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# Evaluating the Effect of Decay and Fission Yield Data Uncertainty on BWR Spent Nuclear Fuel Source Term

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## ABSTRACT

Knowledge of spent nuclear fuel (SNF) source term, for example decay heat, reactivity and nuclide inventory of SNF, is essential in the safe handling and final disposal of SNF. The computational characterization of SNF has many sources of uncertainties. One of these is the uncertainties present in nuclear data. This work continues the identification of the major uncertainty components in the decay and fission yield data in relation to the SNF source term.

The uncertainties of decay and fission yield data are propagated from ENDF-6 file format nuclear data library to the SNF source term using a sampling based technique in the Monte Carlo particle transport program Serpent 2. Studied components of the SNF source term are produced multiple times as functions of burnup and cooling time with randomly perturbed decay and fission yield data.

Similar work has been previously conducted for a VVER-440 type fuel assembly. In this work, a boiling water reactor (BWR) type fuel assembly is studied. The study is conducted varying the void fraction to examine its effect on the uncertainties of the SNF source term components caused by the uncertainties in the decay and fission yield data. Other nuclear data related uncertainties are ignored in this study, and only fixed, nominal depletion conditions are considered.

## 1 INTRODUCTION

An uncertainty sampling method for propagating the ENDF-6 file format decay and fission yield data uncertainties was introduced in Monte Carlo particle transport code Serpent in a previous work [1, 2]. This work continues the study of the SNF source term component uncertainties.

In this work, the methodology is revised from the previous study. A single two-dimensional BWR fuel assembly is studied in fixed nominal depletion conditions having 40 % and 80 % void fractions. The fuel assembly is depleted from 0 MWd/kgU to 80 MWd/kgU burnup, and decay times up to $10^7$ years are studied from burnups of 20, 40, 60 and 80 MWd/kgU.

## 2 METHODOLOGY

The ENDF-6 file format data contain one standard deviation uncertainties of the fission product yield data and radioactive decay data in addition to their respective best estimate values. Serpent 2 was extended to random sample these values in Ref. [2]. The sampling was performed from normal distribution, with a special treatment for possible negative values. In this work, the sampling is performed from log-normal distribution, which prevents the occurrence of negative values. The sampling is still performed for all nuclides, i.e. the user cannot give a specific nuclide list for which the sampling would be performed.

The values used during a single calculation are sampled during the reading of the ENDF-6 files, and therefore their perturbed values are constant during a single calculation. All values are independently sampled, as the ENDF-6 file format does not contain covariance data for these values.

The considered burnup and decay calculations are performed with both the uncertainty sampling off and on with 10 and 300 independent repeats with different random number generator seeds, respectively. The variance caused by the Monte Carlo method and the nuclear data uncertainty are assumed to be independent so that the total variance in the random sampling calculations can be calculated as

$$\sigma_{\mathrm{tot}}^2 = \sigma_{\mathrm{MC}}^2 + \sigma_{\mathrm{ND}}^2 \tag{1}$$

where $\sigma_{\mathrm{MC}}^2$ is obtained from the calculations without the random sampling. Therefore, the final nuclear data one standard deviation uncertainty is obtained with

$$\sigma_{\mathrm{ND}} = \sqrt{\sigma_{\mathrm{tot}}^2 - \sigma_{\mathrm{MC}}^2}. \tag{2}$$

The studied fuel assembly is a 10x10 GE14 design BWR fuel assembly [3, 4]. The fuel assembly geometry plot is presented in Fig. 1. The assembly contains seven $UO_2$ pin types with different U-235 enrichments ranging from 1.6 % to 4.9 % and four pin types with two possible $Gd_2O_3$ contents of 3.0 % and 8.0 % with different U-235 enrichments ranging from 3.95 % to 4.9 %. The studied coolant void fractions are 40 % and 80 %. The fuel pins containing $Gd_2O_3$ are divided into 10 equal volume burnup zones. N-14 and Cl-35 are added as 10 ppm impurities in all fuel materials to estimate the production of C-14 and Cl-36 due to the activation of these impurities. This estimation is based on Ref. [5]. However, only the C-14 content of the fuel is studied later in this work.

