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Nuclear data uncertainties for Swiss BWR spent nuclear fuel characteristics

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Abstract. The effect of nuclear data (fission yields, cross sections and emitted spectra) are quantified for spent nuclear fuel assemblies from a realistic Boiling Water Reactor operated over 25 cycles. Nominal calculations are performed with the CASMO5, SIMULATE-3 and *SNF* codes and the ENDF/B-VII.0 nuclear data library. The uncertainties are calculated with the same codes, using a Monte Carlo propagation method, and the ENDF/B-VII.1 covariance matrices. The conclusions are that (1) the nuclear data have a non-negligible impact for spent fuel quantities (*e.g.* decay heat, neutron emission or isotopic contents); (2) the importance of varying all data together is demonstrated, showing an under or overestimation of uncertainties if fission yields are sampled separately from the other nuclear data; and finally (3) the importance of considering the full irradiation history (multi-cycle assembly life) is also demonstrated, showing also an under or overestimation of uncertainties when performing the nuclear data sampling for a single reactor cycle.

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1 Introduction

In specific cases, nuclear data can be one of the major contributors to uncertainties for a selection of reactor and fuel quantities from the neutronics point of view. It can be expected that in a near future, the calculation of such uncertainties can become part of a normal system analysis, for design, operation or safety analysis. Such an effort is in fact not new and can be traced back to the 70s and 80s [1,2]. During this period of time, a strong limitation was the restricted available computer power, and its recent increase allows today to conveniently perform uncertainty propagation with a limited number of simplifications. Recently, a methodology for nuclear data uncertainty quantification applied to PWR core analysis was proposed in the framework of the Swiss PWR core licensing analysis [3]. Such method was applied to UO_2 and MOX operated cycles, showing either moderate impacts of the nuclear data on many cycle parameters (*e.g.* peaking factors, assembly average and local burnup values), or more pronounced effects, for instance for the moderator temperature coefficient. Additionally, a second study using the same methodology applied to spent fuel characteristics from Swiss power plants (decay heat, neutron/gamma source, activity and isotope inventory) has indicated that the nuclear data uncertainties have a non negligible impact [4,5]. Once such calculation scheme is in place, it was also used to propagate the same type of nuclear data uncertainties to transient systems, as presented in Refs. [6–8]. Such automation also opens the possibility for the propagation over the complete lifetime of the nuclear fuel, from the first irradiation to the long-term repository within specific canister types [9].

Such full core analysis including spent nuclear fuel characteristics (SNF) for nuclear data uncertainty propagation are for the time being not often performed, as it requires a relatively large computational power, as well as all the information on the core parameters, all fuel loading patterns and assembly histories. Therefore many studies have been performed on pincell, or single assemblies, allowing nevertheless to obtain very insightful results (see for instance Refs. [10–20]). As examples of full core analysis, see for instance Refs. [21–24].

To complement the previous work on the impact of nuclear data, this paper presents a similar study as performed in Ref. [3] but dedicated to BWR cycles with a focus on spent nuclear fuels. 25 operated cycles for a specific Swiss BWR are analyzed, as well as the spent fuel assemblies discharged during this operated period of about 15 years (fuel content, decay heat, or neutron emission). In the present work, three groups of nuclear data are considered for the uncertainty propagation: (1) all together (later referred to as "All"), (2) only fission yields (or "FY"), and (3) all nuclear data except FY (or "XS"). As presented later, this last group contains cross sections, emitted particles and spectra. Using these simple definitions, the quantity "All"

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can be defined as the simultaneous variations of FY and XS.
The goal of such differentiation is to answer the first following question: can the variances on fuel quantities, independently induced by XS and FY, be linearly added (separately sampled and propagated through the 25 cycles), or is there an interaction effect preventing such simple sum ? (knowing that in the present nuclear data libraries, there are no correlation between fission yields and other nuclear data quantities such as cross sections). It will be shown that depending on the quantity of interest, there exists an interaction effect, implying that the correct uncertainties can be obtained only by varying simultaneously the FY and XS quantities.
The second question that this paper contributes to answer is related to uncertainties for realistic full core studies through a large number of reactor cycles: are the SNF uncertainties similar if one considers the uncertainty propagation in a single cycle, therefore keeping the nuclear data constant for previous cycles ? If yes, there is no need to simulate a complex system including many reactor cycles with thousands of assemblies. If not, conclusions for simpler systems can not be simply extrapolated to more complex full cycle core analysis. In this paper, we will try to answer these questions in specific cases, when quantities can be compared, and the results will be accompanied with limited discussions or possible future developments.
For readers interested only in the quantifications of uncertainties on SNF quantities considering all cycles, a summary of the results is presented in Table 1 and Table 2. For more details on the above questions, the following sections will present various aspects of the analysis.

Table 1: Total effect of nuclear data (simultaneous variation of FY and XS) in percent for all considered cycles. The "Mean" column is the average uncertainties over all cycles and the "Max" column indicates the maximum uncertainty for a specific cycle or cooling time. See Table 2 for spent nuclear fuel (SNF) isotopic contents.

SNF Quantity	Mean	Max
Decay heat	2.4	6.1
Neutron emission	2.4	6.2
Average burnup	0.2	0.7
Segment burnup	0.9	2.5
Spontaneous fission	5.7	10.8

2 Core and fuel analysis

At PSI, a large database of validated models was built in support of the analysis of core reloads for all Swiss nuclear power plants. Such database, called CMSYS for Core Management SYStem, contains the information for the five Swiss reactors (3 PWR and 2 BWR) from early cycles to nowadays operations. Data from the plant operators are collected (such as cycle lengths, shutdown periods, core loadings, power histories, assembly characteristics, *etc*) and incore measurements (boron concentrations, reaction rates or TIPS). With these data in hand, validated models have been built for the core simulation using CASMO5 and SIMULATE-3 or SIMULATE5 [25–27]. CASMO is a two dimensional characteristics-based neutron and gamma transport lattice physics code with depletion capability. One principal purpose of CASMO is to generate multigroup cross sections and discontinuity factors for SIMULATE. SIMULATE is a three-dimensional multigroup reactor analysis code developed by the Studsvik company. For more details on CMSYS, see Refs. [3,28]. In the present case of a Swiss BWR, these models were also used in reload licensing submittals in support of the national regulator ENSI. Lately, the *SNF* software has been added for the calculations of the spent nuclear fuel characteristics (isotopic inventory, decay heat, source term) [4]. *SNF* calculates decay heats and radiation sources as functions of shutdown time by explicitly tracking all library nuclides: fission products, actinides, and structural elements. It is used in this work in combination with CASMO and SIMULATE, based on the existing validated cycle models. Note that the code *SNF* is identified in italic, whereas the spent nuclear fuel acronym (SNF) is given in normal characters.
In the present analysis, the following case is considered:

