Comparison of nuclear data uncertainty propagation methodologies for PWR burn-up simulations

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Abstract

Several methodologies using different levels of approximations have been developed for propagating nuclear data uncertainties in nuclear burn-up simulations. Most methods fall into the two broad classes of Monte Carlo approaches, which are exact apart from statistical uncertainties but require additional computation time, and first order perturbation theory approaches, which are efficient for not too large numbers of considered response functions but only applicable for sufficiently small nuclear data uncertainties. Some methods neglect isotopic composition uncertainties induced by the depletion steps of the simulations, others neglect neutron flux uncertainties, and the accuracy of a given approximation is often very hard to quantify. In order to get a better sense of the impact of different approximations, this work aims to compare results obtained based on different approximate methodologies with an exact method, namely the NUDUNA Monte Carlo based approach developed by AREVA GmbH. In addition, the impact of different covariance data is studied by comparing two of the presently most complete nuclear data covariance libraries (ENDF/B-VII.1 and SCALE 6.0), which reveals a high dependency of the uncertainty estimates on the source of covariance data. The burn-up benchmark Exercise I-1b proposed by the OECD expert group “Benchmarks for Uncertainty Analysis in Modeling (UAM) for the Design, Operation and Safety Analysis of LWRs” is studied as an example application. The burn-up simulations are performed with the SCALE 6.0 tool suite.

Keywords: uncertainty quantification, burn-up, PWR, UAM, nuclear data uncertainties, NUDUNA, Hybrid Method

1. Introduction

Nuclear transport and depletion codes are the workhorses in the field of nuclear safety, in reactor core design, and for radiation shielding analyzes. Such codes describe the propagation of sub-atomic particles, e.g., neutrons, in matter and simulate the induced change in the material composition, e.g., due to neutron capture, fission, and radioactive decay processes.

A vast variety of experimental and model input data is required in order to parametrize the interaction of sub-atomic particles with the surrounding matter and the induced change in the material composition. Such nuclear data are usually provided in a standardized format, like ENDF-6 (CSEWG, 2013), by nuclear data evaluation groups who release them in the form of nuclear data libraries, such as ENDF/B-VII.1 (Chadwick et al., 2011), JEFF-3.2 (Joint Evaluated Fission and Fusion File (JEFF) project 2014) or JENDL-4 (Shibata et al., 2011). These nuclear data are then processed, filtered, compressed, and reformatted in order to serve as input for specific nuclear transport and depletion codes such as SCALE (Oak Ridge National Laboratory, 2009), ACAB (Sanz et al., 2008), and FISPACT-II (Sublet et al., 2012).

The nuclear input data have limited accuracy which arises both from limited measurement precision and modeling uncertainties, e.g., in regions where insufficient experimental data are available. Hence, it is the objective of the nuclear data community to provide uncertainty estimates that truly reflect the degree of confidence in the nuclear data, and the last years have witnessed great progress in this field.

Besides the fundamental need of guaranteeing conservativeness in safety assessments, there is another major motivation for studying the impact of nuclear data uncertainties. That is replacing very penalizing assumptions in safety assessments with accurate uncertainty estimates,
which will result in an improved economic competitiveness.

Over the last decades, several methodologies have been implemented in code packages to study the impact of nuclear data uncertainties on nuclear transport and depletion problems, such as TSUNAMI, TSURFER, and SAMPLER developed by ORNL (Oak Ridge National Laboratory 2009), XSUSA by GRS (Zwermann et al. 2009), RIB by CEA (Venard et al. 2009), TMC by NRG (Kon- ing and Rochman 2008), FISPACT-II by CCFE (Sublet et al. 2012), NUS by PSI (Wieselquist et al. 2013; Zhu et al. 2014) developed for CASMO-5M (Studsvik Scandpower 2010) and MCNPX (Pelowitz 2005), the Kiwi package by LLNL (Mattoon et al. 2012), the so-called Hybrid Method (García-Herranz et al. 2008) based on ACAB (Sanz et al. 2008), promoted by Universidad Politécnica de Madrid, and the NUDUNA package developed by AREVA Gmbh (Buss et al. 2011). The methods can be divided into first order perturbation theory based methods (TSUNAMI, TSURFER, RIB, FISPACT-II) and Monte Carlo sampling methods (SAMPLER, XSUSA, TMC, Kiwi, Hybrid Method, NUSS, NUDUNA).

A first order perturbation theory method typically requires little extra computation time compared to an analysis without uncertainty quantification. E.g., an adjoint-based sensitivity analysis involving the application of the so-called sandwich rule (Cacuci 2003) requires only as many importance calculations as there are response functions under consideration. Hence, the adjoint-based approach is efficient for a sufficiently small number of response functions. Monte Carlo methods, on the contrary, are not limited to small nuclear data uncertainties because they do not involve any series expansions and, consequently, completely take into account nonlinear effects. Furthermore, they are easy to implement without any major code modification. However, it can be seen as a disadvantage that they usually require elevated CPU time compared to first order approximation approaches, although there are application cases where the increase in CPU time can be rendered negligible (Zwermann et al. 2012; Rochman et al. 2014). Methods also differ by their nuclear data uncertainty input. E.g., the TMC method is directly based on microscopic measurements, while up to now all other methods are based on data from nuclear data evaluations.

When simulating the burn-up of nuclear fuel in a reactor, the problem is usually divided into evaluation of the neutron flux and depletion of the fuel. Fig. 1 shows a typical scheme for such a simulation, which includes the coupling between a transport code, which estimates the energy-dependent neutron flux $\Phi$, and a depletion code, which describes the change of the material compositions. Typically, depletion codes such as MONTEBURNS (Pon- ton and Trellue 1998), TRITON (Oak Ridge National Laboratory 2009), and SERPENT (Leppänen 2007) solve the underlying differential equations with the help of so-called predictor-corrector algorithms.

