Pre- and Post-Test Simulations of the QUENCH-18 Bundle Experiment in the frame of the NUGENIA QUESA Project

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ABSTRACT

Air ingress into the reactor pressure vessel during a severe accident in a nuclear power plant will lead to a mixed atmosphere mainly consisting of air and steam. Due to the strongly oxidizing character of air this mixed atmosphere leads to an enhanced core oxidation and degradation which affects the fission product release from the core to the primary circuit and subsequently to the containment in case of leaks or through relief valves. Several fission products are of high importance because of their high radiotoxicity and their ability to form highly volatile oxides. It is therefore important to understand the phenomena governing cladding oxidation by air as a prerequisite for source term determination. For investigating the oxidation behaviour under mixed air/steam atmospheres two experiments were conducted in the frame of two EU funded projects, QUENCH-18 (ALISA project) and CODEX-AIT3 (SAFEST project).
For both tests, pre- and post-test simulations were done in the frame of the NUGENIA project QUESA (QUEnch experiment with Steam and Air). This paper deals with the analyses for QUENCH-18 conducted at KIT in 2017. The pre-test benchmark was performed by five participants (EDF, GRS, IBRAE, LEI, and formerly of PSI) using four codes (MAAP, ATHLET-CD of AC^2, SOCRAT, twice RELAP/SCDAPSIM) to identify suitable boundary conditions for achieving the targets of the tests, which should consist of the following phases: pre-oxidation, intermediate cooldown, air/steam ingress phase and finally cooldown by water. Additionally, the pre-test analyses were supported by parameter studies from GRS to define the boundary conditions. The results of the pre-test benchmark show mainly comparable behaviour of the simulations except one. Oxygen and steam starvation were predicted, which was one target of the experiment to allow nitride formation as well. For the post-test benchmark nearly the same participants as for the pre-test analyses performed simulations by application of the actual boundary conditions of the experiment. The objective is to evaluate the code capabilities especially related to the air ingress modelling, which is at different development levels for the codes. Primarily the preliminary results of the post-test benchmark and the comparison to the measured data available at the time of this present study will be presented in this paper. The comparison shows in general a good prediction of the measured behaviour by all codes.

KEYWORDS
QUENCH-18, Air Ingress, Severe Accidents, Benchmarks, Code Evaluation

1. INTRODUCTION

During a severe accident in an NPP, air ingress into the vessel will lead to a mixed atmosphere inside the core mainly composed of steam and air. Air is a highly oxidizing atmosphere that can lead to an enhanced core oxidation and degradation affecting the release of Fission Products (FP). Several fission products are

of high importance because of their high radiotoxicity and their ability to form highly volatile oxides. It is therefore of great importance to understand the phenomena governing cladding oxidation by air as a prerequisite for the source term prediction.
Extensive separate-effects tests have been performed recently for better understanding of the mechanisms of air oxidation of zirconium alloys and extraction of corresponding data mainly at IRSN and KIT. The accumulated data have demonstrated that cladding oxidation by air is a remarkably complicated phenomenon governed by numerous processes whose role can depend critically on the oxidizing conditions, the preceding oxidation history and the details of the cladding material specification. A number of air ingress bundle experiments on claddings have been performed under a range of configurations and oxidizing conditions, namely AIT-1, AIT-2, QUENCH-10, PARAMETER SF4 and QUENCH-16.
The QUENCH-10 and QUENCH-16 experiments were performed at KIT with a 21-rod assembly. The target scenario was characterized by:

1. a steam pre-oxidation to reproduce the core uncovery,
2. an air oxidation to reproduce the air ingress into the vessel with a period of oxygen starvation,
3. a reflood initiated at temperatures well below the melting point of the cladding.

