

# OECD/NEA BENCHMARK ON PELLETT-CLAD MECHANICAL INTERACTION MODELLING WITH FUEL PERFORMANCE CODES: IMPACT OF NUMBER OF RADIAL PELLETT CRACKS AND PELLETT-CLAD FRICTION COEFFICIENT

M. DOSTÁL<sup>1</sup>, G. ROSSITER<sup>2</sup>, A. DETHIOUX<sup>3</sup>, J. ZHANG<sup>3</sup>, M. AMAYA<sup>4</sup>, D. ROZZIA<sup>5</sup>, R. WILLIAMSON<sup>6</sup>, T. KOZLOWSKI<sup>7</sup>, I. HILL<sup>8\*</sup>, J.-F. MARTIN<sup>8</sup>

1 - ÚJV Řež, Czech Republic; 2 - NNL, United Kingdom; 3 - Tractebel, Belgium; 4 - JAEA, Japan; 5 - SCK-CEN, Belgium; 6 - INL, United States; 7 - University of Illinois, United States; 8 - OECD/NEA, France

\* corresponding author: [ian.hill@oecd.org](mailto:ian.hill@oecd.org)

## ABSTRACT

The benchmark on Pellet-Clad Mechanical Interaction (PCMI) was initiated by the Nuclear Energy Agency (NEA) Expert Group on Reactor Fuel Performance (EGRFP) in June 2015 and is currently in the latter stages of compiling results and preparing the final report. The aim of the benchmark is to improve understanding and modelling of PCMI amongst NEA member organisations. This is being achieved by comparing PCMI predictions of different fuel performance codes for a number of cases. Two of these cases are hypothetical cases aiming to facilitate understanding of the effects of code-to-code differences in fuel performance models. The two remaining cases are actual irradiations, where code predictions are compared with measured data. During analysis of participants' results of the hypothetical cases, the assumptions for number of radial pellet cracks and the pellet-clad friction coefficient (which can be zero, finite or infinite) were identified to be important factors in explaining differences between predictions once pellet-cladding contact occurs. However, these parameters varied in the models and codes used originally by the participants. This fact led to the extension of the benchmark by inclusion of two additional cases, where the number of radial pellet cracks and three different values of the friction coefficient were prescribed in the case definition. Seven calculations from six organisations contributed results, which were compared and analysed in this paper.

## 1. Introduction

The NEA Expert Group on Reactor Fuel Performance (EGRFP), established within the Working Party on Scientific Issues of Reactor Systems (WPRS), under the auspices of the NEA Nuclear Science Committee, aims at providing expert advice to the nuclear community on the development needs (experimental data, methods, code development, code verification and validation, etc) for fuel performance analysis of existing and proposed fuel designs. Key activities associated with this objective are the identification and preservation of appropriate experimental data, and the dissemination of technical information and knowledge on fuel performance through scientific workshops, benchmark studies and training activities.

The benchmark on Pellet-Clad Mechanical Interaction (PCMI), initiated by the EGRFP started in June 2015 and during the analysis of participants' results of the first two hypothetical cases (preliminary results were presented in [1]), it was pointed out that some of the parameters were in fact not fixed in the case specification. One of them was the number of radial pellet cracks whose effect was observed and described in the past (see e.g. [2]); in particular, the pellet radial deformation is increased and the stress on the cladding when there is pellet-clad contact is concentrated over the cracks. There are different ways to model pellet cracking (lowered elastic constants, smeared model, explicit implementation, etc.) but

the number of radial pellet cracks (pure number or e.g. evolution with linear heat rate) must usually be assumed/prescribed in the model. For the purpose of this benchmark extension the number of radial cracks suggested to be used was set to 8. The second important parameter that was not fixed in the specification is the pellet-clad friction coefficient, which has impact on elongations and hoop stresses generated in the cladding by the pellets. To study its effect in this exercise, three different values were chosen: 0.0 (no friction; unconstrained sliding), infinite (no sliding), and 0.4 (reasonable value simulating the real situation in fresh fuel [3]).

This paper presents the status of the PCMI benchmark and the comparison of the results of the two additional cases where the number of radial pellet cracks and the pellet-cladding friction coefficient were prescribed.

## **2. Benchmark participants and used fuel performance codes**

Participants from more than 20 organisations take part in the benchmark (a full list of participants as of June 2016 was presented in [1]). They include staff from research organisations, national laboratories, regulatory organisations, technical support organisations, universities and international organisations.

