

Modelling Out-of-Pile LOCA Tests on High Burnup Fuel Rods. Results of the fourth SCIP Modelling Workshop

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ABSTRACT

The Studsvik Cladding Integrity Project (SCIP) is an OECD/NEA multilateral international research program. SCIP III is a five-year experimental program carried out from 2014 to 2019 focused on fuel behavior in LOCA and overheating transients. The program brings together 32 organizations in 14 countries in a joint research effort.

In SCIP, modelling and experiment have been brought together in modelling workshops (MWS). Three MWS efforts have been organized previously with the main aim to assess and benchmark fuel rod performance codes under power ramp scenarios investigated within SCIP. Following this successful path, a fourth MWS was implemented in 2017 with the main workshop meeting held in November 2017. The purpose of the MWS was to benchmark results from participating codes on out-of-pile LOCA tests performed on high burnup fuel rods in the Studsvik hot cells. The codes were also used to characterize the fuel rod specimens prior to LOCA testing by modelling the base irradiation for each test rod.

Five LOCA tests were modelled, as well as the base irradiation of three high burnup PWR fuel rods from which the test rods were sampled. In total eight organizations contributed modelling results, although only four carried out the full scope of work. Seven different code systems were represented, including the well-known codes ALCYONE, FRAPCON/FRAPTRAN, TRANSURANUS, ENIGMA, DRACCAR, JASMINE/RELAP and COPERNIC. This paper presents a summary of the modelling results and insights gained from the SCIP III modelling workshop.

1 Introduction

The SCIP III project consists of three main tasks: Task 1 LOCA and overheating transients, Task 2 Pellet-cladding interaction (PCI) and Task 3 Modelling. The main task in SCIP III is Task 1 with the primary objective of determining the experimental thresholds for fine fuel fragmentation and of improving the estimates of fuel dispersal in a LOCA. The degree of fragmentation and the size distribution of the fragments are important parameters determining the amount of fuel that might be released.

The main experimental method employed in SCIP III is semi-integral LOCA testing at the Studsvik Hot Cell Laboratory (HCL). The LOCA test is performed by controlled heating of a refabricated fuel rod specimen in a radiant infrared furnace. The rod is pressurized and when it is heated up above 700 °C the cladding creeps out, balloons and bursts. The rod behavior and the burst characteristics are determined by the internal pressure, temperature ramp rate and the material properties of the test rod specimen. The original test equipment and the test method are described in detail in [1]. More than 20 LOCA test experiments have been carried out in SCIP III. The tests have provided valuable data for correlations as well as an increased understanding of the physical properties controlling fuel fragmentation and dispersal in a LOCA transient.

The objectives of the modelling effort are to support the program with pre- and post-test calculations using existing codes and models, to provide input to the design of test matrices and to the selection of test parameters, to improve evaluation/interpretation of the experimental results and, if possible, to identify model improvements and the data needs for such improvements.

Modelling has always been an important part of SCIP and each project phase has included one or more modelling workshops. Three MWS efforts have been organized previously with the main aim to assess and benchmark fuel rod performance codes under power ramp scenarios investigated within the SCIP. The main results have been reported in [2]-[4]. In line with this experience, a fourth MWS was organized in SCIP III with the main workshop meeting in November 2017.

The direct objective of the MWS was to compare and benchmark results from participating codes on the same test cases. The test cases were based on semi-integral LOCA experiments performed in SCIP III. A wider objective of the MWS was to engage the modelling community to use and interact with the experimental results achieved in SCIP.

2 MWS participants

In total 14 organizations initially signed up for the MWS. Unfortunately, not all organizations could provide calculated results. Finally, contributions from 8 organizations were received with four organisations covering the full scope of test cases. The participating organisations and codes are listed in Table 1. Some participants use codes which manage both quasi-static and time-dependent cases, while others use different codes for quasi-static and time-dependent modelling cases. To perform high fidelity modelling of the Studsvik LOCA test experiments a code with time-dependent modelling capability is needed.