- a Swiss Boiling Water Reactor is selected,
- 25 consecutive cycles are analyzed (spanning over 15 years of operation),
- validated CASMO-5 and SIMULATE-3 models are used (version 2.03.00 with the "e7r0.125.586" library for CASMO5 and version 6.07.17_MOX_4 for SIMULATE-3),
- in addition to CASMO and SIMULATE, the *SNF*-1.6 code is also used to extract different characteristics from the fuel assemblies at the end of each cycle.

From these models, different quantities can be calculated (and eventually compared to measurements) such as values presented in Table 1.
Over the 25 cycles studied here, various types of assemblies were used in the core. Such assemblies were only made of UO_2 fuel and no MOX fuel was considered. The enrichments vary from 3.0 % to 4.2 % with assembly average burnup values up to 65 MWd/kgU. The number of assemblies (used over many cycles) was larger than 1100.

3 Monte Carlo uncertainty propagation and sensitivity

The propagation of nuclear data uncertainties to quantities for large-scale systems (such as reactor cores) is performed in a very simple manner: repeating many times the same calculation, each time randomly changing nuclear data (cross sections, spectra, or/and fission yields). One specific calculation set, based on one realization of random nuclear data, is referred to as a "random run". A random run includes the production of all necessary quantities by CASMO5 for all assemblies, the cycle calculations with SIMULATE-3 over 25 cycles, and finally the

SNF calculations for all assemblies.
Such Monte Carlo approach is relatively widely spread for systems where a sensitivity approach cannot be applied [17,21] and has the main advantage to provide uncertainties on any possible calculated quantities. In return to its generality, it requires relatively large computer power since the number of (similar) calculations N needs to be high enough to ensure a required convergence for a number of moments of the studied distributions.

3.1 Random nuclear data, standard error and standard deviation

In this work, the propagation of nuclear data uncertainties is based on processed covariance matrices from a specific library. In Ref. [3], the SCALE-6.2 library was used and no uncertainties due to fission yields were included. In the present case, the covariance matrices from the ENDF/B-VII.1 library are used. The nuclear data library and covariance matrices are therefore not consistent from a nuclear data evaluation aspect, but this combination results from the available tool setup.
For the fission yields, the uncertainties are also coming from ENDF/B-VII.1, but as no correlations are included in this library, an in-house correlation matrix is used, as presented in Refs. [17,29]. All the important fissioning systems are considered in this study, among which (but not limited to) ^{235,238}U, ^{239,241}Pu.
Three types of calculations are performed regarding the choice of random nuclear data for all cycles:

- all nuclear data varied together: fission yields, cross sections, emitted spectra. A total of 130 random runs are done, and the uncertainties arising from these variations will be referred to as "All",
- only cross sections and emitted spectra are considered: 55 random runs, later mentioned as "XS", and
- fission yields (FY) alone are varied: 85 random runs.

Such separation of inputs allows to estimate the global effect of the fission yields and cross sections (and emitted spectra) alone. Also it is a very convenient way to check if the calculated variance at the core or fuel level is well represented by the sum of the partial variance, or if there are interactions during the cycle simulations which prevent simple summing.
Additionally, for a specific cycle $\mathcal{N}$, the nuclear data are separately varied to quantify the impact of individual reactions or isotopes. This cycle is selected as it is well within the considered 25 cycles, and represents an equilibrium core with respect to the assembly reloading map. This choice is somewhat arbitrary, but it is believed that the results are well representative of similar cycles. A total of 330 random runs are performed for each separated nuclear data, such as ^{235}U(n,f) or ^{238}U(n,γ) cross sections.
Such limited numbers of random runs lead to relatively large standard errors on the means and variances. The standard error on the calculated mean varies as a function of $1/\sqrt{N}$, with N being the number of samples. Possibly more interesting in this work is the standard error on the standard deviation varying as $1/\sqrt{2(N-1)}$, leading to 6 %, 10 % and 8 % for All, XS and FY, respectively. In the case of cycle $\mathcal{N}$ and the 330 random runs for each nuclear data type, the standard error on the standard deviation is about 4 %. In the following, the presented quantities will be named "uncertainties", and are equivalent to one standard deviation.
Other nuclear data, such as decay constants or thermal scattering data are not considered in this work.

3.2 SHARK-X

SHARK-X is a PSI tool to perform CASMO5 calculations with perturbed nuclear data (see for instance Refs. [20, 29]). It is using the covariance matrices from a nuclear data library, assumes Normal distributions for every single nuclear data quantities (cross sections, nubar, prompt fission spectra and fission yields) and produces random nuclear data. The number of energy groups in this work is 19, from 0 to 20 MeV, and in the case of fission yields, additional constraints are added, as presented in Ref. [29].