Based on the SAFEST (CODEX) and ALISA (QUENCH) calls for proposal, the idea was to define a counterpart of QUENCH-16 but with a mixture of air and steam instead of pure air in order to investigate the phenomenology which can occur in a reactor or spent fuel pool scenario.
The technical issues of the NUGENIA QUESA project as well as the proposed air ingress tests QUENCH-18 and CODEX-AIT3 was to extend both phenomenological understanding and the modelling of cladding oxidation under a mixture of air and steam. The project QUESA aims at studying and modelling more precisely the way the oxide layer is formed. It would be also an opportunity to know the influence of this kind of atmosphere on hydrogen production, for instance during bundle reflood. The current status of the phenomenology of air/steam mixtures is give e.g. in [1].

2. QUENCH-18 TEST

In the frame of the EC funded project ALISA (Access to large infrastructures for severe accidents in Europe and in China) the experiment QUENCH-18 on air ingress and aerosol release was successfully conducted at KIT on 27 September 2017. The initiative for this test was proposed by XJTU Xi'an (China) to investigate several topics like absorber rod behaviour, burst of pressurized rods, air ingress with steam and reflooding [2]. The primary aims were to examine the oxidation of M5® claddings in air/steam mixture following a limited pre-oxidation in steam, and to achieve a long period of oxygen and steam starvations to promote interaction with the nitrogen. QUENCH-18 was thus a companion test to the earlier air ingress experiments, QUENCH-10 and QUENCH-16 (in contrast to QUENCH-18, these two bundle tests were performed without steam flow during the air ingress stage). Additionally, the QUENCH-18 experiment investigated the effects of the presence of two Ag/In/Cd control rods on early-phase bundle degradation (comparability to QUENCH-13), and two pressured unheated rod simulators (60 bar, filled with He). In general, the test conduct could be divided into the following phases which were set up together with pre-test simulations (cp. Chapter 3):

- Pre-oxidation,
- Intermediate cooldown,
- Air/steam ingress,
- Quenching.

In Figure 1 the main components of the QUENCH facility are shown (left) together with the implemented bundle as it is specified for QUENCH-18 with M5® claddings. Additionally, the main dimensions of the bundle components are given in Table I. The reactor typical components (rods, absorber rods and guide tubes) are made of M5® or stainless steel with typical dimensions, while components only necessary for the experiment like corner rods (estimation of the oxide layer at different stages of the test sequence) and shroud are made of Zircaloy.

