



Technical Note

Analytical criteria for fuel fragmentation and burst FGR during a LOCA

G. Khvostov

Paul Scherrer Institut (PSI), Forschungsstrasse 111, 5232, Villigen, PSI, Switzerland

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ABSTRACT

Analytical criteria for the onset of fuel fragmentation and Burst Fission Gas Release in fuel rods with ballooned claddings are formulated. On that basis, the GRSW-A model integrated with a fuel behaviour code is updated. After modification, the updated code is successfully applied to simulation of the Halden LOCA test IFA-650.12. Specifically, the calculation with Burst Fission Gas Release during the test resulted in prediction of cladding failure, whereas it could not be predicted at the test planning, before new models were implemented. A good agreement of the current model with experimental data for transient Fission Gas Release in the tests IFA-650.12 and IFA-650.14 is shown, as well.

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1. Introduction

Analytical criteria for the onset of fuel fragmentation and Burst Fission Gas Release (BFGR) in fuel rods with ballooned claddings have been formulated and verified in the current paper. The research presented is deemed to be a follow-up and/or feedback to the latest publications on this topic [1–3]. Specifically, an extension of the model for BFGR during a Reactivity Initiated Accident (RIA) [3] is proposed in the current paper, aiming at analysis of similar phenomena under the conditions of a Loss-of-Coolant Accident (LOCA).

2. Outline of the GRSW-A model

The GRSW-A model was developed to simulate irradiation- and temperature-induced evolutions in the micro-structure of uranium-dioxide fuel, with a view to accounting for the related processes (fission gas release, fuel swelling and densification, thermal conductivity degradation, fragmentation and relocation, etc.) in fuel pellets of Light Water Reactor (LWR) fuel rods, as calculated by integral fuel behaviour analysis codes [4–6].

In general, the GRSW-A model provides numerical solution of a comprehensive set of rate equations, which describes several closely coupled intra-granular and inter-granular processes in the uranium-dioxide fuel under irradiation [6], viz.:

- Fission gas atom generation and migration, resulting in formation and growth of fine (nanometer sized) intra-granular bubbles and gas arrival at the grain boundaries;
- Irradiation- and temperature induced evolution of as-fabricated pores, which is associated with the processes of irradiation-induced densification and high-temperature sintering of the fuel;
- Formation and development of gaseous pores on grain boundaries, including evaluation of grain boundary fractional areas covered by closed and vented pores;
- Fission Gas Release (FGR) to the free volume of the rod due to gas atoms reaching the surfaces of as-fabricated open pores and the emergent, vented pores;
- Formation and development of High Burnup Structure (HBS), including grain subdivision, depletion of intra-granular fission gases, formation and development of HBS specific porosity and eventual release of fission gas by the HBS pores.

The GRSW-A model was implemented and verified at Paul Scherrer Institute (PSI), Switzerland, as part of a research, legacy version of a fuel behaviour code, FALCON MOD01 [7], which has been used at PSI as the platform for further model development. Specifically, the GRSW-A simulation was extended by special models [3] that are expected to have considerable effect on fuel behaviour during RIAs, viz.: (i) a model simulating the pellet-cladding bonding assisted trapping of the released fission gases during the base irradiation; (ii) a model that describes a-thermal release during fast thermal transients, such as RIA, of the fission

E-mail address: grigori.khvostov@psi.ch.

gases retained by the grain boundaries and trapped by bonding after the base irradiation; (iii) a model for specific features of intra-granular gas behaviour, such as inhibited bubble coalescence and enhanced intra-granular gas release to the grain boundaries during fast thermal transients.

In 2012, Electric Power Research Institute (EPRI) released the first version of a so-called redesigned version of the code, FALCON V1 [8] with the source code being updated to FORTRAN 95 and providing a graphical user interface for input and post-processing based on the Hierarchical Data Format (HDF). The current version of the code is FALCON V1.4, which has included the GRSW-A model.

As far as the BFGR is concerned, the model for numerical simulation of this phenomenon during RIAs [3] associates the onset of burst release with the grain boundary fracture due to increase of the de-cohesive stress, normal to a grain face plane, caused by drastic increase of gas pressure in the gaseous pores, so that:

$$R_F \equiv \frac{\sigma_d}{\sigma_{B,gb}} \geq [R_F]_{RIA} = 1.0 \quad (1)$$

where σ_d is the de-cohesive stress due to pore overpressure, normal to a grain face plane, $\sigma_{B,gb}$ the grain boundary fracture strength assumed for the fuel material.

3. Problem statement

The updated GRSW-A is to explain explicit and implicit data on BFGR during the LOCA, viz.: the fact of a rod failing during the Halden LOCA test IFA-650.12, presumably due to unexpected, high level of Rod Internal Pressure (RIP) that was linked with a possible significant BFGR during the test [10,11]. The hypothesis about significant BFGR during test IFA-650.12 was further confirmed by a successful 'non-burst' LOCA test, IFA-650.14, which resulted in cladding being considerably ballooned, but not burst. The main outcome of this experiment was a credible measurement of FGR, which amounted to $\approx 19\%$ of the total gas generation in the tested sample [10].

