

# On the Effective Fuel Temperature of the UO<sub>2</sub> Fuel

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## ABSTRACT

Fuel temperature is an important parameter in the determination of the reactor fuel behaviour, since the neutron cross sections depend on it. In lattice physics calculations, a fuel pellet is usually treated radially as a single region. In this case, the choice of an "effective temperature", which would yield the same response as the actual temperature profile, is very important. There are several known methods for estimating the effective temperature, but they lack generality. In this paper, we investigate how to best preserve the masses of important nuclides such as <sup>235</sup>U, <sup>238</sup>U and <sup>239</sup>Pu on one side and the multiplication factor on the other, by considering the reference results obtained by coupling of neutronic and thermal-hydraulic effects by the coupling of the Monte Carlo code Serpent 2 with the thermal-hydraulic code FINIX. The reference coupled results are compared with burnup calculations using the standalone Serpent 2 runs, keeping the fuel temperature constant in the radial direction. The accuracy of some widely used standard techniques is estimated, while some improvements are proposed.

## **1 INTRODUCTION**

One of our main interests in the Reactor Physics Department of the Jožef Stefan Institute is to simulate the daily operation of reactor cores and predict the key core parameters. Such analyses are performed using the three-dimensional code package CORD-2 [1]. The CORD-2 system is an in-house developed tool, which has been used for verification of Krško NPP cores since 1990. Recently, additional research was performed to improve an existing fuel temperature model of the CHNTMP subroutine. The current model was created based on calculations with the thermo-mechanical PIN code about 25 years ago and uses a precalculated table of average fuel temperatures for different burnup steps and different linear pin power values (power per pin per region length [W/cm]). In this way, the average fuel temperature can be determined for each axial region and for all fuel assemblies for a given operating condition. The calculation scheme within the CORD-2 code aims to reduce the overall calculation time and maintaining an acceptable level of accuracy. It has been demonstrated that the overall accuracy for the initial fuel cycles is on average around 20 ppm for the ARO condition (all rods out) [2]. Recent analysis suggests that updating the precalculated average temperatures by new data obtained from contemporary fuel performance codes could increase the overall accuracy for later fuel cycles.

The analysis for a single 3-D fuel assembly with only one axial region is presented. The reference results obtained by coupling neutronic and thermal-hydraulic codes (by coupling the Serpent 2 Monte Carlo code with the FINIX thermo-hydraulic code) are compared to the Serpent 2 stand-alone burnup calculations. The idea behind the analysis was to compare the

multiplication factors and some isotopic compositions and to evaluate the so-called effective fuel temperature for different burnup steps.

## 2 TEST CASE MODEL OF THE BENCHMARK

For this analysis, a 3D model is used representing the PWR  $16 \times 16$  pin-array configuration of the UO<sub>2</sub> fuel with periodic boundary conditions as it exists in the Krško NPP core. For the presented burnup calculations, the limit in the burnup value is 100 MWd/kgU. Fuel rods are divided in 10 concentric rings in burnup calculations with the following operational conditions:

- Power: 15.985 MW.
- Coolant density: 0.75260 g/cm<sup>3</sup> with constant boron concentration 1000 ppm.
- Fuel density: 10.3029 g/cm<sup>3</sup> and fuel enrichment:  $3.6 \% ^{235}$ U.

Several different calculations were performed. Each calculation is described in the following subsections.

#### 2.1 Reference case calculation

In the reference case, the coupling of Serpent 2 and FINIX is used. The use of the FINIX code has already been described in [3]. It should be mentioned that the coupled FINIX code version does not perform any pin dimensional changes arising from different processes in the fuel, such as fuel densification, pellet swelling, cladding creep etc. As such, the obtained temperatures are not representative for fuel burnout in absolute sense, but are completely adequate for our analysis, where more or less the impact of temperature profile is studied. The goal of the reference case was to calculate the shape of the temperature distribution in a fuel pellet for different burnup steps. In this case, the power is calculated with the Serpent 2 code for each concentric ring (a total of 10 annular regions of equal volume are used). This power is then transferred to the FINIX code, where the temperature distribution is calculated for a given fuel pellet. The temperatures are then returned to the neutron transport calculation, where new power profile is determined. The iteration process is repeated to achieve convergence. This procedure is repeated for each burnup step, with the Serpent 2 nuclide depletion calculation using the same distribution of concentric rings as for power distribution determination. Since the FINIX code calculates the fuel temperature at nodal points (total of 128 points are used), the average temperature of each ring is calculated using the procedure described in [4]. Figure 1 shows the temperature distribution within the fuel pellet for our test case model for two different burnup steps. For each burnup step, the following results are used in further analyses: multiplication factor kinf, average fuel temperature for each concentric ring, average fuel temperature for fuel pellet, and isotopic composition for each concentric ring.

