# TOWARDS A MORE DETAILED MESOSCALE FISSION PRODUCT ANALYSIS IN FUEL PERFORMANCE CODES: A COUPLING OF THE TRANSURANUS AND MFPR-F CODES

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## Abstract

The current study introduces a novel approach for a coupling between the TRANSURANUS (TU) fuel performance code and the Module for Fission Product Release - France (MFPR-F). The new methodology is outlined and first, preliminary results are presented. Simulations have been performed using two versions of TU – the first adopting the existing fission gas module (Fispro 2), while the second being the TU-MFPR-F coupled code. The results for the intragranular concentration of Xe, the fuel centre temperature and fuel-clad gap exhibit consistent trends and comparable magnitudes in each of the two cases (TU-MFPR-F and Fispro 2). Notable differences were observed for the intergranular Xe concentrations. These initial, preliminary results serve as a proof of concept and are the groundwork for the development of a mechanistic multi-scale fuel performance simulation tool.

## 1. Introduction

Nuclear accidents have highlighted the need for improved measures to prevent and mitigate such extreme events. This can only be achieved by understanding and accurately evaluating the evolution and consequences of such off-normal conditions in nuclear power plants (NPPs) [1]. An aspect of paramount significance for the progression of an accident is the behaviour of the fuel. Thus, the amelioration of safety measures would require improved understanding and more accurate predictions of the fuel's performance during normal operation and accident scenarios.[2]

The in-pile performance of nuclear fuel is strongly dependent on its physical properties and these would change during the in-reactor lifetime of the material[3,4]. Such changes include, however are not limited to: 1) swelling due to the generation of fission gas bubbles[5,6]; 2) fuel thermal conductivity degradation due to gas bubble generation, fission product (FP) accumulation and deviations from stoichiometry[3,7]; 3) irradiation enhanced creep[8]. Fuel performance predictions for normal operation, as well as for accidental conditions, are dependent on improving the understanding of these physical processes. The behaviour of the fuel and fission products is coupled and combines phenomena induced by chemical, radiation, thermal and mechanical effects. As a result, a multiphysics-multiscale approach is necessary to confidently predict the fuel's performance in a range of possible reactor scenarios.

In this context the current paper presents a new prototypical coupling between the detailed mechanistic meso-scale code MFPR-F and the conventional fuel performance code TRANSURANUS. The MFPR code was developed by IBRAE with IRSN [12] (IBRAE: models and code development; IRSN code application to interpretation of FP behaviour and benchmarking), and since 2011, the code has been developed independently by both institutes. IRSN is developing its own version MFPR-F which is coupled with TRANSURANUS as presented in this paper. This study is a first step towards improving the predictions of the fission product inventory, swelling and gas release from nuclear fuels, along with the inclusion of more detailed fuel and fission product chemistry in the fuel performance modelling. The work is part of a collaboration agreement between the IRSN and the JRC that started in 2017.

In the next section, the two simulation tools and their coupling scheme are briefly described. The third section discusses the preliminary results obtained from the new tool. For this purpose a simplified irradiation history was used. The coupling's calculations are compared to those obtained by means of the TRANSURANUS code using the already existing fission gas behaviour model (developed in the frame of the FUMEX-III project of the IAEA and published earlier). In the last section, we draw preliminary conclusions and outline future tests and developments related to the coupled code system.

## 2. Methodology

### 2.1. TRANSURANUS fuel performance code

The TRANSURANUS (TU) code calculates key fuel and cladding state variables such as temperature, pressure and associated strain[9]. Additionally, the evolution of actinide nuclides (fissile and fertile) is calculated. The chosen nuclides are considered to be the most significant for the calculation of the heat generation rate. The code calculates all these quantities in a quasi-two-dimensional (1.5-D) manner. The fuel rod is divided into slices of cylindrical geometry. For each of these segments the respective transient governing equations are solved in a 1-D radial geometry. A simplified schematic of the code’s architecture is shown in Figure 1. In particular, the fission gas behaviour and related models are grouped under level 3 in Figure 1. The currently used fission gas module (Fispro 2) was developed by Pastore et al.[6] It describes the creation, diffusion, precipitation and release of fission gases. However, only a limited number of FP elements are taken into account and there is no consideration of FP compounds.

