Comparisons between a priori Uncertainty Quantification and Calculation/Measurement Discrepancies Applied to the MERCI UO_2 Fuel Rod Decay Heat Experiment

S. Lahaye, T-D. Huynh, A. Tsilanizara, J-C. Jaboulay, S. Bourganel

Comparisons between a priori Uncertainty Quantification and Calculation/Measurement Discrepancies Applied to the MERCI UO_2 Fuel Rod Decay Heat Experiment.

S. Lahaye*, T.D. Huynh*, A. Tsilanizara*, J.C. Jaboulay*, S. Bourganel*

**CEA/DEN/DANS/DM2S/SERMA, F-91191 Gif sur Yvette Cedex, France*
sebastien.lahaye@cea.fr

INTRODUCTION

In 2008, an UO_2 fuel rod was irradiated up to ~ 3.5GWd/t_{HL} in the CEA/Saclay research reactor OSIRIS [1] through the MERCI experiment [2]. Some rod's pellets were analysed. Experimental results were obtained:

- fuel rod decay heat measurement by calorimetry (cooling times from 27 minutes to 42 days),
- evaluation of the amounts of some nuclei (U, Pu, Cs, Nd...) by isotopic dilution mass spectrometry,
- nuclide activities.

Comparison of type $(C - M)/M$ where C is the calculated decay heat and M the experimentally measured decay heat was reported in reference [3]. Neutronics flux was computed by CEA TRIPOLI-4 Monte-Carlo or APOLLO2 deterministic transport code system [4, 5]. Irradiation and cooling phases were simulated with CEA DARWIN/PEPIN2 [6] code system. Good agreements were globally shown between numerical simulation results and experimental measurements on total decay heat. Uncertainty propagation in this previous work [3] was established from Rebah's studies [7].

These last years, within the framework of supports to its industrial partners EDF and Areva, the CEA/DEN has implemented two different approaches to propagate nuclear data uncertainties to depletion code outputs. A direct forward deterministic perturbation method using sensitivity profiles was implemented in the French industrial depletion code system DARWIN/PEPIN2 [6]. Meanwhile, a propagation based on Monte Carlo correlated sampling [8] was achieved using the CEA uncertainty platform URANIE [9] and the new generation depletion code MENDEL [10].

Both methods will be described in this article.

Uncertainties on nuclear data (independent fission yields, multigroup microscopic cross sections, radioactive decay constants, radioactive decay branching ratio and radioactive decay energies) are propagated to decay heat and isotopic concentrations.

To match MERCI first study [3], flux computation is realized by APOLLO2. Furthermore, uncertainty quantification (UQ) is re-evaluated by both DARWIN/PEPIN2 and MENDEL codes. It is an important stage in the process of validating both depletion codes with their respective data library.

UNCERTAINTIES ON NUCLEAR DATA

Experimental results are given with a discrepancy, which is assimilated to the standard deviation of the random variable associated to the measurement value.

Uncertainty quantification on numerical simulations aims to compute the standard deviation of the outputs due to the uncertainties on the input data. In this paper, we consider only uncertainties due to nuclear data. Other potential sources of uncertainties are considered perfectly known (geometry, technological data...). Nuclear data without uncertainty data in the evaluation files are associated to a zero standard deviation (no uncertainty).

In the present work, DARWIN/PEPIN2 and MENDEL use uncertainty data from JEFF-3.1.1 [11] for independent fission yields, radioactive decay constants, radioactive decay branching ratios and radioactive decay energies. Table I shows the quantity of uncertain parameters taken from JEFF-3.1.1.

TABLE I. Number of physical parameters with non-zero uncertainty value in JEFF-3.1.1 evaluation.

evaluation	JEFF-3.1.1
Independent fission yields	33668
Radioactive decay constant	3204
Radioactive branching ratios	505
Radioactive decay energies	1554

No correlations are considered between different physical quantities. Radioactive decay periods and radioactive decay energies are two by two independent. Radioactive decay branching ratios are correlated in such a way that the sum of branching ways is equal to 1 (correlation matrix).