The first approach with the above-outlined model for BFGR during a RIA to conditions of LOCA failed to explain important experimental data. Indeed, LOCA transients are much slower, and usually result in significantly lower fuel temperature, than RIA transients do. As a result, the grain boundary fracture ratio, R_F , as calculated with Eq. (1), cannot surpass the earlier established, RIA specific threshold. On the other hand, reduction of the threshold in question would interfere with an adequate prediction of absent BFGR in some RIA tests from the model Verification and Validation matrix [3]. This reveals necessity to extend the model by adding analytical criteria discriminating transients with Pellet Cladding Mechanical Interaction (PCMI) (e.g., RIA) and non-PCMI transients (e.g., LOCA).

In addition, it would be highly preferable if an updated model allowed for evaluation of relevant parameters of fuel state, such as those of fuel fragmentation, as used in modelling of fuel relocation and dispersal during the LOCA [12].

4. Model description

First, a fuel element of interest is divided into idealized equivalent spheres of a radius a_{frag} , with a specific surface area being equal to the specific area of grain-boundary surfaces covered by the vented pores, as calculated by the GRSW-A model [4,6]:

$$4\pi a_{frag}^2 \times \frac{3}{4\pi a_{frag}^3} = \frac{3}{a_{frag}} = 14f_{vn} \left(\pi R_{gF}^2 \right) \times \frac{3}{4\pi R_g^3} \quad (2)$$

where a_{frag} is the radius of equivalent spheres, f_{vn} the grain boundary fractional area (unit less) covered by vented pores, R_{gF} the radius of grain faces, and R_g the grain radius.

Noting that in GRSW-A the grain face radius R_{gF} is linked to the radius of grains as [6].

$$R_{gF} = 0.5558 R_g, \quad (3)$$

an equation for the radius of equivalent spheres is:

$$a_{frag} = 0.9249 \frac{R_g}{f_{vn}} \quad (4)$$

Let us assume that the surfaces of vented pores form a system of loosely coupled domains of the fuel matching the equivalent spheres just mentioned, such that after fragmentation the fuel would be broken into these domains. The above introduced radius a_{frag} is therefore to be interpreted as the averaged radius of the fuel fragments after fragmentation, if any.

A simple geometrical consideration is used to formulate a condition for fuel fragmentation, based on comparison of the mean biased-radial and random displacements of the fragments as they follow radial distension of the cladding due to pellet-cladding bonding:

$$\delta_{ran}(r) \leq \delta_{bias}(r) \quad (5)$$

where r is the initial radial coordinate of the pellet node considered.

Eq. (5) is an analytical criterion that compares two idealized, limiting values, referred to as random- and biased-displacement, δ_{ran} and δ_{bias} , respectively, to evaluate which trend would be more preferential (energetically 'beneficial') – fuel fragmentation or being intact, as schematically shown in Fig. 1.

a_{frag} is the fragment radius; R_0 is the initial pellet radius; ΔG is the increase in a 'mechanical' pellet-cladding gap size; δ_{bias} is the biased radial displacement; δ_{ran} is the random displacement; k_b is the parameter of pellet-cladding bonding.

The random displacement of the fragment, δ_{ran} is defined as an increase in the averaged half-distance between the fragments after their uniform redistribution over the volume under the ballooned cladding:

$$\delta_{ran} = a_{frag} \frac{\Delta G}{R_0} \quad (6)$$

where ΔG is the absolute increase in a 'mechanical' pellet-cladding gap size during the transient of interest, R_0 the initial pellet radius.

The biased radial displacement of the fragments, δ_{bias} is being introduced through an idealized, simplified assumption that a bonding-degree dependent fraction of the fragments will follow the deforming cladding together. Expressing a radial displacement field that would be expected in a solid cylinder with a uniform radial strain yields:

$$\delta_{bias} = r \frac{k_B \Delta G}{R_0} \quad (7)$$

where k_B is the degree of pellet-cladding bonding as introduced in the GRSW-A model [3].

Substitution of Eq. (6) and Eq. (7) into Eq. (5) yields the following analytical condition for local fragmentation:

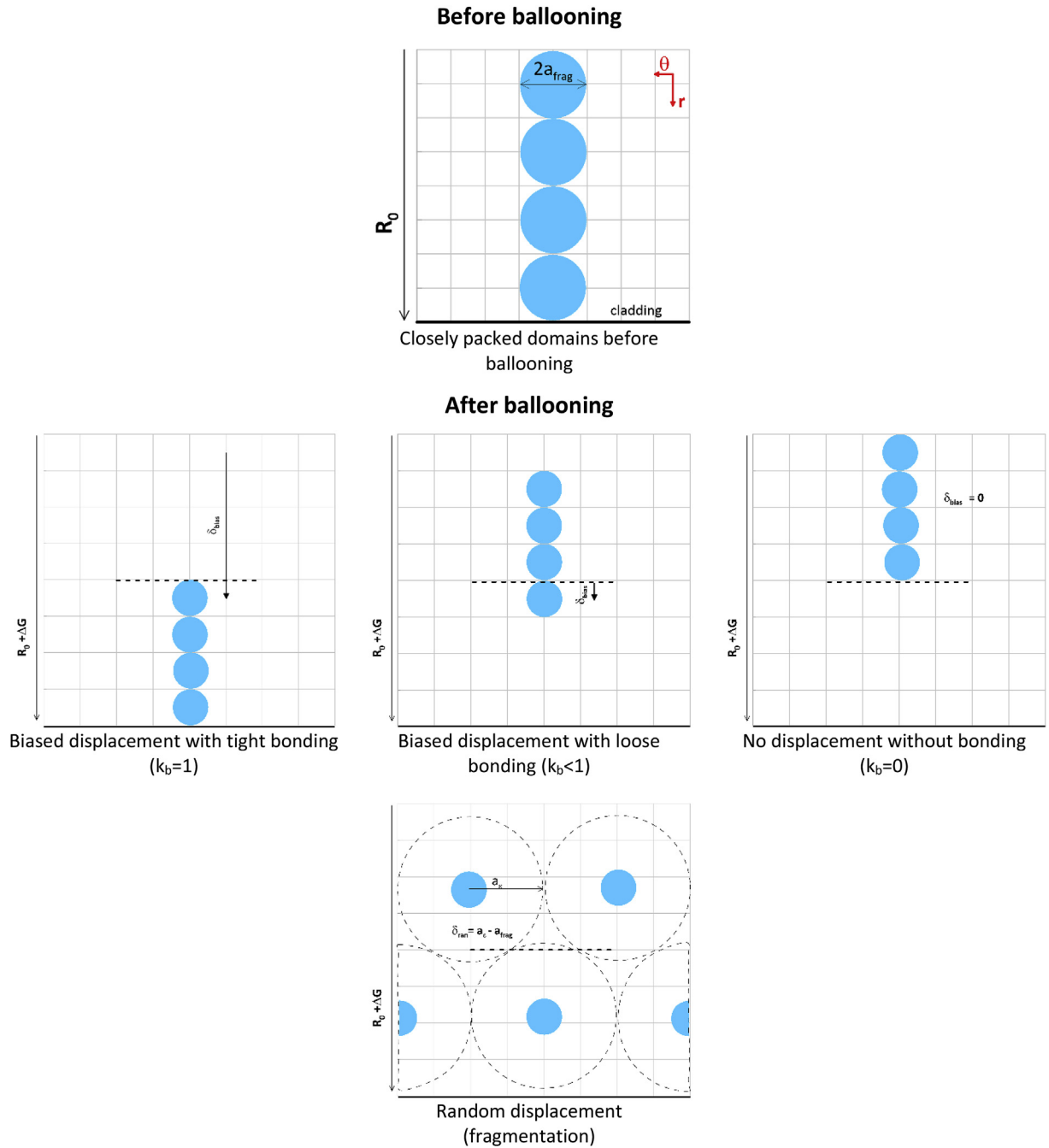


Fig. 1. Model schematics for bonding assisted fragment displacement in a fuel element under the ballooned cladding.

$$a_{frag} \leq k_B r \tag{8}$$

Additionally, it is proposed that the following two conditions relate to a non-PCMI transient, with the RIP driven increase of the pellet-cladding gap in the absence of pellet-cladding contact pressure:

$$P_{con} = 0; \tag{9}$$

$$\frac{k_B \Delta G}{R_0} > 0; \tag{10}$$

where P_{con} is the pellet-cladding contact pressure.

There are a few features in the proposed conditions for local fuel fragmentation to be mentioned here. The most non-trivial one is that the condition of Eq. (8) is independent on a degree of cladding distension, although some positive cladding strain is explicitly required through the conditions of Eq. (9) and Eq. (10). Experimental investigations [9,10] have revealed that axial relocation of fuel fragments during a LOCA requires that a certain threshold of cladding deformation is exceeded. This may suggest that relocation makes the fragmentation more discoverable for Post-Irradiation Examination (PIE).

The conditions of Eq. (10) and Eq. (8) imply some pellet-cladding bonding to occur. In general, the clad ballooning is assumed in the current model to be an important driving force for predicated

fragmentation, as shown in Fig. 1 and depicted in Fig. 2. The RIP driven deformation of the cladding (e.g., ballooning) is converted into the fuel displacement with a degree, which depends on the degree of bonding. This suggests that fragmentation is expected only after irradiation with a pellet-cladding mechanical contact, which is possible in rods with a pellet-averaged burnup higher than ~ 40 MWd/kgU.

The pellet periphery is expected to be more susceptible to fragmentation than the center, for purely geometrical considerations, as seen from the condition of Eq. (8). Besides, the smaller value of a_{frag} and, therefore, a higher susceptibility to fragmentation is correlated by Eq. (4) with higher surface area of the emergent vented pores, which is usually predicted by the GRSW-A model for the High Burnup Structure at the pellet periphery and, eventually, in the pellet center if the fuel has undergone irradiation with elevated Linear Heat Generation Rate (LHGR) and temperature.