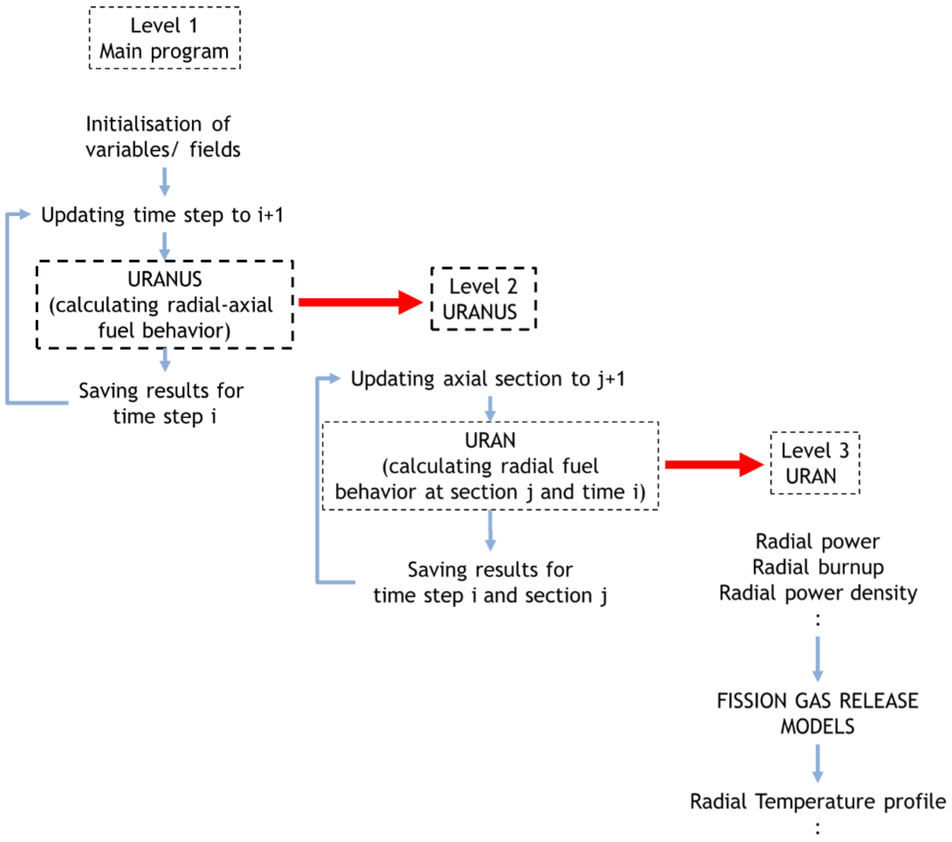

Figure 1. Simplified logic diagram of the TRANSURANUS code structure.

## 2.2. **Module for Fission Product Release - France (MFPR-F)**

MFPR-F simulates solid fuel as an assembly of identical grains[10]. Due to fission, a wide range of FP elements are created in the $UO_2$ matrix. The list of FP elements included in the MFPR-F code is Cs, I, Mo, Ru, Ba, Sr, Zr, La, Ce, Eu, Nd, Nb, Sb, Te, Xe. Elements exist in the $UO_2$ matrix in atomic form. Fission gases, such as xenon, are relatively insoluble and precipitate into bubbles. It is assumed that intragranular bubbles constitute of noble gases only. The behavior of fission gases is strongly linked to the fuel microstructure (point, extended defects and densification) which is described in the code. FP atoms migrate to the grain boundary and in the process some of these (Xe for example) can be captured by mobile intragranular gas bubbles. Irradiation-induced re-solution and thermal re-solution are considered as competing processes during the bubble precipitation process. Chemical interaction between the FP elements and the dissolved oxygen results in the formation of solid precipitates on the grain boundaries. These could subsequently vaporize (generally non-congruently) allowing for additional FPs to be transported to the intergranular gas bubbles. Additionally, the formation of FP compounds impacts the fuel's stoichiometry which has a knock-on effect on various material properties (such as the Xe diffusion coefficient or fuel thermal conductivity). The intergranular bubbles behavior includes face and edge bubbles for which irradiation-induced phenomena are also considered. Finally, grain face bubble saturation occurs once a surface coverage factor of 50 %, resulting in bubble interlinkage and fission gas release via a percolation mechanism.

