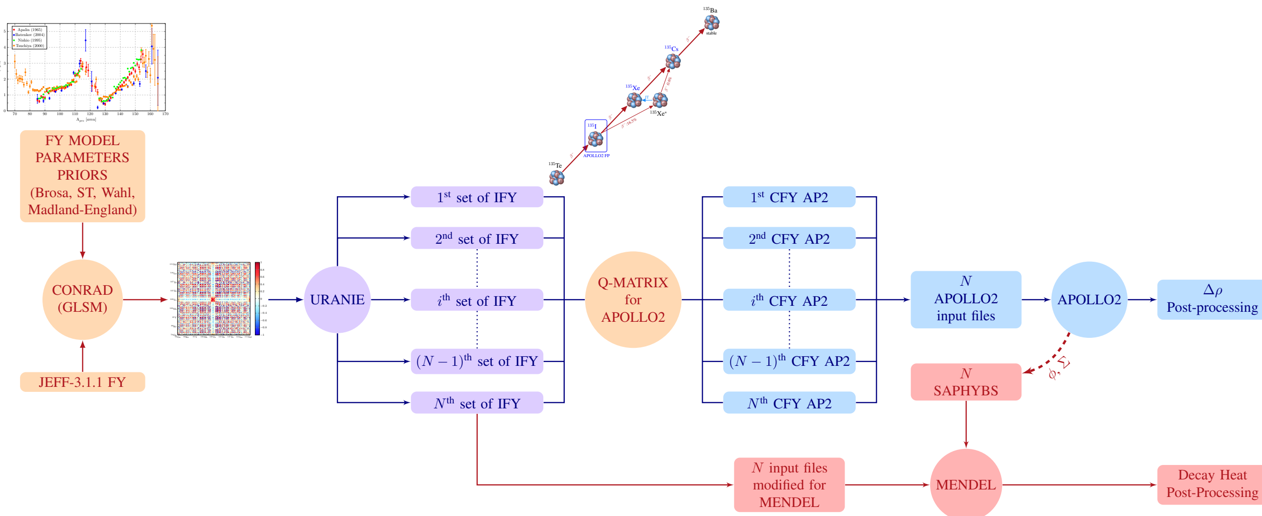


Figure 4. Monte Carlo error propagation flow chart for reactivity and decay heat uncertainty estimation using URANIE. With IFY we indicated independent fission yields, on the other hand we called CFY the cumulative ones.

Libraries for APOLLO2 are based on a selection of specific fission products which have important reactivity effects. Such isotopes are provided with particular fission yields which must be evaluated according to the decay chain dependences specified in the neutronic code library. If a certain isotope is in fact considered as relevant for neutronic purposes, belonging to the list of possible fission products in APOLLO2, the associated yield will be summation of its own independent plus all the other cumulative yields relative to any isotope not included in the APOLLO2 list which can decay directly towards the considered nuclide. For this reason, a special Q-matrix is evaluated to generate cumulative fission yields for APOLLO2. The neutronic calculation gives, using a quasi-static method, flux values and self-shielded cross sections at the different time steps that are provided to MENDEL, in order to perform decay heat calculations. Post-processing will allow to estimate uncertainties on quantities of interest.

3.2. Preliminary Results on Applications

Covariances and variances generated by CONRAD have been tested in uncertainty propagations for reactivity loss and decay heat. In Figures 5(a) and 5(b) the uncertainties due to the ^{235}U(n$_{th}$, f) FY are shown for a UOX-PWR-pin-cell. The comparison between a Monte Carlo uncertainty propagation using a 1000-dimensional sample and the simple application of the sandwich rule induced us to accept linear approximations as precise enough for our purposes. For the PWR-pin-cell problem in fact, FY uncertainty propagation do not present any non-linearity issues that can justify an extensive use of the Monte Carlo method, which is quite time consuming, even if it is straightforward to implement.

