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PROGRESS IN THE MODELING OF HIGH BURN UP STRUCTURE: APPLICATION OF THE TRANSURANUS/MFPR-F COUPLING TO THE NRC-192 STUDSVIK LOCA TEST

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Abstract. The MFPR-F (Module for Fission Product Release – France) code coupled with the TRANSURANUS fuel performance code was applied to the Studsvik NRC-192 Loss of Coolant Accident experiment on a high burnup UO₂ fuel rod. The presented study, conducted in the framework of the R2CA project, focuses on the formation of the High-Burnup Structure during irradiation and on the fission gas release during the LOCA transient. MFPR-F code supplements TRANSURANUS code with a more in-depth description of the local microstructure in the UO₂ matrix, allowing to predict the onset of fuel restructuring [1]. This modelling is used in the present study to calculate the width of the HBS zone in the fuel rod at the end of irradiation, which is found to be 400 µm. Regarding the LOCA transient, the MFPR-F model for fission gas release from the HBS pores, based on an empirical parameter related to the pore over-pressurization, predicts that a large part the gas is released for over-pressure ranging from 150 to 300 MPa.

Keywords: High Burnup Structure, fission gas release, LOCA.

1 Introduction

The increase of the discharge burn up of nuclear fuel requires to improve the understanding of the behavior of high burnup fuel, in particular under accident conditions. To this end, numerical tools able to address the complexity of the phenomena involved in the formation of the High Burnup Structure (HBS) zone during irradiation, and in its role during LOCA, are necessary. The coupling of the fuel performance code TRANSURANUS and of the mechanistic meso-scale code MFPR-F offers that possibility. Indeed, the coupled codes have recently shown their ability to simulate LOCA transient [2]. Furthermore, the MFPR-F code models the formation and growth of HBS zone during irradiation, and the FP release from this zone during thermal transients [1]. Unlike most of the existing models for HBS formation which are based on the empirical concept of effective burn-up [3, 4], the model of MFPR-F, derived

from the work of Veshchunov & Shestak [5], relies on the calculation of radiation damage in the UO₂ matrix, considered as the driving phenomenon for fuel restructuring [6].

In the present work, the TRANSURANUS/MFPR-F coupling has been applied to a high-burnup LOCA case, the NRC Studsvik-192 test, in order to test the predicting capabilities of MFPR-F on the fission gas release from the HBS zone. This study has been conducted in the framework of the R2CA project. The paper is organized as follows: the modeling of HBS in MFPR-F is first briefly described, then the simulation of irradiation of the reference rod is presented, focusing on the formation of the HBS zone predicted by MFPR-F. Finally, the results obtained for the NRC Studsvik-192 test itself are analyzed.

2 Modeling of HBS in MFPR-F

The mechanistic approach adopted in MFPR-F for modeling HBS formation has been described earlier [1, 5], and is here briefly recalled. The main hypothesis is that fuel matrix restructuring is induced by accumulation of dislocations generated by irradiation damage. The level of dislocation density at which the fuel matrix is fully restructured has been estimated at about $\sim 10^{15} \text{ m}^{-2}$ by experimental [6] and numerical means [7]. In MFPR-F, the model for formation of defects in UO₂ matrix provides the evolution, under irradiation, of the dislocation density at each radial location in the pellet. When that quantity reaches the threshold of $2 \times 10^{15} \text{ m}^{-2}$ at a given radius, the fuel matrix is considered as restructured, resulting in a change of the local parameters for microstructure, porosity and gas. Regarding microstructure, the grain diameter is reduced to 0.9 μm , and the concentration of defects (including dislocations) is set to zero. The intergranular porosity is set to 15%, and further evolution of pore radius is fitted on experimental data [8]. Finally, the FG depletion from grain and its accumulation in HBS porosities observed in EMPA measurements performed on irradiated fuel rods [9] or highly enriched fuel discs [10] is reproduced in the MFPR-F HBS model.