Nuclear data uncertainties affect both transport and depletion codes. Uncertainties in cross sections, angular distributions, neutron multiplicities and fission spectra imply uncertainties in the neutron flux and the neutron energy spectrum. This flux and spectrum uncertainty has to be propagated during the depletion analysis which is, additionally, explicitly affected by cross section uncertainties and by decay data and fission yield data uncertainties. After a depletion step, the updated material composition carries an uncertainty which then has to be propagated to the following transport step.

In a full Monte Carlo approach, the nuclear data are sampled at the beginning of the burn-up simulation, then the cycle of transport and depletion is executed for one Monte Carlo sample, then the next sample is generated and used for a next simulation. The statistics of all simulations finally yields the desired uncertainty statements. An approximate way to evaluate the burn-up uncertainty is given by the Hybrid Method (García-Herranz et al. 2008). With this method, flux and spectrum uncertainties are neglected and only the uncertainties in the depletion step are propagated. This has the advantage that it requires performing the transport calculation only once for nominal nuclear data and, consequently, avoids the costly repetitions of the transport code updates.

This work focuses on the impact of different approximations to the propagation of nuclear data uncertainties. As outlined above, the first task will be to check the performance of the first order approximation. The next question that has to be addressed is what is the loss in accuracy related to neglecting either the uncertainties in the transport step or the depletion step. Additionally, the impact of different nuclear data covariance library input is studied by performing the same Uncertainty Quantification (UQ) analysis with two different inputs. For this we have chosen two of the presently most complete nuclear data covariance libraries: ENDF/B-VII.1 and SCALE 6.0. The reference to the approximate methods will be the NUDUNA method which is a Monte Carlo based approach that propagates the uncertainties in a complete fashion. As an example application, we study the burn-up benchmark Exercise I-1 b proposed by the OECD expert group “Benchmarks for Uncertainty Analysis in Modeling (UAM) for the Design, Operation and Safety Analysis of LWRs”. The burn-up simulations are performed with the SCALE 6.0 tool suite.

Note that uncertainties induced by so-called technological parameters, e.g. system dimensions and initial material compositions, and the operating history of a given fuel element, could lead to uncertainty estimations of the same magnitude as the estimations from nuclear data uncertainties (Rochman and Sciolli 2012), but their discussion is beyond the scope of this paper.

This paper is structured as follows. First, the UAM benchmark and the nuclear covariance inputs are discussed. Next, the NUDUNA method is introduced. The main part addresses the impact of different approximations and of different state-of-the-art covariance inputs. Finally, a full UQ analysis for the considered UAM benchmark is pre-
Table 1: List of isotopes whose concentrations are followed throughout the burn-up process.

| Light isotopes | 16O, 90Sr, 95Mo, 109Pd, 109Ag, 109Rh |
|---------------|------------------------------------|
| and fission products | 106Ru, 133Cs, 134Cs, 135Cs, 135I, 135Xe, 139La, 151Eu, 153Eu, 154Eu, 155Eu, 155Gd, 156Gd, 143Nd, 144Nd, 145Nd, 146Nd, 148Nd, 147Sm, 149Sm, 151Sm, 147Pm |
| Heavy isotopes | 234U, 235U, 236U, 238U, 237Np, 238Pu, 239Pu, 240Pu, 241Pu, 242Pu, 243Am, 244Cm |

Figure 1: Calculation scheme for burn-up simulation: coupling of transport and depletion codes.

2. UAM benchmark exercise on nuclear data uncertainties in a pin-cell burn-up calculation

The UAM Benchmark Exercise I-1b is described in Ivanov et al. (2012) Appendix VIII. It consists in performing a UQ study on a typical pressurized water reactor (PWR) pin-cell burn-up calculation. The main specifications are summarized in Fig. 2. Here we only address the most important ones for LWR applications.

3. Nuclear data covariance input

Nuclear data uncertainty quantification is still a developing field, which is demonstrated by the fact that covariance data sometimes significantly change even from one release of a nuclear data library to the other, e.g. when switching from ENDF/B-VI.8 (CSEWG-Collaboration, 2001) to ENDF/B-VII.1, as presented by Ivanov et al. (2012). Since uncertainty estimations from UQ studies reflect the uncertainty data in nuclear data libraries, new developments in nuclear data uncertainty quantification will inevitably lead to different UQ results.

In order to study the impact of different covariance data input, we decided to compare here two of the currently most complete covariance libraries with regard to the data which are important for criticality and burn-up calculations (Rochman et al., 2012; Cabellos, 2013): neutron cross section (including resonant and non-resonant region), neutron multiplicity and neutron emission spectrum uncertainties. Angular distribution uncertainties have not been identified as relevant for this type of analysis (Rochman and Sciolla, 2012), and are not separately investigated in this work. The selected covariance libraries are the SCALE 6.0 covariance library (Oak Ridge National Laboratory, 2009) and the covariances provided in ENDF/B-VII.1 (Chadwick et al., 2011). The SCALE 6.0 covariances have also been selected by the UAM expert group as a reference library for the benchmark exercise after reviewing the state-of-the-art of cross section covariance data (Ivanov et al., 2012; Sec. 2). At the time of that review, the SCALE 6.0 covariance library was the most complete and up-to-date compilation, and only thereafter a considerable amount of additional covariance information was released as part of the ENDF/B-VII.1, JENDL-4.0, and JEFF 3.2 evaluations.

The SCALE 6.0 covariance library consists of two parts:

- “High fidelity” uncertainty data taken from ENDF/B-VI.8 (CSEWG-Collaboration, 2001), ENDF/B-VII.0, a pre-release of ENDF/B-VII.1 and JENDL-3.3 (Shibata et al., 2002) for more than 50 nuclides, including the most important ones for LWR applications.
- “Low fidelity” uncertainty data, estimated independently of a specific data evaluation, retrieved from a collaborative project aimed to provide covariances over the energy range from $10^{-5}$ eV to 20 MeV for materials without covariances in ENDF/B-VII.0. These data were called the “BLO” [BNL-LANL-ORNL] uncertainty data (Little et al., 2008).