For independent fission yields, MENDEL and DARWIN/PEPIN2 can choose different models: no correlation between yields, normalization (sum of yields equal to a constant for each fissile systems) or correlations taking into account the mass yields constraints [12].

Uncertainties for microscopic multigroup cross sections are taken from the COMAC data base [13]. COMAC matrices describe correlations between partial cross sections for one given isotope, and between groups for one given cross section. Data between two distinct nuclei are not correlated. Multigroup data are directly taken into account in URANIE sampling, and multigroup samples are used in MENDEL, while one-group variance and correlations on monocinetic reaction rates are calculated to be used by DARWIN/PEPIN2. It has been shown through inter-comparisons that the effect of the multigroup mesh rather than one group data is of second order.

UNCERTAINTY PROPAGATION METHODS

We describe briefly the propagation methods and hypotheses in this section. Further details will be given in full presentation.

Deterministic Method Used in DARWIN/PEPIN2

DARWIN/PEPIN2 propagates uncertainties from nuclear data to decay heat or isotopic concentrations using a direct forward first order perturbation method. With X the uncertain input variables and Y the uncertain outputs, we can use the following formula:

$$\mathrm{cov}(Y) = S_{Y/X}\mathrm{cov}(X)S_{Y/X}^{T} \qquad (1)$$

where $\mathrm{cov}(X)$ (resp. $\mathrm{cov}(Y)$) stands for the variance-covariance matrix for variable X (resp. Y) and $S_{Y/X}$ stands for the sensitivity matrix of Y regarding X.

The use of a direct forward first order perturbation method implies the hypothesis of linearity of the outputs (as a function of uncertain nuclear data). For small perturbations of the uncertain input parameters (limited to one standard deviation), this approximation is proved to be valid when comparing with propagation approaches not taking this linearity hypothesis, such as stochastic uncertainty propagation approach used in MENDEL.

The uncertainty propagation in DARWIN/PEPIN2 needs the same number of depletion calculations as the number of uncertain parameters for the calculation of sensitivity coefficients. This is performed in parallel mode by DARWIN/PEPIN2 through its INCERD module, which establish the sensitivity matrix before computing the interest output covariance through equation (1).

Stochastic Method Used in MENDEL

MENDEL propagates uncertainty using a correlated sample method. All realizations are generated with URANIE.

For this study, 2000 realizations generated by LHS sampling method were propagated. Most random variables are supposed to be Gaussian if the relative standard deviation is lower than 50% and are supposed to be Log-Normal in the other cases. Fission yields are always considered log-normal. Correlations are taken into account when available, through the use of importance sampling in URANIE.

The sampling method and hypotheses will be described in the full presentation.

DECAY HEAT UNCERTAINTY QUANTIFICATION

We compare numerical calculation discrepancy to decay heat measurements and uncertainty propagation results (likelihood) in Figs 1 and 2. The red plain lines show the $\frac{C-M}{M}$ relative discrepancy between mesurement (**M**) and calculations (**C**). For those computed values, uncertainty on nuclear data has not been taken into account. Grey domain marks an uncertainty zone of 2 standard deviation around the reference value (zero). Note that the decay heat measurement uncertainty is given to $\pm 1\%$ and is included to the grey domain definition.

This grey domain corresponds to a 97.7% likelihood if decay heat is considered to be Gaussian.

Both graphs are similar, and prove a rather good agreement between experimental data and computation. Indeed, for all considered cooling times (from 27 min to 42 days), the two standard deviation domain obtained by uncertainty quantification covers the decay heat discrepancy between experimental data and calculation results.