Table 1. Participating organisations and codes in the SCIP III MWS.

Organization	Code	Cases	Code overall	Transient
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		run		capability
CEA	ALCYONE [6]	1-9	1.5D, 2D, 3D	Yes
Studsвик Scandpower	ENIGMA	1-4	1.5D	No
US-NRC	FRAPCON-4	1-4	1.5D	No
ÚJV Řež	TRANSURANUS [7]	1-9	1.5D	Yes
IRSN	DRACCAR [8]	5-9	1.5D, 2D, 3D	Yes
CNPRI	JASMINE/RELAP	1-9, except 4	1.5D (JASMINE)	No/Yes
Quantum Technologies	FRAPCON-QT-4.0P1 /FRAPTRAN-QT-1.5d [9], [10]	1-9, except 4	1.5D	No/Yes
NPIC	COPERNIC	3	1.5D	No

3 Modelling cases

The LOCA test rodlets are refabricated from full length fuel rods irradiated in commercial power reactors. The modelling cases are thus naturally separated into two categories, i.e. modelling of the base irradiation power history and modelling of the transient LOCA tests. The base irradiation modelling cases are listed in Table 2 and the LOCA modelling cases in Table 3. The fuel rods modelled in cases 1-3 have all reached a burnup of approximately 60 MWd/kgU. However, the detailed power histories are different, and fuel fragmentation experiments performed in SCIP III showed large differences in their fuel fragmentation behavior. Hence, characterization of the condition of the fuel in these rods may shed some light on the fuel fragmentation mechanism, and this is the motivation for selecting these rods for detailed modelling of their base irradiation. The fuel rod in case 4 was part of Task 2 and originally intended to be ramp tested in SCIP III. As the ramp tests cannot be performed within SCIP III due to an unplanned interruption of the Halden reactor operation, modeling data for this rod are not included in this paper.

Test rodlets harvested from the fuel rods in Table 2 were exposed to semi-integral LOCA simulation tests. The LOCA test cases 6 and 7 were performed with the same test parameters. A comparison of the results of these two LOCA tests thus corresponds to differences in the pre-test condition of the test rods. The test parameters for test cases 5 and 6 differ mainly in the temperature history. The temperature in case 5 was increased by 5.7 °C/s to approximately 700 °C, and then by 1.4 °C/s to 880 °C and finally by 0.2 °C/s to 900 °C, after which the furnace was turned off. This heat-up sequence was employed to simulate the temperature curve typically obtained in Halden in-pile LOCA tests [5]. Thus, modelling results from this test case can be compared to SCIP III LOCA tests with constant temperature increase rate, e.g. case 6. Such a comparison supports the understanding of the LOCA test results due to differences in test parameters. Finally, the three last LOCA test cases, 7-9, selected for the MWS were all performed on rodlets refabricated from the same father rod. The tests were also performed using the same rod fill pressure and temperature ramp rate. One test was run to a peak temperature of 1000 °C, while the other two tests were interrupted during the ballooning phase before burst. These three cases, 7-9, provide an opportunity to benchmark model predictions on burst temperature and burst strain.

Table 2. Base irradiation modelling cases in the SCIP III MWS.

Case	Rod name	PWR/BWR	Burnup [MWd/kgU]	Rod diameter [mm]	Cladding type
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1	36U-N05	PWR	61	9.5	M5
2	3V5/Q13	PWR	60	9.55	Zircaloy-4, Duplex
3	R2D5	PWR	63	10.72	M5
4	O2c04	BWR	21	10.05	Zr-2

Table 3. LOCA test cases in the SCIP III MWS.