It provides uncertainties for a total of 401 nuclides in the form of covariance matrices in 44 energy groups for cross-
sections, fission neutron multiplicities $\nu$ and fission neutron energy spectra $\chi$. It also includes covariance data between reactions of different isotopes. Various UQ methodologies use the SCALE 6.0 uncertainty data as input, such as TSUNAMI, XSUSA, and PSI-NUSS.

ENDF/B-VII.1 now also includes comprehensive covariance data and collects efforts of several projects performed between 2006-2011 on nuclear data uncertainties:

- **BOLNA.** A covariance library created by five laboratories (BOLNA = Brookhaven-Oak Ridge-Los Alamos-NRG Petten-Argonne) for the purposes of the international project WPEC Subgroup 26 [Salvatore et al., 2008]. The library represents an ad hoc collection of covariances not tied to any specific evaluated nuclear data library.

- **“Low fidelity” uncertainty data, provided within BLO.**

- **COMMARA-2.0** [Herman et al., 2011]. A library produced by a BNL-LANL collaboration during 2008-2011. It constitutes the backbone of ENDF/B-VII.1 covariances, once adapted to the central values proposed for ENDF/B-VII.1.

Apart from that, re-evaluations were also made for ENDF/B-VII.1, but only for a few nuclides. ENDF/B-VII.1 covariance data have been supplemented by covariance evaluations from JENDL-4.0, providing complete covariance data for a total of 190 nuclides. So, it provides uncertainty data for neutron multiplicities, fission neutron spectra, cross sections and angular distributions. Uncertainties for the unresolved resonance region (URR) are typically included in the cross section uncertainties (i.e. in file 33 of an ENDF-6 tape), and only for very few isotopes there are detailed URR parameter uncertainties given (e.g. $^{232}$Th). JEFF-3.2 was released early in 2014 and includes covariance data for more isotopes than ENDF/B-VII.1, but lacks data for important fuel isotopes. E.g., the $^{239}$Pu cross section file does not provide any non-resonance cross section uncertainties. Thus we have decided to perform our study based on ENDF/B-VII.1, which represents for our field of application the most up-to-date covariance input provided by a nuclear data evaluation group.

4. **NUDUNA program package for nuclear data uncertainty analysis**

The NUDUNA (NUclear Data UNcertainty Analysis) program package has been developed within the last four years by AREVA GmbH. It will be applied as reference method when assessing the impact of different approximations.

NUDUNA provides full Monte Carlo sampling of the nuclear data inputs for transport and depletion calculations. Given such a tool, one can draw random samples of nuclear data and perform a separate transport and/or depletion calculation for each random sample. Then, the distribution of the individual results corresponding to the different random inputs can be analyzed, and uncertainty estimates can be deduced. The flowchart of the NUDUNA random sampling procedure is depicted in Fig. 3.

NUDUNA takes as input the information provided by nuclear data evaluations in the standardized ENDF-6 format [CSEWG, 2013]. Such ENDF-6 formatted files do not only supply best estimate values of cross sections, fission yields, decay data etc., but also their covariances. NUDUNA is capable of drawing random samples of nuclear data based on this covariance information.
At present, NUDUNA is validated for automatic compilation of random input files for the MCNP5 code (X-5 Monte Carlo Team, 2003) and the SCALE 6.0 tool suite, i.e. it can be applied, amongst others, to perform random simulations with the TRITON depletion sequence from SCALE 6.0. However, the NUDUNA output files could also be used as input for other codes, e.g. Serpent or MCNP6.

4.1. Nuclear data stored in ENDF-6 format

The structure of an ENDF-6 tape is hierarchical and sketched in Fig. 4. Each tape contains a library which may have several sections representing different materials (MAT). The library type defines the incoming projectile: there are libraries for photon, neutron, and proton induced events and for decay data. Each material section is structured into several so-called Files. The most relevant files for NUDUNA are Files 1-8 and 31-35. File 1 contains general information and the multiplicities of neutrons for prompt and delayed fission reactions, File 2 contains resonance parameters, File 3 contains non-resonance cross sections, File 4 contains energy and angular distributions of final state particles, File 5 provides thermal scattering data - S(α,β), File 6 provides radioactive decay data and fission product yields. Files 31-35 store the covariance information for Files 1-5. Each file contains sections providing information on a specific reaction type, and the sections themselves are structured in several records.

4.2. Random sampling of nuclear data

NUDUNA is capable of reading nuclear data encoded in ENDF-6 format and of random sampling the following
data according to their covariance information:

- average fission neutron multiplicities $\nu$ (File 1),
- resonance parameters (File 2),
- cross sections (File 3),
- angular distributions (File 4),
- decay data (File 8).

The ENDF-6 format provides only nominal values and covariances, but no further information on the distribution of the data. NUDUNA users can choose between normal and log-normal probability distributions. In this paper, we consider only sampling based on normal distributions. The following paragraph details the sampling procedure. At present, NUDUNA does not consider the covariance information between different nuclides, which usually leads to negligible uncertainty contributions if the thermal energy region of the neutron spectrum is of importance, e.g. for PWR reactors (Cabellos, 2013).

NUDUNA provides random PENDF (point-wise ENDF format) files which are then processed by NJOY and PUFF in order to generate random GENDF, ACE, and AMPX files (cf. Figure 3), which serve as inputs for transport codes.

4.2.1. Fission neutron multiplicity $\nu$

The fission neutron multiplicity $\nu$, i.e. the average number of neutrons per fission, is stored in File 1, which includes information for the total ($\nu_t$), prompt ($\nu_p$) and delayed ($\nu_d$) fission neutron multiplicity. They are connected via

$$\nu_t(E) = \nu_d(E) + \nu_p(E). \tag{1}$$

The multiplicity data are sampled according to their covariances provided in File 31. After the sampling, the sum rule given in Eq. 1 is checked and, if necessary, restored. If the ENDF-6 file provides no information on how this rule should be restored and if there is uncertainty information given for both prompt and total multiplicities, the total multiplicity is re-calculated as the sum of prompt and delayed multiplicities.