The two additional cases (Case1a and Case 2a) were modelled by six participants, namely Tractebel, ÚJV Řež, INL, JAEA, ENEA and University of Illinois, for a total of seven sets of results (ÚJV Řež used two different codes) as shown in Table 1.

A large number of fuel performance codes, with different modelling assumptions, were used (the total number is 19, with several used by more than one organisation; the codes as of June 2016 were listed in [1]). The codes used for modelling the two additional cases are FRAPCON, BISON, TRANSURANUS, FEMAXI and ABAQUS - see Table 1. Code types include 1½-D codes (where the active fuel stack length is divided into axial zones, and predicted quantities – e.g. temperature, hoop stress – are assumed to have only a radial variation within each axial zone), 2-D codes (where predicted quantities are assumed to have both a radial and axial variation), and 3-D codes (where the radial, axial and circumferential variations of predicted quantities can all be calculated).

It is important to understand that the computer codes used in the exercise are not comparable in terms of their level of development (some are under active development, while others are established codes licensed by regulatory authorities) and application domains (which include fuel licensing, research and development, and regulatory activities). In addition, two of the codes (ABAQUS and ANSYS, the first of which was used in modelling the two additional cases) are general finite element codes – that is, they are not dedicated to fuel performance applications. Thus, predictions of the codes should not be compared on a like-for-like basis.

## **3. Specification of the benchmark cases and two additional cases**

The cases analysed in the benchmark are as follows:

- Case 1 is a hypothetical beginning-of-life (BOL) ramp of a short (10 pellet) pressurised water reactor (PWR) rodlet;
- Case 2 is a hypothetical BOL ramp of a full-length commercial PWR rod;
- Case 3 is the BOL ramping of eight rodlets with different pellet designs in the OECD/NEA Halden Reactor Project (HRP) IFA-118 experiment (irradiated in the Halden Boiling Water Reactor (HBWR) from 1969 to 1970) [4];
- Case 4 is the end-of-life (EOL) ramping of a PWR rodlet in the HRP IFA-629.4 experiment (performed in the HBWR in 2004) [5].

The Case 1 ramp consists of a ramp-up over 1 minute (at a constant ramp rate) to a peak pellet rating of 40 kW/m, and a subsequent power hold for 100 hours. The short irradiation is under PWR conditions and for simplicity, uniform axial profiles of power and rodlet surface temperature are assumed. The shortness of the rodlet is to enable reasonable computation times for the case with 3-D codes. The ramp-up time is designed to be sufficiently long for thermal transient (fuel and clad stored heat) effects to be negligible, while being sufficiently short for the effects of other time-dependent phenomena (in particular, fuel creep, clad creep, fuel densification and fuel swelling) to be minimal.

The detailed Case 1 parameters can be found in [1]. The clad inner and outer diameters are both reduced from typical PWR values so that fuel-clad gap closure will occur part-way through the up-ramp.

Case 2 is complementary to Case 1, in that the peak pellet rating versus time behaviour, coolant pressure and fast flux are identical. Non-uniform axial profiles of power and rod surface temperature are assumed; the axial power profile is idealised as a normalised chopped cosine distribution and the rod surface temperature axial profile is set according to the axial power profile via a heat balance calculation and the Jens-Lottes rod-to-coolant heat transfer coefficient correlation [6] (assuming coolant inlet and outlet temperatures of 287 °C and 321 °C, respectively).

The Case 2 rod design is as per the Case 1 rodlet design, except for the active fuel stack length, which is set to a typical value of 12 ft = 3658 mm, and plenum length, which is set to a value of 162 mm.

During analysis of participants' results of the cases [1], the assumptions for number of radial pellet cracks and the pellet-clad friction coefficient (which can be zero, finite or infinite) were identified to be important factors in explaining differences between predictions once pellet-cladding contact occurs. However, these parameters varied in the models and codes used originally by the participants.

In order to study their effects, two sub-cases Case 1a and Case 2a with specified number of pellet cracks (8 radial cracks suggested) and pellet-cladding friction coefficient (0.0, 0.4 and infinite) were added as an extension of the original. The setting of these parameters is not possible in all codes due to different approaches used and only a subset of the participants modelled these two sub-cases. All of the participants were able to use zero and infinite friction coefficient and most of them also 0.4. The codes were used as best as possible to simulate 8 radial cracks, however, it is only with ABAQUS that this could be achieved by prescribing a 45° symmetrical 3D geometry with one radial crack (which corresponds to 8 cracks in a full pellet). FRAPCON and FEMAXI did not explicitly consider any cracks. In both TRANSURANUS calculations four cracks (n=4) were set which lead to lowering the fuel elastic modulus by factor  $(2/3)^n$  and Poisson ratio by factor  $(1/2)^n$ . Smear cracking model assuming radial cracking at any given material point when hoop stress exceeds fracture strength of 130 MPa was used in both BISON calculations.