3.3 Sensitivity

For the purpose of identifying the inputs responsible for the calculated uncertainty, various methods for sensitivity analysis (SA) have been implemented in SHARK-X [30, 31]. They are making use of the calculations already performed, *e.g.* no additional run is needed. Even though uncertainty quantification through the use of random sampling is relatively straightforward, SA based on those random samples is difficult due to the potential non-linearity of the model, to the large number of input variables, as well as to their correlations. Given the low number of samples available, the method based on the determination of Pearson correlation coefficients is used in the present work. In Ref. [32], it is demonstrated that the squared Pearson coefficient is a linearized version of the first order sensitivity index. Such approach has been extensively used in the past by the so-called "GRS method" [33]. Both first order and total sensitivity indices can be determined. No assumption is made with respect to the probability distribution functions of the input/output. However linearity of the output with respect to input perturbations is assumed. It is reviewed briefly below.
In statistics, the Pearson correlation r_p is computed as shown in Eq. (1).

$$r_p = \frac{\sum_{j=1}^{N}(x_i^j - \bar{X}_i)(y^j - \bar{Y})}{\sqrt{\sum_{j=1}^{N}(x_i^j - \bar{X}_i)^2}\sqrt{\sum_{j=1}^{N}(y^j - \bar{Y})^2}} \qquad (1)$$

where i is the input index and j the sample index out of a total of N samples. $\overline{X}_i$ and $\overline{Y}$ are the means of the random variables X_i and Y.
r_p^2 can be interpreted as the coefficient of determination of the relationship between Y and X_i assuming a linear model between X_i and Y [34]. It represents the fraction of

the variance of Y which is explained from approximating Y by a linear combination of the X_i. This interpretation can be used to estimate the first order sensitivity index of the input parameter X_i:

$$S_{X_i} = r_p^2 \tag{2}$$

Those first order sensitivity indices can be generalized to multiple correlation coefficients which correspond to groups of input parameters [33]. Assuming a group of parameters $X_{(1)} = (X_1, ..., X_k)$, the multiple correlation coefficient is defined as Eq. (2).

$$R^2_{(1)} = (r_p(Y, X_1), ..., r_p(Y, X_k)) \times \Sigma^{-1}_{X_{(1)}} (r_p(Y, X_1), ..., r_p(Y, X_k))^T \tag{3}$$

where $r_p(Y, X_i)$ is the correlation coefficient between Y and X_i, $\Sigma^{-1}_{X_{(1)}}$ is the inverse of the covariance matrix for the group of parameters $X_{(1)}$.
The first order sensitivity index for a group of parameters can be defined as $S_{X_{(1)}} = R^2_{(1)}$ and the total index for a group of parameters as $S^T_{X_{(1)}} = R^2 - R^2{}_{(1)}$. $R^2{}_{(1)}$ is the multiple correlation coefficient between Y and the remaining group of input parameters (the ones not included in $X_{(1)}$). R^2 is the total correlation coefficient between Y and the full set of input parameters X.
This sensitivity method is applied in the following to the 330 SIMULATE-3 output samples for cycle $\mathcal{N}$ where only perturbation to cross sections are considered. 5111 input parameters were considered which corresponds to 269 groups of parameters: each group is defined by all the energy boundary of a given nuclide-reaction pair. One case is considered: the number of spontaneous fission calculated by *SNF*. No additional calculation was performed; the outcomes of the study presented below required solely post processing of the existing output samples. This is one of the undeniable strength of this method for SA. Results will be presented in section 4.5.

3.4 Calculation time and storage

In practice, thousands of calculations based on random inputs are often difficult to do within a reasonable amount of time. In the case of simple systems such as criticality benchmarks, N can reach 10 000, but for more complicated cases, only a few tens are sometimes performed. In Ref. [3] where the case of a PWR was studied, a total of $N = 500$ similar calculations was performed, given that for a single one, about 1000 hours of simulation on a single CPU is necessary with 3 Gb of data (for 30 cycles). In the present case, as the BWR core under study is larger and includes more segment calculations than in the case of Ref. [3] (one segment calculation is performed with a single CASMO5 description), about 7200 hours are necessary for $N = 1$ (all lattice calculations, all core cycle calculations and all *SNF* calculations at the assembly level). The lattice calculations represent more than 90 % of the total calculation time. For the data storage, one calculation scheme also is also more voluminous than the PWR case, with almost 30 Gb (for 25 cycles, and again the lattice calculations occupy about 80 % of the total volume).

4 Results

In the following, details for some results presented in Tables 1 and 2 are given. In general, global uncertainties due to nuclear data are provided as a function of assembly burnup. In some cases, the different contributions from various cross sections are also presented. Concerning the results as a function of core cycle, every cycle considers the variations from all previous cycles. There is therefore an uncertainty propagation through all cycles, allowing to follow the trends for various cycles. In addition, cycle $\mathcal{N}$ is considered for the study of uncertainty propagation through a unique cycle and for sensitivity analysis.

4.1 Assembly burnup

The uncertainties due to nuclear data for the average assembly burnup at the end of cycles are presented in Fig. 1. A similar figure was already presented in Ref. [4] for both PWR and BWR assemblies, but for the total effect only (referred as "All" in the figure). As in Ref. [4], all assemblies at the end of every cycle are considered, the assemblies being at their end of life or not. This allows to obtain uncertainties for low burnup values after one irradiation cycle. As observed, the main sources of uncertainties are not the fission yields. Globally, the effect of nuclear data is small on the assembly average burnup. As a point of comparison, the variations obtained by changing the CASMO or SIMULATE version are in the vicinity of 1 or 2 %. The observed trend is a decrease of the uncertainty for higher burnup, reaching relatively small values for assembly burnup usually disposed for short-term storage. Additionally, the linear combination of the variances for XS and FY leads to similar results compared to the variation of all nuclear data together, as presented in the bottom Fig. 1. The plotted difference does not exhibit any pattern linked to possible interactions in the model between the combined variations of XS and FY. The increasing spread with the burnup is simply due to the decreasing uncertainty values.
As for Fig. 1, Fig. 2 is presenting the uncertainties as a function of burnup values, not for the full assemblies, but only for their bottom segment. Looking at a unique segment, especially one at the end of the assembly, provides uncertainties for low burnup values, corresponding to higher contents of fissioning isotopes compared to the rest of the assembly. These parts of the SNF are of relevance in the case of criticality studies as it can correspond to a region of high importance for the neutron population. As observed, the uncertainties can reach up to 3 % in the case of very low burnup values, indicating a similar trend as in Fig. 1. Such higher uncertainties compared to the assembly average values will also translate into higher uncertainties for the segment isotope contents. Finally, as for