Figure 1 shows that the shape of the temperature distribution in a fuel pellet in steadystate operation is approximately parabolic as in a flat power profile case. However, due to resonances and self-shielding, the power profile is not flat and changes when the pellet is irradiated. Furthermore, in lattice physics calculations, a fuel pellet is usually treated as a single region in the radial direction. In this case, the choice of an "effective temperature" that gives the same response as the actual temperature profile is very important.



Figure 1: The temperature distribution within the fuel pellet for the reference case model at three different burnup steps.

Therefore, three different cases were required to analyse the effects of resonances and self-shielding and to evaluate their influence on the temperature:

- case 1: In this case, the same isotopic composition for each annular region as in the reference case was used to calculate the multiplication factor using a flat fuel temperature distribution at each burnup step. These calculations were performed using the stand-alone code Serpent 2, with constant fuel temperature for all annular regions. No depletion calculations were performed.
- case 2: In this case, multiple burnup calculations were performed using the standalone code Serpent 2. Each depletion calculation was performed with a constant fuel temperature over the entire fuel pellet. A set of different fuel temperatures was considered. The depletion calculations were performed with 10 annular regions.
- case 3: This case is the same as case 2, except that the burnup calculations were performed with only one annular region.

The following fuel temperatures [K] were used for each burnup step (case 1) and depletion calculation (cases 2 and 3): 850, 855, 860, 865, 870, 880, 885, 890, 895, 900, 905, 910.

#### **3 RESULTS AND DISCUSSION**

The objective of these three cases is to evaluate the effects of temperature on the multiplication factor and isotopic composition. The main focus is to evaluate the impact of each case compared to the reference case. The following methodology is used:

• Starting from the reference case, the following results are obtained for each burnup step: average fuel temperature (average of 10 rings) and multiplication factor.

- For case 1, the multiplication factors are calculated for each burnup step and each fuel temperature (Figure 2) with isotopic composition from the reference case.
- A linear fit was derived to determine multiplication factor dependency on the temperature. Case 1 interpolated temperature was calculated at the point, where the temperature linear fit intersects the multiplication factor from the reference calculation.
- In addition, the uncertainty in the interpolated temperature are calculated using the 1  $\sigma$  statistical uncertainties of the calculated multiplication factor ( $\Delta k_{inf}$ ) based on the Monte Carlo calculations from the reference case. For different burnup steps, the multiplication factor has an average uncertainty of 9 to 14 pcm.

The same linear fit procedure was used for all three cases for the determination of the interpolated temperature.



Figure 2: Dependency of the multiplication factor on the fuel average temperature (case 1) for burnup step 10 MWd/kgU together with the linear fit.

Figure 3 shows the results of case 1. The calculated interpolated fuel temperature is shown along with the following reference results: centre-line fuel temperature, surface temperature, and the average temperature (average of 10 rings). The centre-line temperature is higher than the temperature on the surface of the fuel by approximately 400 K. It can also be seen that the interpolated fuel temperature results are lower than the average fuel temperature. Figure 4 illustrates a detailed comparison. First, the calculated uncertainties in the interpolated temperature are about 10 K and depend on the 1  $\sigma$  statistical uncertainties in the calculated multiplication factor ( $\Delta k_{inf}$ ) obtained from the Monte Carlo results of the Serpent-FINIX coupling calculations. A statistical uncertainty  $\Delta k_{inf}$  of 10 pcm results in a fuel temperature difference of about 4 K. The temperature difference between the start and end of burnup in the reference case is 16 K, while the interpolated results are around 10 K  $\pm$  14 K. It should be stressed that both cases (reference and the case 1) use the same fuel composition in each of the concentric rings, with the only difference being a difference in fuel temperature.

