

# ANALYSIS OF FRAPCON-4.0's UNCERTAINTIES PREDICTING PCMI DURING POWER RAMPS

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## ABSTRACT

Fuel safety criteria require keeping the integrity of the cladding as the first barrier to confine the fission products. The Pellet-Cladding Mechanical Interaction (PCMI) is a failure-preceding mechanism under operational conditions (driver of Pellet Cladding Interaction, PCI) and, as a consequence, a relevant aspect when the fuel rod thermo-mechanical performance is modelled. Given the current trend towards more flexible modes of operation, PCMI studies are getting focused on operational power ramps.

This study assesses FRAPCON-4.0's uncertainties predicting PCMI under power ramps. Two Halden tests performed on fresh and high burnup fuel have been analysed in terms of cladding elongation. An error less than 20% has been obtained at the end of ramp for fresh fuel, which is within the in-code models' uncertainty band. At high burnup, though, an important deviation has been obtained (overestimation of 50%), which cannot be fully explained by the uncertainty from models and power, unless the uncertainty from the rigid pellet approach would be accounted for. Indeed, the modelling of fuel creep notably improves the accuracy.

## 1. Introduction

The primary safety goal in reactor operation is to prevent the release of radioactive material to the environment. In fact, fuel safety criteria require keeping the integrity of the cladding as the first barrier to confine the fission products. The Pellet-Cladding Mechanical Interaction (PCMI) is related to failure mechanisms which prevention is relevant to the nuclear industry (e.g., Pellet-Cladding Interaction, PCI). Given that the conditions resulting from power ramps foster PCMI, they are the main focus of research, especially due to current trend towards more flexible modes of operation.

The cladding mechanical state (i.e., stress, strain) resulting from PCMI is applied as limiting criterion for reactor operation [1]. Given the key role of fuel performance codes to assure that safety criteria are met, the corresponding modelling has to be soundly checked. In this regard, the PCMI modelling is submitted to continuous evaluation, with the aim of providing accurate predictions of fuel rod mechanical performance.

In 2004, a review of PCI studies was carried out [2]; one of the main conclusions was that despite considerable enhancements of the PCMI modelling had been accomplished, further improvements were required. Since then, a better characterization of the stress due to pellet-cladding interfacial contact has been achieved by accounting for pellet deformation mechanisms like gaseous swelling or fuel creep [3,4,5,6,7,8]. However, the complexity of modelling the coupled behavior of fuel rods introduces the possibility of compounding feedback effects which result in widely varying predictions from various codes for identical cases; this was shown in the benchmark performed under the frame of the SCIP project [9]. Thus, the evaluation of fuel performance codes to predict PCMI is still an issue, especially, given the above mentioned trend to increase power flexibility.

The fuel performance code FRAPCON-4.0 [10] is designed to perform steady state calculations (applied to typical situations of normal operation, including slow power ramps) with the capabilities of fast-running 1.5-D codes. It is based on some assumptions and approximations that imply uncertainty sources; particularly, the one concerning the so-called rigid pellet model (i.e., stress-induced deformation of fuel is neglected) may affect the prediction of PCMI under power ramps [5]. Furthermore, in-code models have a bias that could be other source of uncertainty [11]. Thus, the analysis of the impact that these uncertainties may have on the PCMI prediction under power ramps would allow a more comprehensive evaluation of the code.

The present work is focused on the assessment of FRAPCON-4.0 deviations predicting PCMI under power ramps. It is framed within the OECD/NEA PCMI benchmark [12]. Two ramps from IFA-118 (fresh fuel) and IFA-629.4 (high burnup fuel) Halden tests have been simulated. An uncertainty quantification has been performed by coupling FRAPCON-4.0 with DAKOTA. To do so, it has been accounted for uncertainty sources from in-code models (concerning fuel thermal conductivity, thermal expansion, swelling and relocation recovery, cladding creep, corrosion and irradiation axial growth) and power. The uncertainty related to the rigid pellet model has been also analysed based on the implementation of a fuel creep model.

## 2. Scenarios

### 2.1. Fresh fuel

This case corresponds to the Halden Reactor Project (HRP) IFA-118 experiment, performed in the Halden Boiling Water Reactor (HBWR) [13]. In this experiment, different designs of rodlets clad with Zry-2 were submitted to beginning of life (BOL) ramping. The design of the rodlet considered in this work is the closest to current designs (i.e., dished and chamfered pellets); the corresponding parameters are shown in [13].