4.2.2. Resonance parameters

The resonance region is divided into the so-called Resolved Resonance Region (RRR) and the Unresolved Resonance Region (URR). The parameters that describe the resonances in both sub-regions and their uncertainties are given in File 2 and 32, respectively.

In the RRR regime, NUDUNA supports the most important formalisms (Reich-Moore, Single-level Breit-Wigner and Multilevel Breit-Wigner). It randomizes all parameters according to their covariances and enforces the positivity bounds for the widths and energy parameters. The uncertainties in the URR regime are predominantly treated as non-resonant cross section uncertainties within ENDF/B-VII.1, and the SCALE covariance library does not include explicit URR parameter uncertainties. So explicit URR parameter uncertainties are not considered in this work.

4.2.3. Non-resonance cross sections

Non-resonance cross section data and their uncertainties are stored in Files 3 and 33, respectively. These cross sections have to be added to the resonance cross sections defined by the RRR and URR parameters. As stated in the ENDF-6 format manual, the covariance information provided in the cross section covariance File 33 applies to the sum of non-resonance and resonance contributions. Thus, the resonance cross sections have to be reconstructed and added to the File 3 cross section before the random sampling can be performed.

The covariance data are given for energy ranges, and it is assumed that all points lying in the same energy range are completely correlated. Finally, sum rules have to be fulfilled. In principle, the ENDF-6 format provides with its LTY=0 sections a mechanism for defining how sum rules shall be restored. In case that this information is missing, the following procedure is applied:

- If a cross section is given by the sum of others, e.g. the total cross section, and has no uncertainty information, this cross section is calculated using its sum rule.
- If there is covariance information for the sum and at least for one of the addends, the sum is evaluated as sum of the random draws of all addends.
- If there is uncertainty information for the sum but not for any of the addends, the addends are re-scaled in order to fulfill the sum rule.

4.2.4. Angular distributions

Angular distributions of final state particles and their uncertainties are stored in Files 4 and 34, respectively. Usually, they are expressed as normalized probability distributions given in Legendre representation. The Legendre coefficients are randomized, and the positivity of the distribution is enforced by rejecting samples that lead to negative distributions.

4.2.5. Decay data

Decay data are stored in File 8, Section 457 of an ENDF-6 radioactive decay data sub-library 4. The current ENDF-6 format supports neither covariance matrices for branching ratios nor correlations between data of different isotopes, i.e. the numerical treatment is simple. NUDUNA samples both half-life values and branching ratios. For the branching ratios $\beta_i$, one has to enforce the constraint

$$\sum_i \beta_i = 1. \tag{2}$$
This constraint implies correlations of the different branching ratios. However, ENDF-6 only includes their standard deviations but not their correlation matrix. For cases where there are two branching ratios, the standard deviations for the two channels have to be identical if the constraint of Eq. 2 is taken into account in the uncertainty assessment. If the ENDF-6 file includes a "0" entry for one of two branching ratios, we replace it by the non-zero value of the other branching ratio. If two non-identical standard deviations are provided or if there are more than three decay channels, then the constraint of Eq. 2 is imposed by means of Bayesian updating of the input uncertainties.

The sampled decay data are checked for validity: branching ratios and half-lives have to be positive, and the former cannot get larger than 1. By default, NUDUNA assigns a 100% uncertainty to every decay data entry for which no uncertainty information is provided.

4.3. Converting ENDF-6 files into code-dependent format

NUDUNA currently provides the capability of generating input ACE libraries for MCNP as well as AMPX and ORIGEN libraries for SCALE 6.0. In this paper, we restrict ourselves to SCALE applications.

The AMPX format is a multi-group format, which is compiled by NUDUNA with the help of the NJOY (MacFarlane and Kahler 2010) and PUFF (Wiarda and Dunn 2008) codes, as illustrated in Fig. 3. NJOY is applied to convert ENDF-6 files to group-wise ENDF-6 formatted tapes based on the 238-groups structure and collapsing spectra of SCALE (Oak Ridge National Laboratory 2009) which is suitable for typical PWR reactor applications. Then PUFF is run to convert these files into AMPX files. As stated in Sec. 12 the resonance and non-resonance cross sections have to be summed before the sampling of the cross sections. For this the NJOY module reconr is applied.

The compilation of ORIGEN decay data libraries for SCALE 6.0 is also depicted in Fig. 3. Several limitations of the ORIGEN format have to be taken into account:

- ENDF-6 format can handle multiple particle emission decay modes, while ORIGEN format can store only $\beta^+ + n$. Thus, branching ratios of any multiple particle emission decay mode that involves at least a $\beta^- + n$ are added to the $\beta^- + n$ decay mode.
- ENDF-6 format can provide branching ratios to daughters in excited levels higher than the first, while ORIGEN can only handle decay modes to the first excited (metastable) state. Therefore, branching ratios to higher than the first excited (metastable) states of the daughter isotope are added to the branching ratio to the first excited (metastable) state.
- ENDF-6 format provides neutron emission decay modes (not related to $\beta^- + n$), while ORIGEN does not. Thus this decay mode is omitted in the conversion from ENDF-6 to ORIGEN format.

5. Impact of approximations

In the following, we are going to study the impact of different approximations to nuclear data uncertainty propagation:

- first order approximation,
- neglecting number density uncertainties, and
- neglecting neutron flux and spectrum uncertainties.

