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ScienceDirect

Nuclear Data Sheets 123 (2015) 225–230

Nuclear Data Sheets

www.elsevier.com/locate/nds

Covariance Matrix Evaluations for Independent Mass Fission Yields

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(Received 29 May 2014; revised received 10 August 2014; accepted 15 August 2014)

Recent needs for more accurate fission product yields include covariance information to allow improved uncertainty estimations of the parameters used by design codes. The aim of this work is to investigate the possibility to generate more reliable and complete uncertainty information on independent mass fission yields. Mass yields covariances are estimated through a convolution between the multi-Gaussian empirical model based on Brosa's fission modes, which describe the pre-neutron mass yields, and the average prompt neutron multiplicity curve. The covariance generation task has been approached using the Bayesian generalized least squared method through the CONRAD code. Preliminary results on mass yields variance-covariance matrix will be presented and discussed from physical grounds in the case of ${}^{235}\mathrm{U}(n_{\mathrm{th}}, f)$ and ${}^{239}\mathrm{Pu}(n_{\mathrm{th}}, f)$ reactions.

I. INTRODUCTION

The actual nuclear reactor safety-by-design standards are requiring a more accurate evaluation of engineering parameter uncertainties. Thanks to perturbation theories, now implemented in many reactor analysis calculation tools, sensitivity and uncertainty studies can be carried out for integral reactor parameters describing modern nuclear facilities [1], producing an increasing demand for more accurate and reliable nuclear data.

Recent interest in engineering parameter uncertainty assessment, especially for fast spectrum facilities, has drawn the attention to the deficiencies affecting the present fission yield nuclear data sets [2]. The new requirements for modern applications include improved accuracy and covariance data for fission product yields (FY).

In this work we propose to investigate the possibility to generate variance-covariance matrices for independent fission yields, leaving the cumulative fission yields covariance estimation as a proposal for the future. Our main goal is to reproduce JEFF-3.1.1 nuclear data library results adding covariance information to the existing evaluated FY.

The independent FY represent the secondary fission fragments distribution (after prompt neutron emission). In this work we propose to combine the Brosa model [3], for the distribution before prompt neutron emission (pre-neutron mass FY), and the saw-tooth curve, which describes the average number of prompt neutrons emitted by a primary fission fragment. In the final section preliminary results on mass FY will be presented for the thermal fission of ^{235}U and ^{239}Pu. Covariance estimation has been achieved through the Bayesian approach of the Generalized Least Squared Method (GLSM), implementing new FY features in CONRAD (COde for Nuclear Reaction Analysis and Data assimilation) [4].

II. CALCULATION OF POST-NEUTRON MASS FISSION YIELDS

We start by introducing how independent mass FY can be calculated. A primary fragment of mass A can decrease his mass by several mass units, depending on how many prompt neutrons are evaporated after the scission phase. Therefore we can write

$$Y_{\mathrm{POST}}(A) = \sum_{\nu_i=0}^{\infty} Y_{\mathrm{PRE}}(A+\nu_i) \cdot p_{A+\nu_i}(\nu_i), \qquad (1)$$

where $Y_{\mathrm{POST}}(A)$ and $Y_{\mathrm{PRE}}(A+\nu_i)$ are, respectively, the post-neutron and the pre-neutron mass distributions, while $p_{A+\nu_i}(\nu_i)$ is the probability for a primary fragment of mass $A+\nu_i$ to emit ν_i prompt neutrons during the evaporation process.

It has to be pointed out that the pre-neutron distribution is symmetric. However, the prompt neutron evaporation is a process strongly depending on the fragment mass. The different number of prompt neutrons emitted by heavy and light fragments makes the post-neutron distribution no longer symmetric.

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http://dx.doi.org/10.1016/j.nds.2014.12.039

A. Pre-Neutron Mass Fission Yields

To describe the pre-neutron distribution we used the Brosa model [3]. This model combines the theories of the random neck rupture and of the multi-channels fission, which identifies precise pre-scission shapes according to potential energy minima of the deformed compound nucleus.