The analyses of cases 2 and 3 provide an additional understanding of the temperature impact on resonances and self-shielding on the outer surface of the fuel pellet. Figure 5 illustrates the difference between the reference case and case 2. Case 2 is a simplified case

where no thermo-hydraulic calculations are performed. For all concentric rings and burnup steps, the fuel temperature remains constant. However, different temperatures were used for the different burnup calculations to obtain an interpolated temperature. The temperature was interpolated using the same methodology as in the previous case. Figure 5 shows that the initial average temperature drop in the fuel is larger than in case 1. This happens at burnup step of around 30 MWd/kgU. A drop in interpolated fuel temperature of 60 K is observed. After that the interpolated temperature jump is observed. The reason for this jump is not a post-processing error, but has a physical explanation. At zero burnup, higher temperature induces larger resonance absorption (Doppler effect) and decrease in the multiplication factor, as we would expect. However, with larger resonance absorption, the neutron spectrum become harder. This has an impact on the depletion calculation, since a harder spectrum reduces <sup>235</sup>U consumption and produces more Pu. Such more favourable nuclide composition increases multiplication factor. The effect can also be seen in Figure 6, where the multiplication factor of different temperature cases no longer decreases, but begins to increase as the temperature increases. The change of behaviour occurs at about 30 MWd/kgU. It can also be seen that near 30 MWd/kgU the difference in multiplication factors is less than the statistical uncertainty of the Monte Carlo method at different temperatures, so the linear fitting function might not be appropriate for this case. This explains the sudden jump in calculated temperature shown in Figure 5. It should be noted that the case 2 calculations were done with 10 annular regions, explicitly taking into account high burnup in the outer region.

Figure 7 shows the difference between the reference case and case 3. Case 3 is a simplified case like case 2, but the fuel is not divided into concentric rings as in case 2, so that the impact of rim effect can be studied. The effect of the resonances and self-shielding on the outer surface of the fuel pellet is not explicitly taken into account in the depletion calculation. Again, it can be seen that near a total burnup of about 30 MWd/kgU, a significant drop and jump in the interpolated fuel temperature can be observed. The effect is even larger than in case 2. Case 2 and case 3 comparisons show that the effect of temperature profile and variation of the temperature during the fuel irradiation cannot be compensated with the constant flat temperature alone.



Figure 3: Comparison of the results of case 1 with the reference results.



Figure 4: Detailed comparison of the interpolated temperatures of case 1 with the reference average temperature results.



Figure 5: Detailed comparison of the interpolated temperatures of case 2 with the reference average temperature results.



Figure 6: Average (over 10 concentric rings) total macroscopic cross section in the fuel as a function of the average fuel temperature for selected burnup steps (bottom) and multiplication factor as a function of the average fuel temperature (top).



Figure 7: Detailed comparison of the interpolated temperatures of case 3 with the reference average temperature results.

## 4 **CONCLUSION**

The aim of this work was to evaluate the effect of radial temperature distribution on local reaction rates and multiplication factor by comparing coupled neutronic and thermo-hydraulic model with simplified neutronic simulations. This is important because we commonly use an "effective temperature" approach for the lattice physics calculations, where a fuel pellet is treated radially as a single region.

Many forms of effective temperature formulas can be found in the literature. Usually, a combination of the pellet centre-line temperature and the surface temperature is used. Two important conclusions emerge from our analyses:

- the effective temperature is lower than the average temperature obtained from the realistic power radial distribution,
- the effect of temperature variations on resonances and self-shielding (rim effect) during the fuel depletion cannot be compensated with the fuel temperature correction alone.

Based on these studies, an effective temperature model could be developed applying the total cross sections weighting on the radial temperature profile in the fuel. The results show that the differences in the multiplication factor for each burnup step are small. For burnups less than 12.5 MWd/kgU, the average difference in multiplication factor is around 40 pcm, and for larger burnups the difference is less than 10 pcm. The effect of temperature variations during the fuel irradiation will need a more sophisticated approach. A simple flat constant temperature assumption is not adequate. The possible solution process is limited also by the lattice code constraints. The vast majority of the codes namely does not allow fuel temperature changes within depletion run. The results are exciting and with some additional analysis will be submitted for publication to an international journal.

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