Case	Rodlet name	Fill pressure [bar]	Temp. ramp rate [°C/s]	Burst temp. [°C]	Balloon strain [%]	Peak temp. [°C]
5	36U-N05	72	5.7, 1.4, 0.2	748	61.3	896
6	3V5/Q13	80	5.0	773	40.5	1001
7	R2D5	80	5.0	751	22.9	1000
8	R2D5	80	5.0	No burst	1.5	702
9	R2D5	80	5.0	No burst	11.8	743

4 Results

4.1 Base irradiation cases

Using the provided power histories for cases 1-3, the codes calculated the axial burnup profiles. By comparing with the measured burnup profiles, a measure of the overall fidelity of the management of the input and execution of the calculations is obtained. In general, the calculated burnup profiles are in very good agreement with the measurements, which were evaluated from measured axial Cs-137 activity profiles. The calculated rod average burnups vary between the codes, but all are within ± 2 MWd/kgU of the measured values for each rod. This good agreement shows that all participants have input the power histories appropriately, warranting a high confidence in the code outputs.

The fuel centre temperature as a function of time and the radial fuel temperature profiles at a specific time during irradiation were requested as output to assess the condition of the fuel after irradiation. In general, the fuel temperatures were in good agreement. For example, modelled fuel centre temperatures were within a 100 °C range.

Calculated radial burnup profiles can be compared to cerium data measured by laser ablation, which are normalized to the average pellet burnup, and to the cerium concentration profile measured by SEM-WDS. The latter data exhibit a somewhat sharper increase at the periphery, compared to laser ablation data and calculated profiles. Within the relatively large scatter of the laser ablation data, good agreement is found between all codes and the laser ablation profile. All codes have models for the high burnup peaking at the pellet rim, but the calculated width of the high burnup structure (HBS) shows large variations. In the pellet interior, TRANSURANUS and FRAPCON typically give approximately 5% lower burnup than the other codes. It should be noted that the radial burnup profiles of TRANSURANUS and FRAPCON are similar because they use the same TUBRNP model [11].

The results of the porosity models were requested as a function of fuel radius taken at the axial location of the LOCA test specimens. The radial profiles for total porosity for rod R2D5 are shown in Fig 1. The apparent porosity can be evaluated using light optical microscopy (LOM) and image analysis on polished cross sections. The measured data are labelled LOM in Fig 1. Average porosity for R2D5 was 2.9%. It should be kept in mind, however, that optical microscopy yields lower bounding values, because pores smaller than 0.3 μm are not visible.

The figure shows that the calculated porosity profiles are quite different. The calculated average porosity varies from 3.3% (JASMINE) to 6.1% (ALCYONE). This should be compared to the as-fabricated initial porosity of 3.8%. FRAPCON has a model for porosity increase at the pellet periphery which is the result of the HBS, but it does not describe the porosity evolution inside the pellet. JASMINE has no model for the porosity in the HBS, but it does model the porosity evolution inside the pellet. ENIGMA, TRANSURANUS and ALCYONE have more complete evolution porosity models. At the fuel centre, their porosity results are similar, but in the dark zone, at $1.8 < r < 3.2$ mm, which is characterized by a very high density of intergranular gas bubbles, ALCYONE calculates 50% higher porosity than TRANSURANUS and ENIGMA.

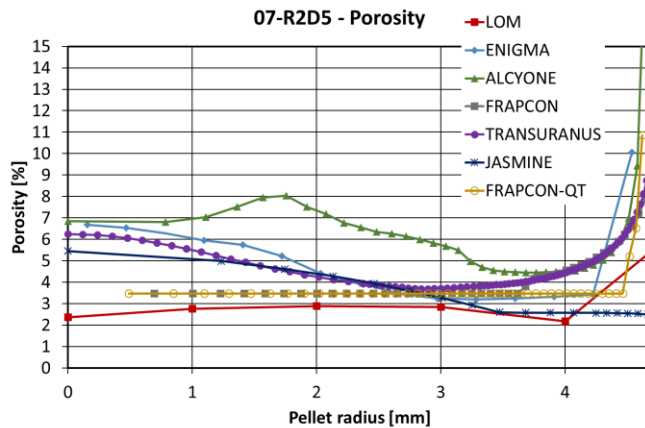


Fig 1. Fuel pellet porosity as a function of radial position.

