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Generation of fission yield covariances to correct discrepancies in the nuclear data libraries

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ABSTRACT

Fission yield uncertainties and correlations should be considered in the uncertainty quantification of burnup responses — e.g. isotopic inventory, effective neutron multiplication factor k_{eff}. Although nuclear data libraries generally provide independent fission yield uncertainties along with the best estimates, currently they lack complete covariance matrices. In addition, several inconsistencies were detected amongst the current fission yield evaluated uncertainties, which could impact on uncertainty quantification (UQ) studies. As a part of this work, we introduced fission yield correlations to sort out the data inconsistency found in the JEFF-3.1.1 fission yield library. Such correlations are produced using an iterative generalised least square (GLS) updating technique, with conservation equations acting as fitting models. The process revises the fission yield estimates and covariances according to reliable evaluations, when available, or conservation criteria.

We chose to work with the PWR fuel rod model of the REBUS international program to test the new covariances, since experimental uncertainties on several concentrations are available. We propagated the original and updated fission yield covariances using a sampling approach and we quantified the uncertainty of k_{eff} and nuclide densities in the chosen burnup problem. The response uncertainty for k_{eff} and nuclide densities showed a sharp drop when using the new set of fission yield covariance matrices.

1. Introduction

Criticality and burnup calculations represent complex systems, where there are many sources of uncertainties. Amongst them, nuclear data uncertainties play a major role for responses such as the k_{eff} and the isotopic inventory. In such cases, cross sections are often considered as the most important sources of uncertainties (García-Herranz et al., 2008; Martinez et al., 2014), although it was shown that the current fission yield uncertainties provided in the major libraries contribute as much to the uncertainties of several fission product densities (Fiorito et al., 2015; Cabellos et al., 2014).

The fission yield files of most of the nuclear data libraries, like JEFF (Kellet et al., 6287) or ENDF/B (Chadwick et al., 2011), contain only best-estimates and uncertainties, without correlations between different isotopes or energy groups. Several efforts have been already made to different extents to provide fission yields with complete covariance matrices. The Working Party on International Nuclear Data Evaluation Co-operation (WPEC)'s Subgroup 37 (SG37) was established to develop "Improved Fission Product Yield evaluation methodologies" (Mills, 2013), with the goal of quantifying the impact of fission yield uncertainties and providing a proper set of variances and correlation matrices.

Amongst the works dedicated to this task, Katakura (2011) introduced a generalised least square method (GLS) to correlate fission yields on the base of the uncertainties of the measured chain yields. Kawano and Chadwick (2013) correlated the ^{239}Pu fission yields of the ENDF/B library using a Bayesian technique and four physical constraints. Schmidt et al. (2014) created correlations using a Monte Carlo perturbation of the fission yield model parameters in the GEF code. Leray et al. (2014) created uncertainties between yields with the same charge. Recently, Pigni et al. (2015) proposed a revision of the ENDF/B-VII.1 fission yield data introducing covariance matrices.

This work follows our previous studies dedicated to the production of fission yield covariance matrices, which are reported in

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Fiorito et al. (2014). The purpose of this work was to generate fission yield correlations for the JEFF-3.1.1 data using a GLS method and the same constraints that were adopted for the production of the JEFF-3.1.1 library, to guarantee consistency. In addition, we introduced further physical constraints in our evaluation, which were not covered in the JEFF-3.1.1 development and which have a large impact on the production of complete fission yield covariance matrices.

After producing adjusted covariance matrices, we assessed their impact through an uncertainty quantification (UQ) study of the k_{eff} and nuclide densities for the REBUS PWR single pin-cell burnup model (Gysemans et al., 2006).

2. State of the problem

2.1. Description of fission yield correlations

Independent fission yields describe the probability of an isotope with a given mass, charge and metastable state to be generated after a single neutron-induced fission. As given in the major nuclear data libraries they are constrained by physical conditions, or conservation equations. Such constraints reflect the real nature of a general fissioning system into a set of equations.

From the physics of a fission event we know that the compound nucleus splits up into, generally, two fission fragments, and it releases neutral particles such as neutrons and photons. However, ternary fissions may also occur, with the production of light charged particles (LCP). Fission products are described by independent fission yield distributions, which abide by global conservation laws and the rules of probability theory.