The burnup calculations were performed with small burnup steps, with a total of 84 steps until the maximum condidered burnup of 80 MWd/kgU. The selected depletion algorithm was the linear extrapolation with quadratic interpolation with 10 substeps in both the predictor and corrector. The neutron population was 100000 neutrons per generation with 100 active and 25 inactive generations. The unresolved resonance probability table sampling was used, energy grid thinning was set to $5 \times 10^{-6}$ tolerance, and Doppler-broadening rejection correction (DBRC) was used for three uranium isotopes and two plutonium isotopes. Upcoming Serpent 2 JEFF-3.2 cross section data files were used with Serpent 1 distributed JEFF-3.1.1 fission product yield and radioactive decay data files. The power density was 28.6 W/gU. The decay calculations were run from burnups of 20, 40, 60 and 80 MWd/kgU.

## 3 RESULTS

As in Ref. [2], the source term components are studied separately for the burnup and decay calculations. The studied components are decay heat (DH), activity (A), spontaneous fission rate

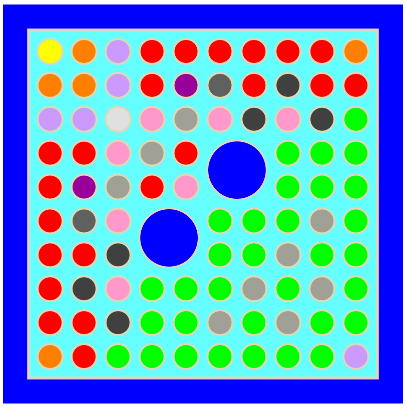


Figure 1: Serpent geometry plot of the studied assembly. The grey colored pins contain $Gd_2O_3$ in addition to $UO_2$, whereas the other colored pins are regular $UO_2$ pins.

(SF) and photon emission rate (PE). Additionally, the mass of C-14 is studied separately during the decay calculations. It is one of the nuclides propagating to biosphere in the TURVA-2012 safety case of Posiva during a 10000 year study time of spent nuclear fuel final disposal in Finland [6].

In all presented figures the coloring and notation is as follows. The mean of the base calculations without uncertainty sampling is plotted with a red line for 40 % void and with a purple line for 80 % void. The blue line represents the mean of the calculations with the nuclear data uncertainty sampling turned on for 40 % void. The blue shaded area around the blue line is the total one standard deviation uncertainty of these results. Additionally, the 5th percentile, median and 95th percentile of the nuclear data uncertainty calculation results are plotted in the figures with dashed blue lines. The similar notation for 80 % void is presented in yellow. The light blue line represents the one standard deviation relative nuclear data uncertainty for 40 % void. This uncertainty is defined as the ratio of $\sigma_{\mathrm{ND}}$ of Eq. (2) and the mean value calculated from the results of the calculations with the nuclear data uncertainty sampling turned on. The similar notation for 80 % void is presented with a green line. All other values are presented on the left $y$ axis, whereas the $\sigma_{\mathrm{ND}}$ values are presented on the right $y$ axis.

### 3.1 Burnup calculation

The studied source term components are plotted in Fig. 2 for the burnup calculation. For all components, the mean values calculated from the sampling calculations were different than the mean values calculated from the base calculations. The maximum relative differences between the means ($\Delta_{\mathrm{mean}}$), the one standard deviation relative nuclear data uncertainties ($\sigma_{\mathrm{ND}}$) and the base Monte Carlo one standard deviations ($\sigma_{\mathrm{MC}}$) are presented in Tab. 1 for the studied variables during the burnup calculation.

The absolute values of all the studied components are higher for the higher 80 % void. The $\sigma_{\mathrm{ND}}$ values are generally slightly higher for the lower 40 % void when compared with 80 % void. The behaviors of the $\sigma_{\mathrm{ND}}$ values are rather similar for both void fractions. The $\sigma_{\mathrm{ND}}$ of the studied components is the highest for the decay heat. The $\Delta_{\mathrm{mean}}$ values are rather small, but they are generally higher for the lower void fraction. The $\sigma_{\mathrm{MC}}$ values are rather insignificant compared with the $\sigma_{\mathrm{ND}}$ values.

