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Comparison of deterministic and stochastic approaches for isotopic concentration and decay heat uncertainty quantification on elementary fission pulse

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Abstract. Uncertainty quantification of interest outputs in nuclear fuel cycle is an important issue for nuclear safety, from nuclear facilities to long term deposits. Most of those outputs are functions of the isotopic vector density which is estimated by fuel cycle codes, such as DARWIN/PEPIN2, MENDEL, ORIGEN or FISPACT. CEA code systems DARWIN/PEPIN2 and MENDEL propagate by two different methods the uncertainty from nuclear data inputs to isotopic concentrations and decay heat. This paper shows comparisons between those two codes on a Uranium-235 thermal fission pulse. Effects of nuclear data evaluation's choice (ENDF/B-VII.1, JEFF-3.1.1 and JENDL-2011) is inspected in this paper. All results show good agreement between both codes and methods, ensuring the reliability of both approaches for a given evaluation.

1 Introduction

These last years, most of depletion code systems have introduced uncertainty propagation functionalities. CEA fuel cycle code systems used in this study have implemented two different methods. DARWIN/PEPIN2 [1] propagates uncertainties using deterministic first order forward perturbations through the INCERD supervisor while MENDEL [2, 3] uses Monte Carlo sampling with samples created by CEA/DEN uncertainty platform URANIE [4].

Three nuclear data evaluations were used: ENDF/B-VII.1, JEFF-3.1.1 and JENDL-2011.

2 Depletion calculations

2.1 Concentrations and decay heat expressions

After an elementary fission pulse, the atom density $N_i(t)$ of the different fission products i is solution of the generalized Bateman equation when all neutronic reactions have been taken out:

$$\frac{\mathrm{d}N_i}{\mathrm{d}t}(t) \quad = \quad -\lambda_i N_i(t) + \textstyle\sum_{j=1}^{N} b_{j,i}\lambda_j N_j(t) \quad ; \quad N_i(0) \quad = \quad \gamma_i \tag{1}$$

where λ_i is the radioactive decay constant of fission product i, $b_{j,i}$ the radioactive decay branching ratio from j to i and γ_i the independent fission yield generating fission product i. Independent fission yields correspond to initial concentration of fission products after the elementary fission pulse.

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For any cooling time t, total decay heat DH is computed as displayed in equation (2), where E_i is the total radioactive decay energy released by nuclide i disintegration (sum of α, β and γ components):

$$\mathrm{DH}(t) = \sum_i E_i \lambda_i N_i(t) \tag{2}$$

2.2 Uncertainty data

In this paper, we consider for radioactive decay constants, radioactive decay energies, radioactive decay branching ratios and independent fission yields all the uncertainty data available in each evaluations (ENDF/B-VII.1, JEFF-3.1.1 and JENDL-2011). If physical parameters are not associated to nuclear data uncertainties in the considered evaluation, its value is considered known without uncertainty. Table 1 summarizes the available uncertainty data in different data sets and evaluations.

Table 1. Number of physical parameters which uncertainty is not equal to 0, in different data sets.

	Decay constant	Total decay energy	Decay branching ratio	Ind. Fission yield (U235T)	Nb of isotopes in decay chain
JEFF-3.1.1	3204	1554	505	918	3849
ENDF/B-VII.1	2233	1285	866	998	3820
JENDL-2011	867	653	590	1067	1142

3 Propagation of uncertainty data

3.1 Correlations between parameters

Two uncertain nuclear data from different parameters types are always considered uncorrelated, as well as two radioactive decay constants or radioactive decay energies or independent fission yields, as no physical correlation are given in evaluation files. For independent fission yields, this assumption will stop as soon as independent fission yields covariance matrices will be available.

Radioactive decay branching ratios corresponding to the different decay processes from the same father are correlated to assure a sum equal to 1, as described in section 3.2.

3.2 Deterministic method

The deterministic method used in DARWIN/PEPIN2 to calculate the propagation of uncertainty is based on the first order Taylor series (linearity hypothesis). In the matrix form, the uncertainty of a variable Y due to the effect of uncertainties on variable X is given by the following formula (3):

$$\mathrm{Cov}(Y) = S_{Y/X} \mathrm{Cov}(X) S_{Y/X}^T \tag{3}$$

where $\mathrm{Cov}(Y)$ (resp. $\mathrm{Cov}(X)$) is the variance-covariance matrix of variable Y (resp. X). $S_{Y/X}$ and $S_{Y/X}^T$ are respectively the sensitivity matrix and its transposed matrix.