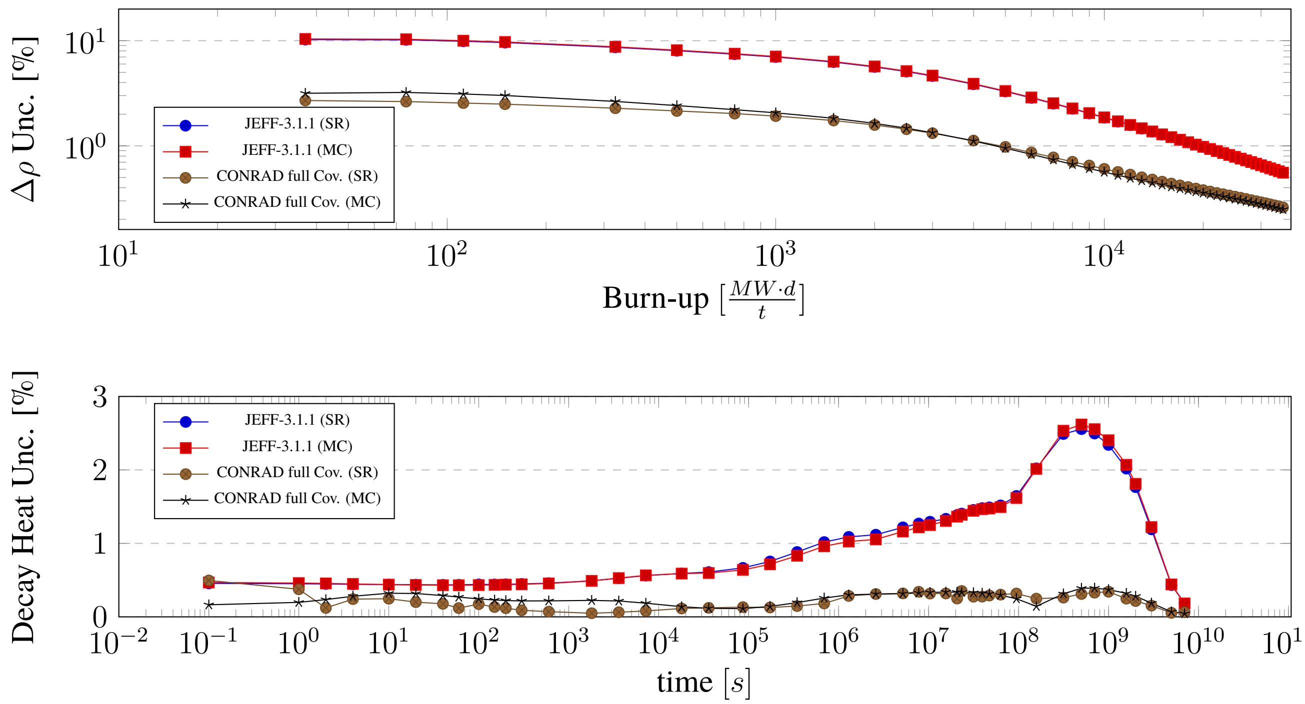


Figure 5. Reactivity loss (top) and decay heat (bottom) uncertainties for a UOX-PWR pin-cell. The propagation of JEFF-3.1.1 $U^{235}(n_{th}, f)$ FY uncertainties using a simple sandwich rule (SR) and the Monte Carlo propagation (MC) has been compared to what we obtained from FY uncertainties generated by CONRAD including correlations.

In Figures 6(a), 6(b) and 7 deterministic uncertainty propagations have been performed for simple PWR-pin-cell geometries to see the impact of correlations and to verify if the methodology adopted was actually able to reproduce the variances of the most problem-sensitive fission product yields evaluated in JEFF-3.1.1. CONRAD can reproduce quite well the variances contained in JEFF-3.1.1 adding correlations which have a significant impact on reactor parameter uncertainty, so further investigations are then necessary. Nevertheless, such covariance testing suggested us that the presented procedure can be actually applied to add covariance information to the existing libraries, even if a truly validation process is still desirable. It has to be emphasized that covariance matrices are not measurable quantities, so an effective and comprehensive validation process could not be possible. However, comparisons to experimental integral measurements and uncertainties might give us indications on how much the proposed covariances are representative of the knowledge we have on FY.