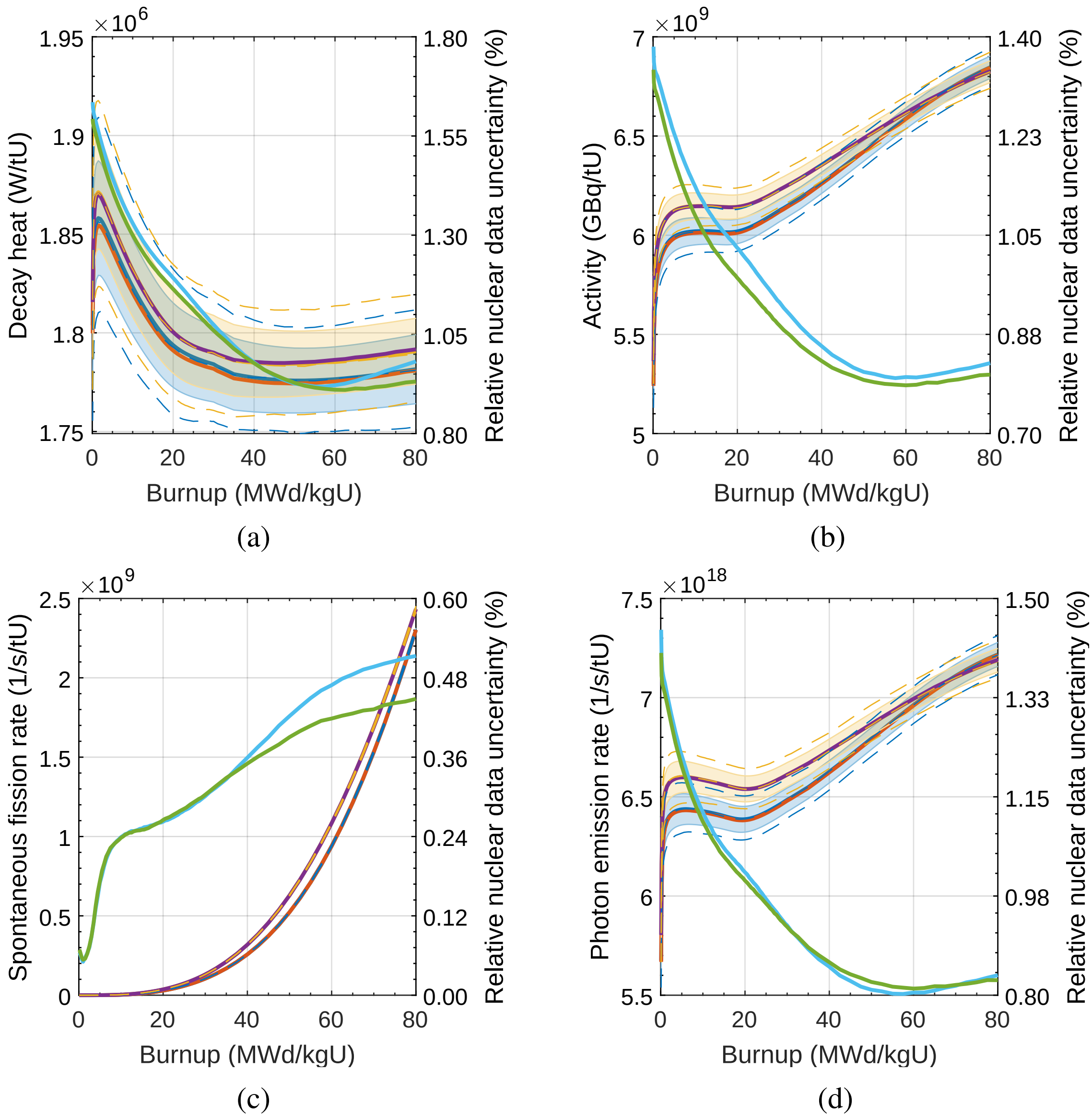