Brosa's results for actinides can be well represented by a summation of five Gaussian distributions related to three fission modes. The first one, called *Super Long*, characterizes the symmetrical pre-scission shape. A non-symmetric shape gives two more fission modes, called *Standard I* and *Standard II*, according to different neck elongations and heavy lobe shapes. The final mass yield distribution for primary fragments can be written as

$$Y_{\text{PRE}}(A) = \sum_c P_c Y_c(A), \quad \sum_c P_c = 1; \tag{2}$$

where

$$Y_c(A) = \frac{1}{\sqrt{2\pi\sigma_c^2}}\Big[e^{-\frac{(A-A_c)^2}{2\sigma_c^2}} + e^{-\frac{(A-A_f+A_c)^2}{2\sigma_c^2}}\Big]. \tag{3}$$

The index c stands for the fission modes (St.I, St.II, SL). Each fission mode is described by a Gaussian distribution centered in A_c on the heavy side and its corresponding light partner, and it is characterized by three parameters: the deviation from the center $D_c = A_c - A_f/2$, where $A_f/2$ is half of the compound nucleus mass, the width σ_c and a weight P_c. Since the *Super Long* is centered in $A_f/2$ and $\sum_c P_c = 1$, the number of free parameters is reduced to 7.

B. Neutron Evaporation Probability

As it is well known, the prompt neutron emission depends mainly on the mass and on the available excitation energy of the fragments after their full acceleration. The average number of prompt neutrons emitted by a fragment of mass A follows what is known as the *saw-tooth* curve, which shows the dependency of the average $\bar{\nu}_p$ as a function of the primary fragment mass.

We supposed the neutron evaporation probability distributed as a Gaussian. The discrete probability to emit ν neutrons for a fragment of mass A was found integrating the Gaussian distribution between $\nu - 0.5$ and $\nu + 0.5$, or between zero and 0.5 if we were considering zero prompt neutrons emitted. The integration is quite straightforward and gives

$$p_A(\nu) = \frac{N}{2}\cdot[V - W], \tag{4}$$

with

$$V = \text{erf}\Big(\frac{\nu + 0.5 - \bar{\nu}(A)}{\sqrt{2}\sigma}\Big) \tag{5}$$

and

$$W = \text{erf}\Big(\frac{\nu - 0.5 - \bar{\nu}(A)}{\sqrt{2}\sigma}\Big), \tag{6}$$

where N is the normalization factor and $\bar{\nu}(A)$ and σ are respectively the central value and the width of the Gaussian distribution describing the neutron evaporation probability. We assume the same σ ($\sigma = 0.9$) for all the $p_A(\nu)$ referring to different fragment masses. $\bar{\nu}(A)$ is, instead, related to the primary fragment mass and can be found once the average number of prompt neutrons $\bar{\nu}_p(A)$, given by the experimental saw-tooth, is known. $\bar{\nu}(A)$ is, in fact, very close to $\bar{\nu}_p(A)$ when this is sufficiently greater than zero, such that the normalization does not affect the symmetry of the distribution. $\bar{\nu}(A)$ can be found solving iteratively $\sum_{\nu_i} \nu_i \cdot p_A(\nu_i) = \bar{\nu}_p(A)$.

In Fig. 1 the saw-tooth curve for ^{235}U is shown. In the figure some experimental sets are reported, such as the experiments performed by A. S. Vorobyev [5], Nishio [6] and Boldeman [7] as well as the Wahl saw-tooth evaluation [8].

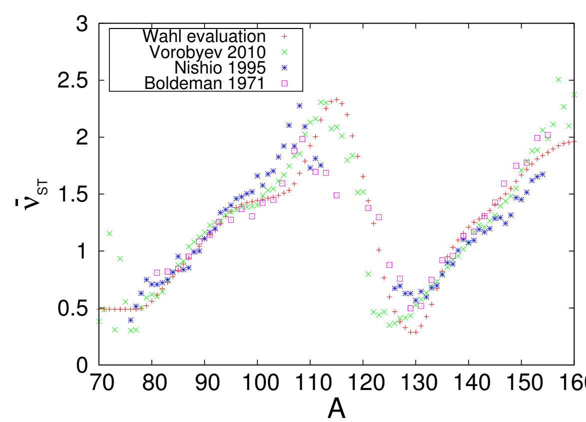

FIG. 1. (Color online) Experimental data sets [5–7] and Wahl evaluation [8] for the average number of prompt neutrons emitted by a primary fragment of mass A produced by thermal fission of ^{235}U.

It should be emphasized that this kind of experiment is not straightforward and the data reduction is most of the time complex. The mass resolution of this experiment is typically 2-3 *amu* and a x-error bar should be added. Discrepancies between experiments are visible in some mass regions, making the saw-tooth curve not very well known.

To faithfully represent the JEFF-3.1.1 mass FY, the saw-tooth values $\bar{\nu}_p(A)$ and the width σ were taken as free parameters for the prompt neutron emission probability in the adjustment procedure.