MFPR-F also comprises a model for FG release from the HBS pores under thermal transient, based on the assumption that the release is driven by the over-pressurization of the pores. This assumption is grounded by thermal transient experiments carried out on very high burn-up fuel in a vacuum chamber [11]. In the current state of the model, the release occurs when the over-pressurization of HBS pores reaches a critical threshold ΔP_{crit} . This leads to the following criterion:

$$P_g = 2\gamma/R_{pore} + P_h + \Delta P_{crit}$$

with P_h the hydrostatic pressure, γ and R_{pore} the surface tension and radius of a pore, respectively, and $P_g = EoS(N, V, T)$ the pore gas pressure, determined by temperature T , pore volume V and the number N of gaseous atoms and molecules in the pore, via the equation of state EoS . In the present work, several hard-sphere equations of state have been tested, such as Carnahan-Starling and Perkus-Yevik, adapted to the extreme conditions (very low molar volumes) encountered in the HBS pores [12].

3 Formation of HBS zone under irradiation

3.1 Irradiation of the reference rod

The characteristics of the NRC Studsvik-192 test element (rodlet) are summarized in Table 1. The sample comes from a UO₂ fuel rod irradiated during 4 cycles in a PWR. A simulation of this irradiation period is performed with the TRANSURANUS//MFPR-F coupling, providing a proper initial state for the subsequent LOCA simulation.

Table 1. Irradiated test element characteristics.

Parameter	Value
Height	300 mm
Free volume	10.4 cm ³
Filling gas pressure	8,2 MPa
Initial ²³⁵ U enrichment	3.99 % wt.
Mean burn up	78 MWd/kgU

The irradiation simulation is based on a TRANSURANUS dataset prepared by SSTC NRS in the framework of the FUMAC project [13]. The irradiation history obtained in the simulation is shown in Fig. 1.

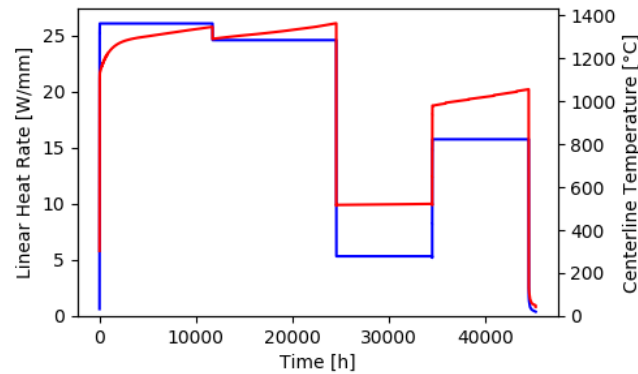


Fig. 1. Power history (W/mm, in blue) and pellet center temperature (°C, in red) at rod mid-section.

The final burnup of 72 MWd/kgU (part of test element) is sufficient for a HBS zone to develop. The dislocation density profile obtained at different instants during the last cycle of irradiation at rod mid-section is represented in Fig. 2. The profile is relatively

flat except for radii higher than 3mm, where the dislocation density increases with radius, as expected from the evolution of conditions toward the pellet rim (fission rate increase and temperature decrease). The dislocation density eventually reaches the restructuring threshold of $2 \times 10^{15} \text{ m}^{-2}$, at a given radius delineating the interior limit of the HBS zone. As the burnup increases, the levels of dislocation density become more important, and the limit of the HBS zone moves toward the interior of the pellet, materializing the growth the HBS zone. Note that, the dislocation density inside the HBS zone being null, it is not represented on the figure.

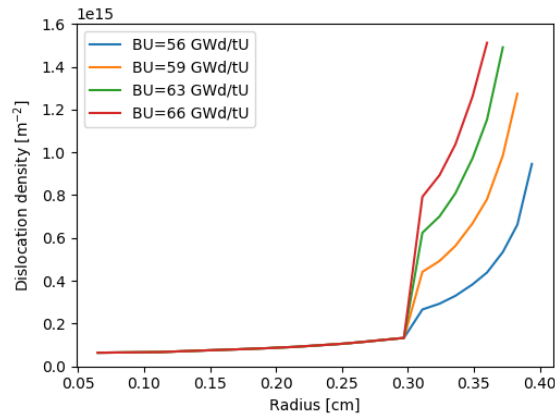


Fig. 2. Radial profiles of dislocation density [m^{-2}] calculated by MFPR-F at different instants (labelled by the pellet burnup) during the last irradiation cycle.