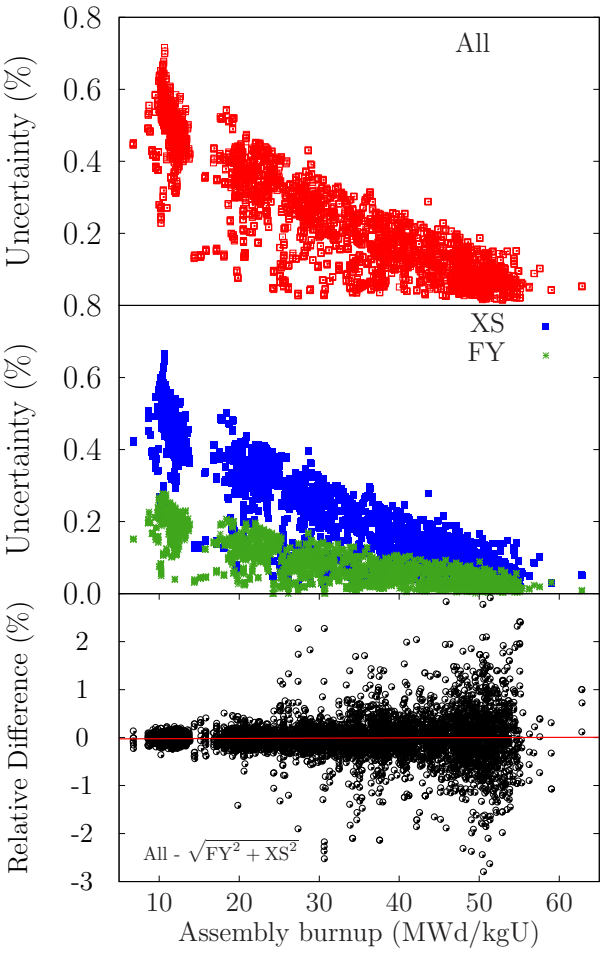

Fig. 1: Uncertainties due to nuclear data on the average assembly burnup; Top: all nuclear data sampled together; Middle: FY and XS sampled separately; Bottom: differences in terms of relative uncertainties between sampling together and separately. The red line is a fit of the differences. Each dot indicates a specific assembly at the end of a specific cycle.

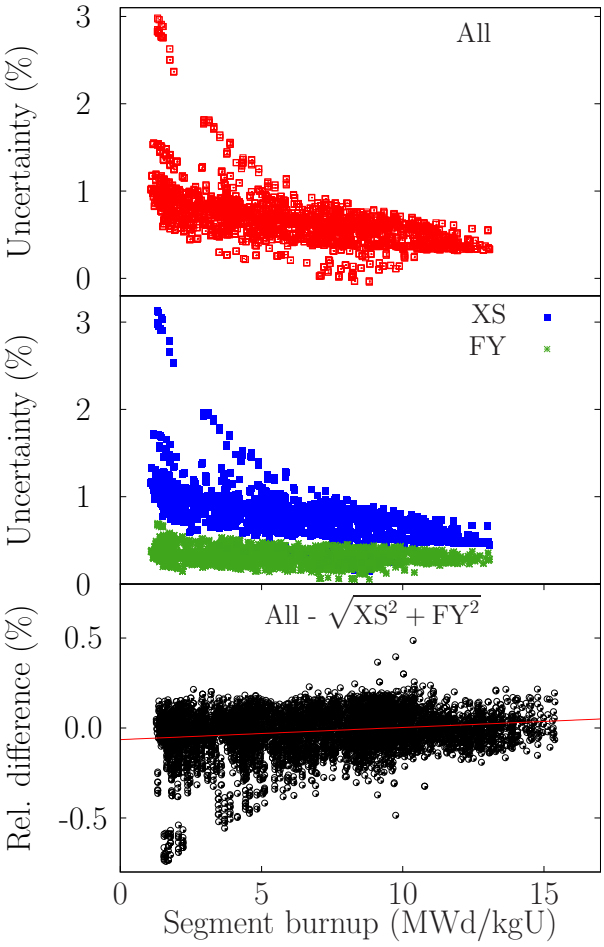

Fig. 2: Same as Fig. 1 but for a specific assembly segment (bottom of the assemblies) instead of assembly average.

the average assembly burnup values, there is no strong difference in considering together or separately the FY and XS quantities.

4.2 Assembly decay heat

The impact of nuclear data on the decay heat (as well as neutron and gamma emission) was partially already presented in Ref. [4]. In the following figures, the particular case of the studied BWR is illustrated with greater details. Fig. 3 presents the effect of nuclear data on a large amount of assemblies, as a function of the cooling time at the end of each considered cycle. In this figure, each curve represents a specific assembly, and the cooling time starts at the end of each considered cycle. There is no distinction if the assembly is used in a next cycle of not. For the sake of simulations, calculations of the decay heat are performed for every assembly and every cycle. This leads to the notion of "assembly-cycle", as it is presented in Figs. 3 and 6. The same idea was presented in Ref. [4].

As noticed, the total uncertainty on the decay heat (and neutron emission) is more significant compared to the case of the core parameters [3]. The values of 5 % and higher are reached between 1 and 10 years of cooling time. Some differences as a function of the assembly burn-up value can also be observed and are explained by looking at the impact of the fission yields and cross sections separately. As seen in the middle of Fig. 3, the uncertainties on cross sections play a more dominant role at long cooling times, whereas the impact of fission yields is higher below 1000 years. If the impact of the cross sections is increasing with the burn-up, almost independently of the cooling time, it is rather different for fission yields. The contribution to the fission products from minor actinides (originally not present in the fresh fuel) tends to decrease the knowledge below 1 year. A similar effect can be observed in Fig. 6 for the neutron emission.