Since overpressurisation of fission gas bubbles and pores most probably is an important factor for fuel fragmentation in a LOCA transient, the fission gas distribution and partition are of specific interest. A normalized laser ablation profile of the retained Xe-132 gas is compared to calculated profiles for rod R2D5 in Fig 2. In general, there is good agreement between measured and calculated retained gas concentrations. TRANSURANUS and FRAPCON, however, calculate gas release from the periphery large enough to turn the curve downward which contradicts the measurement. Furthermore, the retained gas concentration calculated by ENIGMA appears somewhat low in the pellet centre. The measured high peaks in the dark zone region, are probably caused by large gas bubbles opened by the laser, which thus leads to a somewhat overestimated amount of retained gas in this region.

The difference between generated and retained fission gas is the released fission gas. The fission gas release (FGR) calculated by the different codes for rod R2D5 varies from 2.9 to 8.3%, to be compared to the measured value of 6.5%. For all rods, most calculated results fall within $\pm 1\%$ of the calculated average value. However, for each rod, there is one or two outliers. The measured FGR is in the range of predictions for rods R2D5 and 36U-N05, but for rod 3V5/Q13 all calculated FGR values are lower than the measurement.

The partitioning of fission gas in different components, such as released fission gas, fission gas at grain boundaries and fission gas in precipitated intragranular gas bubbles is important to accurately model fission gas behavior. High-power operation of rod R2D5 has resulted in both significant FGR from the fuel centre, but also in a prominent dark zone with a high concentration of precipitated large gas bubbles. By comparing measured SEM WDS Xe concentrations along the pellet radius with calculated gas in solution, it was found that only ALCYONE results agreed with the measured data. The reason is that the codes do not

properly take the precipitated gas bubbles into account. The bubbles, whose gas content cannot be measured by SEM WDS, thus make up the difference between calculations of gas in solid solution and measured gas in solution for most codes. This difference is particularly important for the dark zone and could be important for the development of fuel fragmentation models. Since fuel fragmentation occurs by fracture along the grain boundaries [5], the gas at the grain boundaries is also important for the development of any fuel fragmentation model. Most of the codes in the MWS include gas partition models which calculate the gas at grain boundaries. The calculated radial distribution of grain boundary gas for each code is shown in Fig 3 for rod R2D5. There is a large variation between the results of different codes, indicating model differences. Several models calculate peaks in the fraction of gas at grain boundaries in the dark zone. This indicates a high concentration of gas at grain boundaries, which may make the dark zone more susceptible to fuel fragmentation. In any case, a mechanistic model of fuel fragmentation surely would need to consider the gas bubbles and the microstructural development of the dark zone.

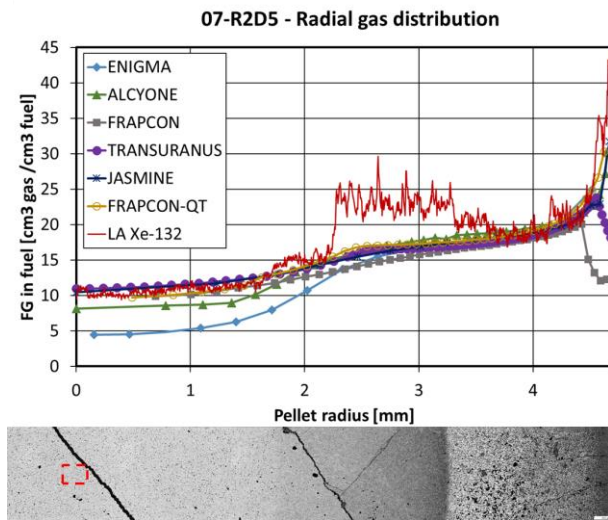


Fig 2. Fission gas distribution in the fuel pellet as a function of radial position for rod R2D5.