## 2.3. **TU-MFPR-F coupling interface**

In this work a coupling between the aforementioned codes is proposed. A schematic is shown in Figure 2. Figure 2A shows the multi-scale nature of the coupling. MFPR-F is used to simulate the FP behaviour on the grain scale. It is integrated at the local radial level of each fuel slice in TU (level 3 in Figure 1). As part of the coupled tool MFPR-F is substituting the current fission gas release module (Fispro 2). Figure 2B highlights the two-way principle of the coupling. The physical parameters calculated by TRANSURANUS and subsequently provided as input for MFPR-F are also shown in Figure 2B. These include temperature, fission rate density, hydrostatic pressure, fission yield, porosity, the time interval, mesh location and volume, as well as grain size. Utilising this information MFPR-F then calculates and transfers the fission product concentrations, swelling and updated grainsize back to TRANSURANUS at a particular radial location in an axial fuel rod slice. It must be noted that for the purpose of this preliminary (simplified) coupling dislocations have not been considered.

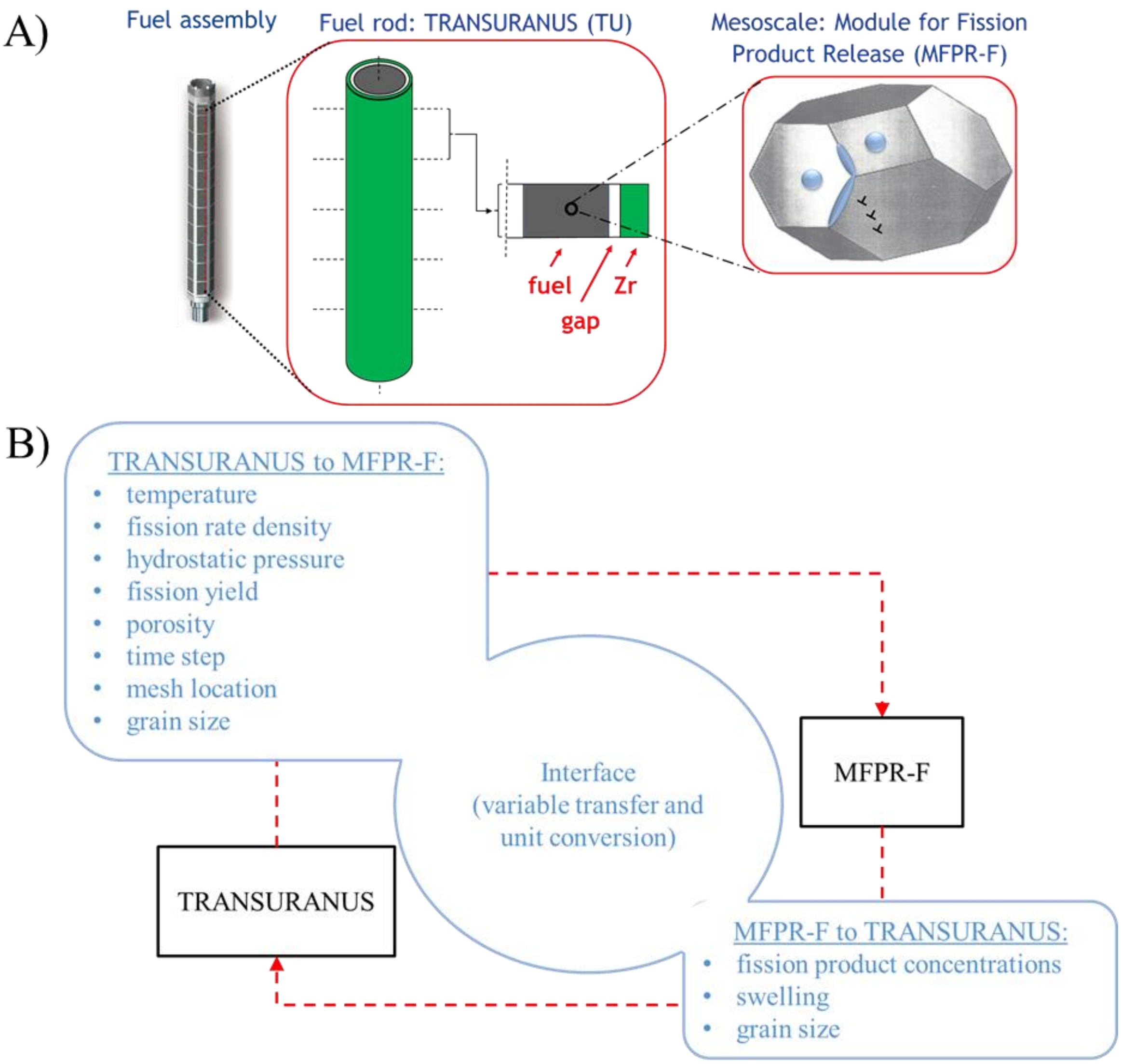

Figure 2. Schematic of the TU-MFPR-F coupling approach. A) Diagram showing the multiscale nature of the methodology. MFPR-F describes the fission product behaviour at grain level, while TU uses this information during its fuel rod simulation. B) Depiction of the two-way coupling between the codes. The respective transfer variables have been listed as bullet points.