The above conditions are being proposed as the criteria for fuel fragmentation, which is deemed to be a prerequisite for the onset of BFGR during a LOCA. The criterion for BFGR *per se* remains to be the surpassing of a postulated critical threshold by the grain boundary fracture ratio [3], which is set to a reduced, LOCA specific value, $[R_F]_{LOCA}$:

$$R_F \geq [R_F]_{LOCA} \approx 0.35 \quad (11)$$

The proposed value for a critical fracture stress ratio under conditions of LOCA, $[R_F]_{LOCA}$, is based on model calibration, which is discussed in the next section. Qualitatively, the reduction of the threshold value in question is due to the mutual effect of grain-boundary pore overpressure and additional mechanical impact of clad ballooning on the pellets in the presence of pellet-cladding bonding. If the conditions of Eq. (8), Eq. (9) and Eq. (10) are not fulfilled, the unchanged condition of Eq. (1) is being used as the criterion for predicting the on-set of BFGR.

Similar to the model for BFGR during a RIA [3], the current simulation assumes that the bonding induced gaseous ‘pockets’ are being opened upon a BFGR is predicted with the above relationship in the outermost node of the pellet, with immediate release of the fission gas trapped in these pockets after the base irradiation.

5. Model calibration and verification

The above-described analytical criteria for predicting fuel fragmentation and BFGR under LOCA conditions were implemented in the GRSW-A model integrated into the FALCON fuel behaviour code [6]. After modification, the updated code has been verified using, as

the main experimental basis, available data of the Halden LOCA testing program [10].

First, evaluation of the radial zones in a base-irradiated pellet, susceptible to fragmentation and burst FGR under conditions of a hypothesized LOCA was done for the two test cases with high-burnup fuel samples from the GRSW-A Verification and Validation matrix:

- The CIP0-1 RIA test using a rodlet refabricated from the rod pre-irradiated in a PWR to high burn-up [3], noting that base irradiation during the last fuel cycle was characterized by a relatively high linear power density;
- The Halden LOCA test IFA-650.12 using a fuel sample base irradiated in the BWR Leibstadt to high burnup at a relatively low linear power density [10,11].

The fuel fragment sizes after base irradiation, as calculated with Eq. (4), are shown in Fig. 3 against the fragmentation threshold as defined by the condition of Eq. (8). The pellet zones that can contribute to BFGR, once the condition of Eq. (11) is fulfilled, are shown in pink in Fig. 3. The quantities of grain boundary gas contributing to BFGR from the affected zones in question can be evaluated from the GRSW-A calculated grain-boundary gas retention, as shown in Fig. 4.

The results of Fig. 3 underline the difference between fragmentation and BFGR related conditions at the End-of-Life (EOL) in rods with high- and low-power at the end of base irradiation, in agreement with the summary for appropriate experimental data, as provided in Chapter 3 of Ref. [13]. The high-power irradiated pellets in CIP0-1 show extensive zones of fragmentation, both in the center and the periphery. A potential fragmentation into the small particles with sizes less than $200 \mu\text{m}$ is predicted, which is commonly referred to as fuel pulverization [14]. Here, significant BFGR from the pores of the High Burnup Structure (HBS) and grain boundary pores in the central pellet zone during LOCA is expected. In the very center of the pellet, the calculation points out to reduced susceptibility to fragmentation and BFGR due to high-temperature induced vanishing of the grain-boundary pores.

In the case of low-power irradiated rod used in IFA-650.12, pulverization and BFGR is shown to be possible in a wide zone at the pellet periphery only. However, the fuel sample in question was base irradiated in a BWR, where a specific bonding induced trapping of the released fission gas is expected [3]. The trapped gas just mentioned will be eventually released during the LOCA, additionally to BFGR of the gas retained by grain boundary pores.

According to Eq. (11), an empirical, LOCA specific threshold of

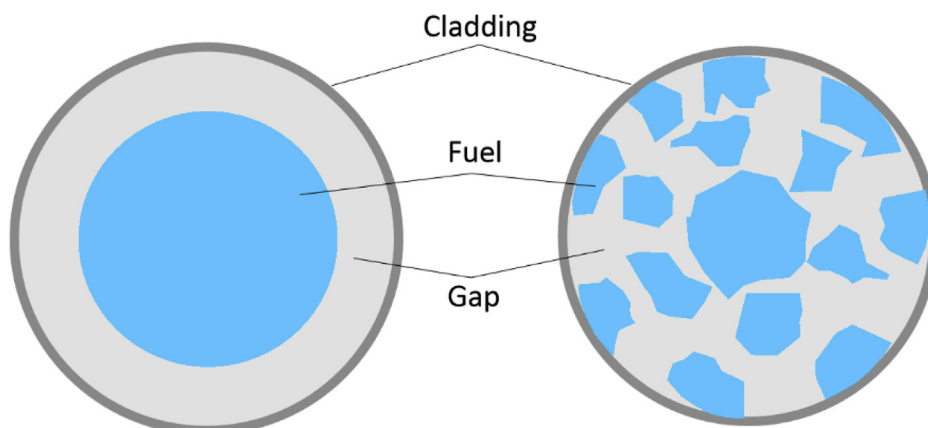


Fig. 2. Model schematics for forced fuel fragmentation in a ballooned cross section of the rod without (left) and with (right) pellet-cladding bonding.