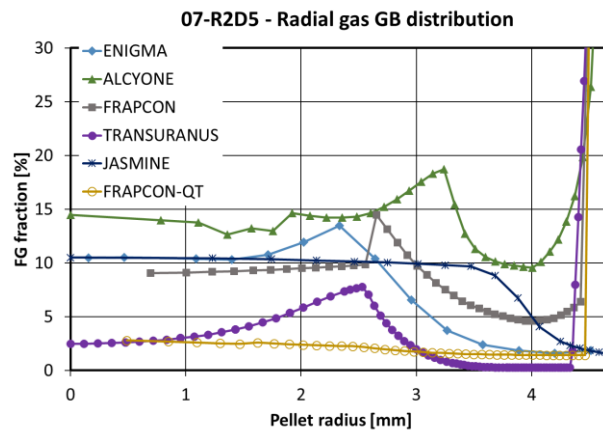


Fig 3. Calculated grain boundary gas fraction for rod R2D5.

4.2 LOCA test cases

The requested output from LOCA test modelling included time traces of cladding and fuel temperatures and rod internal pressure. The rod temperatures all showed good fidelity to the measured data in the LOCA test experiments. The calculated pressure showed quite good agreement with measured pressure, except for RELAP, which strongly overpredicted the pressure increase in all cases. Rod burst is calculated to occur at slightly different times, resulting in different burst temperatures. The burst temperatures are summarised in Fig 4. Overall, calculated burst pressures and temperatures agree well with the measurements. The main exception is RELAP, which calculates too high burst pressure and thus too low burst temperature. After burst, all codes calculate instant pressure drop to ambient pressure, which does not agree with measurement. It takes a few minutes for the pressure to decrease. This shows that no participating code models the gas communication in the rod and the gas flow out from the rod. Modelling the gas communication may be important both in predicting the burst, but also to model fuel dispersal from the rod.

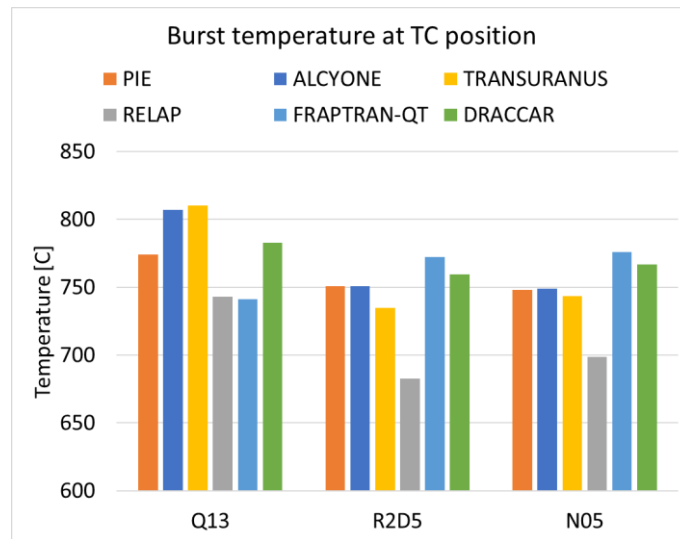


Fig 4. Burst temperatures for LOCA tests 5-7.