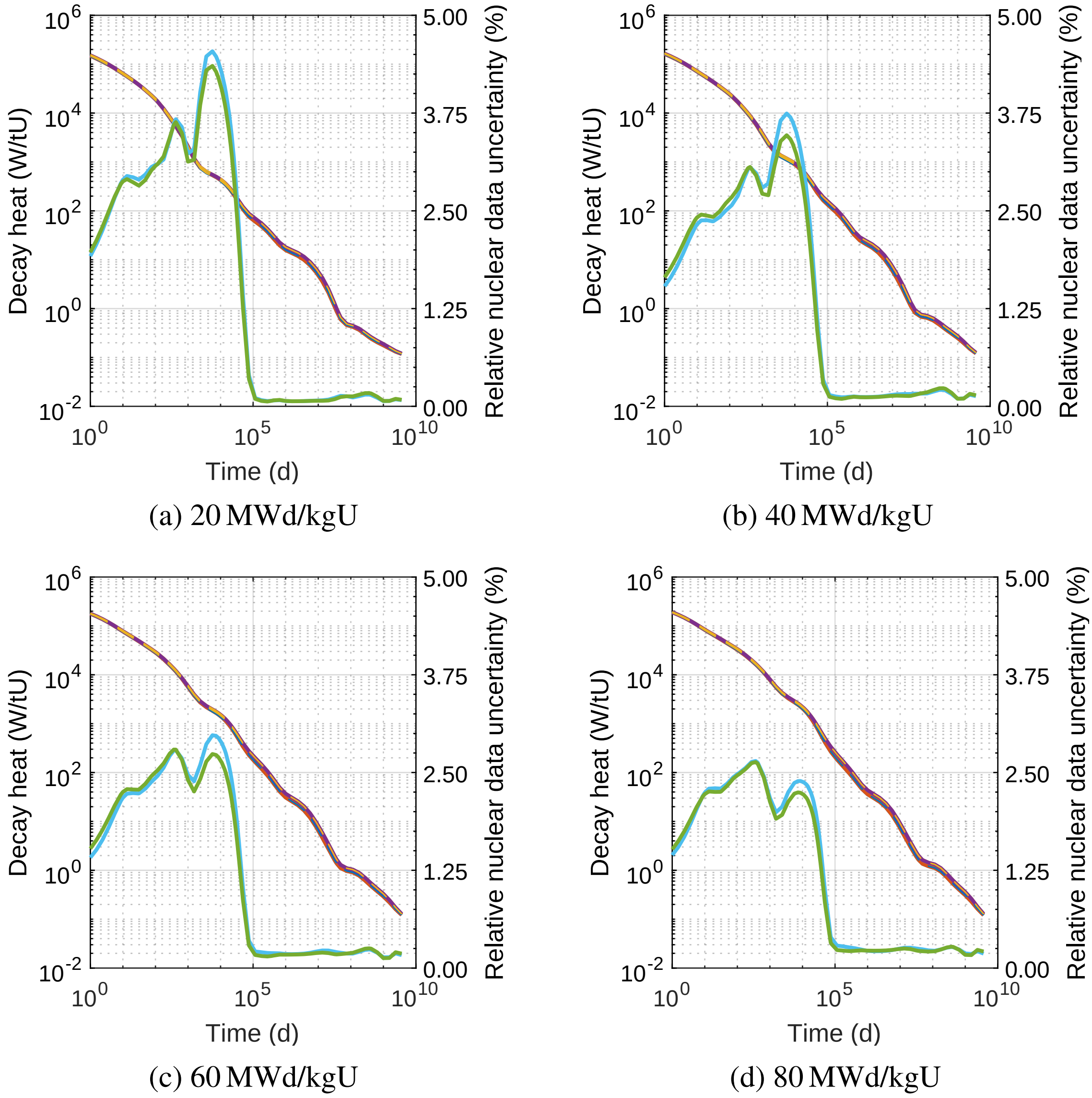