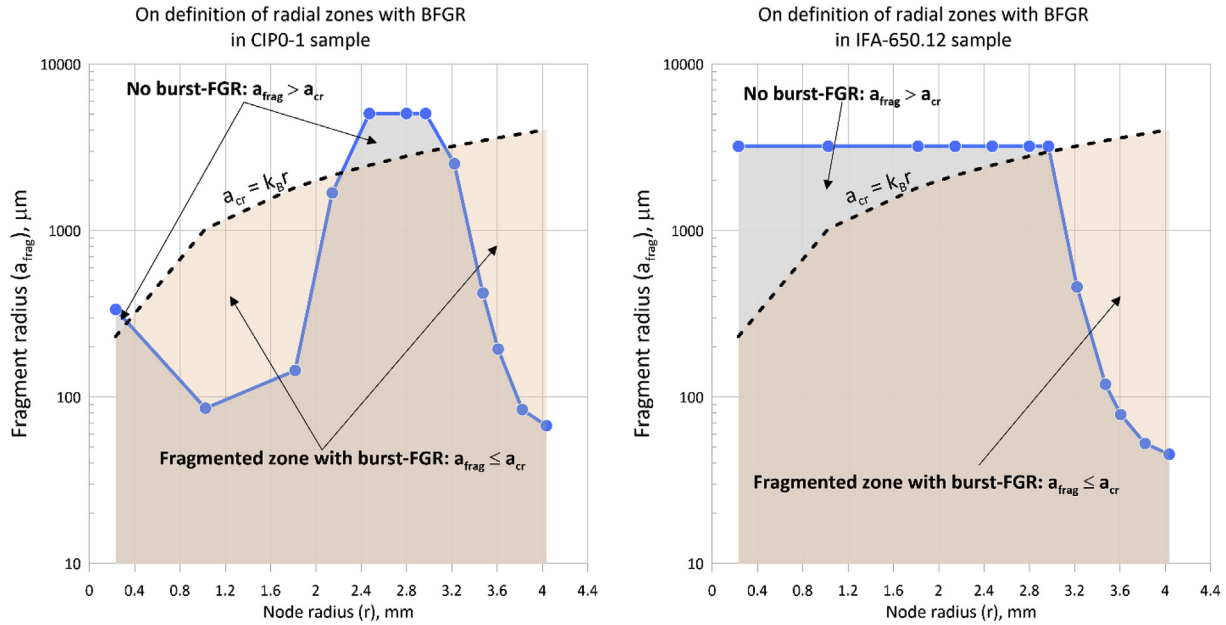


Fig. 3. Results of calculation for parameters of fuel structure after base irradiation related to the model of fragmentation and BFGR in fuel samples used in CIP-01 (left) and IFA-650.12 (right) experiments.

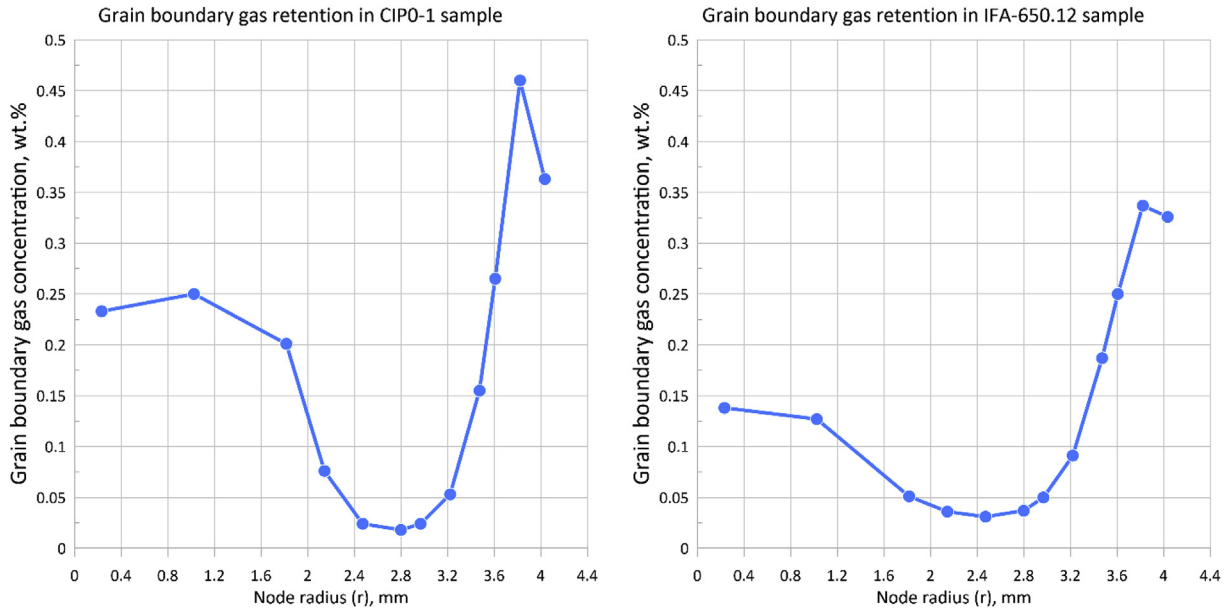


Fig. 4. Calculated initial radial distribution of the grain-boundary retained fission gas in CIP-01 (left) and IFA-650.12 (right) samples.