Although the whole test irradiation is composed by a number of ramps, this work has focused the analysis on the first ramp, in which an increase rate close to 3 (kW/m)/h is applied, from zero power to a maximum value of 53.4 kW/m. The average linear power,  $q'$ , during the ramp and the axial power profile applied are represented in Figure 1.

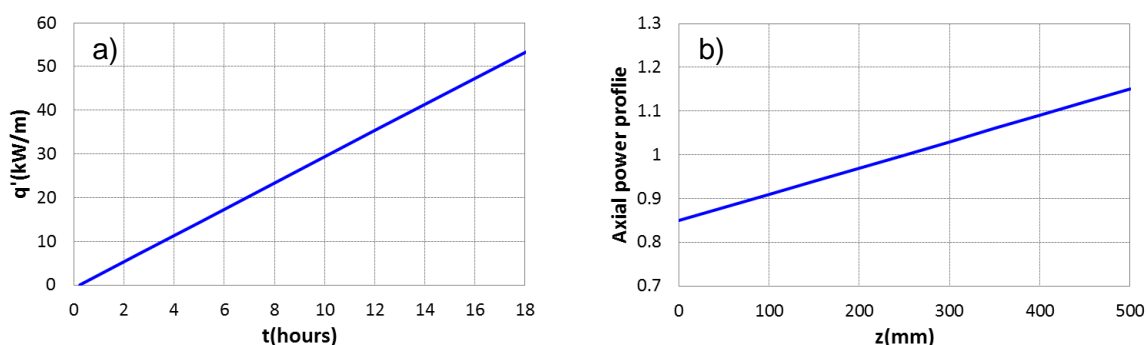


Figure 1. Power ramp (a) and axial power profile (b) in fresh fuel case.

### 2.2. High burnup fuel

The ramp studied in this case corresponds to an end-of-life (EOL) ramping in the HRP IFA-629.4 experiment (performed in the HBWR) of a PWR rodlet clad with Zry-4 (re-fabricated segment of a base irradiated commercial rod). The details about irradiation and fuel design are shown elsewhere [14,15]. A burnup around 60 GWd/tU has been estimated.

Figure 2 represents the power evolution of the ramp analysed in this study; a variable power increase rate was applied with maximum values up to 10 (kW/m)/h. The power axial profile has been considered uniform. Note that fuel rod temperatures were measured with thermocouples at the top of the fuel stack; the penetration extended to 4 pellets, approximately, and the inner diameter of the drilled pellets was 2.5 mm. This has been taken into account in the simulation.

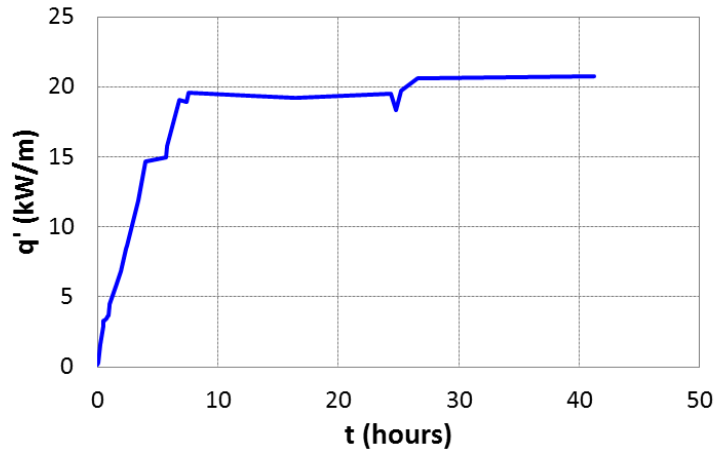


Figure. 2. Power ramp in high burnup fuel case (initial time subtracted).

### 3. Methodology

#### 3.1. Best estimate

The scenarios described above have been simulated with FRAPCON-4.0. It is the NRC steady-state fuel performance code, developed by PNNL to be applied to in-reactor operational conditions [10]. The code architecture is based on the coupling of the thermal, mechanical and fission gas release (FGR) modules; the two latter can be modelled through different options. The models chosen in this study are the ones recommended by the code developers: FRACAS-I and Massih for the mechanical and FGR modules, respectively.