Results obtained with approximate methods are compared to results obtained with NUDUNA which solves the problem in a complete manner based on Monte Carlo sampling and is free of the above approximations. These studies are based on SCALE 6.0 covariances, and, for the sake of simplicity, only $^{235}\text{U}$ and $^{239}\text{Pu}$ uncertainties are propagated, and covariances for total, elastic, $(n,\gamma)$, $(n,2n)$, fission and inelastic cross section, plus correlations between elastic-fission, elastic-$(n,\gamma)$ and $(n,\gamma)$-fission are included. Correlations between cross section reactions of different isotopes are not included, as they have been shown to be irrelevant (Cabellos 2013).

5.1. First order approximation

In first order approximation, the uncertainty of a desired response function is obtained by applying the so-called sandwich formula (Cacuci 2003, Sec.III.F), which involves sensitivity coefficients and covariances. Current tools that apply first order approximation can tackle transport and depletion problems - however, a complete implementation that couples the two problems, as needed for the simulation of burn-up, is not yet available. Cabellos (2013) has attempted to solved this issue, but the method still misses some effects.

One of the best known tools for uncertainty propagation in transport calculations is the TSUNAMI tool which is part of the SCALE package. It is based on first order approximation and can only estimate uncertainties of transport problems. Nevertheless, we can use it to study the performance of this approximation. For this we neglect the isotopic number density uncertainties, and perform at each burn-up step a TSUNAMI and a NUDUNA analysis for given inventory using identical SCALE 6.0 covariance input. Thus only the uncertainty due to flux and spectrum uncertainty will be obtained. Fig. 5 shows the predicted $k_{\text{eff}}$ uncertainty with TSUNAMI (data from Cabellos 2013) and NUDUNA, where the upper panel gives the uncertainty induced by $^{235}\text{U}$ and the lower panel the one induced by $^{239}\text{Pu}$ input data uncertainties. Good agreement between the TSUNAMI and NUDUNA results is found for $k_{\text{eff}}$, which might suggest that a first order treatment is generally appropriate, at least for thermal light water systems. However, one has to keep in mind that nonlinear effects become more important for larger nuclear data uncertainties. Hence, first order results are expected to be less accurate for application cases sensitive to isotopes with large cross section uncertainties, such as the Gadolinium isotopes $^{155}\text{Gd}$ and $^{157}\text{Gd}$.
5.2. Neglecting the isotopic concentration uncertainties

NUDUNA is capable of propagating uncertainties through the complete burn-up process and thus considers both isotopic and flux uncertainties. However, one can also perform a limited analysis where the isotopic concentration uncertainties are neglected (cf. previous section). In the following, we are going to study the impact of such an approximation with special focus on the uncertainty contributions coming from cross section and neutron multiplicity data.

5.2.1. Impact of cross section uncertainties

Fig. 6 and 7 show uncertainties in $k_{\text{eff}}$ and in the isotopic concentrations of $^{235}\text{U}$ and $^{239}\text{Pu}$ induced by $^{235}\text{U}$ and $^{239}\text{Pu}$ cross section uncertainties, respectively. The lower panels show the isotopic concentrations and their uncertainties as obtained with the full NUDUNA analyzes. The upper panels compare the uncertainty estimates obtained with and without including isotopic concentration uncertainties induced by the depletion step. As can be seen, neglecting the uncertainties of isotopic concentrations leads to a considerable underestimation of the overall uncertainty.

When propagating $^{235}\text{U}$ uncertainties, the impact of isotopic concentration uncertainties becomes relevant above 10 GWd/MTU, and increases with increasing $^{235}\text{U}$ concentration uncertainty. When propagating $^{239}\text{Pu}$ uncertainties, the omission of isotopic concentration uncertainties shows an effect already at the very beginning and reaches a maximum between 20 and 50 GWd/MTU.

The lower panels of Fig. 6 and 7 also show that $^{235}\text{U}$ data uncertainties induce isotopic concentration uncertainties on $^{239}\text{Pu}$, and vice versa. The reason is that a change in the cross section of one isotope induces changes in neutron flux and spectrum, which modifies the reaction rates of the other isotope whose nuclear data are not modified.
5.2.2. Impact of fission neutron multiplicities

Fig. 8 presents uncertainties induced by fission neutron multiplicity ($\nu$) uncertainties. Each panel shows a curve obtained by propagating all uncertainties and a curve obtained by neglecting isotopic number density uncertainties.

One observes a very good agreement of the two approximations for $k_{\text{eff}}$ uncertainties. In fact, it shows that $\nu$ uncertainties have no impact on the depletion step, and also the implicit impact of $\nu$ uncertainties on isotopic compositions via the induced flux uncertainty is negligible.

5.3. Neglecting neutron flux and spectrum uncertainties

The last section discussed the impact of neglecting the uncertainties on isotopic concentrations. Now we are going to neglect flux uncertainties.

Again, NUDUNA is applied to provide the full uncertainty, and the Hybrid Method (HM) (García-Herranz et al., 2008; Díez et al., 2014) is used to propagate nuclear data uncertainties only in the depletion step. HM is based on Monte Carlo sampling of nuclear data uncertainties, and for each random draw a complete depletion calculation is performed. However, the flux input is kept at its nominal value, and so no additional transport calculations have to be carried out which implies savings in computing time. Consequently, neutron flux and spectrum uncertainties are not taken into account.