the grain boundary fracture ratio for the onset of BFGR from fragmented fuel amounts to ca. 35% of the threshold during PCMI (e.g. under RIA conditions) [3]. This value was established based on comparison of the results of calculation and experimental data [10] for the Halden LOCA test IFA-650.12. Specifically, the selected threshold value corresponds to the calculated grain boundary fracture ratio, as shown in Fig. 5, at a cladding temperature for which the onset of BFGR was detected from the measured RIP.

The onset of BFGR coincides with the bending point in the calculated fracture stress ratio in the fragmented zone of the pellet (the pellet periphery) in Fig. 5. After reaching the LOCA-specific threshold (0.345) for the grain boundary fracture ratio, the gas

pressure in the opened pores starts decreasing due to gas loss.

In the unfragmented zones of the pellets, e.g. in the pellet center, as shown in Fig. 5, the fracture ratio increases throughout the simulated period of the test. The rate of the increase is controlled by the mutual effect of the fuel temperature and the external pressure (i.e., RIP). Specifically, the temperature induced increase in calculated ratio levels off after the increase in RIP due to transient FGR (Fig. 6 – left), and is accelerated during further fast decrease in RIP due to clad-ballooning and burst (Fig. 7 – left). However, the grain boundaries in the unfragmented zones of the pellets remain sub-critical, meaning that the predicted fracture stress ratio does not reach the corresponding threshold, which is set to unity for non-

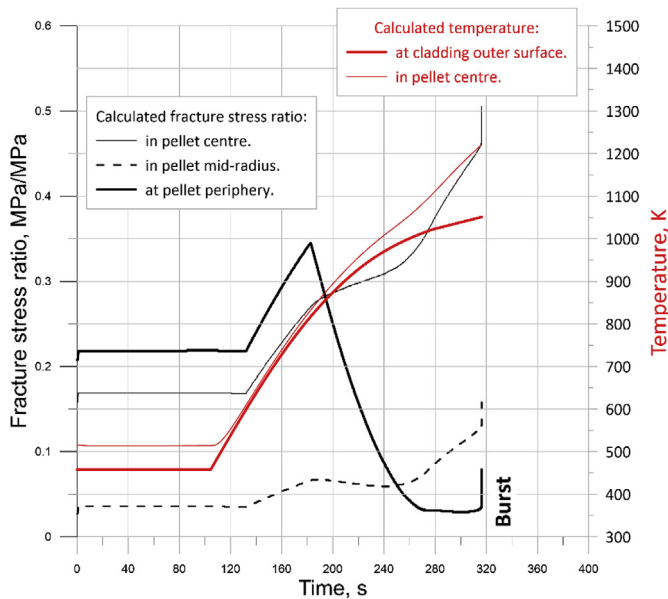


Fig. 5. Calculated grain boundary fracture ratio at fuel stack mid-height against fuel and cladding temperature during Halden LOCA test IFA-650.12.

fragmented fuels [3].

Integral calculation of the LOCA test IFA-650.12 using the GRSW-A model with updated analytical criteria for BFGR predicts discernible FGR (13.8% in the moment of cladding burst) during the test (Fig. 6 – left), which compares well with a value estimated in Ref. [11] on the basis of measured RIP (13.3%). The model assumes a certain time lag between the moment of grain boundary fracture and fission gas reaching the free volume of the rod, which is controlled by time constants [3], τ_1 and τ_2 , for the gas in grain-boundary pores and bonding assisted traps (pockets), respectively. In this specific calculation, both parameters just mentioned were set to 50 s. The selected value for the time constants in the equations for the kinetics of BFGR during LOCA seems to result in a reasonable agreement of the calculation with the experimental data for the dynamics of RIP increase after the onset of release (see

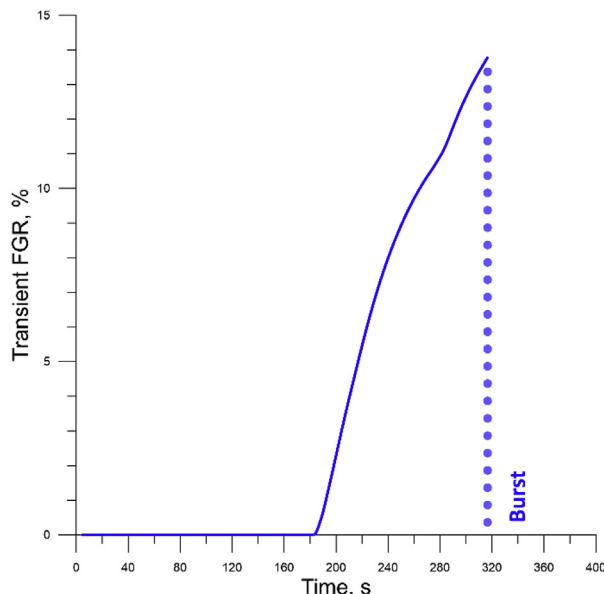


Fig. 7 – left), as well as with the estimated BFGR in the moment of cladding failure.

