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Fission yield covariance generation and uncertainty propagation through fission pulse decay heat calculation

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ABSTRACT

Fission product yields are fundamental parameters in burnup/activation calculations and the impact of their uncertainties was widely studied in the past. Evaluations of these uncertainties were released, still without covariance data. Therefore, the nuclear community expressed the need of full fission yield covariance matrices to be able to produce inventory calculation results that take into account the complete uncertainty data.

State-of-the-art fission yield data and methodologies for fission yield covariance generation were researched in this work. Covariance matrices were generated and compared to the original data stored in the library. Then, we focused on the effect of fission yield covariance information on fission pulse decay heat results for thermal fission of ^{235}U. Calculations were carried out using different libraries and codes (ACAB and ALEPH-2) after introducing the new covariance values. Results were compared with those obtained with the uncertainty data currently provided by the libraries. The uncertainty quantification was performed first with Monte Carlo sampling and then compared with linear perturbation. Indeed, correlations between fission yields strongly affect the uncertainty of decay heat. Eventually, a sensitivity analysis of fission product yields to fission pulse decay heat was performed in order to provide a full set of the most sensitive nuclides for such a calculation.

1. Introduction

Nowadays, any engineering calculation performed in the nuclear field should be accompanied by an uncertainty analysis. In such analysis, different sources of uncertainties are taken into account. Works, such as those performed under the UAM project (Ivanov et al., 2013), treat nuclear data as a source of uncertainty: in particular cross-section data for which uncertainties given in the form of covariance matrices are already provided in the major nuclear data libraries. Meanwhile, fission yield uncertainties were often neglected or treated shallowly, because their effects were considered of second order compared to cross-sections (Garcia-Herranz et al., 2010).

However, the Working Party on International Nuclear Data Evaluation Co-operation (WPEC)—dedicated to assess the needs of nuclear data improvement—initiated a new interest on fission yield data within its Subgroup 37 (SG37), with the goal of developing "Improved Fission Product Yield evaluation methodologies" (Mills, 2013), not only in order to quantify the impact of such uncertainties, but also to provide a proper set of variances and correlation matrices.

Fission yield data are of critical importance in decay heat applications (Katakura, 2012). The calculation of the decay heat and of its uncertainty has a deep impact on a series of industrial challenges like the design of emergency cooling systems, the design of transport waste casks and storage facilities or the cooling time that is needed before maintenance. The uncertainty on decay heat raises from the propagation of variance and covariance values of the nuclear data. Individual fission yield uncertainties, where no correlation is taken, are regarded as the main contributors to the fission pulse decay heat uncertainty (Diez et al., 2011). However, the use of covariance data may have a huge impact on the final result.

The purpose of this study was to present and summarise the information on fission yield data and their uncertainties provided in the major nuclear data libraries: ENDF/B-VII.1 (Chadwick et al., 2011), JEFF-3.1.2 (Kellet et al., 2009) and JENDL-4 (Katakura, 2012). The current proposed methodologies for generation of fis-

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sion yield data covariances, mainly presented at the WPEC-SG37 kick-off meeting, were studied and described. Covariance matrices were generated using both ENDF/B-VII.1 and JEFF-3.1.2 libraries. fission pulse decay heat (FPDH) calculations for ^{235}U thermal fission were carried out to assess the impact of these new covariance matrices. The uncertainty quantification (UQ) was performed with both Monte Carlo sampling and perturbation theory.

2. Fission yield data and covariance generation

Fission yields (FYs) characterise the probability of a particular nuclide or mass to be formed after fission. Accurate FY measurements and/or predictions, as well as the knowledge of the carried uncertainties, are essential to many applications in nuclear technology. The most used general-purpose evaluated nuclear data libraries: JEFF, ENDF/B and JENDL, provide these data in the ENDF-6 format (CSEWG, 2013) along with their uncertainties as standard deviation. To date, no correlation between FYs is supplied in such libraries, but several institutions/projects are putting a great effort to develop methodologies to generate full covariance matrices.

This section aims to point out the differences on neutron FY data and uncertainties in the latest release of the already mentioned libraries, namely, ENDF/B-VII.1, JEFF-3.1.2 and JENDL-4. Different methodologies for FY covariance data generation, mainly proposed in the framework of WPEC-SG37, are described and applied here for ^{235}U thermal fission.