Figure 2: Various SNF source term components during the burnup calculation.

Table 1: Maximum values during the burnup calculation of the relative difference between the mean values of sampling and base calculations, one standard deviation relative nuclear data uncertainty and base Monte Carlo one standard deviation uncertainty.

| | Void (%) | $\Delta_{\text{mean}}$ (%) | $\sigma_{\text{ND}}$ (%) | $\sigma_{\text{MC}}$ (%) |
|---|---|---|---|---|
| DH | 40 | 0.226 | 1.64 | 0.018 |
| | 80 | 0.064 | 1.59 | 0.013 |
| A | 40 | 0.184 | 1.38 | 0.026 |
| | 80 | 0.052 | 1.34 | 0.017 |
| SF | 40 | 0.030 | 0.51 | 0.049 |
| | 80 | 0.040 | 0.45 | 0.054 |
| PE | 40 | 0.125 | 1.44 | 0.028 |
| | 80 | 0.056 | 1.40 | 0.019 |




(a) 20 MWd/kgU
(b) 40 MWd/kgU
(c) 60 MWd/kgU
(d) 80 MWd/kgU

Figure 3: Decay heat during the decay calculation at different burnups.

### 3.2 Decay calculations

The decay heat is plotted in Fig. 3 for the decay calculations starting from all studied burnups as an example of the decay calculation SNF source term component results. For all studied SNF source term components, the mean values calculated from the sampling calculations were different than the mean values calculated from the base calculations. The maximum relative differences between the means ($\Delta_{\mathrm{mean}}$), the one standard deviation relative nuclear data uncertainties ($\sigma_{\mathrm{ND}}$) and the base Monte Carlo one standard deviations ($\sigma_{\mathrm{MC}}$) are presented in Tab. 2 for the studied variables during the decay calculations. The decay times of the maximum nuclear data uncertainties are also shown in the table.

For decay heat, the maximum $\sigma_{\mathrm{ND}}$ decreases with the increasing burnup. The maximum $\sigma_{\mathrm{ND}}$ is higher for the lower 40 % void fraction than for the higher 80 % void fraction. The behavior of the maximum $\sigma_{\mathrm{ND}}$ is similar for both void fractions. The second local maximum of $\sigma_{\mathrm{ND}}$ is consistently higher for the lower void fraction. This causes the maximum $\sigma_{\mathrm{ND}}$ to be at an earlier decay time for the higher void fraction at 60 MWd/kgU. The maximum $\Delta_{\mathrm{mean}}$ values