The time constants used for FGR are different from those used in Ref. [3]. The difference is about two orders of magnitude; 50 s instead of 0.1 and 1.0 s used in Ref. [3]. On the other hand, the data used in calculation of [3] was limited to FGR after the RIA tests, as measured by puncturing. An on-line measurement for RIP in tested rodlets was not conducted. Consequently, a similar calibration for the time parameters in question was not possible. Because the power pulses analyzed in Ref. [3] were very short (a few-millisecond wide), the assumed time parameters could not considerably affect predicted BFGR already in ca. 100 s after the simulated pulses, let alone days pasting till puncturing. Recalculation of the RIA tests from the code Verification and Validation matrix has shown that the current modification in time constants has not affected the conclusions drawn in Ref. [3].

Due to the time lag, just mentioned, not all the fission gases retained by grain boundary and traps could be released by the moment of cladding burst, as shown e.g. in Fig. 6 (right). Should more time be available, e.g. in the case of cladding not being failed until the end of the experiment, the amount of fission gas released would be a few percent higher. This result, qualitatively, agrees with the measured FGR ($\approx 19\%$) in a successful non-burst Halden LOCA test, IFA-650.14, which was carried out using a similar fuel sample and similar design of the experiment [10]. The relevant results of calculation with the current model for the IFA-650.14 test are presented in Fig. 8, showing good agreement with the experimental data for BFGR in the test in question. Besides, the relatively low value predicted for Cumulative Damage Index (CDI), which is used as an analytical measure of cladding damage [11], is consistent with the cladding not being failed during this experiment.

After implementation of the new model, simulation of Halden LOCA test IFA-650.12 has been a success, as well. As shown in Fig. 7, the calculation with BFGR during the test has resulted in prediction of cladding failure (cladding burst), whereas it could not be predicted when the test was planned [11] before an appropriate model was implemented. Indications of the predicted cladding burst in Fig. 7 are the instantaneous drop of RIP to the level of external coolant pressure (0.2 MPa), and the fast increase in CDI, reaching the postulated threshold for cladding burst [11].

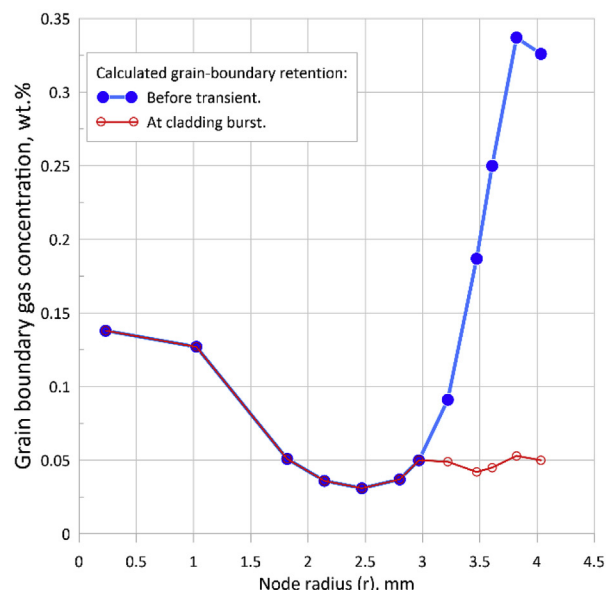


Fig. 6. Calculated BFGR (left) during Halden LOCA test IFA-650.12 against grain-boundary gas retention before the test and in the moment of cladding burst (right).