## 3. Preliminary results

In this section the first preliminary results of the coupling are compared to the existing fission gas module in TRANSURANUS (Fispro 2 – developed by Pastore et al.). Simulations were performed for each version of TU using identical input parameters, including the same linear heat rating history (see Figure 3). All calculations have been performed for the mid-section of a fuel rod split into five axial meshes for 40 000 h. The power history consists of three stages: 1) ramp-up (0 h to 177.6 h); 2) constant power level (177.6 h to 10 000 h); 3) ramp-down (10 000 h to 40 000 h). This simplified case is suitable for the initial stages of testing. The red dots in Figure 3 indicate the time instants 177.6 h and 5000 h, respectively. At these time steps radial profiles of the Xe concentrations and swelling strains are compared by using the two different modules (MFPR-F vs. Fispro 2). Despite the fact that the calculation ran successfully for the entire irradiation history, we discuss here only results up to 5000h in order to avoid the complexity brought abought by the high burnup structure (HBS) formation. A specific model for the HBS is under development and will be considered separately in a later stage of the code coupling.

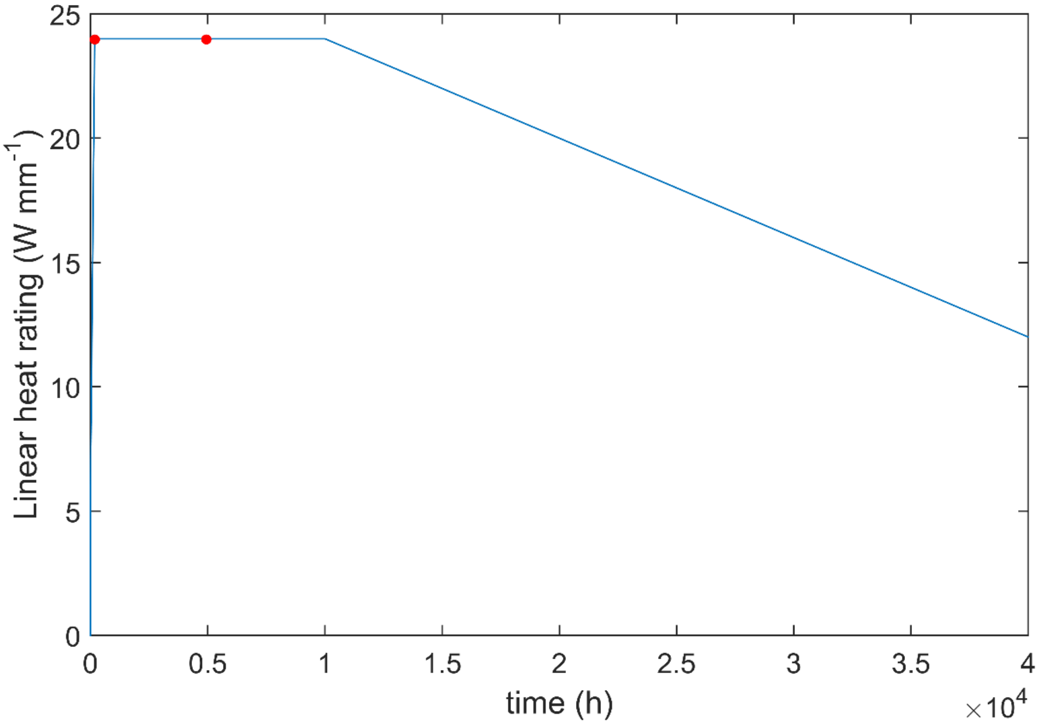

Figure 3. The linear heat rating (W mm$^{-1}$) vs. time (h) (serving as input for all TU calculations).