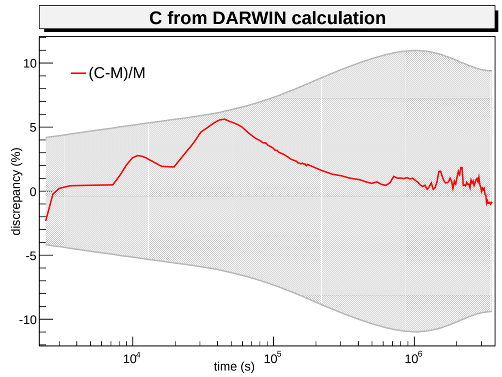

Fig. 1. In red, decay heat discrepancy between experiment data and DARWIN. In grey, the 2 standard deviation from deterministic method used in DARWIN/PEPIN2 domain.

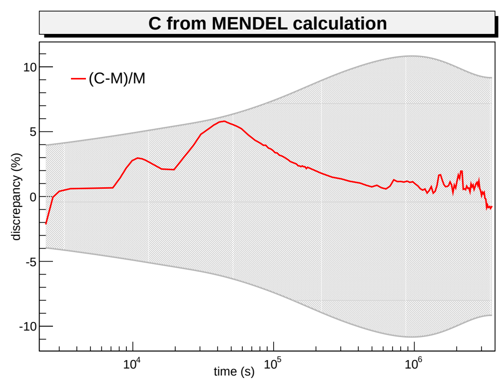

Fig. 2. In red, decay heat discrepancy between experiment data and MENDEL. In grey, the 2 standard deviation domain from stochastic method used in MENDEL.

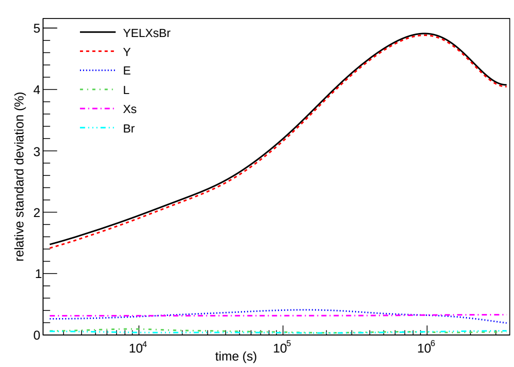

Fig. 3. Contributions of each type of nuclear data to total decay heat. Main contributors are fission yields uncertainties.

Contributions by type of nuclear data are shown in Fig. 3. The main contributor to decay heat uncertainty among nuclear data are the uncertainties due to independent fission yields (in red). We considered here for both codes that fission yields are normalized so that the sum for one fissile system is constant. We do not take here in consideration the correlations resulting from mass yields constraints [12]. For this small burnup, other contributors are negligible, especially radioactive decay branching ratios and radioactive decay periods.

Full presentation will analyze more precisely uncertainty quantification and sensitivity analysis, in particular the effects of correlation hypotheses on fission yields.

ISOTOPIC DENSITY UNCERTAINTY QUANTIFICATION

Experimental ratios of concentrations were measured for both heavy nuclides (U, Pu) and fission products (Cs, Nd). Those values, associated to experimental measurement error bars, enable to verify the actual burnup of the fuel rod, in particular when considering Neodymium isotopes.

We show in graph 4 experimental values and MENDEL uncertainty quantification propagation values for Neodymium ratios. DARWIN/PEPIN2 uncertainty propagation results are coherent with MENDEL ones for all isotopes.

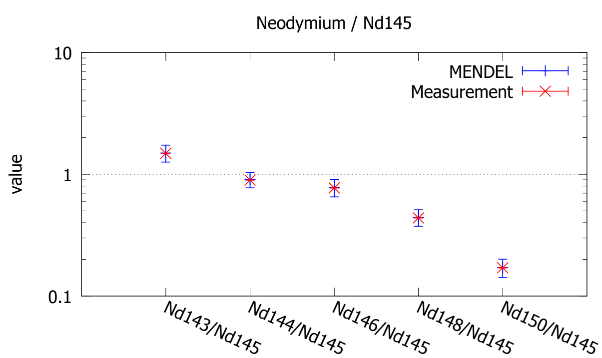

Fig. 4. MERCI experimental data and MENDEL uncertainty quantification for Neodymium isotopes.