**Comment [RGD1]:** need Jinzhao and Masaki to expand on this

Organisation	Code	Chosen number of cracks for suggested value of 8 <sup>(2)</sup>	Chosen friction coefficient for suggested value of 0.0	Chosen friction coefficient for suggested value of 0.4 (not used in all cases)	Chosen friction coefficient for suggested value of infinite
Tractebel	FRAPCON 3.5-FEA	No explicit value	0.0	0.4	infinite
ÚJV Řež	TRANSURANUS v1m3j12	4	0.0	0.4	infinite
ÚJV Řež	ABAQUS 6.12-3	8	0.0	0.4	2.0
INL	BISON V1.2 <sup>(1)</sup>	No explicit value	0.0	0.4	infinite
JAEA	FEMAXI-7 V7.1.123	No explicit value	0.0	0.4	10 <sup>6</sup>
ENEA	TRANSURANUS v1m3j12	4	0.01	0.4	10 <sup>3</sup>

University of Illinois	BISON V1.2	No explicit value	0.0	0.4	infinite
------------------------	------------	-------------------	-----	-----	----------

<sup>(1)</sup> Commit a911ae6 derived from v1.2 Jan, 21, 2016

<sup>(2)</sup> See section 3 for more details

Tab. 1 List of participating organizations and codes used in PCMI benchmark Cases 1a, 2a

## 4. Results of the two additional cases

### 4.1. Predictions for Case 1a

The predictions requested for Case 1a (and Case 1) were as follows:

- Fuel stack elongation along pellet centreline as a function of time from start of irradiation.
- Clad elongation along inner wall as a function of time from start of irradiation.
- Maximum (axially, therefore including any pellet hourglassing effects) clad outer diameter as a function of time from start of irradiation.
- Maximum (axially, therefore including any pellet hourglassing effects) clad hoop stress at inner wall as a function of time from start of irradiation (no information about the circumferential variation in the hoop stress was requested, so predictions are either maximum circumferential values over a radial pellet crack (where predictable) or average circumferential values (otherwise)).

The results are illustrated in Figs. 1 and 2.

#### *Clad and Pellet Elongation:*

The clad elongation initially increases slightly with time as the clad undergoes thermal expansion due to the increasing clad temperature with increasing power. The cladding elongation decreases after establishing pellet-cladding contact for zero friction coefficient due to pellet diameter increase and consequential clad diameter increase (Poisson's effect); for infinite friction there is generally a sharp jump in the rate of increase with time due to the tensile forces applied to the clad in the axial direction by the thermal expansion of the pellets; for a 0.4 friction coefficient the results are intermediate to the zero and infinite friction results. These effects apply for all received results which suggests reasonable behaviour of the models. All calculations predict the highest cladding elongation change for infinite (or sufficiently high) friction coefficient. The fuel stack elongation exhibits the opposite behaviour: its change is highest for zero friction coefficient and lowest for infinite friction. It is observed that the difference between 0.4 and infinite is not large (parametric calculations have shown that with increasing friction coefficient its influence decreases).

The starting point of fuel elongation differs between the predictions much more than the cladding elongation initial value. The difference of peak and initial fuel elongation is however similar (~0.5 mm) for most of the predictions when comparing zero friction. This was already observed in preliminary results comparisons [1] and is usual for a large number of compared codes (see e.g. [7], [8]), because: (a) the thermal expansion correlations differ in the codes; (b) the calculation initialization is computed differently in some cases (the initial elongations are meant to include the thermal expansion contribution from 20 °C to 330 °C, but this may not have been done correctly in all cases); and (c) variations in the predicted radial location of pellet-pellet contact (due in part to the complications of the pellet end geometry) affect the elongations. On the other hand, cladding elongation starting values spread is much smaller (0.1 to 0.26 mm), since only (a) and (b) above apply.

