

The Effect of Calculation Parameters on Spent Nuclear Fuel Source Term

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ABSTRACT

1 INTRODUCTION

For the safe handling, interim storage and final disposal of spent nuclear fuel (SNF) knowledge of the source term (decay heat, reactivity, nuclide inventory etc.) is essential. However, the estimation of the source term using computational methods has several sources of uncertainty such as uncertainties in the nuclear data, uncertainties in the operation history, choice of calculation parameters etc. In this work the focus is on the effect of calculation parameters when the built-in burnup capability of Serpent 2 [1] is used to estimate the source term.

2 METHODOLOGY

Estimating the source term with Serpent requires running a burnup calculation to obtain the nuclide inventory in SNF and for this calculation several parameters have to be specified. In this work the effect of the following parameters on the source term is studied: depletion zone division, burnup steps, unresolved resonance probability table sampling, Doppler-Broadening Rejection Correction (DBRC) and energy dependent branching ratios. As a test case a 2D BWR assembly was modelled. First a burnup calculation was executed up to a burnup of 60 MWd/kgU followed by a decay calculation up to 10^7 years starting from the maximum burnup. These simulations were repeated for different variations of the studied parameters and since the use of Monte Carlo method introduces statistical uncertainty, each variation was repeated five times to obtain an estimate for the uncertainty. The following source term components were considered when investigating the effect of the studied parameters: total decay heat, photon emission rate and spontaneous fission rate. These components are automatically calculated by Serpent when running a decay calculation.

In the burnup calculations 10^7 active neutron histories divided into 100 cycles of 10^5 source neutrons were simulated in each transport calculation. JEFF-3.2 based cross section data

files were used with JEFF-3.1.1 fission product yield and radioactive decay data files. Linear extrapolation with linear interpolation using 10 substeps in both predictor and corrector was used as a depletion algorithm.

In more detail the test case is a 10x10 BWR fuel assembly based on the GE-14 design [3][4]. The assembly contains UO_2 fuel rods with several different U-235 enrichments ranging from 1.6 to 4.9 %. 18 of the rods have Gd_2O_3 mixed in the fuel. The coolant has a 40 % void fraction. The geometry is shown in Figure 1 in which each fuel type has a different color. Reflecting boundary conditions were used and the power density was set to 28.6 W/gU.

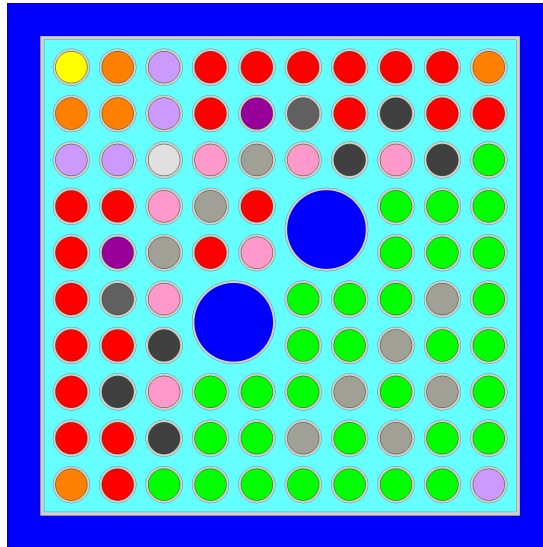


Figure 1: Serpent geometry of the GE14 type assembly.

3 VARIATIONS

In the following sections the studied variations are described.

3.1 Depletion zones

The following depletion zone divisions (listed from the coarsest to the finest) were studied:

1. Each fuel material as a separate depletion zone
2. Fuel pins as separate depletion zones
3. Gd pins divided into 10 rings with equal volumes, regular pins with a 0.3 mm surface layer
4. Gd pins divided into 10 rings with equal volumes, regular pins with a 0.3 mm surface layer, subdivision into 4 azimuthal sectors in each pin

The division with sectors (4.) is used as reference when the results of the different divisions are compared. When the effect of the other parameters was studied, the division with rings (3.) was used.

3.2 Steps

Step length variations presented in Table 1 were studied. In all variations shorter steps were taken until gadolinium was completely depleted at 22.5 MWd/kgU. The variation with 64 steps is used as reference. When the effect of the other parameters was studied, the variation with 34 steps was used with the exception of depletion zones in which case 64 steps was used.