The calculated Xe concentrations, both in the grain and at grain boundaries are shown in Figure 4 at two different time instants. From Figure 4A and Figure 4C it is evident that the intragranular gas concentration predicted by the new coupled system is slightly higher compared to the result obtained with Fispro 2. As a result the coupling predicts a lower concentration of Xe at grain boundaries (see Figure 4B and Figure 4D). This is likely to be the result of irradiation induced resolution of grain boundary bubbles. In the case of Fispro 2 only intragranular bubbles undergo this process, while MFPR-F allows for both intra- and intergranular bubbles to shrink due to irradiation. In both cases the intragranular concentration increases towards the pellet periphery. The higher fission product source term towards the pellet edge justifies the steep increase in the intragranular Xe concentrations. Furthermore, the radial temperature profile of the fuel is nearly-parabolic, with the central temperature being higher under normal operating conditions. As the temperature along the radius drops, fission gases become less mobile and fewer of these are able to migrate towards the grain boundaries. Hence, more fission products are retained inside the grain at the pellet periphery compared to the fuel centre. Due to this thermal diffusion mechanism, the Xe intergranular concentrations should be higher in the centre and lower at fuel edge. This can be seen in Figure 4B and Figure 4D when performing the TU simulation using either Fispro 2 or MFPR-F.

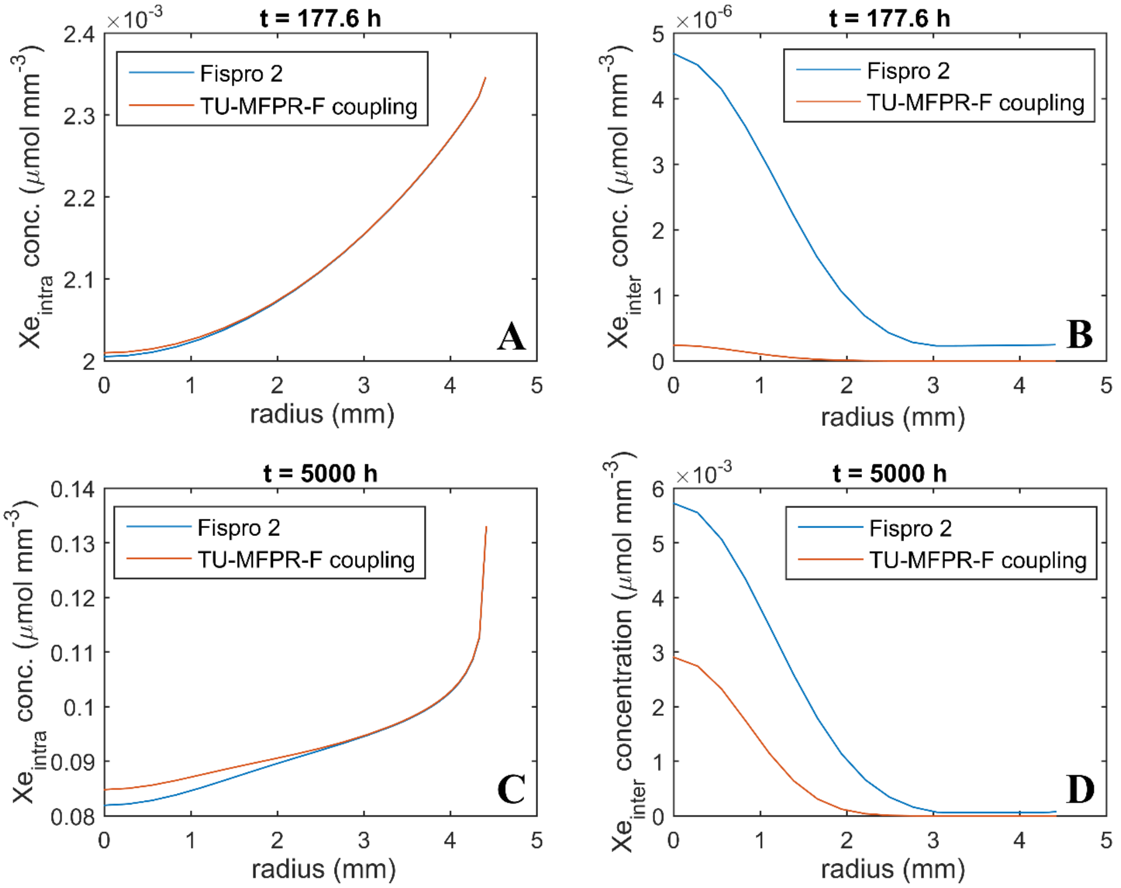

Figure 4. Xe concentrations vs. radius predicted by means of two TRANSURANUS simulations. The Xe behaviour of the coupled system is compared with the already existing fission gas module in TU (Fispro 2). A) intragranular Xe concentration at 177.6 h; B) intergranular Xe concentration at 177.6 h; C) intragranular Xe concentration at 5000 h; D) intergranular Xe concentration at 5000 h.