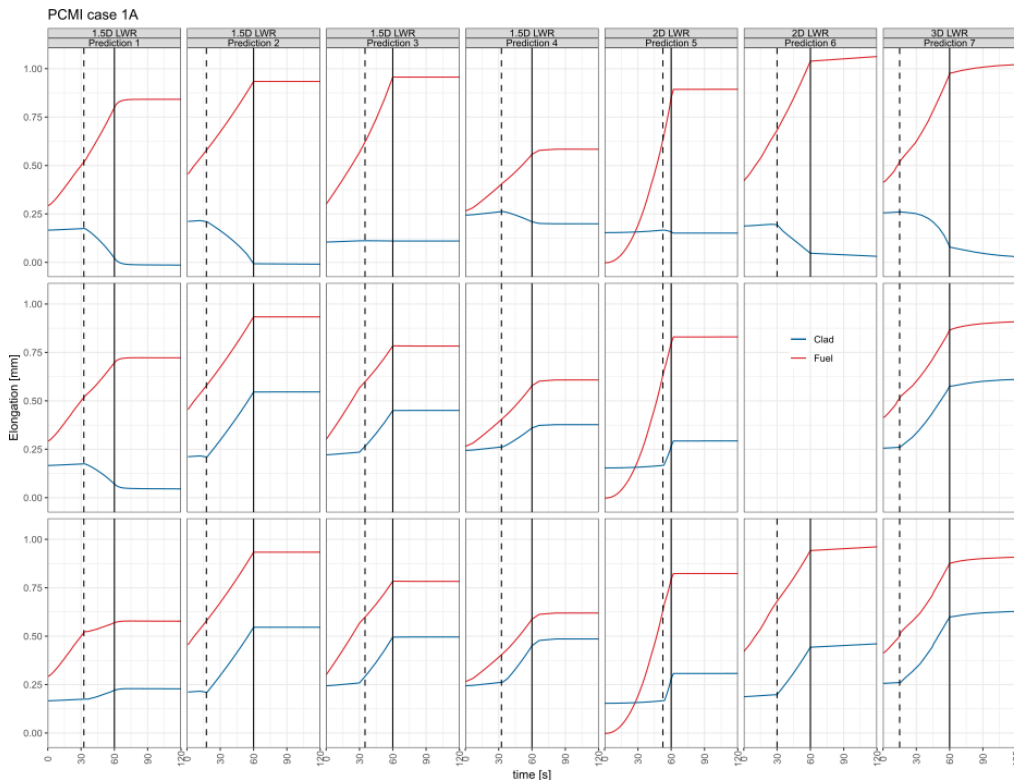


Fig. 1 Case 1a - cladding and fuel stack elongation over the first 120 seconds of the irradiation - zero friction top figures, friction 0.4 middle figures, infinite friction bottom figures (dashed vertical lines indicate estimated times of pellet-clad contact)

#### Cladding Diameter and Hoop Stress:

Predictions of cladding diameter during the power ramp start at almost the same level, however the peak value and time of pellet-clad contact (that is, time of gradient increase) differ significantly. A very weak trend of outer diameter increase with time before contact (thermal expansion effect) is observed for almost all predictions.

Initial (open gap condition) hoop stress value is again almost the same for all predictions ( $\sim -90$  MPa) and the increases during the power ramp after pellet-clad contact correspond to the diameter increases (in one case with very small diameter increase hoop stress remains negative). Before pellet-clad contact, the hoop stress increases slightly with time in some cases; this is thought to be caused by a slight increase in rod internal pressure with increasing power (which is in turn due to an increasing gas temperature in, and decreasing volume of, the fuel-clad gap with increasing power). In other cases the hoop stress decreases slightly with time; the reasons for this are unclear. There is some influence of friction coefficient on peak hoop stress, which tends to be higher for higher friction coefficient.

2D and 3D simulations extracted mid-pellet and pellet-pellet interface values confirming the higher ones at the pellet-pellet interface. The individual pellets were modelled with contact (i.e. no mutual bonding) in 3D prediction which lead to higher difference in mid-pellet and pellet-pellet cladding diameter values (Fig. 2) compared to 2D predictions where the fuel stack is held in axial contact by bonding adjacent pellets at a point (or ring in 3D) corresponding to the outer radial edge of the dish region.

The influence of the friction coefficient on the elongation and hoop stress relaxation after 120 seconds, which does not differ significantly for different friction coefficients, depends on the used cladding creep, fuel creep and fuel densification models, which are not the same for the different codes, hence it is not shown or discussed in this paper.