Fig. 3 Bottom presents the effect of varying either simultaneously cross sections and fission yields, or separately. If there is no interactions (from the uncertainties on decay heat) between cross sections and fission yields, then it would be equivalent to randomly change these quanti-

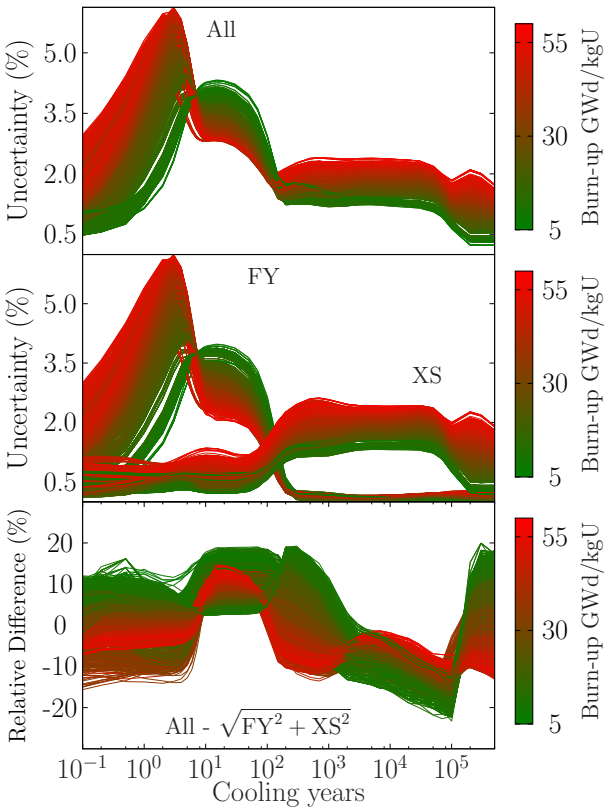

Fig. 3: Uncertainties due to nuclear data on the assembly decay heat; Top: all nuclear data sampled together; Middle: FY and XS sampled separately; Bottom: differences in terms of relative uncertainties between sampling FY and XS together and separately. Each curve represents a specific assembly and the color line is proportional to the assembly burnup.

ties together or not, and Fig. 3 Bottom would show only statistical variations around zero. But as observed, there is a structure in this figure, indicating that different total uncertainties are obtained if cross sections and fission yields are varied together or separately. Negative values in this figure indicate that there is an overestimation of the uncertainty if quantities are separately varied.
It is also interesting to study the effect of considering (or not) previous cycles for the SNF uncertainty propagation. The method is rather simple: perform two separated calculations: one where the nuclear data are varied from the first considered cycle and for all cycles, and another one where the nuclear data are varied only at the beginning of the considered cycle. The example for the uncertainties on decay heat, considering or not the cycle prior to cycle $\mathcal{N}$ is presented in Fig. 4. The relative difference between the uncertainties for all cycles, minus the ones for cycle $\mathcal{N}$ only are plotted as a function of cooling time, for all assemblies considered in cycle $\mathcal{N}$. Some of these assemblies were used in previous cycles and are therefore partly burned at the beginning of cycle $\mathcal{N}$. Others are fresh. This distinction can be seen with the burnup values also presented in this figure. A negative value for the relative uncertainty indicates that the uncertainty considering cycle

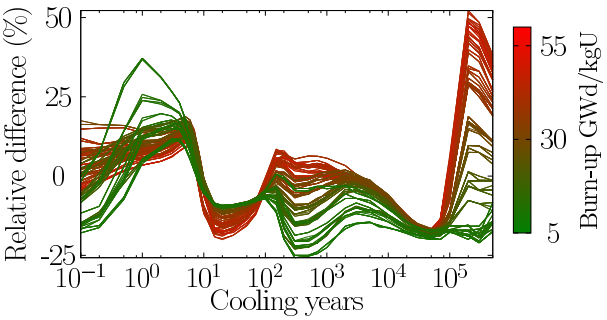

Fig. 4: Relative difference for the decay heat of assemblies considered in cycle $\mathcal{N}$ between (1) varying nuclear data for all cycles, and (2) varying nuclear data only for cycle $\mathcal{N}$. Each curve represents a specific assembly.

$\mathcal{N}$ only is larger than by considering all previous cycles (and cycle $\mathcal{N}$). As observed, the bias in the uncertainty estimations has a complex behavior as a function of cooling time and assembly burnup. This figure indicates anyway that different uncertainties can be obtained depending on the number of considered cycles: to avoid any under or overestimation of uncertainties for the decay heat, it is preferable to consider all previous cycles.
As explained in the section 3, additional calculations were performed for cycle $\mathcal{N}$ where specific nuclear data were varied alone: *e.g.* capture and fission cross sections for ^{235}U and ^{239}Pu. The effects are presented in Fig. 5 in the case of XS only (no variations of FY), for two specific assemblies: one with a low burnup (top of the figure), and one with a high burnup (bottom of the figure). The global effect of the XS does not have the same amplitude for both cases (higher for higher burnup), partly coming from the increasing role of the minor actinides. The impact of the capture cross section on ^{238}U is also important and increasing with burnup. For the low burnup case, the inelastic ^{238}U cross section is the second or third source of uncertainties. It is interesting to notice that the same cross section was mentioned in Ref. [5] as the origin of the a non-linear effect on the peak pin power: in the present case, it is also a cross section having an relative impact. Finally, one can also see that the ^{239}Pu(n,f) and ^{235}U(n,f) cross sections are important contributors to the XS uncertainties. In the context of a desire to reduce uncertainties due to nuclear data, these results indicate the isotopes and cross sections of interest.

4.3 Assembly neutron emission

The effect of nuclear data for the assembly averaged neutron emission is presented in Fig. 6. The maximum uncertainty is similar to the assembly decay heat, reaching a bit more than 5 % at 10 years of cooling time. The separation of the FY and XS effect is opposite to the decay heat case. Because neutrons are mainly emitted by actinides with half-lives from a few years to a few hundreds of years, the FY have a limited impact on the assembly neutron emission. There is also an increase of uncertainty

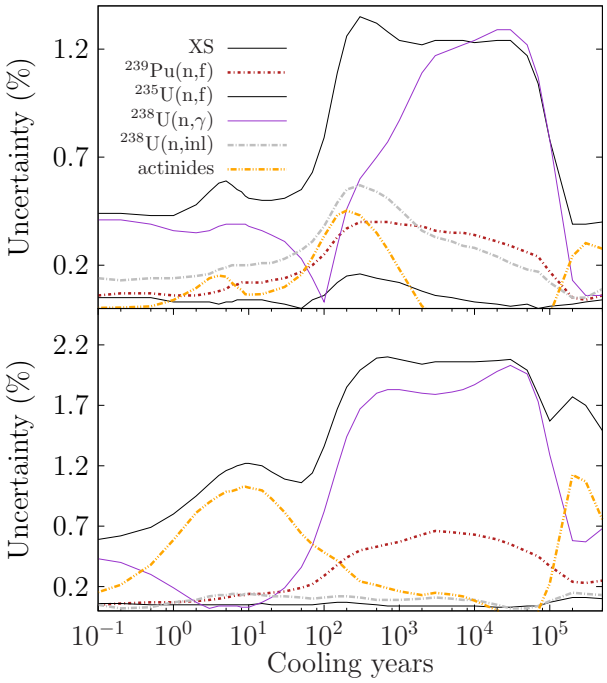

Fig. 5: Effect on decay heat of separated (independently sampled) nuclear data for two specific assemblies: bottom figure with high burnup (about 40 MWd/kgU); top figure with a low burnup (about 12 MWd/kgU).