Error bars correspond to one standard deviation. We observe a good agreement for all ratios, all experimental error bars being fully included in MENDEL uncertainty quantification standard deviation.

For Plutonium, only Pu242/Pu239 experimental value is outside the one standard deviation of calculation results, due to the very low amount of Pu242, leading to a bad evaluation of the quantities during the isotopic dilution mass spectrometry.

For Cesium and Uranium isotopes MERCI experimental results are inside the one standard deviation of calculation results, as will be shown in full presentation.

CONCLUSION

Comparisons between codes and experimental measurement give globally good agreement.

Other isotopic concentration uncertainty propagation results and analysis of correlation hypotheses consequences on decay heat uncertainty will be given in the full presentation.

This work is a new contribution for the validation of both MENDEL and DARWIN/PEPIN2 codes for isotopic concentration and decay heat computations, as well as both deterministic and probabilistic methods to propagate nuclear data uncertainty to those quantities.

ACKNOWLEDGMENTS

The authors thank EDF and AREVA for their financial support to the developments of DARWIN/PEPIN2 and MENDEL code systems.

REFERENCES

1. S. LOUBIÈRE ET AL., "OSIRIS Reactor for Fuel, Material and Other Irradiation," in "12th Int. Group on Research Reactor, Beijing, China," (October 28-30 2009).
2. C. BLANDIN ET AL., "MERCI-MOSAIC: Experimental Tools for Residual Power Measurement in OSIRIS Reactor," in "12th Int. Group on Research Reactor," (2009).
3. J. C. JABOULAY and S. BOURGANEL, "Analysis of MERCI Decay Heat Measurement for PWR UO_2 Fuel Rod," *Nuclear Techonology*, **177**, 73–82 (January 2012).
4. E. BRUN ET AL., "Systematic Uncertainty Due to Statistics in Monte Carlo Burnup Codes: Application to a Simple Benchmark with TRIPOLI-4-D," *Prog. in Nucl. Sci. and Technol.*, **2**, 879 – 885 (2011).
5. R. SANCHEZ ET AL., "APOLLO2 year 2010," *Nuclear Engineering and Technology*, **42**, *5*, 474–499 (2010).
6. A. TSILANIZARA ET AL., "DARWIN: an Evolution Code System for a Large Range of Applications," *Nucl. Science Technol. Suppl.*, **1**, 845 – 849 (2000).
7. J. REBAH, *Uncertainty on Decay Heat Power Due to Fission Product Data Uncertainty*, Ph.D. thesis, CEA-N-2387 PhD thesis (1998).
8. A. TSILANIZARA ET AL., "Probabilistic approach for decay heat uncertainty estimation under URANIE platform by using MENDEL depletion code," *Annals of Nuclear Energy*, **90**, 62–70 (2016).
9. F. GAUDIER, "URANIE: the CEA/DEN Uncertainty and Sensitivity platform," *Proc. - Social and Behavioral Sciences*, **2**, *16*, 7660–7661 (2010).
10. S. LAHAYE ET AL., "First Verification and Validation Steps of MENDEL Release V1.0 Cycle Code System," in "PHYSOR 2014," (2014), Kyoto, Japan.
11. M. KELLET, O. BERSILLON, and R. MILLS, *The JEFF-3.1/-3.1.1 Radioactive Decay Data and Fission Yields Sub-libraries*, OECD (2009).
12. T. R. ENGLAND and B. F. RIDER, "ENDF-349, Evaluation and Compilation of Fission Product Yields 1993," Tech. Rep. LA-UR-94-3106 (1994).
13. C. DE SAINT-JEAN ET AL., "Estimation of Multi-Group Cross-Sections Covariances for $^{235,238}U$, ^{239}Pu, ^{241}Am, ^{56}Fe, ^{23}Na and ^{27}Al," in "PHYSOR 2012," (2012).