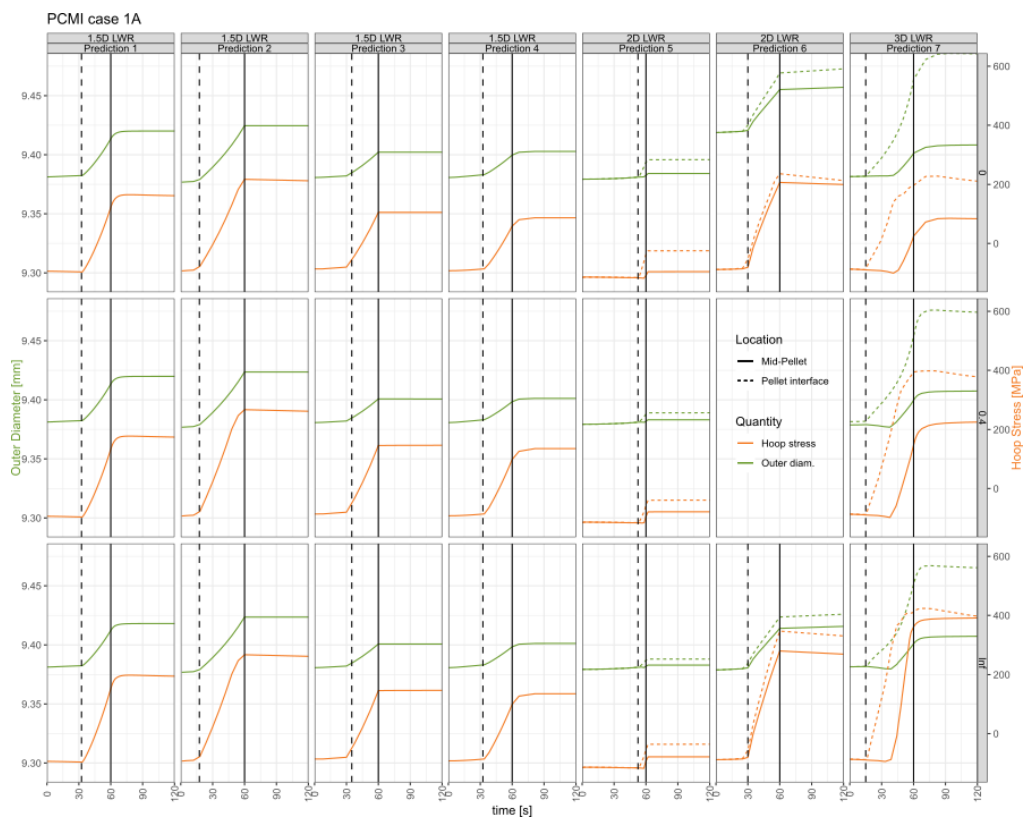


Fig. 2 Case 1a - cladding hoop stress and cladding outer diameter over the first 120 seconds of the irradiation - zero friction top figures, friction 0.4 middle figures, infinite friction bottom figures (dashed vertical lines indicate estimated times of pellet-clad contact)

## 4.2. Predictions for Case 2a

The predictions requested for Case 2a (and Case 2) are as follows:

- fuel stack elongation along pellet centreline as a function of time from start of irradiation;
- clad elongation along inner wall as a function of time from start of irradiation;
- maximum (axially, therefore including any pellet hourglassing effects) clad outer diameter as a function of time from start of irradiation;
- maximum (axially, therefore including any pellet hourglassing effects) clad hoop stress at inner wall as a function of time from start of irradiation;
- clad outer diameter as a function of elevation from bottom of active fuel stack at end of up-ramp (that is, at start of hold period);
- inner wall clad hoop stress as a function of elevation from bottom of active fuel stack at end of up-ramp (no information about the circumferential variation in the hoop stress was requested, so predictions are either maximum circumferential values over a radial pellet crack (where predictable) or average circumferential values (otherwise)).

The results are illustrated in Figs. 3 to 5. Similar behaviour is observed for the cladding and fuel elongation as for Case 1a. The scatter between the predictions for the ramp increase (peak minus initial) is slightly smaller, but the absolute values are higher and differ more due to the 3.7 m fuel stack height (Fig. 3).