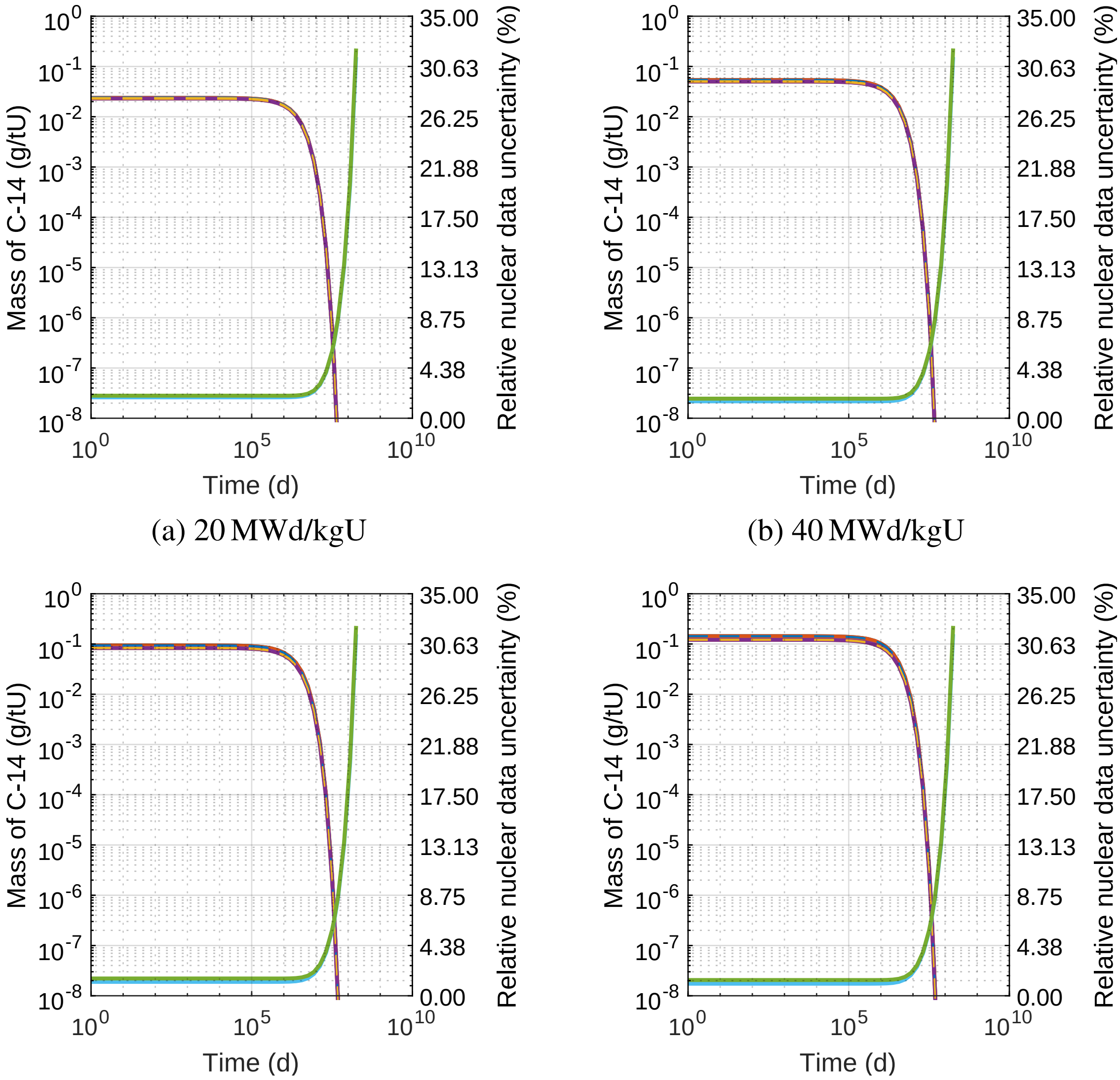
Table 2: Maximum values during the decay calculation for the relative difference between the mean values of sampling and base calculations, one standard deviation relative nuclear data uncertainty and base Monte Carlo one standard deviation uncertainty.

| | Burnup (MWd/kgU) | Void (%) | $\Delta_{\text{mean}}$ (%) | $\sigma_{\text{ND}}$ (%) | $\sigma_{\text{MC}}$ (%) | Time of max $\sigma_{\text{ND}}$ (a) |
|---|---|---|---|---|---|---|
| DH | 20 | 40 | 0.336 | 4.54 | 0.009 | 15 |
| | 20 | 80 | 0.736 | 4.35 | 0.010 | 15 |
| | 40 | 40 | 0.221 | 3.74 | 0.016 | 15 |
| | 40 | 80 | 0.664 | 3.47 | 0.013 | 15 |
| | 60 | 40 | 0.141 | 2.98 | 0.017 | 15 |
| | 60 | 80 | 0.571 | 2.79 | 0.016 | 1.0 |
| | 80 | 40 | 0.126 | 2.65 | 0.024 | 1.0 |
| | 80 | 80 | 0.489 | 2.63 | 0.023 | 1.0 |
| A | 20 | 40 | 0.327 | 5.13 | 0.012 | 70 |
| | 20 | 80 | 0.633 | 4.98 | 0.014 | 70 |
| | 40 | 40 | 0.240 | 4.66 | 0.015 | 70 |
| | 40 | 80 | 0.612 | 4.46 | 0.014 | 70 |
| | 60 | 40 | 0.214 | 4.34 | 0.016 | 70 |
| | 60 | 80 | 0.578 | 4.15 | 0.016 | 60 |
| | 80 | 40 | 0.207 | 4.16 | 0.021 | 70 |
| | 80 | 80 | 0.545 | 4.02 | 0.020 | 60 |
| SF | 20 | 40 | 0.018 | 0.49 | 0.059 | 2.7 |
| | 20 | 80 | 0.052 | 0.44 | 0.071 | 70 |
| | 40 | 40 | 0.016 | 1.03 | 0.051 | 100 |
| | 40 | 80 | 0.094 | 1.06 | 0.070 | 320 |
| | 60 | 40 | 0.029 | 2.08 | 0.051 | 320 |
| | 60 | 80 | 0.263 | 2.43 | 0.055 | 320 |
| | 80 | 40 | 0.054 | 2.56 | 0.053 | 210 |
| | 80 | 80 | 0.255 | 2.91 | 0.053 | 24000 |
| PE | 20 | 40 | 0.461 | 8.53 | 0.020 | 24 |
| | 20 | 80 | 0.561 | 8.03 | 0.022 | 24 |
| | 40 | 40 | 0.363 | 7.55 | 0.026 | 30 |
| | 40 | 80 | 0.490 | 6.97 | 0.042 | 30 |
| | 60 | 40 | 0.356 | 6.87 | 0.023 | 30 |
| | 60 | 80 | 0.424 | 6.37 | 0.030 | 30 |
| | 80 | 40 | 0.351 | 6.44 | 0.047 | 37 |
| | 80 | 80 | 0.387 | 6.09 | 0.031 | 30 |