The code recommended values for the minimum time step and the maximum linear power increment/decrement are 0.1 days and 5 kW/m, respectively; that is to say, a maximum ramp rate around 2 (kW/m)/h. Even though slower than the experimental ramp rates to be addressed, it is rather close to the one of the fresh fuel test and in the same order of magnitude of the high burnup one.

The fuel deformation modelling with FRACAS-I is characterised by:

- Thermal expansion, swelling (due to solid and gaseous fission products), densification and radial relocation (related to cracking) as contributions to the strain.
- No stress-induced deformation of fuel (rigid pellet model). Particularly, creep is not modelled.
- Isotropic mechanical properties.
- Axi-symmetric strains.
- No ridge effect (i.e., hourglassing of the pellets).

Concerning cladding deformation, the main features are:

- Thermal expansion, elasticity, plasticity (creep) and irradiation axial growth as contributions to the strain.
- Internal stress determined from internal pressure and fuel contact (if gap is closed), accounting for stress relaxation.
- Stress and strain are uniform throughout clad thickness (thin shell approach).

- No fuel-cladding slippage if gap is closed (cladding elongation estimated from fuel elongation, which is used in the stress calculation).
- Axi-symmetric strains.

It is worth noting that when the gap is closed, the hard contact (i.e., PCMI) is simulated once the fuel radial relocation modelled is 50% recovered. This relocation recovery accounts for fuel inwards deformation due to cracks. However, fuel inwards strain within other significant voids, particularly pellet dishes [16], is not considered according to the approximation of the rigid pellet model. This may affect not only the cladding mechanical performance during PCMI but also the PCMI onset, which in turns affects the cladding deformation (i.e., the longer the PCMI duration, the greater the deformation).

### 3.2. Uncertainty sources

The uncertainty sources taken into account in this study are classified in three categories:

- Boundary conditions. Focused on the power of the experiments simulated; although the power uncertainty was not reported in the corresponding experimental descriptions [13,14,15], an uncertainty of  $\pm 5\%$  has been taken into account based on data from other experiments carried out in the HBWR [17]. The probability distribution applied has been uniform.
- In-code models (details shown in section 3.2.1).
- Approximations. Focused on the rigid pellet model (details shown in section 3.2.2). Note that the architecture of FRACAS-I makes it difficult to address approximations like the ones concerning fuel-cladding slippage or ridge effect.

#### 3.2.1. In-code models

FRAPCON-4.0 gives the option to bias the models used for fuel thermal conductivity, thermal expansion, swelling (related to solid fission products), FGR, cladding creep, irradiation axial growth, corrosion and hydrogen pick up. Except the latter, the rest of the models may affect the PCMI prediction according to the code modelling.

The models uncertainty is expressed through the standard deviation obtained from the supporting database of each model. Table 1 shows the standard deviation of the models taken into account in this study. The corresponding bounds have been set according to the 95% confidence level, assuming normal probability distribution functions.

Furthermore, the percentage of relocation recovery can be changed through the input deck, so it has been included as an additional uncertainty. Particularly, uniform distribution is considered within the range 0-100%.

Table 1. Standard deviation of models [10].

Model	Standard deviation
Fuel thermal conductivity	0.088
Fuel thermal expansion	0.103
Fission gas release	1
Fuel swelling	0.114
Cladding creep	0.145
Cladding irradiation axial growth	0.223
Cladding corrosion	0.4

### 3.2.2. Rigid pellet model

The uncertainty related to the rigid pellet model has been analysed through the in-code implementation of a fuel creep model (i.e., additional contribution to fuel inwards deformation, added to the fuel pellet size calculation along with the other pellet deformation mechanisms). To do so, the MATPRO's fuel creep law [18] has been used. Given the scarce effect of fuel thermal creep under operational conditions [16], only irradiation fuel creep has been considered in this study; the irradiation creep rate is expressed as:

$$\dot{\epsilon}_{irr} = 3.72 \cdot 10^{-35} \cdot \sigma \cdot \phi \cdot \exp\left(\frac{314.72}{T}\right) \quad (1)$$

where  $\sigma$  is the stress (Pa),  $\phi$  is the fast neutron flux ( $n/m^2/s$ ) and  $T$  the fuel temperature (K).

Given that the fuel creep effect related to cracks can be taken into account through the relocation recovery, the creep modelling has been focused on the dishes (main contribution to fuel internal void). According to this, the fuel can creep into this volume and then other deformation mechanisms such as thermal expansion will cause a smaller increase in the pellet size.

