Modelling nuclear fuel assembly with thermal-hydraulic feedback and burnup using WIMS-PANTHER-Serpent

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Abstract. State-of-the-art deterministic code sequence WIMS-PANTHER and Monte Carlo particle transport code Serpent are employed in this work for computationally modelling the UK EPR nuclear reactor core’s fuel assembly with and without thermal-hydraulic feedback, the results of which targets the government energy policymakers and wider academic community.

1. Introduction

As the key component of a nuclear power plant, reactor core modelling has a significant potential for impact in terms of both neutron economy [1] and safety competency [2] that assist the government in the energy policy decision making. In principle, a nuclear fission reactor core can be computationally modelled following a standard two-step methodology from two dimensional (2D) to three dimensional (3D), i.e. from burnup and operating conditions dependent cross-section library generated by deterministic [3] or Monte Carlo approach [4], towards 3D nodal-diffusion [5] calculations incorporating thermal-hydraulic feedback [6] with the core height.

This work pioneers the employment of the WIMS-PANTHER-Serpent codes sequence in the 3D assembly analysis for a European Pressurised Reactor (EPR). The data library of homogenised group constants used by PANTHER is generated from a matrix of WIMS calculations, covering multiple dependencies on burnup and thermo-hydraulic parameters, namely, moderator and fuel temperatures, coolant density, boron concentration, and rod cluster control assembly (RCCA) insertion. Prior to building the full-core model, analysing a single 3D assembly in PANTHER is very useful, not only because it can be tested with Serpent Monte Carlo code, but on the other hand it includes all the important phenomena, e.g. spatially distributed burnup and thermal-hydraulic conditions.

Work begins by creating an infinitely reflected node in PANTHER without thermal-hydraulic feedback. By demonstrating that the effective multiplication factor ($k_{\text{eff}}$) calculated by PANTHER matches with WIMS, realistic boundary conditions and thermal-hydraulic feedback are applied. Serpent is used to validate the 2D assembly results obtained by WIMS in order to check the reliability of the WIMS model assumptions. It is expected from the modern lattice codes to predict the multiplication factor of a single assembly with a few hundred pcm accuracy (pcm = delta-rho×10\textsuperscript{5}). Identical fuel compositions (in terms of atomic number fraction) and operating conditions are set for the two codes to avoid inconsistencies. Note that the macroscopic cross sections generated by Serpent...
are in cm⁻¹, whereas the WIMS library feeding PANTHER is converted to m⁻¹, as all PANTHER data are held on the internal database (IDB) in SI units.

2. Lattice physics simulation of burnup dependent cross sections using WIMS and Serpent

As presented in Figure 1, both the assemblies with and without burnable poison Gadolinia (Gd) are examined in the cross-section parameterisation with respect to burnup by solving neutron transport criticality equation and burnup matrix. Finer irradiation sub-steps are strategically chosen at the beginning of life (BOL) to accurately capture the relatively fast changes in material compositions. The results of the assemblies with burnable poisons zoning are shown in Figure 1 (b), characterised by the use of a higher number of discrete time steps at the BOL to precisely simulate the depletion of Gd. As evidenced in the benchmarking comparison between the two codes, Serpent’s burnup calculation results with and without Gd agree well with WIMS. The deviation could be due to the different depletion algorithms adopted by the two different codes.

![Figure 1](image)

**Figure 1.** Comparison of assembly $k_{inf}$ with burnup: WIMS vs. Serpent (a) no Gd (b) with 8 Gd.

On the basis of few-group cross sections production for all the assembly types and state points by WIMS and benchmark against Serpent, subsequent calculations in PANTHER are performed, i.e. 3D core nodal diffusion calculation including pin power reconstruction.

3. 3D assembly simulation without thermal-hydraulic feedback using PANTHER

The 2.1wt% assembly (0 Gd) is firstly examined using prescribed operating conditions adhering to the UK Office for Nuclear Regulation [7]. Implementing the strategies as stated in the introduction section, PANTHER successfully reproduces the WIMS result as shown in Table 1 for the beginning of cycle (BOC). The effect of polynomial expansion order in PANTHER is investigated in Figure 2.

**Table 1.** Steady-state flux calculation results comparison: WIMS vs. single-node PANTHER for 2.1wt% assembly, BOC, 1000 ppm boron, order of polynomial expansion = 16, RCCA out.

| Burnup steps (GWd/t) | Multiplication factor $k_{eff}$ | Deviation (pcm) |
|----------------------|---------------------------------|-----------------|
| 0.0                  | 1.08705                         | 0.93            |
| 0.1                  | 1.08242                         | 0.85            |
| 0.5                  | 1.07480                         | 0.87            |
| 1.0                  | 1.06913                         | 0.96            |
| 4.0                  | 1.03701                         | 1.02            |
| 10.0                 | 0.97562                         | 1.05            |
Figure 2. Effect of varying the order of polynomial expansion in PANTHER on the $k_{\text{eff}}$ deviation between WIMS and PANTHER.