2.1. Fission yield data libraries

Fission yield data from the latest release of the following libraries are compared:

- JEFF (Joint evaluated fission and fusion file) fission yield evaluation has been mainly compiled by Mills, James and Weaver (James et al., 1991; Mills, 1995). The most recent release JEFF-3.1.2 takes the fission yield data from the previous JEFF-3.1.1 which is developed from the UKFY3.6A database (Kellet et al., 2009).
- ENDF/B (United States evaluated nuclear data file) fission yield evaluation was mainly compiled by England and Rider (1993). The last release ENDF/B-VII.1 takes its data from ENDF/B-VII.0 (copied from ENDF/B-VI) (Chadwick et al., 2006) with the ^{239}Pu fission yields for fast and 14 MeV fissions being re-evaluated (Chadwick et al., 2011).
- JENDL (Japan evaluated nuclear data library) introduced data from the ENDF/B-VII.0 fission product yield files into its JENDL/FPY-2011 (Fission Product Yields Data File), and adjusted fission yield libraries based on the data in JENDL/FPD-2011 (Fission Product Decay Data File). Then, ternary fission yields were added. Data, mainly by Katakura, are the same as in JENDL-4 Fission Yield Sublibrary (Katakura, 2012).

Table 1 lists the data stored in the three libraries according to the fissioning nuclide and neutron energy.

ENDF/B-VII.1 includes 60 sets of neutron FY data and provides FYs for heavy nuclides at different neutron energies. JENDL-4 resorts to the same evaluation as ENDF/B-VII.1, covering the same 60 sets of FYs, but includes the products of ternary fissions, not handled in ENDF/B-VII.1. JEFF-3.1.2 copies its data from JEFF-3.1.1, which stores 41 sets of FYs and includes ternary yields as well.

Table 1
Fission yield data available in ENDF/B-VII.1, JEFF-3.1.2 and JENDL-4 as function of the incident neutron energy. T, H, and F stand for Thermal (0.0253 eV), Fast (500 keV), High-energy (14 MeV) neutron fission and S for Spontaneous fission. The total number of fission products (FP) in each evaluation is reported in the last line.

Nuclide	ENDF/B-VII.1	JEFF-3.1.2	JENDL-4
Th227	T	–	T
Th229	T	–	T
Th232	FH	FH	FH
Pa231	F	–	F
U232	T	–	T
U233	TFH	TFH	TFH
U234	FH	FH	FH
U235	TFH	TFH	TFH
U236	FH	FH	FH
U237	F	–	F
U238	FHS	FH	FHS
Np237	TFH	TF	TFH
Np238	F	TF	F
Pu238	F	TF	F
Pu239	TFH	TF	TFH
Pu240	TFH	F	TFH
Pu241	TF	TF	TF
Pu242	TFH	F	TFH
Am241	TFH	TF	TFH
Am242m	T	TF	T
Am243	F	TF	F
Cm242	F	S	F
Cm243	TF	TF	TH
Cm244	FS	TFS	FS
Cm245	T	TF	T
Cm246	FS	–	FS
Cm248	FS	–	FS
Cf249	T	–	T
Cf250	S	–	S
Cf251	T	–	T
Cf252	S	S	S
Es253	S	–	S
Es254	T	–	T
Fm254	S	–	S
Fm255	T	–	T
Fm256	S	–	S
FPs	1321	1355	1241

2.1.1. Description of fission yields

There exist different definitions of FYs:

The *Independent fission yield* (IFY), $y(A,Z,M)$, is defined as the number of atoms of nuclide with mass A, charge Z, and isomeric state M produced directly from one fission, after the emission of prompt neutrons, but before the emission of delayed neutrons. It can be written as the product of three factors (Eq. (1))

$$y(A,Z,M) = Y(A)f(A,Z)r(A,Z,M) \tag{1}$$

where

- $Y(A)$ represents the total *mass fission yield* (MFY), that is, the sum of independent fission yields of all fission products with mass number A, before delayed neutron emission.
- $f(A,Z)$ is the *fractional independent yield* of all isomers with mass A and charge Z.
- $r(A,Z,M)$ is called an *isomeric yield ratio* and represents the fraction of fission products (A,Z) produced as isomeric state M.

To calculate IFYs the said coefficients need to be known for each fission system, but even those chains with the highest coverage of measured data do not provide values for all parameters. It is indeed necessary to resort to semi-empirical models and interpolation/extrapolation methods for both mass and fractional yields.

The *cumulative fission yield* (CFY) $C(A,Z,M)$ is the total number of atoms of nuclide with mass number A, charge Z and isomeric state M produced over all time after one single fission. That is, the total number of atoms of that nuclide generated both through one single direct fission and radioactive decay of all the precursors. CFYs have a strong relationship with fission products decay chains, which means that they can be calculated from IFYs and decay data