The main stress when PCMI occurs has been considered in the hoop direction,  $\theta$ , due to the compressive effect related to the cladding resistance azimuthally. In order to simplify the stress calculation, the dishes have been assumed as formed by cylindrical volumes (i.e., pile of cylinders centered in the axial axis of the dish), in a way that the lower the dish height, the greater the corresponding cylinder radius, and the higher the hoop stress at this level (i.e., thinner pellet thickness). In the creep calculation an average stress is applied (10 levels chosen by default). Note that low sensitivity of PCMI to the number of levels has been checked.

The hoop stress calculation is given by (thick wall approximation):

$$\sigma_{\theta} = \frac{P_{PCMI} \cdot r_p - P_i \cdot r_c}{r_p - r_c} \quad (2)$$

where  $P_{PCMI}$  is the pellet-cladding interfacial pressure,  $r_p$  is the pellet radius,  $P_i$  is the gas internal pressure and  $r_c$  is the radius of the cylinder considered. Note that  $P_{PCMI}$ ,  $r_p$  and  $P_i$  are provided by the code along the irradiation period. Regarding the thermal term of equation 1, the temperature used has been the average given by the code (the effect on irradiation creep of the radial gradient of the pellet temperature has been checked, showing scarce impact). Based on this modelling, the fuel creep calculated would directly impact on the PCMI onset and the cladding hoop strain, whereas the cladding axial elongation would be affected through the PCMI onset.

Since the strains calculated by the code in each axial node are considered as an average, the strain contribution per node concerning the fuel creep modelled ( $\epsilon_{irr}(z)$ , focused on dishes) is calculated as:

$$\epsilon_{irr,avg}(z) = \frac{\epsilon_{irr}(z)}{(h_p / 2 \cdot h_d)} \quad (3)$$

where  $h_p$  and  $h_d$  are the pellet and dish height, respectively.

Based on this adaptation, the uncertainty related to the rigid pellet model has been expressed as an uniform distribution between 0 and 100% of the fuel creep estimated.

### 3.3. Uncertainty quantification

A commonly tool used to propagate uncertainties in FRAPCON-4.0 is DAKOTA. It is an interface between simulation codes and iteration methods, which contains algorithms for uncertainty quantification with sampling-based methods. A detailed explanation of a probabilistic uncertainty analysis applied to FRAPCON-4.0 by using DAKOTA can be found elsewhere [19,20].

In this work, it has been applied the simple random sampling method with 1000 samples (based on [19]). The output uncertainty band has been determined by adopting a confidence level of 95% [21].

## 4. Assessment

### 4.1. Best estimate

The target variable in the assessment carried out is the cladding elongation, in order to compare with the experimental data made available [15]. Figure 3 represents the predictions and measurements for the ramps analysed. The initial elongation has been subtracted to focus on the ramp related effects. According to the curves shown, predictions have given rise to the expected trend from a qualitative point of view (i.e., transition from free thermal expansion to strong cladding elongation driven by fuel expansion, that is to say, elongation slope becomes steeper after the PCMI onset).

From a quantitative point of view, an overestimation at the end of both ramps is observed, being moderate in the fresh fuel ramp (17.6%) and relevant in the high burnup fuel ramp (50.2%). Focusing on the PCMI onset and the elongation increase rate during PCMI, the following observations can be made:

- Prediction delays the early PCMI onset measured in the fresh fuel ramp (discrepancy of 5.6 kW/m) (Figure 3a). This means that a slower fuel-cladding accommodation is modelled by the code.
- PCMI onset predicted in the high burnup fuel ramp is faster than measured (discrepancy of 0.94 kW/m) (Figure 3b). Thus, a faster fuel-cladding accommodation is modelled by the code.
- In both ramps, the elongation increase rate during PCMI is overestimated (Figure 4), which is somewhat more noticeable in the high burnup fuel ramp (average slope overprediction of 38.5% against 33% in the fresh fuel ramp). According to that, the PCMI modelled is stronger than the measured one in the fresh fuel ramp, whereas in the high burnup fuel ramp the faster PCMI onset modelled could be other reason of the overprediction observed.