Table 1: Different step length variations

Steps	Lengths of the steps (MWd/kgU)									
14	0.1	0.1	0.3	0.5	1.5	5 x 4.0	7.5	3 x 10.0		
20	0.1	0.1	0.3	0.5	1.5	10 x 2.0	2.5	5.0	3 x 10.0	
34	0.1	0.1	0.3	0.5	0.5	21 x 1.0	2.5	7 x 5.0		
64	0.1	0.1	0.2	0.3	0.3	43 x 0.5	1.0	1.5	14 x 2.5	

3.3 Unresolved resonance probability table sampling

The effect of unresolved resonance probability table sampling was studied by modelling the test case with unresolved resonance probability table sampling switched on and off. The variation with the probability table sampling switched on is used as reference and it was also switched on when the effect of the other parameters was studied.

3.4 Doppler-broadening rejection correction

The effect of DBRC was studied by modelling the test case with DBRC switched on and off. DBRC was applied for U-234, U-235, U-238, Pu-239 and Pu-240. The variation with DBRC switched on is used as reference and it was also switched on when the effect of the other parameters was studied.

3.5 Energy-dependent branching ratios

In burnup calculations branching ratios to isomeric states are used for the production of long-lived meta-stable nuclides. By default, Serpent uses constant branching ratios which have been calculated from energy-dependent branching ratios in the JEFF-3.1 activation file in a PWR flux spectrum. Results obtained using these constant branching ratios were compared against results obtained using energy-dependent branching ratios from the JEFF-3.1 activation file. The variation with constant branching ratios is used as reference and constant branching ratios were also used when the effect of the other parameters was studied.

4 RESULTS

As noted previously, each simulation was repeated five times and in the following the presented results are mean values or relative differences between mean values during the decay calculation. For each source term component i.e. decay heat, photon emission rate and spontaneous fission rate four figures are shown. In the first of these figures the time development of the component is plotted based on the results from the simulations which used the finest depletion zone division with sectors. In the other three figures relative differences between the reference variation and other variations are presented for depletion zone division, burnup

steps and DBRC. Differences resulting from the use of unresolved resonance probability table sampling or energy dependent branching ratios were significantly smaller. Therefore, they are not presented with figures and instead maximum absolute relative differences during the decay calculation are given. Statistical uncertainty is illustrated in the relative difference figures using a curve labeled as "Max RE" which represents the maximum relative error over the variations at each time step. The relative errors were calculated as

$$RE = \frac{\sigma_{\bar{x}}}{\bar{x}}, \tag{1}$$

where $\sigma_{\bar{x}}$ is the standard deviation of the mean and \bar{x} is the mean.

4.1 Decay heat

Results for the decay heat are presented in Figure 2. For all three parameters the relative differences between the reference variation and the other variations are small. Largest absolute relative difference of approximately 0.6 % is observed for the depletion zone variation with material-wise depletion zones approximately 7 years after discharge. Maximum absolute relative differences for the unresolved resonance probability table sampling and energy dependent branching ratios were approximately 0.06 % and 0.01 %, respectively.

