PHYSOR 2016 – Unifying Theory and Experiments in the 21st Century
Sun Valley Resort, Sun Valley, Idaho, USA, May 1 – 5, 2016, on CD-ROM (2016)

# COMPARISON OF FISSION YIELD PERTURBATION METHODOLOGIES ON NUCLIDE COMPOSITION OF A PWR UO2 FUEL ASSEMBLY

O. Leray[a], L. Fiorito[b],
D. Rochman[a], H. Ferroukhi[a], A. Pautz[a],
A. Stankovskiy[b], G. Van den Eynde[b]
[a] Laboratory of Reactor Physics and System Behavior
Paul Scherrer Institut, Switzerland
[b] Institute for Advanced Nuclear Systems
SCK•CEN, Belgium
olivier.leray@psi.ch
lfiorito@sckcen.be

## ABSTRACT

The assessment of the fission yield uncertainty on neutronic parameters is of great interest for criticality and spent fuel behavior studies. In this work, several fission yield perturbation methodologies are used to propagate the uncertainty on a PWR fuel assembly. The resulting k-inf uncertainty versus the exposure and the nuclide density uncertainties at 60 GWd/MT are assessed and discussed.

*Key Words:* **Fission Yield perturbation, SHARK-X, GEF.**

## 1. INTRODUCTION

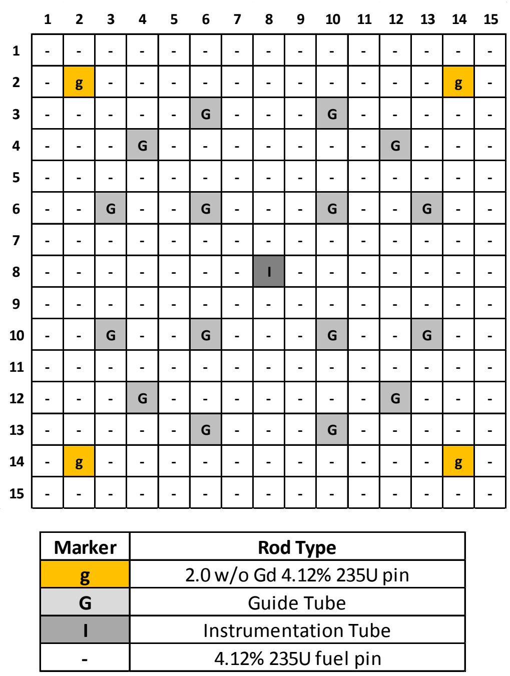
The assessment of biases for Best Estimate calculations needs precise quantification of the uncertainties. Nuclear data uncertainties such as cross-sections are now perturbed using the Variance-Covariance Matrices. It means that not only the uncertainties but also the correlations between reactions, energies and sometimes isotopes are taken into account. Even if uncertainties are given for fission yields in the international evaluations, no correlations are provided.

This paper presents the results of the propagation of fission yield uncertainties to nuclide compositions of a UO2 burned fuel. Different methodologies to perform the perturbation with and without correlations are first described and then used.

## 2. CASE DESCRIPTION

### 2.1. The TMI-1 Fuel Assembly Lattice

This section describes the UAM Benchmark Phase II case 2a (TMI-1). The studied case is composed of a PWR UO2 lattice described in Figure 1. The calculations are performed at Hot Full Power (HFP) with a constant power density of 33.75 W/gU up to 60 GWd/MT and an average boron concentration of 900 ppm. The specifications can also be found in [1].



| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 2 | - | g | - | - | - | - | - | - | - | - | - | - | - | g | - |
| 3 | - | - | - | - | - | G | - | - | - | G | - | - | - | - | - |
| 4 | - | - | - | G | - | - | - | - | - | - | - | G | - | - | - |
| 5 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 6 | - | - | G | - | - | G | - | - | - | G | - | - | G | - | - |
| 7 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 8 | - | - | - | - | - | - | - | I | - | - | - | - | - | - | - |
| 9 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 10 | - | - | G | - | - | G | - | - | - | G | - | - | G | - | - |
| 11 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |
| 12 | - | - | - | G | - | - | - | - | - | - | - | G | - | - | - |
| 13 | - | - | - | - | - | G | - | - | - | G | - | - | - | - | - |
| 14 | - | g | - | - | - | - | - | - | - | - | - | - | - | g | - |
| 15 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - |

| Marker | Rod Type |
|---|---|
| g | 2.0 w/o Gd 4.12% 235U pin |
| G | Guide Tube |
| I | Instrumentation Tube |
| - | 4.12% 235U fuel pin |

**Figure 1. TMI-1 fuel assembly lattice.**

### 2.2. The SHARK-X tool

The SHARK-X [2] platform embeds the 2D deterministic lattice physics code CASMO-5 [3] wrapped in Perl-based scripts and allows the perturbation of nuclear data. The classical stochastic sampling method using Variance-Covariance Matrices (VCM) is used to generate relative perturbation factors p (Equation (1)).

$$\boldsymbol{\sigma}^{*} = \boldsymbol{p}.\boldsymbol{\sigma} \tag{1}$$

Recently, the perturbation of nuclear data has been extended to fission yield in SHARK-X [3]. Nevertheless, due to restrictions from the CASMO-5 code, the initially implemented fission yield perturbation methodology includes approximations [5]. To overcome these, a new SHARK-X development allows external sources of perturbed fission yields. Hence any set of perturbed fission yields in an ENDF-6 format [6] can now be used for uncertainty propagation and applied on the ENDF/B-VII.0 fission yields (only library available in CASMO-5).

## 3. FISSION YIELDS PERTURBATION

This section presents the different methodologies used to perturb the fission yields (from several nuclear data evaluations). Sets of ENDF-format files with perturbed fission yields are produced and relative perturbation factors based on those are then created. The relative perturbation factors are finally employed with the CASMO-5 code to propagate the uncertainty on the nuclide composition (section 4).

### 3.1. Fission Yields perturbation from TENDL-2011

The TENDL-2011 [7] evaluation provide a set of perturbed independent (MT454) and cumulative (MT459) fission yields. The perturbations are performed on the parameters of the systematics of fission yields (Wahl). The resulting perturbed thermal fission yields for $^{235}$U, $^{239,241}$Pu and the fast (500 keV) perturbed fission yields for $^{238}$U are then normalized to 2 and no correlation information is used (the VCM is then a diagonal matrix).

### 3.2. Fission Yields perturbation from the GEF code

The thermal random fission yields for $^{235}$U, $^{239,241}$Pu and the 500 keV random fission yields for $^{238}$U are produced using a modified version of the GEF code [8]. In the GEF code, fission yields, among other fission observables, are produced based on theoretical background using parametrizations of different nuclear physics observables. Two main advantages can be noticed: (1) the available empirical information is used to develop a general description of the fission process, and (2) the theoretical frame assures that the model is able to quantitatively predict many fission observables (such as fission yields).

Such parametrizations is based on a limited number of theoretical parameters, from which mean values and standard deviations can be obtained by comparisons with experimental data. The mean values were determined to globally reproduce the experimental data. For standard deviations, a “short list” of 21 parameters was selected and they were independently randomly varied following Normal distributions. Considering the experimental spread of data and their uncertainties, uncertainties on these parameters were obtained as presented in [8], Table 7.

In the present work, the GEF code is modified in the following way: parameters presented in Table 7 of Ref. [8] are independently sampled (also considering Normal distributions) and fission yield calculations are performed with GEF, not starting from the nominal values of the 21 parameters, but from the sample values. This process, repeated n times (n larger than 1000) produces random fission yields. This process gives the advantage to produce random fission observables based on theoretical background, as in the Total Monte Carlo approach [9].