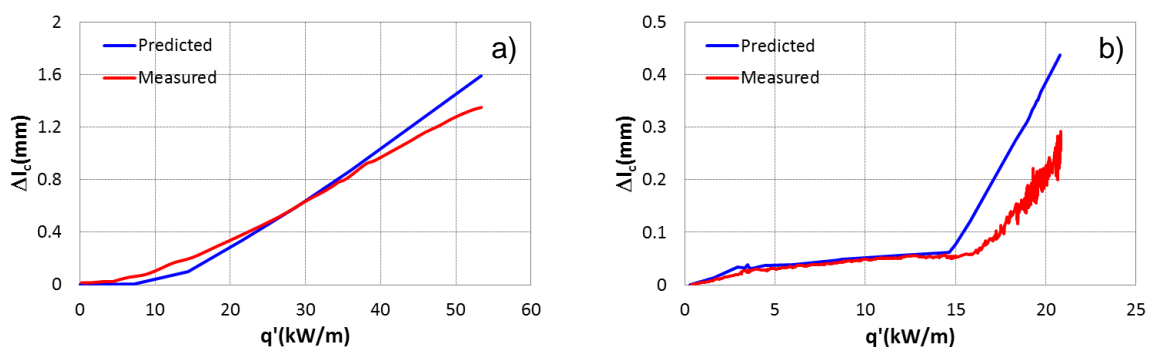


Figure. 3. Cladding elongation vs linear power during fresh fuel ramp (a) and high burnup fuel ramp (b).

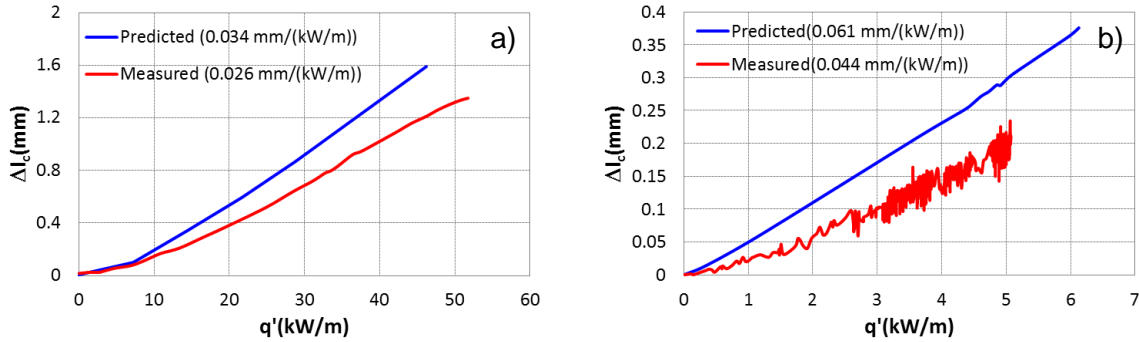


Figure. 4. Cladding elongation after PCMI onset vs linear power (PCMI onset power subtracted) during fresh fuel ramp (a) and high burnup fuel ramp (b). Average slope shown in brackets.

In the case of high burnup fuel ramp, the availability of fuel centerline temperature measurements (at the top of the fuel stack) has allowed ruling out the thermal modelling as the reason of the discrepancy found (relative errors lower than 5%). Other factor that might contribute to the stronger PCMI predicted is the gaseous swelling model (relevant impact shown on PCMI at high burnup [22]). In this case, the predictions with gaseous swelling (by default) and without it are nearly identical. Thus, at the relatively low power conditions in the high burnup fuel ramp, the temperatures attained (lower than 1220 K) are not enough to activate the fuel gaseous swelling model (activation from 1233 K [10]).

Concerning the approximation of no fuel-cladding slippage, even if a friction coefficient reduced the elongation slope during PCMI, the discrepancies found in the PCMI onset would not be resolved.

## 4.2. Uncertainty and sensitivity

In order to figure out the sources of the discrepancies found in the ramps studied, an uncertainty analysis has been done taken into account the uncertainties shown in section 3.2.

Figure 5 represents the measured evolution of the cladding elongation along with the best estimate plus uncertainty (BEPU) prediction in each ramp. Regarding the fresh fuel ramp (Figure 5a), the uncertainty covers the maximum elongation measured. However, it does not capture the early PCMI onset observed; this may be due to the lack of ridge effect modelling. It should be noted that the pellet height in this case (around 1.5 times greater than current heights) promotes the ridge effect [13]; thus, the observations made in the PCMI onset should be checked with a current design. Concerning the elongation during PCMI, the average slope is close to the measured one in the lower uncertainty bound predicted (0.029 mm/(kW/m)); anyhow, the discrepancy found in the PCMI onset prevents from doing a precise analysis during the PCMI period.