Modelling of the Studsvik LOCA tests has also shown the differences in cladding and fuel temperatures due to the external furnace heating. The difference in fuel temperature between external and internal heating of the fuel in a LOCA test is quite modest, except at the time when the pellet-cladding gap is at its largest. In this case, the fuel is temporarily isolated from the external heating and the temperature at the fuel periphery may be 50 °C lower than at the cladding inner surface. This suggests that fuel fragmentation in an in-pile experiment should be similar or slightly more severe than an out-of-pile experiment, considering only the fuel temperature impact on fragmentation. The comparison of temperatures after burst also shows differences in heat transfer models. Steam may enter the fuel rod after burst and affect the heat conduction over the pellet-cladding gap. TRANSURANUS and ALCYONE shows low fuel outer temperature at high cladding temperature, which is consistent with poor heat transfer by steam in the gap. Comparing calculated fuel outer and centre temperatures after burst shows that DRACCAR and FRAPTRAN-QT calculate high fuel outer temperature compared to the fuel centre. FRAPTRAN-QT models the thermal effects of crumbling of the fuel pellet stack into the balloon. When the pellet stack crumbles, the fuel stack radial temperature distribution in FRAPTRAN-QT changes because of reduction of the pellet-cladding distance and reduction of the thermal conductivity of the crumbled fuel. The combined effect is that the fuel center

temperature increases while the surface temperature decreases after the pellet stack has collapsed.

For each LOCA modelling case, the cladding permanent hoop strain along the test rodlet was calculated. The permanent strain, as a function of axial position for burst test case 5, is shown in Fig 5. Most codes show quite good agreement with the measurement. However, the strain calculated by TRANSURANUS scattered significantly, and most codes significantly underestimated strain. In TRANSURANUS, there is no model available for M5 cladding and instead a model for E110 cladding was used. This may explain the low permanent strain calculated by TRANSURANUS in Fig 5. Moreover, the LOCA correlation in TRANSURANUS is now being revised. The three modelling cases 7-9, which were all performed on specimens from fuel rod R2D5, are of special interest for predictions of the ballooning strain since two tests were interrupted before burst. For case 7, all codes calculated burst with large strains in agreement with the experiment. For case 8, all codes calculated non-failure with small strain in agreement with the experiment. For case 9, ALCYONE, TRANSURANUS and RELAP indicated burst, while FRAPTRAN-QT and DRACCAR indicated non-burst. This test was non-burst and the differing predictions thus illustrate just how close to burst this test was. Despite calculating burst in cases 7 and 9, TRANSURANUS underestimates the ballooning strain. It seems that the burst criterion and the strain calculation are not consistent. ALCYONE overestimates strain in case 9, but since ALCYONE indicated burst for this test, the calculated strain is consistent with the prediction of burst.

Except for ALCYONE and FRAPTRAN-QT, the participating codes lack models for transient gas release. For case 6, the total transient gas release was 4.7% (FRAPTRAN-QT) and 3.8% (ALCYONE). By comparing with the calculated time of burst, it was found that approximately half of the calculated transient FGR occurs before burst. The values correspond to the release from the full length of the rodlet. However, most gas will be released at the location of the peak temperature and this is also the most likely location of the balloon. Considering the slow axial gas communication in most parts of the rod, a significant gas release at the balloon may be important for cladding burst. It was not part of the MWS, but clearly a study of the transient gas release at the balloon would support understanding of this issue.

In LOCA test case 6, FRAPTRAN-QT calculates a spike in the gas release just 5-6 seconds before burst. For ALCYONE, the release is more gradual and starts 50 s earlier. The calculated transient gas release as a function of fuel outer temperature is shown in Fig 6. This figure illustrates that for case 6, ALCYONE calculates start of the gas release at a lower temperature than FRAPTRAN-QT. For each modelled LOCA test case, FRAPTRAN-QT predicted larger transient gas release than ALCYONE. Gas release at low temperature is associated with grain boundary fracture and release of the gas available there. For thermal diffusion to become important for fission gas release, the fuel temperature must exceed 800 °C. The conclusion is that fission gas released by diffusion would not be able to contribute to ballooning and burst in the Studsvik LOCA tests. Grain boundary fracture with transient gas release can also be associated with fuel fragmentation. Thus, the transient gas release models in FRAPTRAN-QT and ALCYONE may support development of a fuel fragmentation model. However, none of the participating codes yet includes such a model.