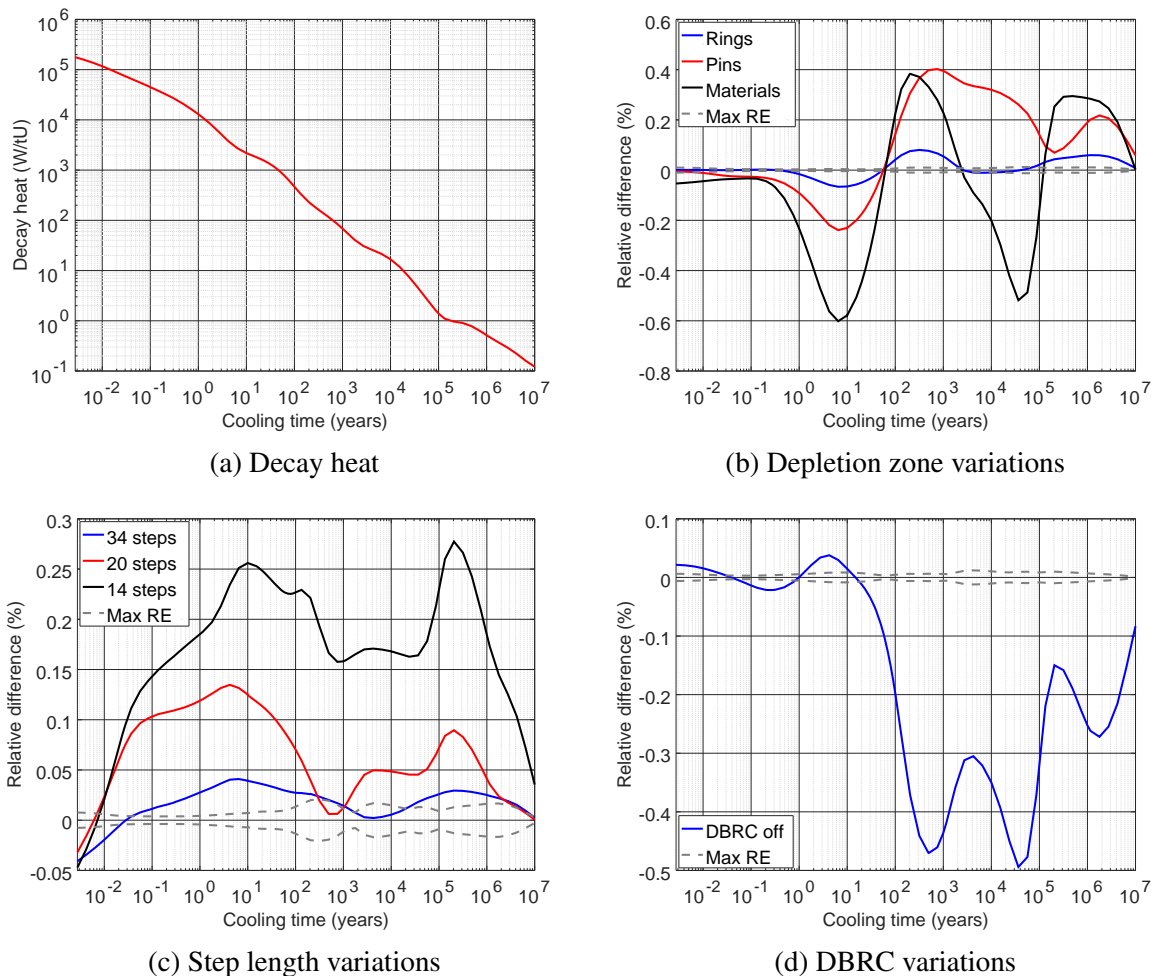


Figure 2: Results for the decay heat.

4.2 Photon emission rate

Figure 3 shows the results for the photon emission rate, and similar to decay heat the calculated relative differences are small and the largest absolute relative difference compared to the reference variation is observed for the depletion zone variation with material-wise depletion zones. This maximum value of approximately 1.1 % is observed at a cooling time of approximately 7000 years. Maximum absolute relative differences for the unresolved resonance probability table sampling and energy dependent branching ratios were approximately 0.08 % and 0.02 %, respectively.