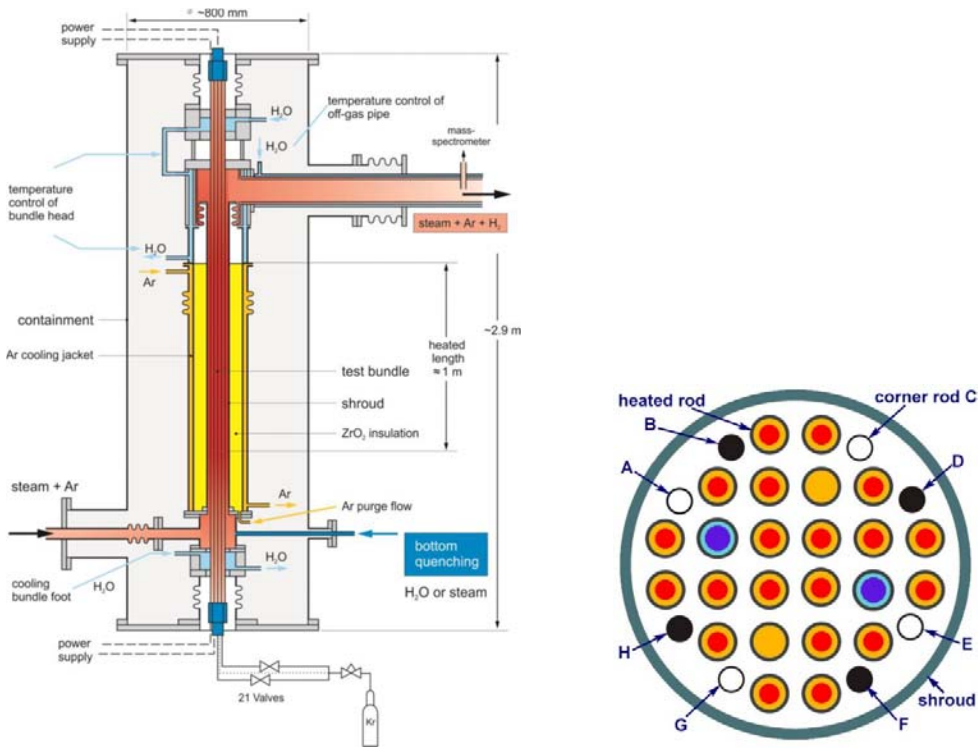

Figure 1, QUENCH facility (left) [3] and bundle (right) [2]

Table I. Main parameter of the QUENCH-18 bundle components [2]

Component	No.	Material properties	Outer diameter (mm)	Inner diameter (mm)
Rod Cladding	22	M5®	9.50	8.36
SIC Absorber Rod	2	Ag 80%, In 15%, Cd 5% density: 10.17 g/cm³	7.65	
Absorber Cladding	2	Stainless Steel	9.68	7.72
Absorber Guide Tube	2	M5®	12.45	11.25
Corner Rod	8	Zry-4	6.00	
Shroud	1	Zry	89.00	83.00

The applied boundary conditions for flow rates and power are given in Figure 2 together with the temperature at 950 mm which is in general one of the elevations where the highest temperatures can be observed in QUENCH tests. After the commissioning phase before 0 s the heat-up of the bundle and the pre-oxidation was realized by a power increase and a constant steam and argon mass flow rate. For the intermediate cooldown the power was reduced again. With this power and a reduced steam mass flow rate together with air (20% O_2 and 80% N_2) the mixed steam/air phase was initiated at 7540 s and takes 4789 s before quenching and power decrease was started to cool the bundle.