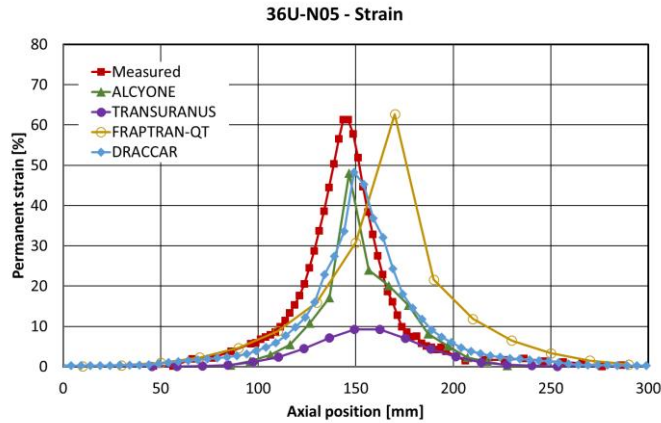


Fig 5. Axial distribution of cladding permanent hoop strain on the LOCA test specimen from rod 36U-N05, i.e. case 5.

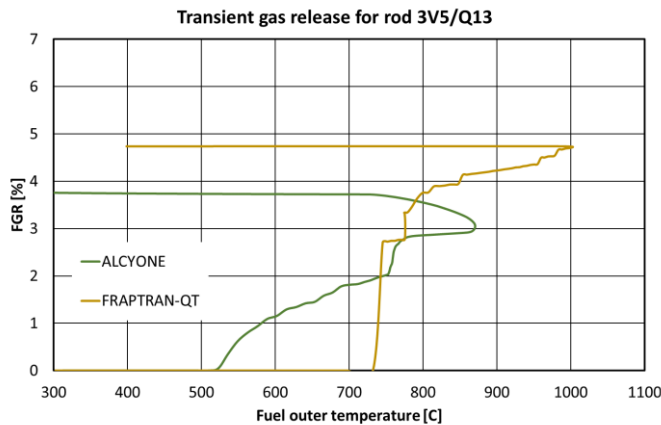


Fig 6. Calculated transient gas release in LOCA case 6.

5 Summary and conclusions

As part of the OECD/NEA international research project SCIP III, a modelling workshop was organized. The purpose of the MWS was to benchmark results from participating codes on out-of-pile LOCA tests performed on high burnup fuel rods in the Studsvik hot cells. Five LOCA tests were modelled, as well as the base irradiation of three corresponding high burnup PWR fuel rods. Eight organisations contributed modelling results, applying the code systems ALCYONE, FRAPCON/FRAPTRAN, TRANSURANUS, ENIGMA, DRACCAR, JASMINE/RELAP and COPERNIC.

In general, the results from base irradiation modelling show good agreement between calculated and measured values. Differences were noted for porosity and gas distributions. ALCYONE has the most advanced gas partition model, which provides the best agreement with measurements by laser ablation and SEM WDS. There is a large difference in the calculated gas at the grain boundaries by different codes and this is likely due to a lack of experimental data. Improved models for bubble precipitation and microstructural evolution in the so called dark zone may support development of thresholds for fine fragmentation.

LOCA test modelling showed overall good agreement with Studsvik LOCA test results, regarding burst/no burst, burst pressure, burst temperature and peak permanent strain. However, the MWS also revealed a lack of models in many codes for several of the parameters of interest for prediction of fuel fragmentation, relocation and dispersal (FFRD), e.g.

- Burst opening size
- Fuel fragmentation
- Length of relocation (only FRAPTRAN-QT)
- Packing ratio (only FRAPTRAN-QT)
- Transient gas release (only FRAPTRAN-QT and ALCYONE)
- Gas flow / pressure drop after burst
- Fuel dispersal

SCIP III and the Studsvik LOCA tests provide data on most of the phenomena above. The data will be useful for developing correlations and models for FFRD. SCIP III will end in 2019, but the experimental work on FFRD is planned to continue in SCIP IV with more detailed examinations and focus on separate effects studies.

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