To take into account the correlation $r_{j,k}$ between radioactive decay ratio branches $b_{i,j}$ and $b_{i,k}$ from a given radioactive nuclide i, we introduce a unique correlation coefficient r_i between all radioactive decay branching ratio from the same father isotope i, with respect of the physical constraint $\sum_{j=1}^{N} b_{i,j} = 1$. It is deduced from equation (4):

$$\mathrm{Var}\left(\sum_{j=1}^{N} b_{i,j}\right) = 0 \tag{4}$$

Which leads to:

$$r_{jk} = \text{const} = \frac{-\sum_{j=1}^{N} \mathrm{Var}(\mathrm{b_{i,j}})}{2\sum_{1\leq j<k\leq N}\sqrt{\mathrm{Var}(b_{i,j})\mathrm{Var}(b_{i,k})}} \tag{5}$$

The uncertainty propagation in DARWIN/PEPIN2 involves the supervisor module INCERD. INCERD gathers all user's data and uncertainties data of physical parameters and launches depletion calculating in parallel mode (using MPICH2/OPENMPI) to determine the sensitivity coefficient values ($S_{Y/X}$). Then, INCERD performs the uncertainty propagation as described by equation (3).

3.3 Stochastic method

The stochastic method implemented in MENDEL propagates the uncertainty on output data using sampled input data. For each uncertain nuclear data parameter, sampling is done using the CEA/DEN uncertainty platform URANIE.

Decay branching ratios cannot be sampled using the correlation factor from equation (5), as incoherence in the evaluation data creates for ENDF/B-VII.1 and JENDL-2011 correlation coefficients outside $[-1, 1]$. MENDEL assumes all standard deviations are equal for a given father isotope, which leads to $r_i = -1/(N-1)$. All other parameters are sampled independently.

Radioactive decay energies, radioactive decay periods and radioactive decay branching ratios are considered to have positive Gaussian distribution (truncated) if their relative standard deviation is less than 50%, lognormal distribution if it is bigger. Due to large number of high relative standard deviation for fission yields, they are sampled by a lognormal distribution. Those assumptions enable to assure the positivity of the distributions and a good estimation of mean value and standard deviation.

All results shown in this paper result from a use of 2000 realisations.

4 Results and Discussion

4.1 Uncertainty quantification for decay heat

When propagating uncertainty data to total decay heat for the three nuclear evaluations, DARWIN/PEPIN2 and MENDEL results both show a very good agreement, but also huge differences between evaluations, as shown in figure 1.

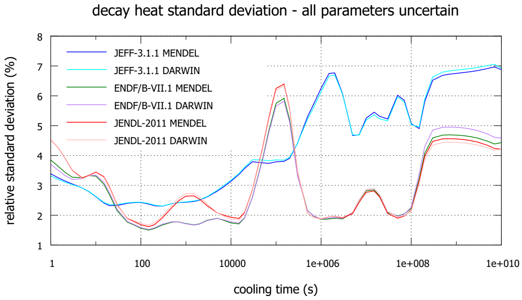

Figure 1. Uncertainty quantification of decay heat due to all parameters.

When observing the impact of each parameter separately, both codes for all evaluations show with the assumptions adopted here that fission yields is the most important contributor, followed by energies. Discrepancies are observed only for decay branching ratios, due to the differences in adopted correlations. This discrepancy can be important, as shown in the botom left of Figure 2.