Neglecting neutron flux and spectrum uncertainties implies that the concentration uncertainty of a given isotope is only influenced by its own cross section uncertainty and by those of isotopes that are part of a transmutation chain that results in the given isotope. Fig. 9 presents the dominant contributions to the $^{235}\text{U}$ and $^{236}\text{U}$ concentration uncertainties. Indeed, the $^{235}\text{U}$ concentration addressed in the upper panel is not affected by $^{238}\text{U}$ or $^{239}\text{Pu}$ data uncertainties within the HM framework. Propagating also flux uncertainties, as NUDUNA does, leads to sizable contributions of $^{238}\text{U}$ and $^{239}\text{Pu}$ data uncertainties to the $^{235}\text{U}$ concentration uncertainty, as shown by the dashed and dashed-dotted curves in the upper panel of Fig. 9. So the HM method is not capable to predict the $^{235}\text{U}$ concentration uncertainty since it provides uncertainty estimations much lower than actual ones. The combined effect of propagating at the same time the uncertainties in $^{235}\text{U}$, $^{238}\text{U}$ and $^{239}\text{Pu}$ cross sections has been also addressed, show-
Two major conclusions can be drawn from these results. First, the uncertainty estimates for $k_{\text{eff}}$ strongly depend on the choice of the input source: the $\sigma$ contributions based on ENDF/B-VII.1 uncertainties are very different from those based on SCALE 6.0 uncertainties. The could at least be used to study a limited set of isotopes.

6. Impact of covariance data input

The previous section was solely based on SCALE 6.0 covariance data input in order to compare NUDUNA results to SCALE TSUNAMI and Hybrid Method results. Next, the impact of different covariance data input on the obtained uncertainty estimates is addressed. As outlined in Sec. 3, ENDF/B-VII.1 provides the most modern covariance evaluation which also includes all fuel isotopes. The SCALE 6.0 and ENDF/B-VII.1 libraries show major differences for the important $^{235}\text{U}$ and $^{239}\text{Pu}$ fuel isotopes, and the following paragraphs address these isotopes as examples to demonstrate the need for consistent covariance data input.

6.1. ENDF/B-VII.1 and SCALE 6.0 uncertainties for $^{235}\text{U}$ and $^{239}\text{Pu}$

The upper panels of Fig. 10 show $^{235}\text{U}$ $\sigma$-uncertainties as provided by ENDF/B-VII.1 and SCALE 6.0. ENDF/B-VII.1 gives covariance data for both prompt ($\sigma_p$) and total ($\sigma_t$) neutron multiplicities. However, the two covariance matrices are not consistent: the difference between the covariance matrices is too large to be explained by the delayed neutron multiplicity $\sigma_t$ whose contribution to the total multiplicity is only approx. 0.64%. Hence, the total and prompt covariance matrices should be almost identical. There are also major differences between SCALE 6.0 and ENDF/B-VII.1 covariance data for $\sigma$. With regards to $^{235}\text{U}$ cross section uncertainties, only small differences are found among ENDF/B-VII.1 and SCALE 6.0.

The lower panels of Fig. 10 show the $\sigma$ uncertainties for $^{239}\text{Pu}$. For ENDF/B-VII.1, the covariance matrices for the total and prompt multiplicities are identical and, consequently, only the one for the total multiplicity is presented. Again, very large differences are observed between ENDF/B-VII.1 and SCALE 6.0. Additionally, the ENDF/B-VII.1 and SCALE 6.0 cross section uncertainties differ for $(n,\text{fission})[E>1\text{eV}], (n,\gamma) [1-100\text{eV}]$ and the cross-correlation between $(n,\text{fission})$ and $(n,\gamma)$.

6.2. Propagating ENDF/B-VII.1 and SCALE 6.0 uncertainties for $^{235}\text{U}$ and $^{239}\text{Pu}$

Fig. 11 presents the $k_{\text{eff}}$ uncertainties induced by $^{235}\text{U}$ and $^{239}\text{Pu}$ cross section and $\sigma$ uncertainties as predicted by NUDUNA. The SCALE uncertainties have been obtained by creating an ENDF-6 formatted file that represents a fusion of ENDF/B-VII.1 nominal information and SCALE uncertainty information.

Two major conclusions can be drawn from these results. First, the uncertainty estimates for $k_{\text{eff}}$ strongly depend on the choice of the input source: the $\sigma$ contributions based on ENDF/B-VII.1 uncertainties are very different from those based on SCALE 6.0 uncertainties. The
Figure 10: Covariance data for $^{235}$U (upper panels) and $^{239}$Pu (lower panels) fission neutron multiplicities from ENDF/B-VII.1 and SCALE 6.0, presented in the SCALE 44-group structure.
second conclusion is related to the fact that in ENDF/B-VII.1 the uncertainties for total and prompt $\sigma$ for $^{235}$U are inconsistent (cf. Sec. 6.1), so that one has to choose between sampling the $\sigma$ data based on the total or on the prompt uncertainties. As shown by a comparison of the red solid and the red dashed-dotted curve in Fig. 11(a), this arbitrary choice induces a large ambiguity in the predicted contribution of the $^{235}$U $\sigma$ uncertainty to the $k_{\text{eff}}$ uncertainty.

Fig. 11 also shows results for propagating cross section uncertainties, i.e., for propagating File 33 (MF33) covariance information. For $^{235}$U, the ENDF/B-VII.1 and SCALE 6.0 results are very similar, as could be expected from their similar covariance information. However, the results are also very similar for $^{239}$Pu, in spite of the fact that there are significant differences in the $^{239}$Pu covariances. Here it seems that differences between individual cross sections counteract each other.

To summarize, depending on the choice of uncertainty data input, ENDF/B-VII.1 or SCALE 6.0, very different UQ results are obtained. Even the most important uncertainty contributors may change. Additionally, the inconsistency in $\sigma$ uncertainties for $^{235}$U in ENDF/B-VII.1 has to be addressed.

### 7. Full UQ analysis based on ENDF/B-VII.1

In the following, an UQ analysis with focus on nuclear data is performed, which includes almost all contributions to nuclear data uncertainty. The contribution from $S(\alpha,\beta)$ uncertainties is, however, not included, since these uncertainties are not yet fully quantified and not yet provided within evaluated nuclear data libraries. Currently, methodologies are being developed for estimating them (Rochman and Koning 2012; Holmes and Hawari 2014), and there are also first impact estimates available, e.g., by Cabellos et al. (2014a) for PWR reactor cores.