### 3.3. Fission Yields perturbation using a generalized least square (GLS) updating procedure

A new NJOY-wrapping numerical code was developed at SCK•CEN to perform the sensitivity analysis (SA) and uncertainty propagation (UQ) of nuclear data. Amongst its capabilities, such code generates covariance matrices for independent fission yields using a generalized least-square (GLS) approach. After collecting best-estimate and uncertainty values from the ENDF-6 files, such data are constrained to comply with the conservation equations of a fission event – e.g. conservation of mass, charge and number of fission fragments, symmetry, correlation between independent and chain fission yields.

Hence, covariance matrices are produced and independent fission yields are upgraded. Such an update tackles the need for more consistency of fission yield uncertainties in the major general purpose libraries (JEFF, ENDF/B), which only loosely abide by the conservation laws at the current stage.

Then, given an upgraded array of best-estimate independent fission yields Y and a covariance matrix C, random samples are drawn from a multivariate normal probability density function (pdf) N(Y,C) using a standard Monte Carlo sampling procedure. The new random sets of independent fission yields replace the original values in "perturbed" ENDF-6 files. In each "perturbed" file, cumulative fission yields are also recalculated using the random independent yields and the Q-matrix equation.

In this work, we created "perturbed" files for the U and Pu fissioning systems of ENDF/B-VII.1.

## 4. RESULTS

### 4.1. Nuclide composition uncertainty at high burnup

The above described methodologies have been used to create 500 samples each which have been propagated in CASMO-5 to the TMI-1 fuel assembly. The uncertainties on the density of the main nuclides due to the fission yields perturbations are presented in Table 1. From these results the GEF code gives rather high uncertainties on the nuclides compositions compared to TENDL-2011 whereas it uses correlations between the fission yields. One has to keep in mind that the GEF uncertainties are propagated from the fission observable parameters and are independent from the other uncertainties (coming from the international evaluations).

**Table 1.** Nuclide composition relative uncertainties due to different fission yield perturbation methodologies (one standard deviation) at 60 GWd/MT.

| Nuclide | TENDL 2011 | GEF | JEFF 3.1.1 | ENDF/ B-VII.1 | Nuclide | TENDL 2011 | GEF | JEFF 3.1.1 | ENDF/ B-VII.1 |
|---|---|---|---|---|---|---|---|---|---|
| $^{90}$Sr | 1.34% | 3.66% | | | $^{145}$Nd | 1.36% | 4.60% | | |
| $^{95}$Mo | 1.37% | 2.94% | | | $^{146}$Nd | 1.25% | 5.51% | | |
| $^{99}$Tc | 1.40% | 2.33% | | | $^{148}$Nd | 1.86% | 8.23% | | |
| $^{101}$Ru | 4.62% | 3.81% | | | $^{147}$Sm | 1.92% | 6.97% | | |
| $^{103}$Rh | 2.32% | 7.23% | | | $^{149}$Sm | 2.20% | 7.71% | | |
| $^{109}$Ag | 36.43% | 13.45% | | | $^{150}$Sm | 2.10% | 8.68% | | |
| $^{129}$I | 59.01% | 14.31% | | | $^{151}$Sm | 2.30% | 9.86% | | |
| $^{131}$Xe | 2.59% | 7.24% | | | $^{152}$Sm | 1.95% | 11.55% | | |
| $^{135}$Xe | 4.18% | 2.16% | | | $^{153}$Eu | 1.84% | 12.24% | | |
| $^{133}$Cs | 22.94% | 4.11% | | | $^{154}$Eu | 1.92% | 12.89% | | |
| $^{134}$Cs | 22.28% | 4.12% | | | $^{155}$Eu | 2.19% | 13.27% | | |

| | | | | | |
|---|---|---|---|---|---|
| $^{137}$Cs | 1.51% | 2.71% | $^{155}$Gd | 2.22% | 14.30% |
| $^{144}$Ce | 1.53% | 3.60% | $^{156}$Gd | 2.97% | 15.42% |
| $^{142}$Nd | 1.89% | 2.83% | $^{157}$Gd | 7.08% | 17.87% |
| $^{143}$Nd | 1.39% | 2.32% | $^{158}$Gd | 12.12% | 22.64% |
| $^{144}$Nd | 0.93% | 3.39% | | | |

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