The sensitivity analysis carried out from the Pearson coefficient in the fresh fuel ramp (Table 2), highlights fuel thermal conductivity and thermal expansion models as the main contributors to the elongation uncertainty (the sum of the squares of Pearson coefficients is 0.922, where the total sum is 0.992). The contribution of the power uncertainty is also noticeable, although less important than the cited models; in fact, the uncertainty band without the power uncertainty also covers the maximum elongation measured. Note that this scenario does not have the influence of irradiation related models like fuel creep or swelling, as expected.

Concerning the high burnup fuel ramp, Figure 5b shows that the uncertainty band covers both the PCMI onset and the elongation attained during PCMI. Thus, the propagation of the

uncertainties taken into account explains the error obtained in the elongation. In this case, the Pearson coefficient (Table 2) highlights the sensitivity to power, fuel swelling model and rigid pellet approach (the sum of the squares of Pearson coefficients is 0.961, where the total sum is 0.969). Particularly, the deviation observed in the best estimate is mainly due to the uncertain power and the rigid pellet approach, being the latter the most influential. In fact, it has been checked that the uncertainty band related to power and in-code models (i.e., without the contribution of fuel creep) is not enough to cover the maximum elongation measured.

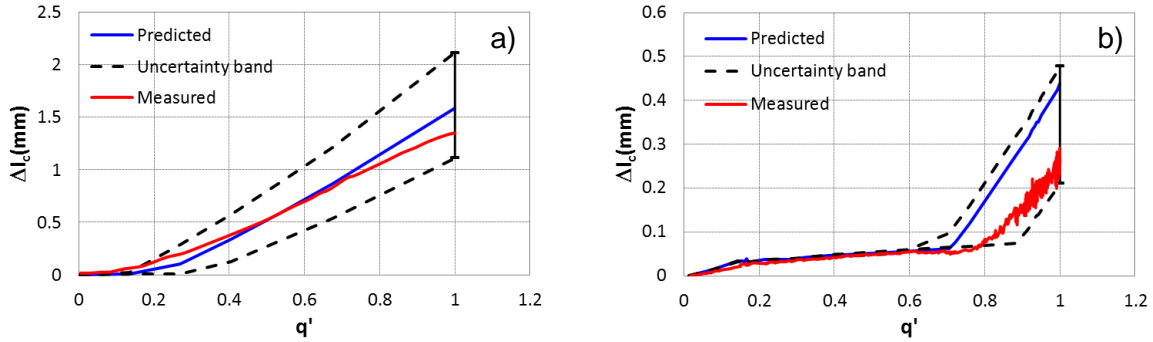


Figure. 5. Cladding elongation vs normalized linear power during fresh fuel ramp (a) and high burnup fuel ramp (b) (prediction uncertainty included).

Table 2. Sensitivity analysis.

Uncertain factor	Pearson coefficient	
	Fresh fuel	High burnup fuel
Power	0.254	0.551
Fuel thermal conductivity	-0.447	-0.016
Fuel thermal expansion	0.850	-0.022
Fission gas release	-0.002	0.031
Fuel swelling	-0.001	0.377
Cladding creep	0.005	-0.034
Cladding irradiation axial growth	0.002	-0.002
Cladding corrosion	0.045	0.065
Relocation recovery	-0.060	-0.013
Rigid pellet approach	-0.003	-0.719

Given the impact shown by the rigid pellet approach in the high burnup fuel ramp, a parametric case has been simulated taken into account the fuel creep modelled (i.e., 100% of the contribution), keeping the rest of uncertain variables in the best estimate values. Figure 6 and 7 show the results obtained in terms of cladding elongation (measurement included) and stress (hoop and axial); the code's best estimates are also included. As it can be observed, the elongation calculated notably improves the prediction made by default: the PCMI onset is well captured and similar elongation is estimated during PCMI. Note that the smaller elongation slope predicted with fuel creep is due to a late pellet-cladding contact in the upper part of the rodlet (i.e., drilled pellets), that happens quite later than the PCMI onset predicted (related to the rest of the rodlet). It should be highlighted an important reduction of the hoop and axial stresses (around 45%) when the approach of rigid pellet is avoided.



