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Probabilistic approach for decay heat uncertainty estimation using URANIE platform and MENDEL depletion code

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ABSTRACT

The knowledge of the decay heat quantity and the associated uncertainties are important issues for the safety of nuclear facilities. Many codes are available to estimate the decay heat. ORIGEN, FISPACT, DARWIN are part of them. MENDEL is a new depletion code developed at CEA, with new software architecture, devoted to the calculation of physical quantities related to fuel cycle studies, in particular decay heat.

The purpose of this paper is to present a probabilistic approach to assess decay heat uncertainty due to the decay data uncertainties from nuclear data evaluation like JEFF-3.1.1 or ENDF/B-VII.1. This probabilistic approach is based both on the MENDEL code and URANIE software which is a CEA uncertainty analysis platform. As preliminary applications, single thermal fission of Uranium 235 and Plutonium 239 are investigated.

1. Introduction

The decay heat is an important parameter in the analysis of nuclear power plant safety, both in normal operation and accidental situation. The study of the uncertainty assigned to its best estimate value answers economic issues, such as reactor design or during fuel cycle discharge, fuel cycle transport and reprocessing, waste storage…

Many codes are available to calculate the decay heat. ORIGEN (Ludwig et al., 2002), FISPACT (Forest, 2007), DARWIN (Tsilanizara et al., 2000) are among them. MENDEL is a new depletion code developed at CEA, with new software architecture, dedicated to the calculation of physical quantities related to fuel cycle studies, in particular decay heat.

The decay heat uncertainty has several origins: nuclear data, technological data, reactor operation data… The present paper focuses only on the estimation of the decay heat uncertainty due to nuclear data.

The most widely used method to perform uncertainty calculations is based on first or second order Taylor series expansion (Smith, 1991; Kalfez and Bruna, 1977; Rebah et al., 1998; Gandini, 1987). Sensitivity profiles S are then calculated and combined to parameters covariance data to obtain the final uncertainties. If we note $Y = F(X)$, the response depending on X parameters, we have:

$$Cov(Y) = {}^{t}S(Y/X) \cdot Cov(X) \cdot S(Y/X)$$

Diagonal terms of $Cov(Y)$ represent the uncertainty of the Y components. Thanks to the significant increase of the computer power, a second method has gained a great interest among scientists. It is based on a global analysis where input variables of the problem are random variables in accordance with their uncertainties. The input variables are sampled according to appropriate probability density functions. A large number of simulations is done, and the resulting empirical distribution of Y can be used to estimate various statistical properties: mean, variance, probability to exceed threshold, α-quantiles, confidence intervals, etc. This paper uses this latest approach to perform the decay heat uncertainty due to the uncertainties of decay branching ratio, decay constant, independent fission yield and decay energy, as they appear in both JEFF-3.1.1 (Kellet et al., 2009) and ENDF/B-VII.1 (Chadwick and Herman, 2011) nuclear data libraries.

2. Decay heat expression

After the reactor shutdown, decay heat $P_{res}(t_c)$ can be calculated at each cooling time t_c by the summation method:

$$P_{res}(t_c) = \sum_i \lambda_i N_i(t_c)\overline{E_i} \tag{1}$$

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λ_i	:	decay constant of nuclide i
t_c	:	cooling time after the reactor shutdown
$N_i(t_c)$	:	atom number density of nuclide i at t_c
$\overline{E_i}$	:	total mean energy released by nuclide i disintegration, sum of α, β and γ components.

The atom density $N_i(t)$ of different nuclides i in a homogenized fissile material region is the solution of generalized Bateman equations:

$$\frac{dN_i(t)}{dt} = -(\lambda_i + \tau_{i,i})N_i(t) + \sum_{j \neq i}(b_{j,i}\lambda_j + \tau^r_{j,i})N_j(t) + \sum_k \gamma_{k,i}\tau^f_k N_k(t) \qquad (2)$$

$b_{j,i}\lambda_j$	:	partial decay rate of nuclide j to nuclide i
$\tau_{i,i}$	:	total disappearance rate of nuclide i by nuclear reactions induced by neutrons
$\tau^r_{j,i}$	:	transmutation rate of nuclide j to nuclide i by nuclear reaction r induced by neutrons
$\gamma_{k,i}$	:	fission yield of fissile nuclide k creating the fission product i
τ^f_k	:	fission rate of fissile nuclide k

3. Tools description

3.1. URANIE uncertainty platform

The URANIE (Gaudier, 2010) platform provides powerful functionalities which cover all necessary needs to perform uncertainty studies. It is based on the ROOT (ROOT, 2008) framework developed at CERN for the analysis of the Large Hadron Collider's data. On top of ROOT's functionalities, URANIE provides various modules for data manipulation and visualization, construction of designs of experiments, statistical modeling, optimization, sensitivity analysis, etc. It also provides tools to automatically launch external code on internal data, retrieve the results and store them internally for further analysis.