Increasing the order of polynomial expansion manually in PANTHER, the flux representation is almost flat in an infinitely reflected node. Nearly zero pcm difference between PANTHER and WIMS is observed. Based on demonstrating the validity of the WIMS-PANTHER model setup, realistic conditions of EPR are applied to the single-channel analysis. Setting the boundary condition as radially reflected but axially open, cosine-shaped axial flux distribution is obtained at the BOC as shown in Figure 3 below. The axial power distribution with burnup but without thermal-hydraulic feedback is firstly examined by feeding the WIMS cross-sections database without branches to PANTHER. Twenty-one axial layers (with a height of 0.2 m for each mesh) are used to precisely simulate the axial power distribution over the core life.

Figure 3. EPR single-channel calculation of axial power profile without thermal-hydraulic feedback using PANTHER.

Without thermal-hydraulic feedback on neutronics, fuel and moderator temperatures are uniformly distributed axially at the BOC, i.e. there is no variation in the water density. Thus, the cross sections are not affected by the core height, and the spectrum hardening does not occur at the upper part of the core. Therefore, the reaction rate and hence the power is completely symmetric with respect to the center of the core, i.e. the typical axial power shape biasing towards the bottom at the BOC due to
density difference with core height is not observed. However, the spatial burnup effect is clearly visible in Figure 3 shown above. Due to higher flux at the middle core height at BOC, fuel at the center has higher burnup and more fission products building up with time. With lower burnup at the BOC, the fuel at the top and bottom contribute to two power peaks progressively from the middle of cycle (MOC) towards the end of cycle (EOC), when the fuel at the center core height has burnt out, depressing the power in the center. When the fuel at the top and bottom finally burns down (EFPD = 402), the spatial burnup becomes nearly uniform, and the axial form factor is reduced as reported in Figure 4.

![Figure 4](image)

**Figure 4.** EPR single-channel calculation of axial form factor vs. burnup (without thermal-hydraulic feedback) using PANTHER.

For the benchmarking purpose, the Serpent 3D single-channel analysis is carried out and compared with PANTHER (switching off the thermal-hydraulic feedback). As illustrated in Table 2, the difference in predicting the effective multiplication factor between PANTHER and Serpent is largely within 100 pcm over cycle 1, hence verifying the 3D model setup.

| Burnup steps (GWd/t) | Multiplication factor $k_{eff}$ | Deviation $\Delta$ (pcm) |
|---------------------|---------------------------------|--------------------------|
|                     | PANTHER 3D                      | Serpent 3D               |
| 0.0                 | 1.08172                         | 1.08255 (±0.00014)       | 71          |
| 0.1                 | 1.07832                         | 1.07937 (±0.00014)       | 90          |
| 1.0                 | 1.07007                         | 1.07120 (±0.00015)       | 99          |
| 10                  | 0.99410                         | 0.99507 (±0.00016)       | 98          |
| 24                  | 0.92685                         | 0.92778 (±0.00017)       | 108         |

4. **3D assembly simulation with thermal-hydraulic feedback and burnup using PANTHER**

In the final part of the study, the 3D simulation of the same single assembly is repeated but with thermal-hydraulic feedback switched on. It is worth noting that the updated axial power shaping results depicted in Figure 5 below exhibit an asymmetric peak at the BOC, and double peaks towards the end of life (EOL) of cycle 1, with the detailed analysis explained below.
At hot zero power (HZP), the axial distribution of water density is nearly uniform, resulting in the flux peak at the centre of the core height. When it comes to hot full power (HZP) at the BOC, coolant temperature varies with core height, i.e. the outlet is higher than the inlet. Due to the thermal expansion, the atomic number ratio of moderator to fuel, i.e. $\frac{\text{H}_2\text{O}}{^{235}\text{U}}$, in this work decreases with core height. The decreasing coolant density from bottom to top leads to less efficient moderation above the core mid-plane, and hence the neutron spectrum is hardened and leakage is increased, shifting the flux peak from the centre towards the lower part (at about 40% of the core height). With more fission reactions occurring due to the higher thermal flux, the fuel at the bottom achieves a higher burnup. Axial power re-distribution occurs with the bottom fuel burning down faster and higher concentration of Xenon building up at the bottom compared with the fuel at the top. This progressively leads to another skewing of the flux profile, i.e. peaking towards the top as evidenced in the results from MOL to EOL. The results well agree with nuclear reactor physics, demonstrating that the cross-sections generation with thermal-hydraulic branches functions well by the proposed novel sequence of WIMS-PANTHER-Serpent to inform in-core safety instruments and fuel-loading optimisations.

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