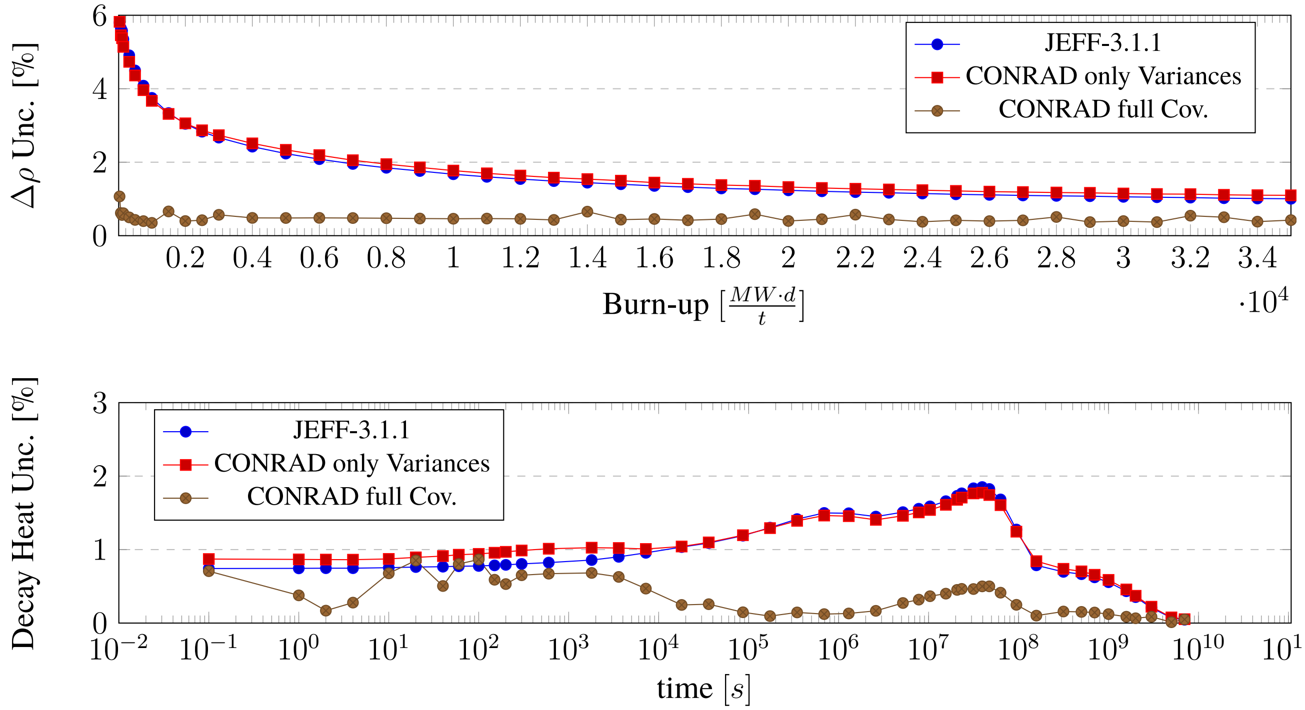


Figure 6. Reactivity loss (top) and decay heat (bottom) uncertainties for a PWR-MOX pin-cell. The propagation of JEFF-3.1.1 $Pu^{239}(n_{th}, f)$ FY uncertainties is compared to what we obtained from FY uncertainties generated by CONRAD, with and without correlations.