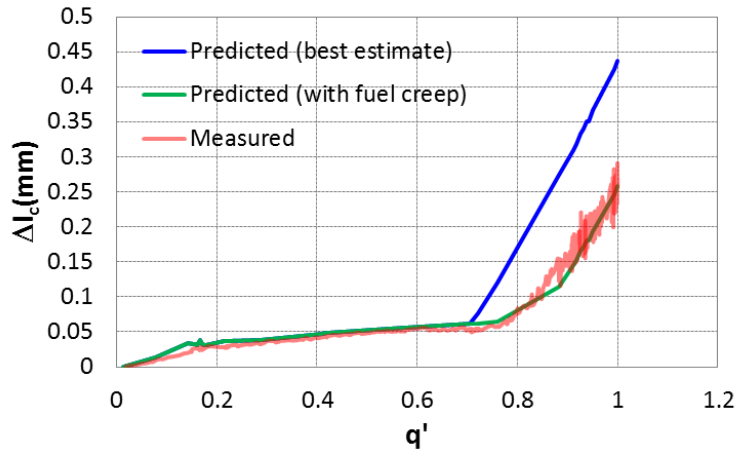


Figure. 6. Cladding elongation vs normalized linear power during high burnup fuel ramp.

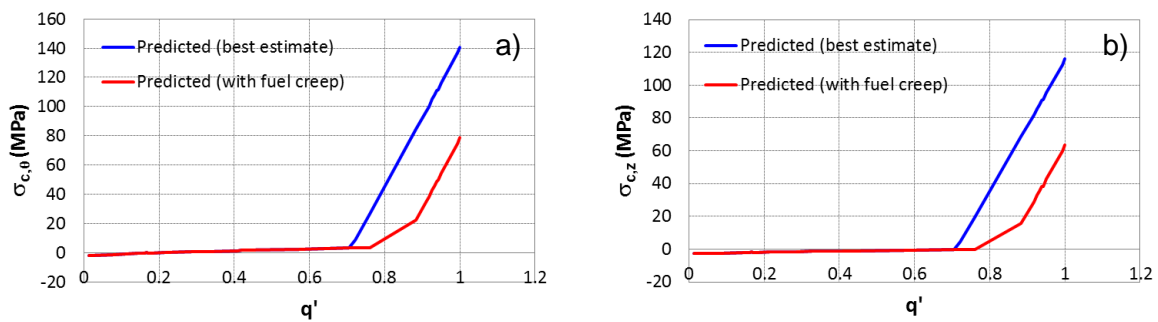


Figure. 7. Prediction of cladding stress vs normalized linear power during high burnup fuel ramp, in hoop (a) and axial (b) direction.

## 5. Conclusions

The present work has been focused on assessing FRAPCON-4.0 capabilities to predict PCMI in LWR fuel rods submitted to power ramps, both for fresh fuel and high burnup fuel. To do that, two power ramps tested in the Halden reactor have been simulated; the assessment has been done in terms of the cladding elongation (predicted vs measured), taking into account the uncertainty of power and in-code models. The uncertainty related to the rigid pellet approach has been also analysed through the implementation of a fuel creep model (focused on dishes zones).

The analysis from the best estimate allows concluding that the code response to different conditions of rod design and power ramp is consistent, in spite of being out of the recommended ramp rate limit ( $> 2$  (kW/m)/h). Nonetheless, an important error has been found in the high burnup fuel ramp (overprediction of 50% at the end of ramp), being less than 20% in the fresh fuel ramp. From the uncertainty analysis carried out, it should be highlighted:

- The uncertainty from the in-code models is the main cause of the deviation found in the fresh fuel ramp. Nevertheless, more accurate predictions of PCMI onset would have been obtained if the ridge effect had been accounted for in the modelling.
- The rigid pellet approach is shown to be the main reason, along with the power uncertainty, of the high overestimation observed in the high burnup fuel ramp. The power and in-code models related uncertainty is not enough to explain the total error.

Therefore, the rigid pellet model used by the code may lead to excessive conservatism in the PCMI predicted at high burnup, which can be notably reduced through the implementation of a fuel creep model. The cladding stress obtained when the fuel creep is modelled (around 45%

less than the best estimate of the default code), allows concluding that the uncertainties of the code associated to its overall approach should be considered when the scenario modelled is prone to highlight PCI as a major threat for fuel rod integrity.

Further work is foreseen to keep on verifying the conclusions made with further ramps. Moreover, a critical review of the experimental data made available (representativeness, uncertainty from measurements) would be valuable to carry out a sounder analysis.

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