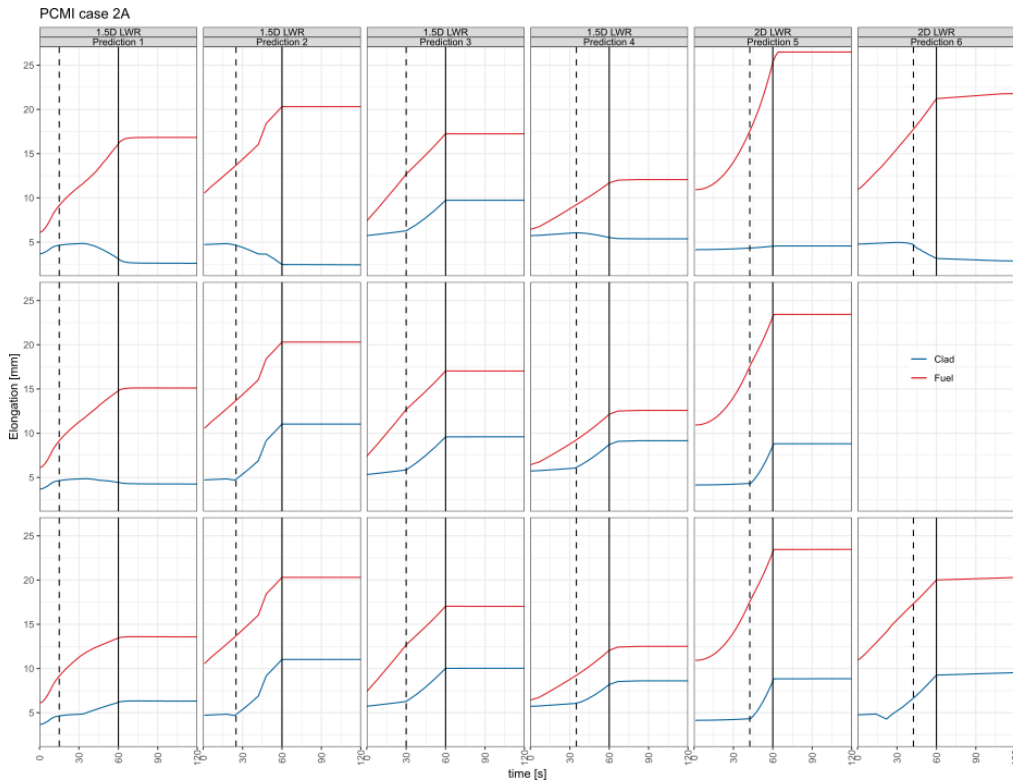


Fig. 3 Case 2a - cladding and fuel stack elongation over the first 120 seconds of the irradiation - zero friction top figures, friction 0.4 middle figures, infinite friction bottom figures (dashed vertical lines indicate estimated times of pellet-clad contact)

Cladding diameter and hoop stress at the maximum (axially) (Fig. 4) have nearly the same peak values as in Case 1a, however no general trend could be observed because some predictions show higher stress/diameter than the other ones. All predictions show higher peak hoop stress for higher friction coefficient.

Cladding outer diameter profile predictions (Fig. 5) can be divided into two groups according to the influence of the friction coefficient: for 1.5D simulations there is almost no impact, while 2D simulations show significant differences for zero and infinite friction. The other observation is that the height of ridges tends to be dependent on the friction coefficient value.