In order to perform the UQ analysis, the incident neutron data and the decay data were sampled according to ENDF/B-VII.1 uncertainty data. The decay data sampling considered all isotopes included in the ORIGEN input, while the incident neutron data sampling was limited to the most important isotopes presented in Table 2 and data for the minor isotopes were not sampled but taken from the nominal ENDF/B-V library of SCALE 6.0.

A reference calculation is presented in Fig. 12 which is based on nominal ENDF/B-VII.1 decay data, nominal ENDF/B-VII.1 neutron data for the isotopes in Table 2 and nominal ENDF/B-V neutron data for the other isotopes. The evolution of the neutron multiplication factor $k_{\text{eff}}$ presented in Fig. 12 shows the typical PWR pin-cell behavior.

The following paragraphs discuss the impacts of incident neutron and decay data uncertainties separately in order to illustrate their individual contributions.

#### 7.1. Impact of ENDF/B-VII.1 incident neutron uncertainties

Fig. 13 shows the $k_{\text{eff}}$ uncertainty estimate that has been obtained based on the ENDF/B-VII.1 incident neutron data covariances for the list of isotopes given in Table 2. This estimate includes uncertainties of $\sigma$, resonance parameters, cross sections, and angular distributions. The $\sigma$ values are sampled based on the covariance information for the prompt multiplicities if there is covariance information for both prompt and total multiplicities.

Fig. 13 also presents the individual contributions due to $^{235}$U, $^{238}$U and $^{239}$Pu uncertainties. The $^{238}$U data uncertainty causes a prominent almost constant $k_{\text{eff}}$ uncer-
The neutron data are taken from ENDF/B-VII.1 for nuclides given in Table 2 and from the SCALE 6.0 ENDF/B-V multi-group cross section library for all others. Decay data are taken from ENDF/B-VII.1 for all isotopes.

The above estimate does not include uncertainties induced by the fission neutron spectrum \( \chi \) and by the fission yields since their sampling has not yet been implemented in NUDUNA. However, we have estimated the fission neutron spectrum with the aid of TSUNAMI. The contribution of the \( ^{235}U \) \( \chi \) uncertainty to \( k_{\text{eff}} \) decreases from 100 pcm at BOC to 50 pcm at EOC, and the \( ^{239}Pu \) \( \chi \) uncertainty contribution increases from 36 pcm at 10 GWd/THM to 150 pcm at EOC. Adding these contributions quadratically to the pure NUDUNA estimates results in the uncertainty estimates of approximately 450 pcm at EOC.

The impact of decay data uncertainties on isotopic compositions is also limited, and only for three isotopes the induced uncertainty exceeds 0.3%: \( ^{133}Cs \), \( ^{134}Cs \) and \( ^{151}Eu \). The large uncertainty of \( ^{151}Eu \), whose number density uncertainty is almost constant at 9.3% throughout the whole burn-up period, has been identified before in (Cabellos et al. 2014b), and it is mainly produced by neutron capture in \( ^{151}Sm \) and its daughter \( ^{151}Gd \). Additionally, the \( (n,\gamma) \) reaction in \( ^{151}Gd \) has uncertainties of approx. 10%.

7.2. Impact of ENDF/B-VII.1 decay data uncertainties

Now we are going to study the uncertainties induced by ENDF/B-VII.1 decay data uncertainties, i.e. uncertainties of half-lives and branching ratios.

Any data without uncertainty specification in ENDF/B-VII.1 is assigned a 100% uncertainty in the NUDUNA random sampling procedure. Even with this conservative assumption, the resulting \( k_{\text{eff}} \) uncertainty is completely negligible and does not exceed 6 pcm during the whole burn-up period.

The impact of decay data uncertainties on isotopic compositions is also limited, and only for three isotopes the induced uncertainty exceeds 0.3%: \( ^{133}Cs \), \( ^{134}Cs \) and \( ^{151}Eu \). The large uncertainty of \( ^{151}Eu \), whose number density uncertainty is almost constant at 9.3% throughout the burn-up period, has been identified before in (Cabellos et al. 2014b), and its large uncertainty comes from the 6.67% uncertainty on the \( ^{151}Sm \) half-life.

The \( ^{133}Cs \) and \( ^{134}Cs \) uncertainties are presented in Fig. 14. For \( ^{134}Cs \) the decay of its parent \( ^{134}Xe \) plays a minor role since \( ^{134}Xe \) is almost stable (half-life \( 5.8 \times 10^{22} \) years), and it is mainly produced by neutron capture in \( ^{133}Cs \). Thus, the \( ^{134}Cs \) uncertainty follows the \( ^{133}Cs \) uncertainties. \( ^{133}Cs \) is a stable isotope and its number density uncertainties are generated by the decay data uncertainties of its parents \( ^{133}Xe \), \( ^{133}I \), and \( ^{133}Te \). These parent isotopes have small half-life values and cause already at BOC quite a large uncertainty of their \( ^{133}Cs \) daughter number density.

Table 4 shows the uncertainty estimates for the number densities after 300 years of cooling. They are only sizable for the \( ^{137}Cs \), \( ^{125}Eu \), \( ^{151}Sm \), and \( ^{241}Pu \) isotopes. These results are in agreement with the ones provided by Martínez et al. (2014) who also applied a Monte Carlo
Table 3: Isotopic composition uncertainties as a function of burn-up when propagating incident neutron data uncertainties according to ENDF/B-VII.1 covariance data (only those isotopes are shown for which the uncertainty exceeds 1%).