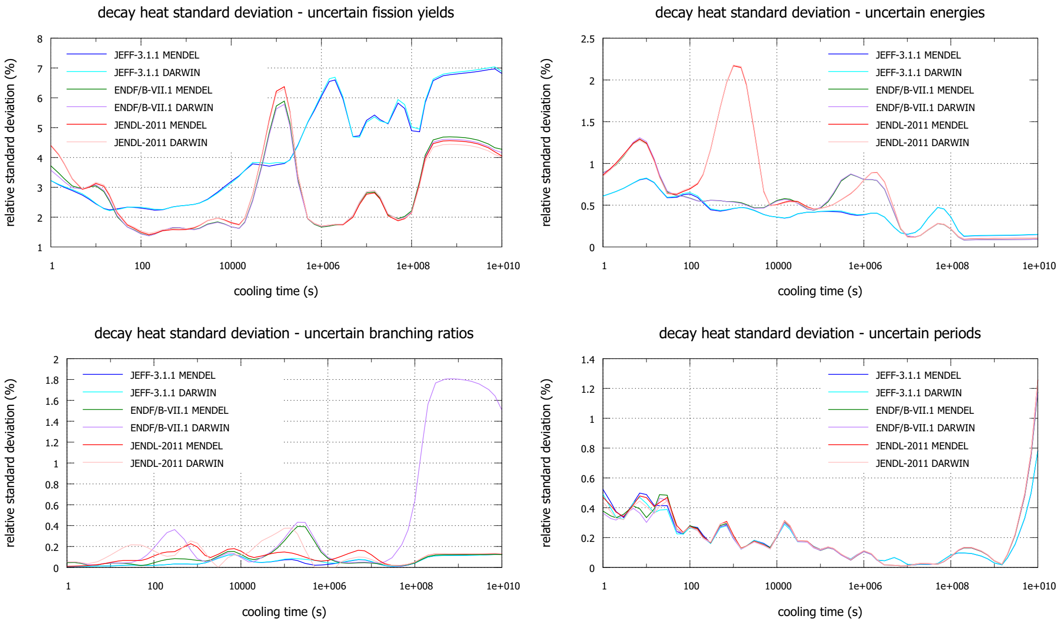

Figure 2. Uncertainty quantification of decay heat due to each parameter parameters.

4.2 Uncertainty quantification for nuclide density

DARWIN/PEPIN2 and MENDEL were used in this study to propagate uncertainty data to isotopic concentration of various fission products. Results are presented in this paper for Iodine-131 only but are representative of results for other nuclei. Uncertainty on Iodine-131 is due on independent fission yields (initial concentration), radioactive decay branching ratios and radioactive decay periods.

This work has been done assuming that uncertainty data not present in the evaluation corresponds to physical data known without uncertainty. This leads to no uncertainty of Iodine-131 concentration due to radioactive decay branching ratios for JEFF-3.1.1 in the bottom left of Figure 4.

Numerical precision effects can appear for when concentrations tends to 0 as MENDEL works in double precision and DARWIN/PEPIN2 in simple precision. MENDEL results where truncated to match DARWIN/PEPIN2 accuracy, but differences can still be seen for radioactive decay branching ratios around 10^8 s, when DARWIN/PEPIN2 goes down to zero before MENDEL.

5 Conclusion

This work validates DARWIN/PEPIN2 and MENDEL uncertainty quantification of isotopic concentrations for a Uranium-235 elementary thermal fission pulse.

The importance of differences between evaluations on uncertainty data leads several new needs from evaluation files. Correction on uncertainty levels incoherences like for ENDF/B-VII. and

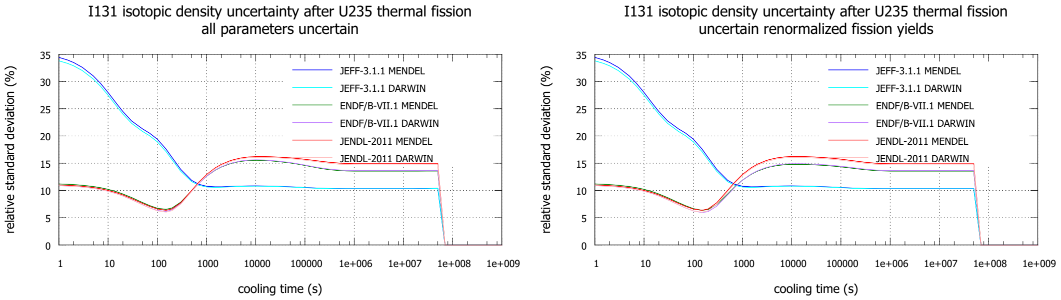

Figure 3. Uncertainty quantification of Iodine-131 concentration due to all parameters (left) and independent fission yields (left).

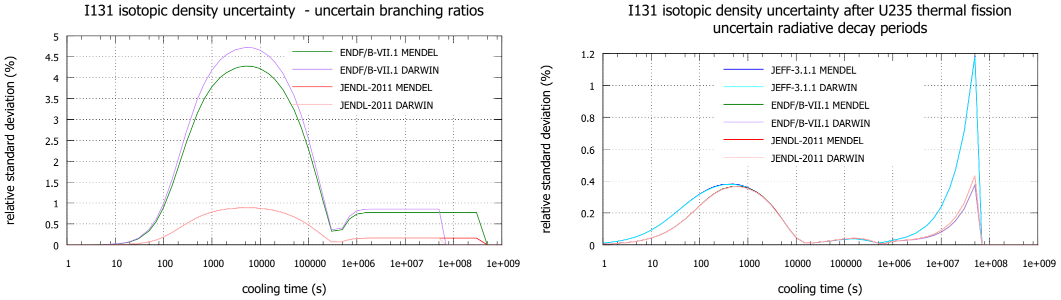

Figure 4. Uncertainty quantification of decay heat due to branching ratios (left) and periods (right).

JENDL-2011 radioactive decay branching ratios is needed to be able to use completely the data. Availability of covariances data on fission yields is expected, as well as the completion of uncertain data not present in the current evaluations.

Acknowledgement

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