3.2 Fission gas repartition

The fission gas repartition over the pellet radius obtained at the end of irradiation is shown on

Fig. 3. In the non-restructured zone of the pellet (white domain on the figure), most of the gas remained inside the grain. It can be noticed that in the central zone of the pellet, due to high temperature levels encountered during irradiation, part of the gas diffused out of the grain and have been released. In restructured zone (blue domain), a strong depletion of the intragranular gas occurred and resulted in a high quantity of gas trapped in the (intergranular) HBS pores, in line with experimental observations (see section 2).

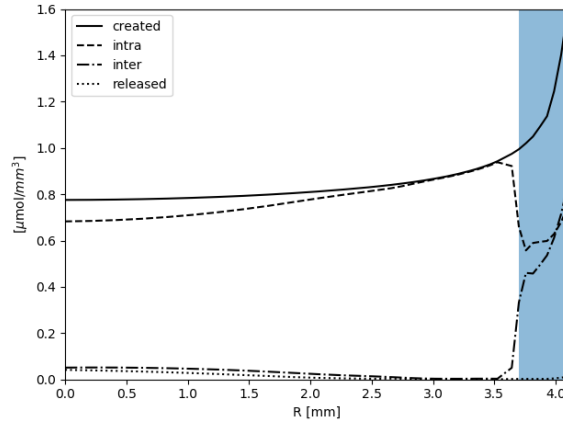


Fig. 3. Radial profile of the fission gas created (plain), intragranular (dash), intergranular/HBS pores (dash-dot), and released (dot) at the end of irradiation. The blue stripe corresponds to the extent of the HBS zone.

4 FG behavior in HBS zone during LOCA transient

4.1 The NRC Studsvik 192 test

The NRC Studsvik-192 test was performed in 2011 in the LOCA facility of the Studsvik nuclear laboratory in Sweden. The test element consists of a 0.3m section cut from the reference rod. The element is externally heated by infrared radiation in a clamshell furnace, where a flow of steam is applied. The test element is initially filled with Helium gas at 8MPa and 573 K, corresponding to the internal PWR rod pressure at the end-of-life. A temperature ramp is then applied at a rate of 5 K/s up to a maximum of 1446 K (peak cladding temperature) held during 5s before cooling and quenching. The LOCA transient is displayed on Fig. 4.

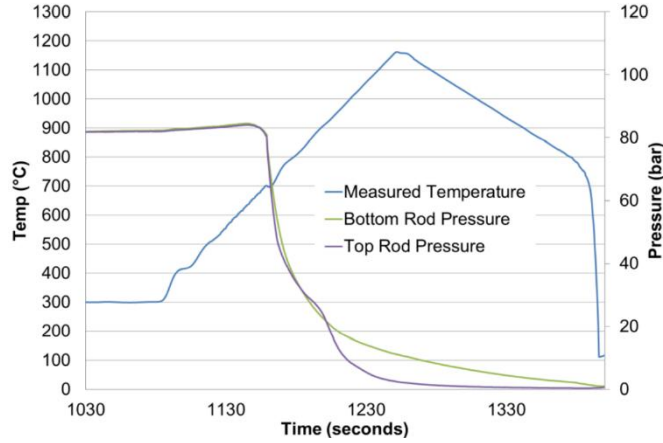


Fig. 4. Pressure and temperature evolution measured during the LOCA transient [3].

The internal pressure drop indicates a clad rupture 81 s after the start of heating, at a temperature of 981 K. The clad ballooning and rupture occurred slightly above mid-plane. The slit dimension is 9x22.7mm. About half of the fuel mass was ejected from the rod as fine fragment, 32 % of which are less than 0.125mm in size.

4.2 TRANSURANUS//MFPR-F simulations

The LOCA transient were simulated with the TRANSURANUS//MFPR-F coupling in restart mode, using the results provided by the irradiation calculation as initial state. As described in section 2, the model for FG behavior in the HBS zone allows the usage of different equations of state. Simulations have thus been performed with either Perkus-Yevik (PY) and Carnaham-Starling (CS) equations of state to assess their impact on the results. Several values of the FGR threshold over-pressure ΔP_{crit} have also been tested. Finally, a standalone TRANSURANUS calculation has been performed for reference. The simulations are summarized in Table 2.

Table 2. LOCA simulations and associated parameters of model for FG behavior in HBS.