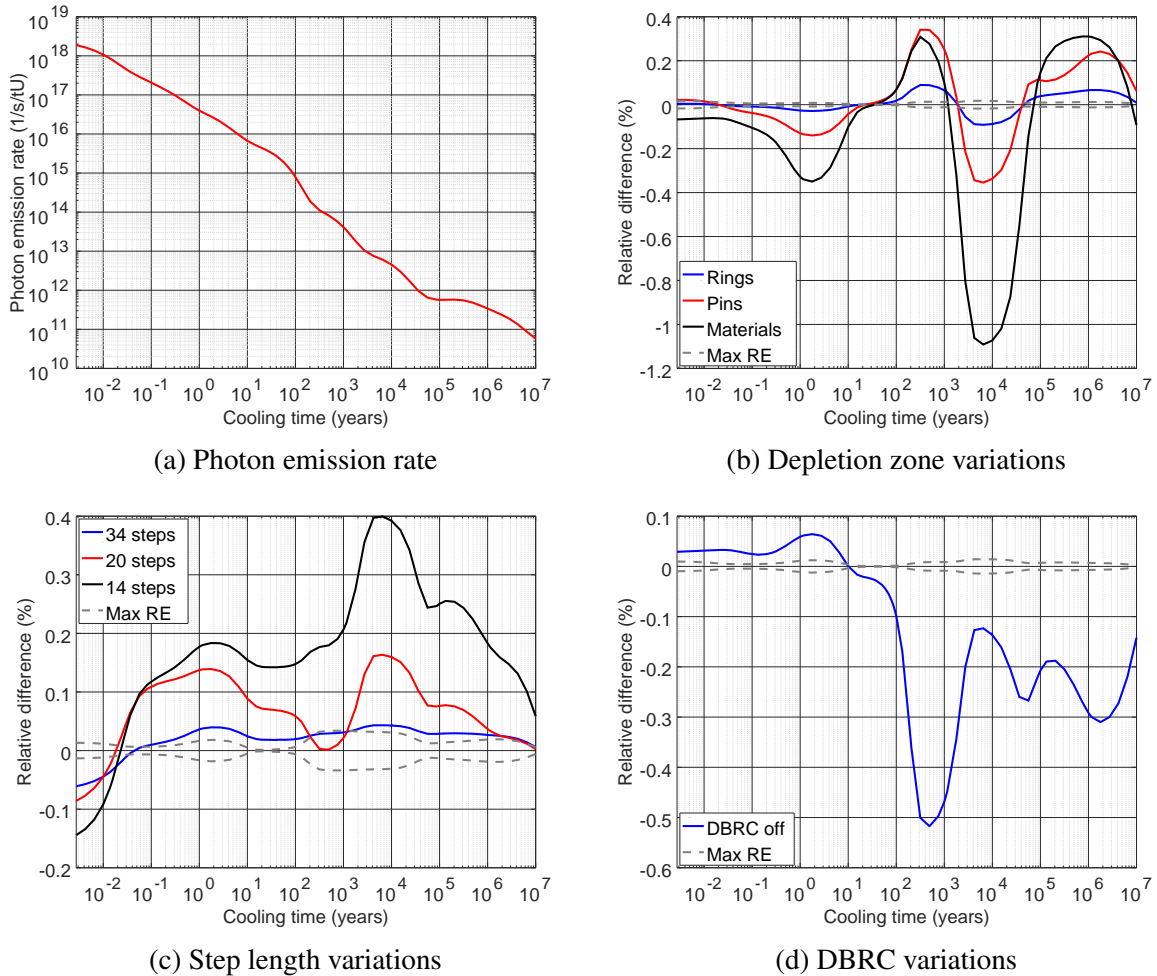


Figure 3: Results for the photon emission rate.

4.3 Spontaneous fission rate

Results for the spontaneous fission rate are presented in Figure 4. Compared to the ones obtained for decay heat and photon emission rate the relative differences for the depletion zone variations are clearly larger. For the variation with material-wise depletion zones relative differences of nearly 8 % are observed few hundred years after discharge. Maximum absolute relative differences for the unresolved resonance probability table sampling and energy dependent branching ratios were both approximately 0.02 %.