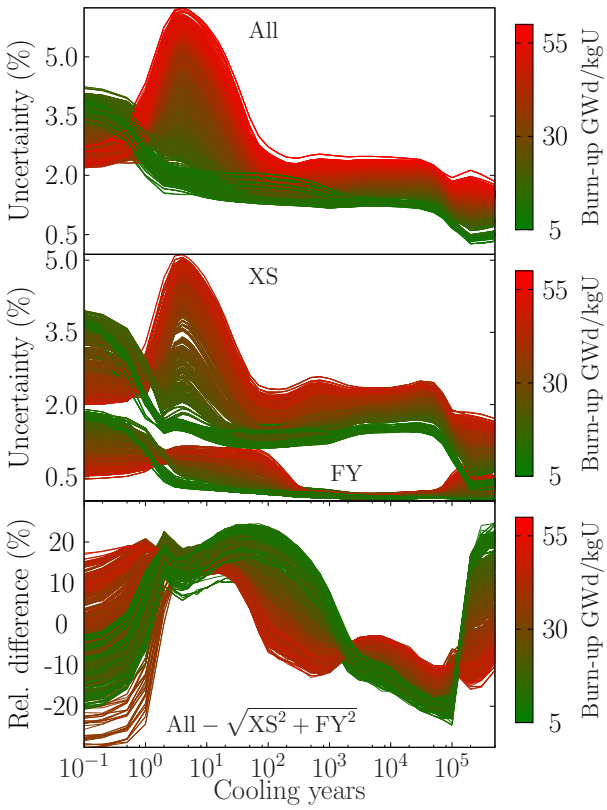

Fig. 6: Same as Fig. 3 but for neutron emission.

with the assembly burnup, due to the fact that minor actinides are building up with higher burnup and that their production (from successive capture, partly compensated by fission) is also not well estimated from the nuclear data knowledge.

Concerning the simultaneous or separated variations of FY and XS, Fig. 6 Bottom indicates different results from a "zero line", as oberved for the decay heat. It is therefore advised to perform a simultaneous variation of these quantities.

As for the decay heat, one can evaluate the effect of considering all previous cycles or only the one of interest for the uncertainty propagation. Fig. 7 presents the relative difference for the neutron emission. For important neutron

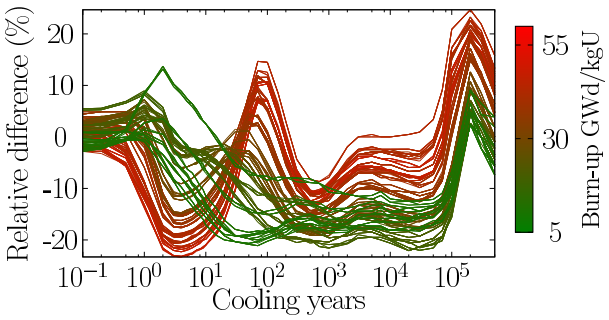

Fig. 7: Relative difference for the neutron emission of assemblies considered in cycle $\mathcal{N}$ between (1) varying nuclear data for all cycles, and (2) varying nuclear data only for cycle $\mathcal{N}$. Each curve represents a specific assembly. Only the XS nuclear data are considered (no FY).

emission (at cooling time less than 100 years), the relative differences can change from negative to positive values . Therefore not considering previous cycle and focusing only on the last will lead to an incorrect total uncertainty.

As for the case of the decay heat, partial contributions to the uncertainties induced by XS only are presented in Fig. 8. The total XS uncertainties also increase with the burnup value, mainly due to the increasing minor actinide contribution. In this case too, the capture cross section on ^{238}U is an important contributor. One can notice the growing importance of the minor actinides. To go further in this analysis, it is necessary to separately vary the cross sections for each minor actinides, but such work was not performed due to the limited computer resources. The impact of ^{244}Cm is nevertheless visible at about 10 years of cooling time, as this isotope has a half-life of 18.1 years and partially decays by spontaneous fission (emitting between 2 and 3 neutrons for each fission event).

4.4 Assembly isotopic contents

The isotopic contents of the spent fuel at the end of cycle are important quantities as they determine the source term for different calculations such as the criticality of spent fuel pool or transport and storage canisters, or the

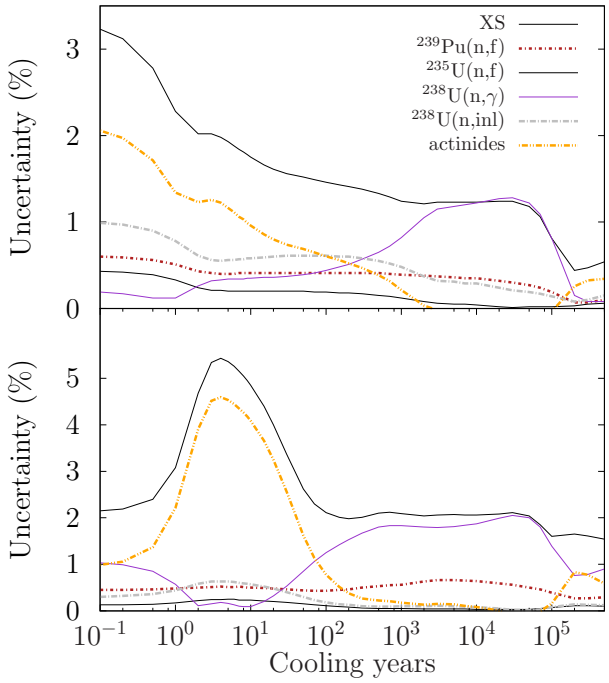

Fig. 8: Effect on neutron emission of separated (independently sampled) nuclear data for two specific assemblies: bottom figure with high burnup (about 40 MWd/kgU); top figure with a low burnup (about 12 MWd/kgU).