Name	Eq. of State – FGR threshold over-pressure ΔP_{crit}
CS15	Carnaham-Starling – 150 MPa
PY15	Perkus-Yevik – 150 MPa
PY30	Perkus-Yevik – 300 MPa
TU	[Standalone Transuranus calculation]

Thermo-mechanics. The thermo-mechanical behavior of the test element is very similar between the simulations, as seen on Fig. 5 representing internal pressure and external clad temperature evolution for the different simulations. Temperatures are

indeed identical, whereas small differences are noticed, for coupled simulations, on the pressure rise before burst. The standalone TRANSURANUS simulation exhibits slightly higher pressure levels all along the transient, which can be explained by a different state at the end of the irradiation, in terms of pellet/clad deformation as well as fission gas release, resulting in a higher pressurization of the rod free volumes.

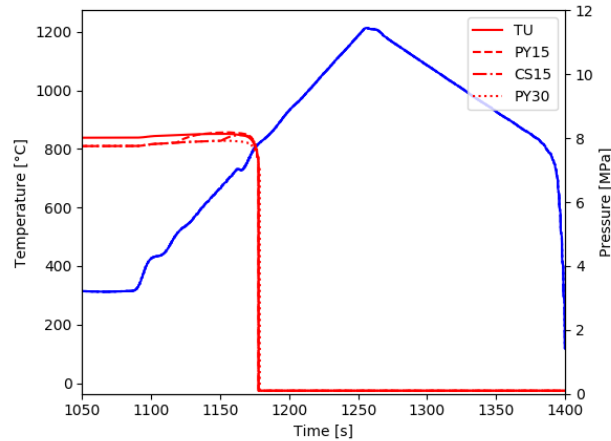


Fig. 5. Pressure [MPa, in red] and external clad temperature [°C, in blue] evolution during the simulated LOCA transients.

Table 3 presents the calculated burst times for various equations of state. The burst event is primarily influenced by the external/internal pressure difference, which is a constituent of the tangential stress, and the temperature of the cladding, which is a constituent of the burst stress of the cladding material. Under LOCA transient conditions, the rising temperature of the cladding is the main cause of burst propagation in the examined cases. Since the calculations are performed with the same cladding temperature, the variance in burst times is minimal. However, differences in the results can be attributed to the release of FG.

Table 3. Calculated burst time of the cladding.

Name	Burst time, s
CS15	1173.4827
PY15	1173.6035
PY30	1174.5000
TU	1173.7399

Fission gas release. The internal pressure rise before burst is due to FG released from fuel and over pressurizing the gas in the rod free volumes. The differences observed

in rod pressure evolution can thus be attributed to differences in the onset of FGR, represented on Fig. 6. It appears indeed that switching from CS to PY equation of state advanced the FGR onset (CS15 vs PY15 curves), whereas raising the over-pressure threshold from 150 to 300 MPa delayed it (PY15 vs PY30 curves).

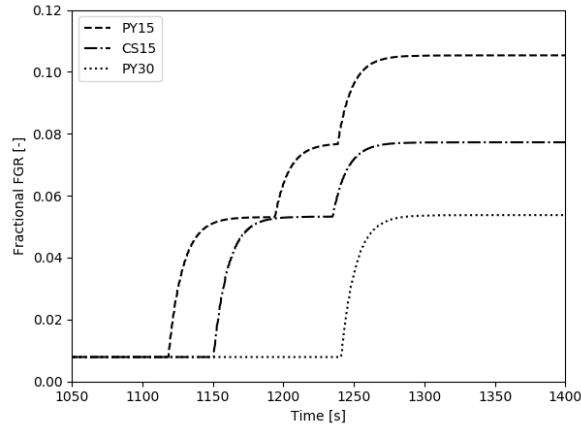


Fig. 6. Fractional fission gas release during the simulated LOCA transients.