Figure *5* compares the gaseous swelling as a function of radius for the simulations performed using Fispro 2 and the TU-MFPR-F coupling, respectively. Towards the pellet periphery the swelling values obtained by the two cases are nearly identical. However, the results obtained via the TU-MFPR-F coupling exhibit lower swelling strain values in the fuel centre when compared to Fispro 2. This is consistent with the lower intergranular gas inventory predicted by the coupled system.

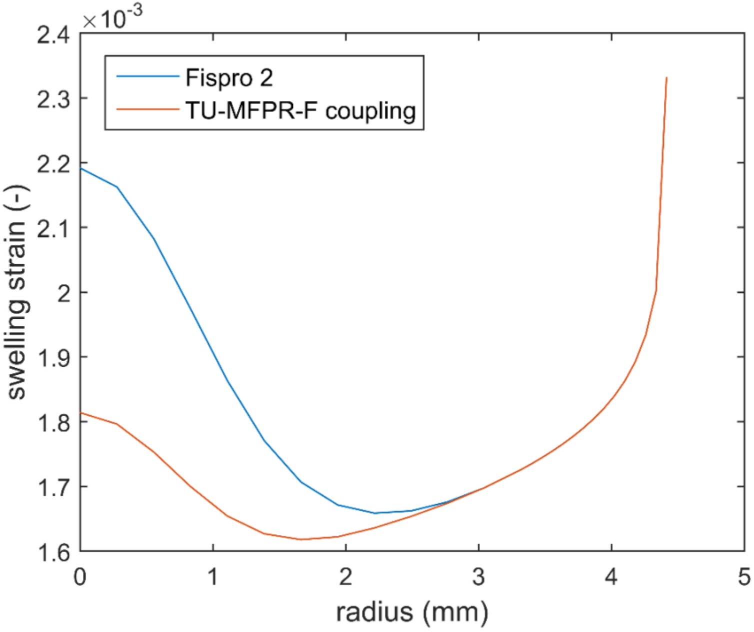

Figure 5. Strain due to swelling as a function of pellet radius at 5000 h. The results of the TU-MFPR-F coupling are compared to Fispro 2.

Figure 6 compares the temperature profiles obtained with the coupled version of TRANSURANUS and the one utilising the Fispro 2 module. The calculated temperatures are in excellent agreement throughout the whole simulation time.