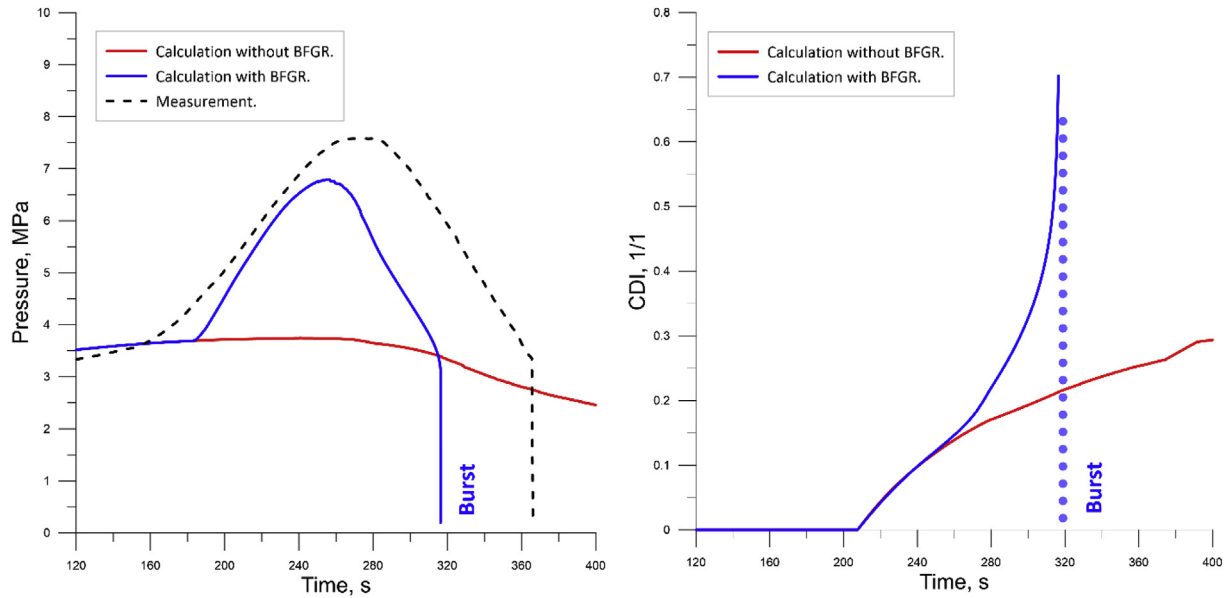


Fig. 7. Calculated RIP (left) and cumulative damage index (right) during the cladding heat-up phase of Halden LOCA test IFA-650.12. The measured values for peak RIP and RIP in the moment of burst are 7.6 MPa and 3.5 MPa, respectively [10,11].

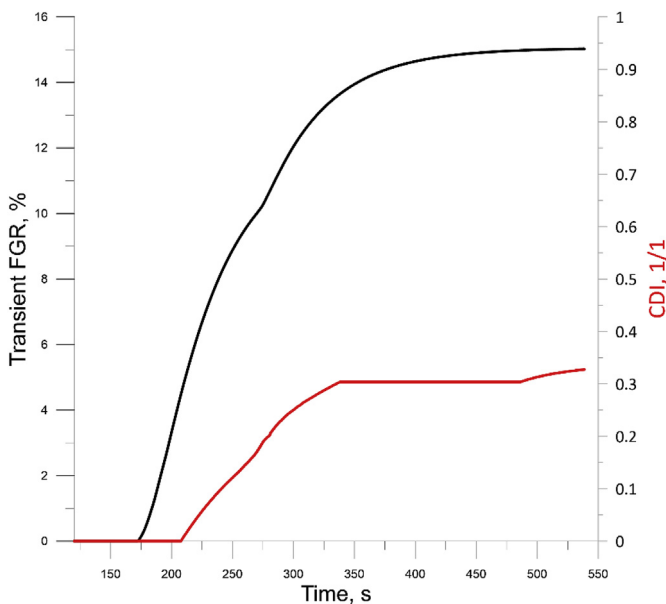


Fig. 8. Calculated BFGR (black) and cumulative damage index (red) during the cladding heat-up phase of Halden LOCA test IFA-650.14. The measured FGR was 15.9% just after puncturing and stabilized at 18.6% in ca. 3 min. after puncturing [10]. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article).

6. Conclusions and outlook

The current paper presents the results of an activity on 'Model Development and Verification for Fission Gas Release (FGR) from the LWR High-Burnup Fuel during a LOCA', which has been carried out at Paul Scherrer Institute (PSI). Analytical criteria for the onset of fuel fragmentation and Burst Fission Gas Release (BFGR) in fuel rods with ballooned claddings are formulated and verified. On that basis, the GRSW-A model integrated with a fuel behaviour code is updated.

Susceptibility of fuel pellet zones to fragmentation and,

eventually, pulverization is correlated with an increased specific surface area of the emergent vented pores, as calculated by the GRSW-A model. Fuel fragmentation is considered as a prerequisite for the onset of BFGR under LOCA conditions. The criterion for BFGR remains to be the surpassing of a postulated critical threshold by the grain boundary fracture ratio. The proposed analytical criteria can be used in safety analysis of LWR fuel behaviour during LOCA.

After implementation of the new model, simulation of the Halden LOCA test IFA-650.12 has been a success. Specifically, the calculation with BFGR during the test has resulted in prediction of cladding failure (cladding burst), whereas it could not be predicted when the test was planned, i.e. before an appropriate model was implemented. A good agreement of the current model with the data for BFGR in the tests IFA-650.12 and IFA-650.14 has been shown, as well.

In the future, the updated GRSW-A model and fuel behaviour code will be coupled with a new version of the FRELAX code [15], which takes into consideration the effects of axial bulk-flow and diffusion of the gas into the rod free volume during the clad-ballooning phase of LOCA transients. The updated codes will be employed for integral LOCA analysis. Additional calculations are being planned for the cases from the FRELAX verification matrix dealing with full-length rod behaviour under postulated LOCA conditions.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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