amount of emitted radiations. It is naturally connected to the decay heat (see previous section), but the uncertainties on specific isotopes can greatly vary, whereas the decay heat is an integrated value.
As for the previous calculated quantities, the uncertainties due to nuclear data can be presented for each assembly, at the end of each cycle and for various cooling times. A summary is presented in Table 2 for important isotopes at two different assembly burn-up values. Similar results can be found in Ref. [5].

The values of the uncertainties are clearly isotope dependent. As shown in Ref. [5], they can also vary as a function of the cooling time, depending if a specific isotope disappears by decay, or is produced by the decay of other ones.
In the case of actinides, their uncertainties tend to be high either when concentrations are low (^{235}U at high burn-up), or for minor actinides (^{244}Cm).
The effect of the separation of FY and XS for uncertainties is more direct than for other quantities: the FY almost do not affect the actinide compositions whereas they are an important factor for the fission products. As pointed out in Refs. [4,17,29], the correlation matrix for fission yields will play an important role, and users have a certain degree of freedom as such matrices are not included in the nuclear data libraries.
Following the method for the neutron emission in the previous section, the impact of considering all cycles or only a specific one for the uncertainties on the isotopic contents can be calculated. The selected cycle is again the same cycle $\mathcal{N}$. It was presented in Ref. [4] that the uncertainties on the isotopic contents do not strongly vary as a function of cooling time, as long as their concentrations do not vary. It is not the same for the relative difference between considering all cycles and only the last one, and such differences are not negligible. Some examples are presented in Fig. 9. Again, the relative differences can be important,

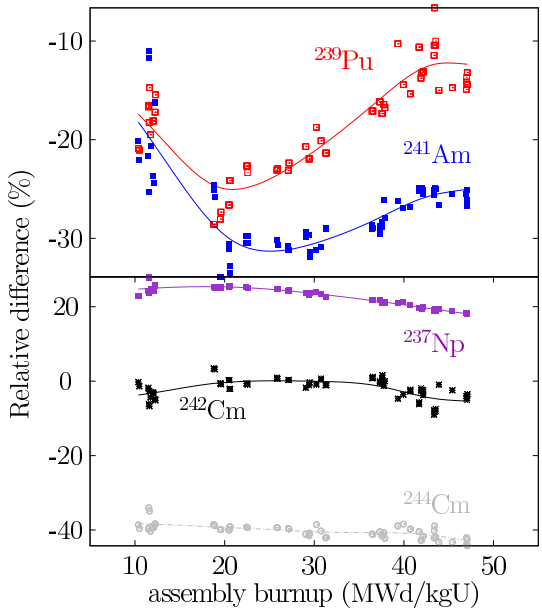

Fig. 9: Same as Fig. 7 for specific actinide contents from assemblies considered in cycle $\mathcal{N}$. The solid lines are spline fits.

strongly vary from one isotope to the other (large variabilities are also observed for isotopes such as ^{239}Pu or ^{235}U). This confirms that in the case of the SNF isotopic contents, the complete irradiation history of the considered assembly needs to be taken into account to properly calculate uncertainties due to nuclear data.

4.5 Spontaneous fission

Uncertainties for the calculated average spontaneous fission of the assemblies are presented in Fig. 10, similarly to the decay heat and neutron emission uncertainties. The two main contributors to the spontaneous fission uncertainty are ^{242}Pu and ^{244}Cm capture cross sections. ^{244}Cm is the leading source of uncertainty for small and large cooling time while ^{242}Pu plays a large role for cooling times between 100 and 10^4 years.
Again, the effect of considering or not all cycles for the uncertainty propagation is presented in Fig. 11. As in the previous cases, the variations as a function of the cooling time are not simple and can change sign. As a conclusion, similarly for the other studied quantities, one needs to take into account previous cycles in an integrated calculation scheme in order to obtain less or no biased uncertainties. The method presented in section 3.3 to obtain

Table 2: Maximum uncertainties due to all nuclear data for the isotopic content of spent assemblies at two specific burnup values (40 and 55 MWd/kgU). These maximum values can be obtained at various cooling times.

	40 MWd/kgU	55 MWd/kgU		40 MWd/kgU	55 MWd/kgU		40 MWd/kgU	55 MWd/kgU
	uncertainty	uncertainty		uncertainty	uncertainty		uncertainty	uncertainty
Isotope	(%)	(%)	Isotope	(%)	(%)	Isotope	(%)	(%)
^{234}U	2.1	3.6	^{235}U	1.9	4.0	^{236}U	1.6	1.6
^{237}U	3.0	2.9	^{238}U	0.02	0.04	^{237}Np	3.3	3.7
^{238}Pu	4.6	5.2	^{239}Pu	2.2	2.7	^{240}Pu	2.1	2.5
^{241}Pu	1.9	2.6	^{242}Pu	3.4	3.8	^{241}Am	3.5	5.1
^{242m}Am	3.2	4.2	^{243}Am	9.2	7.6	^{242}Cm	2.6	2.3
^{243}Cm	11	11	^{244}Cm	10	9	^{245}Cm	14	12
^{85}Kr	0.6	0.5	^{87}Rb	0.3	0.5	^{90}Sr	0.8	0.7
^{91}Y	0.8	1.3	^{93}Zr	0.7	0.5	^{95}Zr	0.9	1.2
^{95}Nb	0.9	1.2	^{99}Tc	1.3	1.6	^{103}Ru	1.3	1.6
^{106}Ru	1.4	1.5	^{107}Pd	0.7	0.7	^{126}Sn	11	12
^{129}I	2.4	3.2	^{134}Cs	30	26	^{135}Cs	10	7.0
^{137}Cs	7.9	7.0	^{141}Ce	0.5	0.8	^{144}Ce	0.5	0.7
^{147}Pm	7.6	9.2	^{147}Sm	6.9	8.2	^{148}Nd	0.4	0.4
^{154}Eu	2.9	2.2						