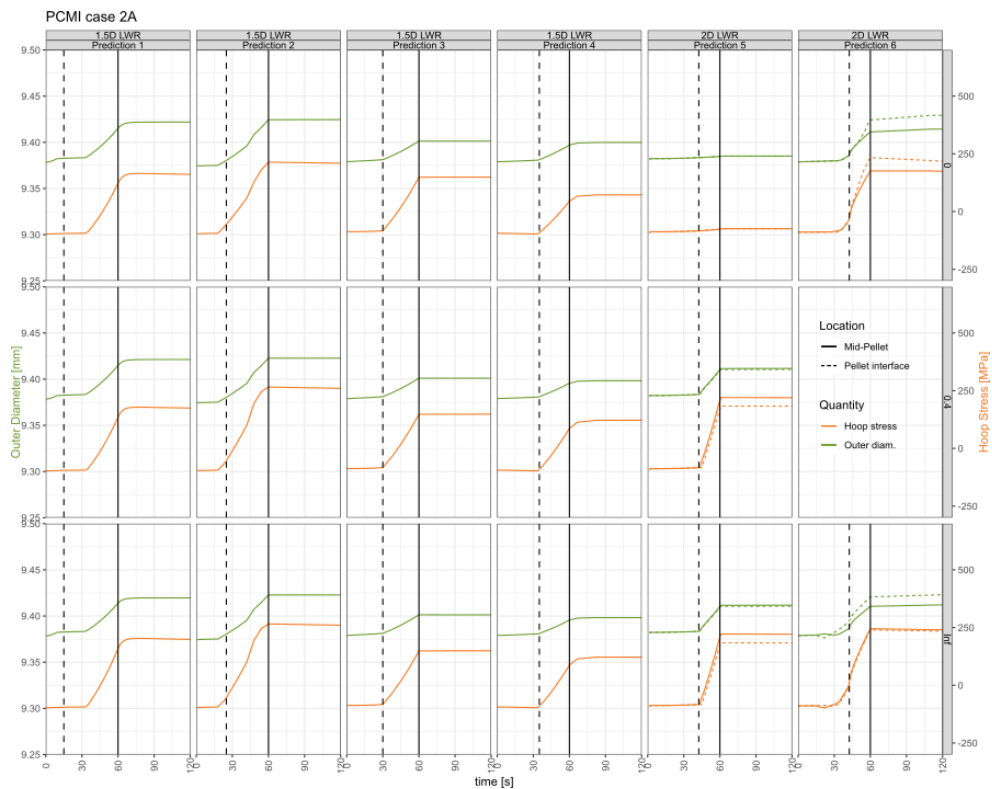


Fig. 4 Case 2a - cladding hoop stress and cladding outer diameter over the first 120 seconds of the ramp - zero friction top figures, friction 0.4 middle figures, infinite friction bottom figures (dashed vertical lines indicate estimated times of pellet-clad contact)

The cladding inner wall hoop stress profile (Fig. 5) confirms the previous statement about the higher peak value for higher friction coefficient. Moreover, the shape appears 'wider' than the diameter one, i.e. is less peaked than diameter.



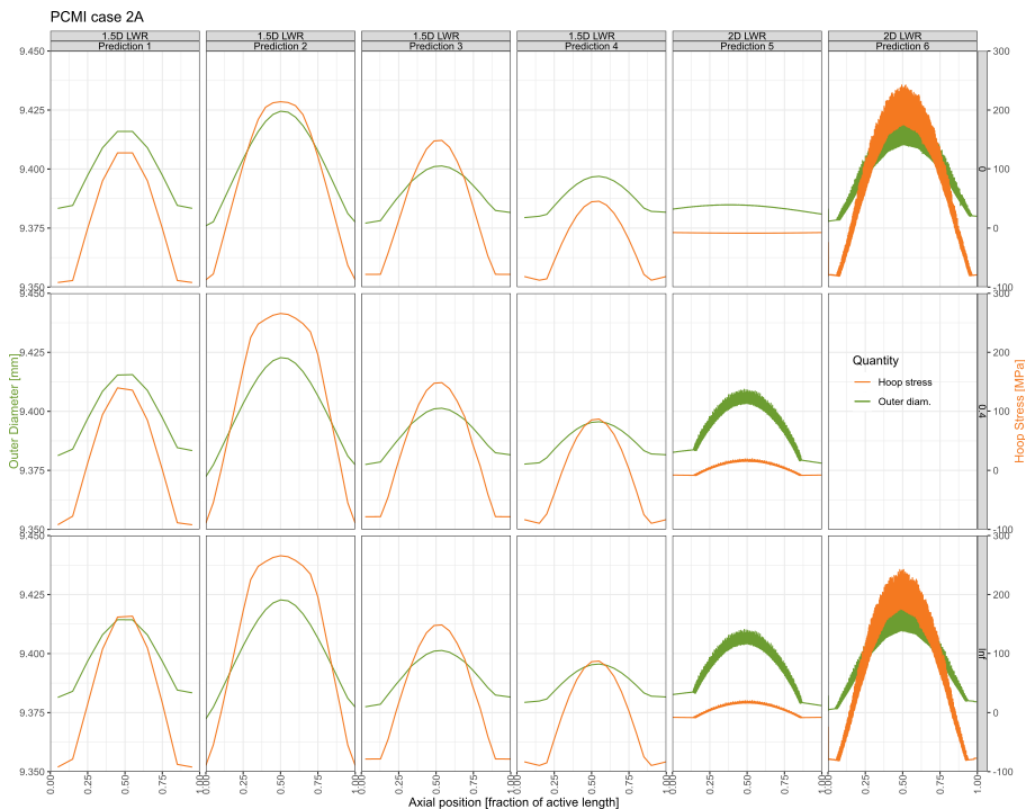


Fig. 5 Case 2a - cladding outer diameter and inner wall cladding hoop stress as a function of elevation from bottom of active fuel stack at end of up-ramp (that is, at start of hold period) - zero friction top figures, friction 0.4 middle figures, infinite friction bottom figures.