The conservation laws say that the charge and mass of the compound nucleus (CN) must be conserved, as described by Eqs. (1) and (2):

$$\sum_i A_i Y_i = \mathbf{A}^t\mathbf{Y} = A_{\text{CN}} - \bar{\nu}_p(E) - A_{\text{LCP}} \tag{1}$$

$$\sum_i Z_i Y_i = \mathbf{Z}^t\mathbf{Y} = Z_{\text{CN}} - Z_{\text{LCP}} \tag{2}$$

where **A** and **Z** are design vectors containing the mass number and charge of each possible fission product, respectively. All together, the mass values of the fission products multiplied by their yields of production **Y** add up to the mass of the compound nucleus A_{CN}, to which one must subtract the mass carried away by the light charged particles (LCP) emitted in ternary fission $A_{\text{LCP}} = \sum_{\text{LCP}} A_i Y_i$ and the prompt neutrons $\bar{\nu}_p(E)$. Analogously, also the charge Z_{CN} of the compound nucleus must be preserved in the fission yield distribution. Here, $Z_{\text{LCP}} = \sum_{\text{LCP}} Z_i Y_i$ is the charge carried away by the light charged particles emitted by ternary fission.

In addition, since an independent fission yield represents the probability of its corresponding nuclide to be generated immediately after a single fission event, it is evident that, for fission events that do not include ternary charged products, the sum of all the independent fission yields must be equal to two, for two are the fragments of the fission. Thus we introduce the third conservation equation:

$$\sum_i Y_i = \mathbf{I}^t\mathbf{Y} = 2 \tag{3}$$

where **I** is the design array for the given equation, which in this specific case is a unit vector. Light charged products are not included in the left-hand side of Eq. (3).

Then, the binary fission of the compound nucleus produces asymmetrical daughter products. The heavy fission product is generated with mass $A \geqslant \frac{A_{\text{CN}} - \bar{\nu}_p(E)}{2}$. We can express the conservation law with Eq. (4):

$$\sum_{A_i \geqslant \frac{A_{\text{CN}} - \bar{\nu}_p(E)}{2}} Y(A_i) = \mathbf{H}^t\mathbf{Y} = 1 \tag{4}$$

where **H** is a sensitivity vector with unit coefficients for products with mass $A \geqslant \frac{A_{\text{CN}} - \bar{\nu}_p(E)}{2}$ and zero elsewhere.

These four constraints apply to the global independent yield distributions. However, there are further constraints that apply only individually to a number of yields. Mills (1995) proposed individual constraints on the charge yields – i.e. the total fission yield of all the fission products with the same charge Z^*:

$$\sum_{Z=Z^*} Y_i = Y_{Z^*} \tag{5}$$

For any two nuclides with complementing charges Z_1 and Z_2, which obey the condition $Z_1 + Z_2 = Z_{\text{CN}}$, the charge yield of the lighter charge should be equal to the charge yield of the heavier charge:

$$Y_{Z_1} = Y_{Z_2} \tag{6}$$

These individual constraints were applied to the charges with the largest yields – i.e. those belonging to the peaks of the charge distribution – for each fissioning system in JEFF-3.1.1.

Mills (1995) used the general conservation equations and the individual charge constraints to produce the independent fission yield database of the UKFY3 data library, which was later introduced into JEFF-3.1.1. Then, fission yield data sets were created for the major fissioning systems at thermal (0.0253 eV) and/or fast (400 keV) and/or high (14 MeV) incident neutron energies. Every fission yield was given with an evaluated uncertainty. However, no correlation between yields of different nuclides, nor different energy levels were introduced.

Chain fission yields and uncertainties are retrievable both for JEFF and ENDF/B even though they are not directly provided in the libraries. As a consequence, we can add a further constraint using the chain yield data.

A chain yield Ch_i represents the total yield for a given decay chain and although at first sight it may be confused with the so-called mass yield, the two can differ by a few percent (James et al., 1991). As a matter of fact, the latter represents the sum of the yields with the same mass as they appear immediately after fission, but before the delayed neutron emission. On the other hand, chain yields are evaluated after both prompt and delayed neutron emission. Eq. (7) describes the relation between independent and chain fission yield.

$$\mathbf{D}^t\mathbf{Y} = \mathbf{Ch} \tag{7}$$

For any mass value A^*, the design matrix **D** represents the constraint $\sum_{A_i=A^*} Y(A_i) = Ch(A^*)$, with the mass of the independent fission yields corrected by the emission of delayed neutrons.

Also cumulative fission yields **C** are provided by the general purpose libraries. They are the isotopic yields generated after a neutron-induced single fission, followed by infinite decay, therefore they account for the production of delayed neutron and radioactive decay. Cumulative yields can be calculated from the independent yields using the Q-matrix notation (James et al., 1991):

$$\mathbf{Q}^t\mathbf{Y} = \mathbf{C}. \tag{8}$$

Their uncertainty can be calculated with the moment propagation equation, or "sandwich" equation:

$$\mathbf{S}^t\mathbf{V}_P\mathbf{S} = \mathbf{V}_R \tag{9}$$

In this case, **S** is the Q-matrix and the parameter and response covariances $\mathbf{V}_P$ and $\mathbf{V}_R$ are the independent and cumulative yields covariance matrices, respectively.