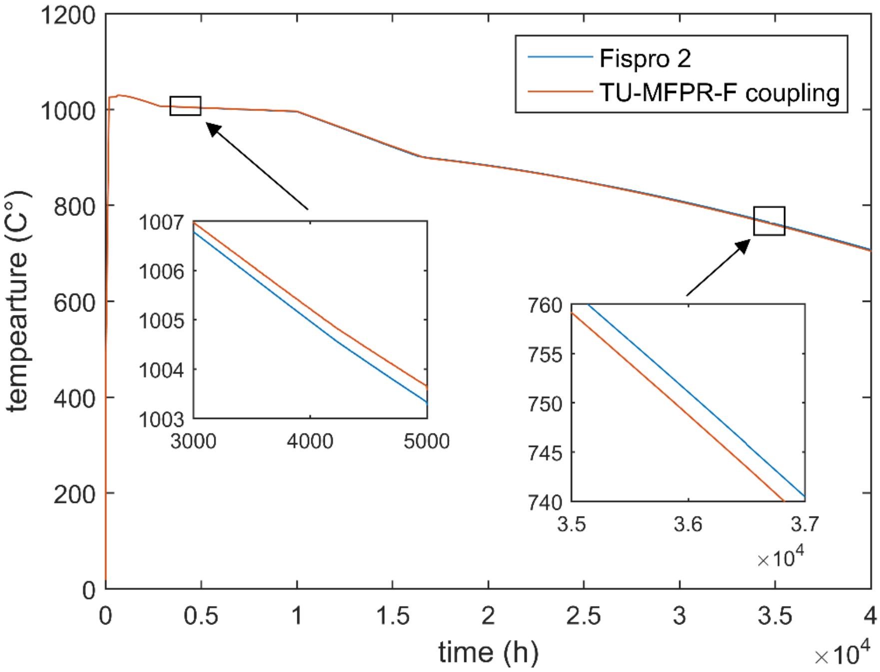

Figure 6. Fuel centre temperature as a function of time (h). The results of the TU-MFPR-F coupling are compared to Fispro 2.

Figure 7 shows the calculated fuel – cladding gap adopting the coupling and using the Fispro 2 module in TRANSURANUS. The two simulations exhibit nearly identical results. Fispro 2 predicts a slightly more accelerated gap closure. A smaller gap is consistent with the higher swelling strain (see Figure 5) and lower fuel centre temperature predicted by TRANSURANUS when using the Fispro 2 module[11] (see Figure 6).

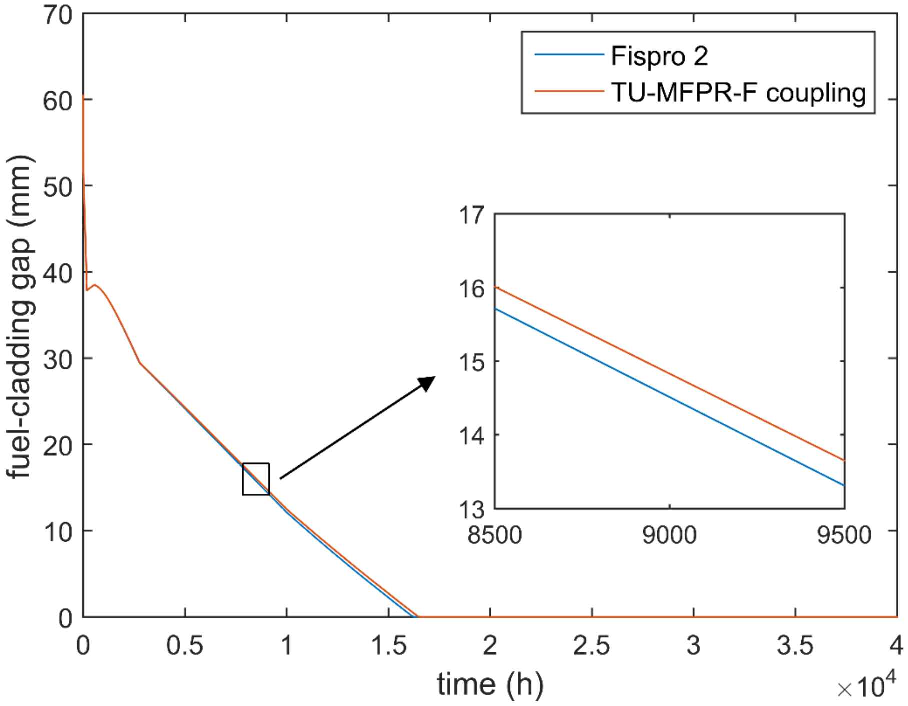

Figure 7. Evolution of the fuel- cladding gap (mm) as a function of time (h). The results of the TU-MFPR-F coupling are compared to Fispro 2.

## 4. Conclusion

This work presents the preliminary status of a new coupling between the TRANSURANUS fuel performance code and the detailed mechanistic MFPR-F fission product code. The TU-MFPR-F version has been compared against the existing version of TU (utilising a conceptually similar fission gas module - Fispro 2). The results for the intragranular concentration of Xe, the fuel centre temperature and fuel-clad gap exhibit consistent trends and comparable magnitudes in each of the two cases (TU-MFPR-F and Fispro 2). Notable differences were observed for the intergranular Xe concentrations. Overall, these first results serve as a proof of concept and are only the initial stage in the development of a mechanistic multi-scale fuel performance simulation tool. Future work would include: 1) extending the fission product inventory transferred from MFPR-F to TRANSURANUS to more elements and compounds; 2) performing separate effect and sensitivity studies using the coupled system; 3) considering the effect of dislocations on the transport and release of fission products, and 4) comparing the coupling to other codes and experimental data.

## 5. References

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