HBS zone. A better insight in the FG behavior in the HBS zone can be obtained by comparing radial profiles of the FG repartition before and after the LOCA transient. Such repartition is represented on Fig. 7 for the different simulations, focusing on the external part of the pellet. The HBS zone extends from $R=3.7$ to 4.1 mm (blue domain). As mentioned in section 3.2, before the LOCA transient (Fig. 7a) about half of the gas in the HBS zone is localized in the intergranular domain (in the HBS pores) and may be subsequently released after the transient. It appears from Fig. 7b-d that the release occurred in the exterior part of the HBS zone only, while in the interior part the gas remains in the pores. This behavior could be expected considering that, in the current state of the model, the pore gas content is higher in the exterior part of the HBS, hence a higher build-up of pore pressure during the transient. Accordingly, the extent of the HBS region where the release occurs depend on the parameters of the release model. For example, raising the over-pressure threshold from 150 to 300 MPa (PY15 vs PY30) decreases the extent of this region, as seen from Fig. 7b) and c). Similarly, using the CS equation of state, which predicts lower pressure levels than the PY one, reduces the extent of the region, as seen from Fig. 7b) and d) (PY15 vs CS15).

a)

b)

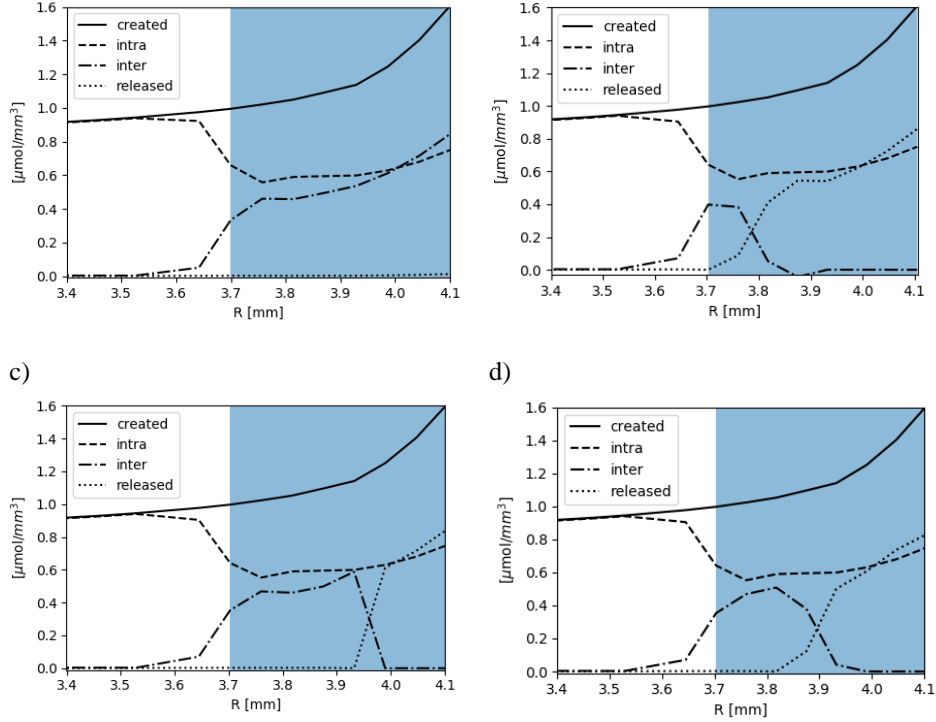


Fig. 7. Radial profiles of the fission gas repartition (see caption of

Fig. 3); a) before LOCA, b) PY15, c) PY30, d) CS15

5 Summary and conclusion

In this work, simulations of the NRC-192 Studsvik LOCA test were performed with the coupling of the fuel performance code TRANSURANUS and of the mechanistic meso-scale code MFPR-F. The coupled code was first used to simulate the irradiation of the reference rod and predicted the formation of a HBS zone 400 μm wide. Restart calculations were then performed to simulate the LOCA transient, using different set of parameters of the model for FG release from the HBS zone. All the calculations provided coherent results in terms of thermo-mechanical behavior of the rod, the evolution of central temperature and pressure in the free volume being almost identical to that obtained by a standalone TRANSURANUS calculation. Noticeable differences were observed solely in the pressure rise before burst, attributed to the fission gas release from the HBS zone, across the simulations. The FGRs were found to strongly depend on the over-pressure threshold ΔP_{crit} , and to a lesser extent on the equation of state applied in the HBS pores. This last point highlighted the importance of a precise evaluation of the pore pressure, which depends – in addition to the equation of state –

on the initial gas content and volume of the HBS pores, for which analytical models such as [14] should be applied. Regarding the over-pressure threshold for FGR, the empirical parameter currently used in the model should be replaced by a mechanical criterion accounting for the HBS zone fragmentation, which is expected to be responsible for the FG release [15].



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