## 5. Conclusions

The NEA/EGRFP benchmark on Pellet-Clad Mechanical Interaction (PCMI) was launched in June 2015 to improve understanding and modelling of PCMI amongst NEA member organisations. The analysis of the preliminary results indicated the potential impacts of some of the parameters that were unspecified.

Two additional cases, Case 1a and Case 2a, were thus defined for hypothetical beginning-of-life ramps with specified number of radial pellet cracks and pellet-clad friction coefficient values, and the results have been presented and discussed. The conclusions are as follows:

- The majority of the predictions of fuel stack elongation, clad elongation, clad outer diameter and clad hoop stress versus time exhibit similar behaviour, although, somewhat surprisingly given the simplicity of the cases, there is a significant variation in predictions at time zero (i.e. before any pellet-cladding interaction), in particular with respect to fuel stack and clad elongation.
- More precise specification of pellet crack number led to lower differences between individual codes' results compared to original cases without specification.
- The effect of the assumed friction coefficient on the cladding elongation and cladding hoop stress is clear in all codes.
- The peak clad hoop stress for these simple cases varies from ~ 0 - ~ 400 MPa (Case 1a - more predictions are included than in Case 2a) and ~ 50 - ~ 250 MPa (Case 2a). This is an important finding because peak clad hoop stress is a key parameter in understanding PCMI (and therefore in fuel licensing) and because its prediction cannot be directly validated with measured data (and so which prediction is 'right')

cannot be directly determined). It should be stressed that the cases were deliberately designed to minimize the differences caused by the models of the fuel and cladding mechanical properties (creep, plasticity) and it was expected that the variation of these results would be lower.

- 'Prediction sets' – that is, two or more predictions generated with the same fuel performance code – suggest that the way in which cases are modelled via code input (including selection of models) is influencing the results, in addition to the differences in the codes themselves.

The PCMI benchmark as a whole is currently in the phase of results analysis and final report preparation. The objective is to publish the final report in 2019.

## 6. Acknowledgement

The participants of OECD/NEA EGRFP PCMI benchmark are acknowledged for fruitful discussions.

## 7. References

- [1] G Rossiter, et al., "OECD/NEA benchmark on pellet-clad mechanical interaction modelling with fuel performance codes", OECD/NEA Workshop on Pellet-Cladding Interaction (PCI) in Water Cooled Reactors, 22-24 June 2016, Lucca, Italy.
- [2] M Oguma, "Cracking and relocation behavior of nuclear fuel pellets during rise to power". Nuclear Engineering and Design. Vol. 76, p. 34-45, 1983.
- [3] T Tachibana, D Narita, H Kaneko and Y Honda, "Measurement of the friction coefficient between  $UO_2$  and cladding tube," Proc. of the Fall Meeting of the Atomic Energy Society of Japan, PNCT 831-78-02, October 1977.
- [4] H G Walger, K D Knudsen, E Rolstad, K Svanholm, K D Olshausen and A Hanevik, "A parametric study of the influence of important fuel design parameters on the elongation and bamboo-ridge formation of Zr-2 clad  $UO_2$  fuel rods", OECD Halden Reactor Project report HPR-141, August 1971.
- [5] H Koike, N Murakami, E Kolstad and T Tverberg, "Ramp tests with two high burnup  $UO_2$  fuel rods in IFA-629.4", OECD Halden Reactor Project report HWR-769, November 2004.
- [6] W H Jens and P A Lottes, "Analysis of heat transfer, burnout, pressure drop and density data for high pressure water", ANL-4627, May 1951.
- [7] NEA/CSNI/R(2013)7, "RIA Fuel Codes Benchmark- Volume 1", Nuclear Energy Agency, OECD, Paris, France, 2013.
- [8] NEA/CSNI/R(2016)6, "Reactivity Initiated Accident (RIA) Fuel Codes Benchmark Phase II - Volume 1: Simplified Cases Results – Summary and Analysis", Nuclear Energy Agency, OECD, Paris, France, 2016.