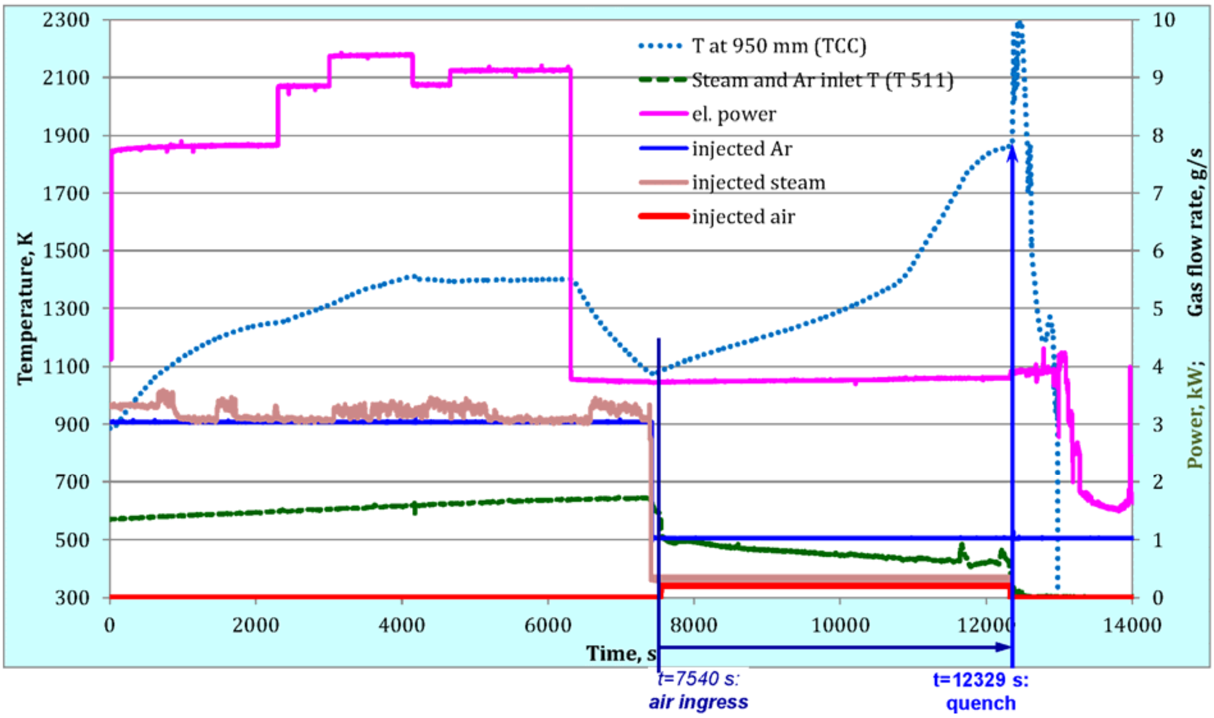

Figure 2, QUENCH-18 test conduct [2]

3. PRE-TEST BENCHMARK

In the frame of the NUGENIA QUESA project pre-test simulations of the QUENCH-18 experiment were performed to investigate and confirm planned initial and boundary conditions to achieve the targets of the test. In this phase four different codes were applied by five participants:

- EdF MAAP
- GRS ATHLET-CD as part of the code system AC^2
- IBRAE SOCRAT
- Jon Birchley RELAP/SCDAPSIM
- LEI RELAP/SCDAPSIM

while both simulations with RELAP/SCDAPSIM were done with version 3.5 including different updates [4,5]. Besides that, parameter studies were performed with ATHLET-CD after the initial simulations for identifying suitable initial and boundary conditions for the final pre-test benchmark, which is shortly described in the following. Detailed information about the pre-test benchmark is given in [4,5].

The results of the pre-test calculations show that all participants predict a comparable behaviour during the pre-oxidation and the intermediate cooldown phase. Afterwards for a long period of the mixed steam/air ingress phase most predictions – except LEI – show a similar behaviour, but at the end the different level of modelling of the phenomena during this phase leads to differences (Figure 3). The different temperatures at the end of the mixed phase lead to a temperature increase during reflooding in some calculations with maxima of more than 2000 K.

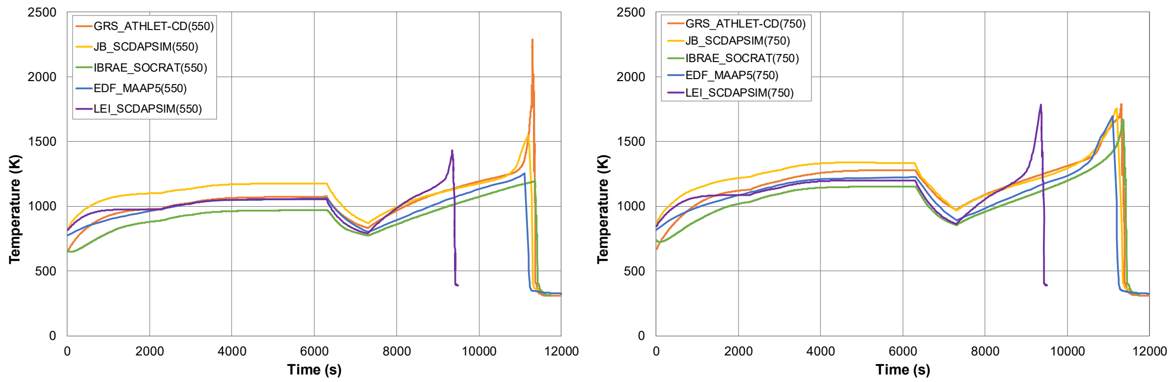

Figure 3, Calculated cladding temperatures at 550 mm (left) and 750 mm (right) of the pre-test benchmark

The specified objectives of the experiment like oxygen and steam starvation are predicted by the simulations for a comparable point of time with some differences in the evolution of the mass flow rate at the outlet of the bundle (Figure 4). For the codes (ATHLET-CD and SOCRAT), which have models for nitride formation, also nitrogen consumption is calculated with good agreement (Figure 5). Unfortunately, the points of starvation are very close to each other, which makes the identification of different phenomena and interactions harder. Figure 5, right side, shows that hydrogen generation is predicted for pre-oxidation, mixed steam/air phase and subsequent flooding by each code in a more or less pronounced way.