Like ROOT, URANIE's tools are accessible through the scripting language CINT (whose syntax is close to C++) and Python. The platform itself is written in C++.

3.2. MENDEL

MENDEL is a new code based on deterministic depletion solvers developed at CEA which is dedicated to radioactivity calculations related to neutron irradiation. MENDEL is developed in C++ with new software architecture which allows it to share its capabilities with other CEA codes more easily. For example, MENDEL provides its depletion solvers to deterministic transport code (APOLLO3®, Golfier et al., 2009) as well as to Monte-Carlo transport code (TRIPOLI-4®, Brun et al., 2011), in order to carry out homogeneous materials depletion in burnup or activation calculations. In addition, in its autonomous operation, MENDEL performs depletion calculations from specific database provided by transport codes such as APOLLO2 (Sanchez et al., 2010) (with the named *Saphyb* database) or APOLLO3® (with the named *M.P.O* "*Multiple Parameters Outputs*" database). To perform the propagation of the nuclear data uncertainties by the probabilistic approach, two C++ classes have been created. The first is an upstream interface class with URANIE. It provides methods which allow acquisition of the random variables observations from a data file generated with URANIE, and the setting of the physical quantity of interest in appropriate MENDEL classes. The second is a downstream class which provides methods used to export results to URANIE. The details about the different sources of uncertainties considered, the sampling methods and the assumptions made are given in the following sections.

4. Calculation methodology

The probabilistic uncertainty propagation method relies on a large number of simulations. Eqs. (1) and (2) point out the parameters of which depends the total decay heat estimation. To estimate the uncertainty on the total decay heat, the uncertainties of the four parameters listed below are coming from nuclear data libraries used:

- average decay energies (α, β and γ components),
- independent fission yield,
- decay constant,
- decay branching ratio.

A complete filiation chain is considered in our study leading to a large amount (several thousand) of random variables to sample.

4.1. Input data sampling

Decay branching ratio, decay constant, decay energy and fission yield are assumed independent of each other. It is the same for radioactive nuclide decay constants. The precursor decay branching ratios are negatively correlated with correlation coefficient equal to $-1/(n-1)$ where n is the number of decay branches from

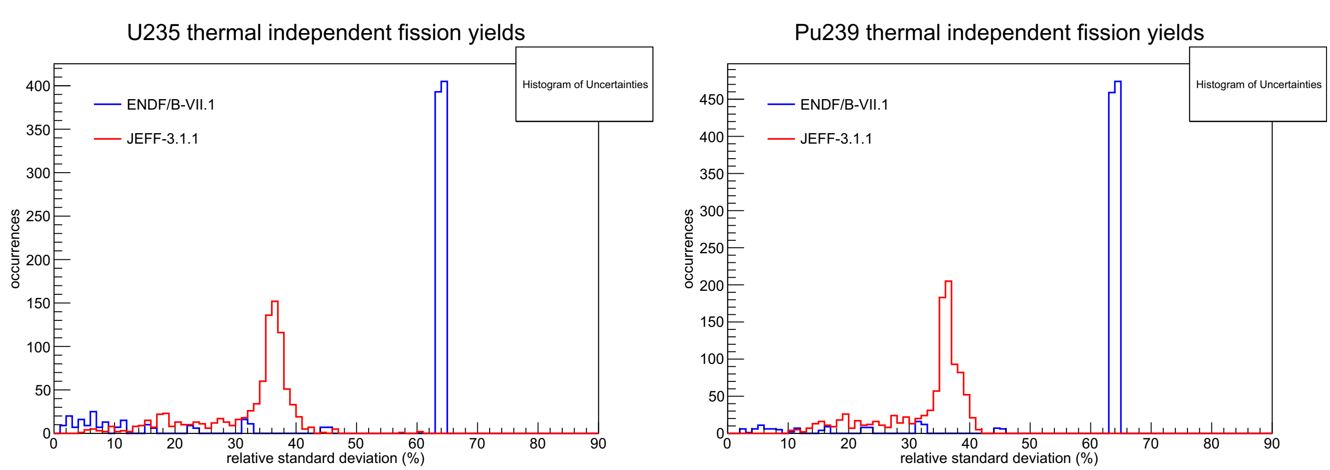

Fig. 1. Histogram of independent fission yield uncertainties for ^{235}U and ^{239}Pu thermal fissile systems.