are rather high for the studied case. The values are greater for the higher void fraction.

For activity, the maximum $\sigma_{\text{ND}}$ decreases with the increasing burnup, but less than for the decay heat. Again the values are slightly higher for the lower void fraction. The behavior of the maximum $\Delta_{\text{mean}}$ is similar as with the decay heat.

For spontaneous fission rate, the maximum $\Delta_{\text{mean}}$ values are generally much smaller than for decay heat and activity. The only higher values are for the higher void fraction at the two highest burnups. The maximum $\sigma_{\text{ND}}$ values increase with increasing burnup. The values are




(a) 20 MWd/kgU (b) 40 MWd/kgU (c) 60 MWd/kgU (d) 80 MWd/kgU

Figure 4: Mass of C-14 during the decay calculation at different burnups.

higher for the greater void fraction for all but the lowest considered burnup.

For photon emission rate, the maximum $\sigma_{\mathrm{ND}}$ values are highest of all four studied components. The values decrease with increasing burnup. The values are slightly higher for the lower void fraction. Again, the maximum $\Delta_{\mathrm{mean}}$ values are rather high for all studied burnups and void fractions.

The mass of C-14 during the decay calculations is presented in Fig. 4. The figures are cropped so that a maximum of eight orders of magnitude are shown. The actual magnitude of the C-14 masses depend on the original mass of the parent nuclide N-14 assumed to be in the fuel as impurity. The Monte Carlo base calculation relative standard deviation $\sigma_{\mathrm{MC}}$ was under 0.006 % of the mean values. The $\sigma_{\mathrm{ND}}$ values are rather similar for decay calculations from all burnups. The values are slightly higher for the higher 80 % void fraction. The uncertainties stay at rather constant value until some 2000 years of decay time, where the values start increasing. When the actual nuclide masses decrease by orders of magnitude, the relative nuclear data uncertainties increase sharply.

## 4 SUMMARY

A previously implemented radioactive decay data and fission yield uncertainty sampling method was revised to use log-normal distribution and applied to a BWR fuel assembly. Burnup calculations were performed until 80 MWd/kgU and decay calculations from four different burnups. The relative nuclear data uncertainties of the studied spent nuclear fuel source term components were obtained by performing the Monte Carlo calculations with the nuclear data uncertainty sampling off and on. The calculations were performed with 40 % and 80 % void fractions.

The maximum one standard deviation nuclear data uncertainties of decay heat, activity, spontaneous fission rate and photon emission rate were under 1.7 % during the burnup calculations. The uncertainties were higher during the decay calculations, where the maximum values ranged from 2.9 % to 8.6 %, depending on the component. There were slight differences between the different void fractions. The means of the uncertainty sampling calculations and calculations without the sampling were rather different for some components, especially during the decay calculations. The reason for the differences in the mean values were not investigated further in this work. The behavior of C-14 mass was similar with both studied void fractions and with all studied burnups.

In this work the uncertainty sampling was performed for all nuclides. The study of the importances of the nuclear data uncertainties of single nuclides is left for future work.

## ACKNOWLEDGMENTS

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