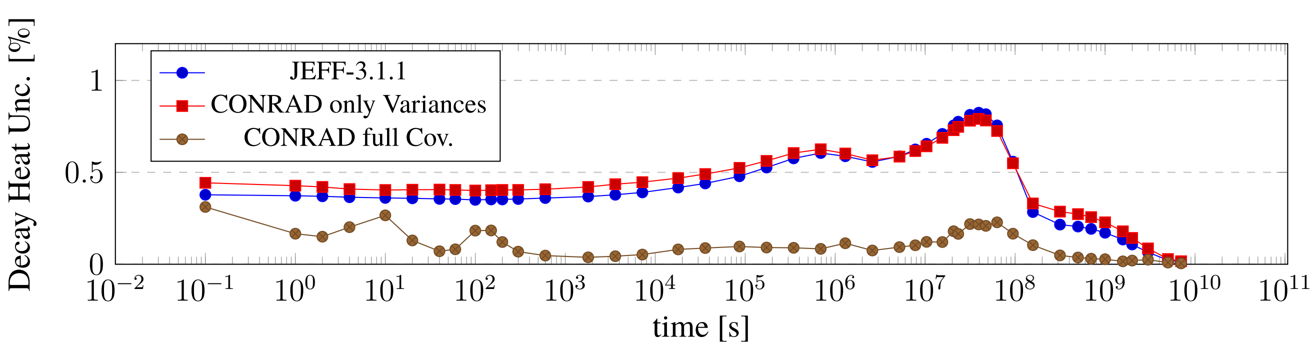


Figure 7. Decay heat uncertainty for a PWR-MOX pin-cell. The propagation of JEFF-3.1.1 $^{241}Pu(n_{th}, f)$ FY uncertainties on the decay heat is compared to what we obtained from FY uncertainties generated by CONRAD, with and without correlations.

In Figure 8 the impact of the $^{235}U(n_{th}, f)$ covariance matrix is shown for the reactivity loss of the JHR, confirming what we observed for simple geometry cases.

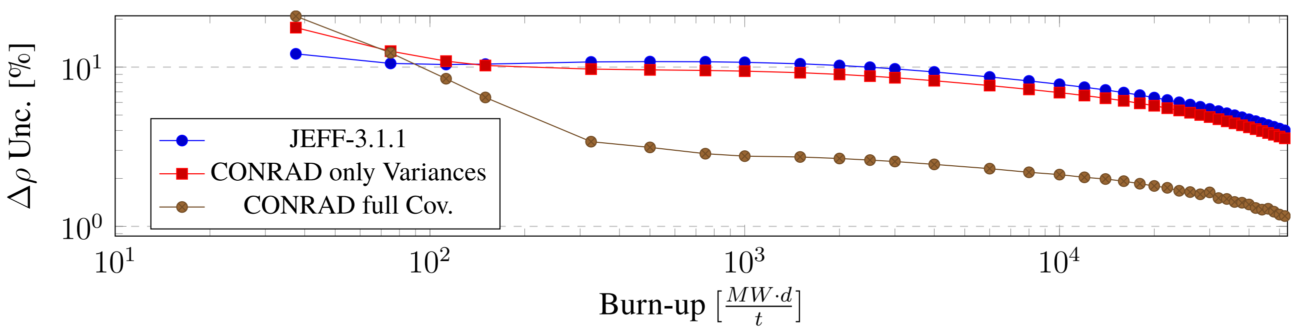


Figure 8. Relative reactivity loss uncertainty as a function of the burn-up for the JHR. The propagation of JEFF-3.1.1 $U^{235}(n_{th}, f)$ FY uncertainties on the reactivity loss is compared to what we obtained from FY uncertainties generated by CONRAD, with and without correlations.

4. CONCLUSION

FY covariance matrices have been consistently generated for several fissioning systems using the CONRAD code. The main goal was to reproduce JEFF-3.1.1 FY library and add covariance information. Such matrices have been tested in nuclear reactor applications for reactivity loss and decay heat uncertainty estimations. The results showed the possibility to effectively propose the CONRAD-generated matrices as additional uncertainty information to the existing evaluations. A comprehensive uncertainty validation should be performed. Only a detailed comparison with experimental integral measurements and related uncertainties might help to conclude if the proposed covariance information are actually representing the knowledge we have on FY data.

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