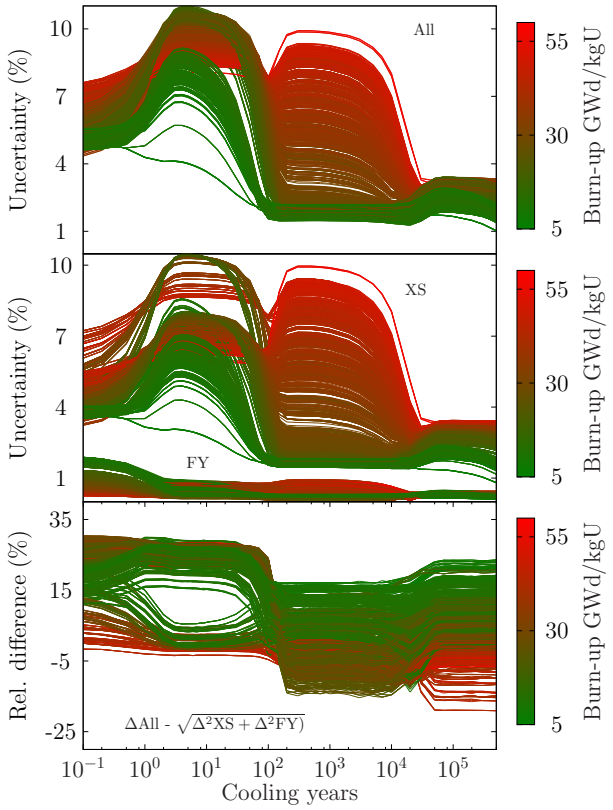

Fig. 10: Same as Fig. 6 but for the average spontaneous fission for each assembly.

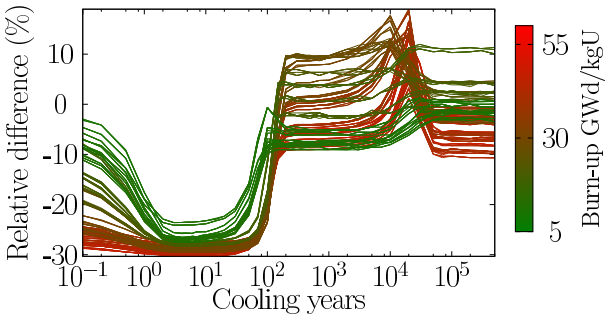

Fig. 11: Same as Fig. 7, but for the spontaneous fission.

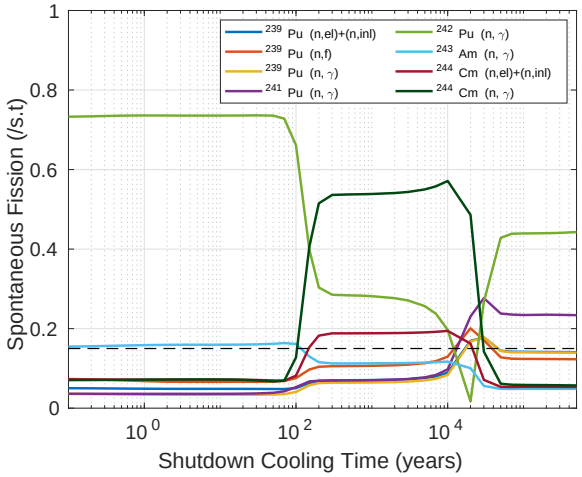

Fig. 12: Evolution of the spontaneous fission sensitivity indices during shutdown cooling.

sensibility vectors is applied here and results are presented in Fig. 12. The capture and scattering cross sections of the other minor actinides leading to the production of ^{244}Cm and ^{246}Cm appear as contributors even though at lower magnitude. In order to reduce the uncertainty in the spontaneous fission prediction, the uncertainties associated with the ^{242}Pu and ^{244}Cm capture cross sections should be reduced. This exercise demonstrates that the capabilities of the methods available at PSI to extract sensitivity information from the output samples of the forward

uncertainty propagation for BWR core follow calculations with SIMULATE-3 and long term shutdown cooling with *SNF*. Such analysis does not require the production of additional output samples even though it is approximate as it assumes linearity of the computational model.

5 Conclusion

This work presents the impact of nuclear data on a Swiss BWR, considering validated full core models and a large number of consecutive cycles. It is a second of its kind for the propagation of nuclear data using such integrated scheme (following Ref. [4]). It demonstrates that full core and SNF uncertainty propagation over multiple cycles can be performed, and eventually leads to uncertainties on all calculated quantities.

Apart from the medium-size computer cluster required for this work, another challenging aspect is the amount of produced data. Indeed, to consider the full power of this type of integrated approach, one can calculate the isotopic contents not only for each assembly (as performed here), but also for each rod and eventually each (vertical) assembly segment. Such data can in a following step be used to populate a Monte Carlo model for full core steady-state calculations or for canister calculations with criticality studies [9]; the advantage of a Monte Carlo model being the limited number of approximations. Such efforts are currently ongoing at our laboratory, revealing issues with the large amount of data to build such Monte Carlo models, and also to store and efficiently access the raw information.

A general trend in this work is the non-negligible impact of nuclear data for spent nuclear fuel quantities. This is not new, but is now confirmed for BWR.

The original contribution of this work, apart from being a dedicated study for a realistic BWR, concerns the impact of (1) considering separately or together various nuclear data, and (2) considering or not many reactor cycles for the calculation of uncertainties. It was demonstrated with many examples in this paper that to avoid decreasing or increasing uncertainties simply due to the calculation method, it is important to consider all varied nuclear data together, and also to consider the full history of cycles. Therefore such conclusions are important in the context of "Best Estimate Plus Uncertainties" calculations.

There are still some additional efforts to perform such type of studies on a routine basis for any licensing analysis, but realistic perspective can now be considered.

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