| Isotopes  | 0 GWd/MTU (at./barn-cm) | 10 GWd/MTU (at./barn-cm) | 30 GWd/MTU (at./barn-cm) | 50 GWd/MTU (at./barn-cm) | 60 GWd/MTU (at./barn-cm) |
|-----------|-------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
|           | unc. (%)                | unc. (%)                 | unc. (%)                 | unc. (%)                 | unc. (%)                 |
| 134Cs     | 4.442E-07               | 3.362E-06                | 7.824E-06                | 1.034E-05                | 3.89                     |
| 149Sm     | 1.228E-05               | 3.237E-05                | 4.399E-05                | 4.879E-05                | 1.97                     |
| 151Sm     | 4.014E-07               | 5.858E-07                | 6.966E-07                | 7.381E-07                | 6.98                     |
| 151Eu     | 5.963E-10               | 9.179E-10                | 9.634E-10                | 9.538E-10                | 7.26                     |
| 155Eu     | 4.567E-08               | 2.126E-07                | 4.789E-07                | 6.133E-07                | 35.58                    |
| 155Gd     | 5.243E-10               | 2.456E-09                | 4.752E-09                | 7.540E-09                | 26.74                    |
| 234U      | 1.166E-05               | 8.153E-06                | 6.231E-06                | 5.406E-06                | 2.15                     |
| 235U      | 1.126E-03               | 1.076E-04                | 1.402E-04                | 1.480E-04                | 1.39                     |
| 236U      | 5.137E-04               | 1.448E-04                | 3.111E-04                | 1.970E-05                | 3.03                     |
| 237Np     | 8.397E-06               | 3.343E-06                | 1.622E-05                | 1.648E-05                | 2.68                     |
| 238Pu     | 2.020E-06               | 3.411E-06                | 6.985E-06                | 7.009E-06                | 2.89                     |
| 239Pu     | 1.218E-07               | 3.405E-07                | 6.145E-07                | 7.425E-07                | 2.12                     |
| 240Pu     | 8.256E-05               | 1.488E-04                | 1.639E-04                | 1.648E-04                | 2.00                     |
| 241Pu     | 9.675E-06               | 4.005E-05                | 6.514E-05                | 7.425E-07                | 2.12                     |
| 242Pu     | 3.802E-06               | 1.434E-05                | 1.639E-04                | 1.648E-04                | 2.00                     |
| 243Am     | 1.066E-08               | 2.595E-06                | 4.334E-06                | 7.028E-06                | 2.26                     |
| 244Cm     | 6.472E-10               | 1.900E-07                | 1.802E-06                | 3.678E-06                | 2.67                     |

8. Conclusions

This work presented an uncertainty quantification study for the burn-up of a typical PWR pin-cell, focusing on uncertainties induced by nuclear data uncertainties. Different approximations to uncertainty assessment were studied by evaluating their performance in the burn-up analysis of the UAM Exercise I-1b pin-cell benchmark.

An analysis of the $k_{eff}$ uncertainty for transport calculations at different burn-up points based on first order approximation leads to results that are very similar to the exact results obtained by Monte Carlo sampling when propagating $^{235}$U and $^{239}$Pu uncertainties. Note that in (Cabellos, 2013) and (Sabouri et al., 2014) first order uncertainty propagation methods are proposed that include both uncertainties of transport and depletion. However, these schemes yield higher $k_{eff}$ uncertainty estimates than the exact Monte Carlo schemes.

Neglecting either flux or isotopic number density uncertainties in the burn-up simulation is both problematic and may lead to considerable underestimations of the total uncertainty. Neglecting uncertainties in the isotopic number densities leads to sizable deviations for the $k_{eff}$ uncertainty, especially at EOC. Neglecting the flux uncertainties, as proposed by the Hybrid Method, leads to an underestimation of the overall isotopic number density uncertainty. The magnitude of the underestimation is hard to predict, and so it is not clear when such an approximation can be applied in order to perform fast UQ studies for burn-up problems. Future HM developments for defining applicability criteria and for including a reactor power constraint in the random sampling are desirable. Overall,
we conclude that accurate uncertainty quantification studies should always fully propagate flux and isotopic number density uncertainties.

Additionally, the impact of different covariance input data was analyzed with NUDUNA. For $^{235}\text{U}$, an inconsistency between total and prompt $\nu$ uncertainties is found for ENDF/B-VII.1, which leads to ambiguous results for the resulting $k_{\text{eff}}$ uncertainty. Owing to the large differences between SCALE 6.0 and ENDF/B-VII.1 $\nu$-uncertainties, the $k_{\text{eff}}$ uncertainty study based on SCALE 6.0 yields much higher uncertainties than the one based on ENDF/B-VII.1.

Finally, a complete uncertainty quantification was performed with NUDUNA for the UAM benchmark based on ENDF/B-VII.1 covariances. The $k_{\text{eff}}$ uncertainty amounts to approx. 450 pcm at BOC and approx. 530 pcm at EOC. The most important contributions stem from $^{235}\text{U}$, $^{238}\text{U}$, $^{239}\text{Pu}$ data uncertainties: the $^{235}\text{U}$ contribution decreases and the $^{239}\text{Pu}$ contribution increases as burn-up increases, and the contribution of $^{238}\text{U}$ is almost constant until EOC. The impact of decay data on the $k_{\text{eff}}$ uncertainty is negligible.

The incident neutron data uncertainties lead to uncertainties in isotopic concentrations. The number density uncertainties typically do not exceed 4% for heavy isotopes and 8% for fission products. Only for $^{154}\text{Eu}$ and $^{152}\text{Gd}$ higher values of up to 35% are obtained. Decay data uncertainties induce additional sizeable uncertainties for the $^{137}\text{Cs}$, $^{151}\text{Eu}$, $^{151}\text{Sm}$, and $^{241}\text{Pu}$ isotopes, and the results for the uncertainties 300 years after shutdown are in good agreement with the ones obtained by Martínez et al. (2014).

Monte Carlo schemes are up to now the only ones capable of including both uncertainties of neutron transport and depletion calculations. The presented Monte-Carlo scheme may also be extended to uncertainty assessments on a fuel assembly or reactor level.

Note that this work represents an exemplary UQ study based on currently available covariance data. The study should be repeated once updated covariance data are provided or new ENDF/B or SCALE libraries are released.

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