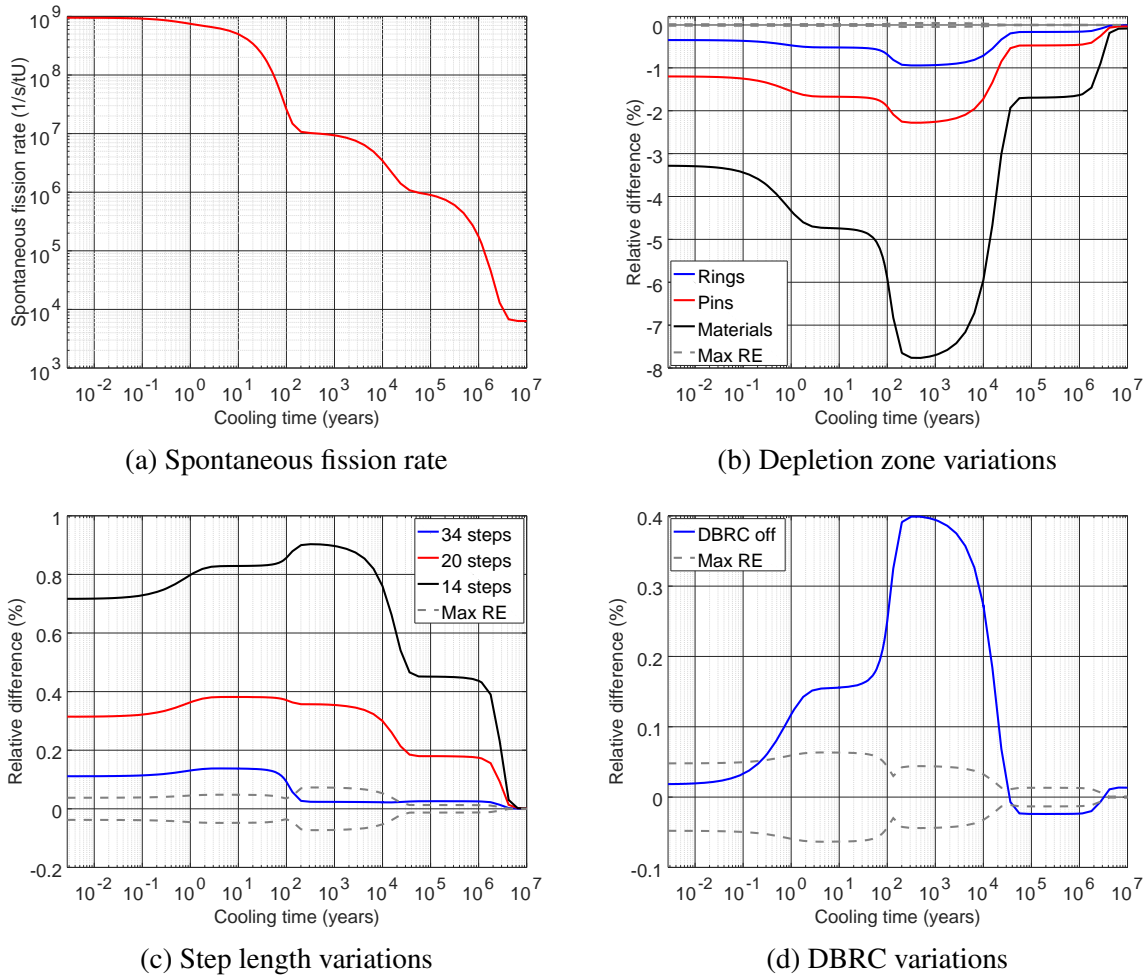


Figure 4: Results for the spontaneous fission rate.

5 CONCLUSIONS

The effect of five calculation parameters on decay heat, photon emission rate and spontaneous fission rate was studied by modelling a 2D BWR assembly using the built-in burnup calculation capability of Serpent 2. The studied parameters were depletion zone division, burnup steps, unresolved resonance probability table sampling, DBRC and energy dependent branching ratios. A burnup calculation and a subsequent decay calculation were repeated for the different variations of the studied parameters.

In general the differences resulting from the use of different parameter variations were small for all three studied source term components. For the decay heat largest absolute relative difference was approximately 0.6 % and for the photon emission rate approximately 1.1 %. For the spontaneous fission rate maximum absolute relative difference of nearly 8 % was observed in the depletion zone variations.

Overall, the unresolved resonance probability table sampling had little effect in this calculation case which is not surprising due to the thermal spectrum in the BWR assembly. A somewhat more interesting discovery is the generally insignificant effect of replacing the default constant isomeric branching ratios used by Serpent with energy dependent branching ratios from the JEFF-3.1 activation file. Generally, the branching ratios do affect the equilibrium concentrations of the isomeric states but it seems that the effect is mostly lost in longer time

decay calculations. The effect of the Doppler broadening rejection correction is rather clear and indicates that it should be switched on in all calculations. The variations on spatial and temporal discretization used in the burnup calculation indicate that the ring-based spatial division and 34 step burnup calculation reproduce the reference results with a good accuracy.

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