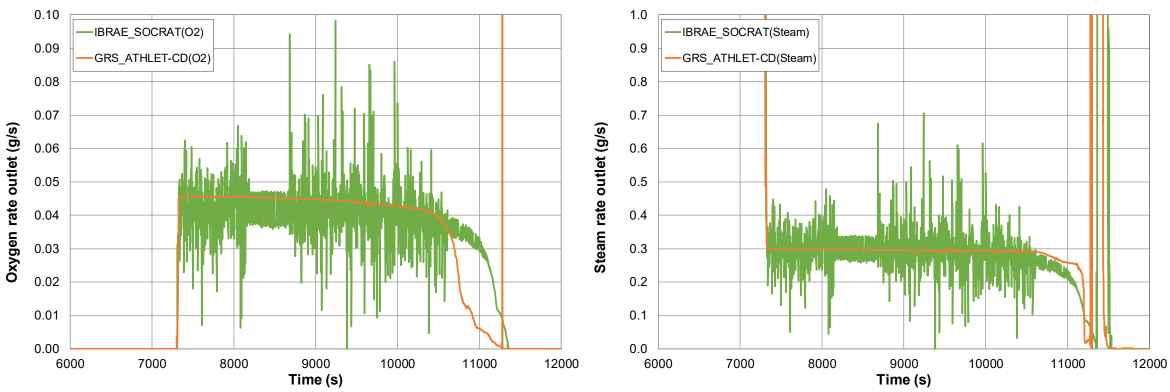

Figure 4, Calculated oxygen (left) and steam (right) flow rate at the outlet of the pre-test benchmark

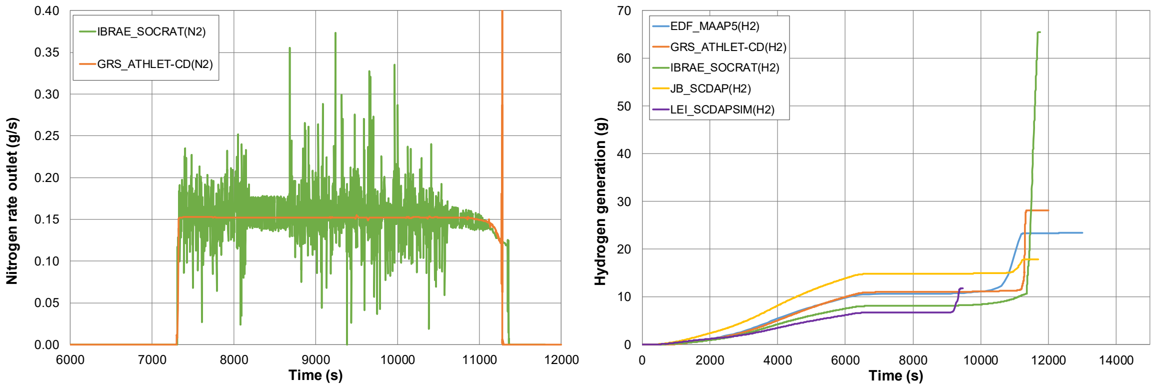

Figure 5, Calculated nitrogen flow rate at the outlet (left) and hydrogen generation (right) of the pre-test benchmark

4. POST-TEST BENCHMARK

The following chapter deals with the post-test benchmark about the QUENCH-18 experiment in the frame of the NUGENIA project QUESA. At first, the used codes and chosen model options by each participant are shown. The discussion and evaluation of the achieved results in comparison to the experimental data, as far as they are available, is done by main events at certain stages of the experiment and by time depending parameters.

4.1. Used Codes and Model Options

The post-test calculations were performed by four different participants using three different severe accident tools:

- GRS ATHLET-CD as part of the code system AC^2
- IBRAE SOCRAT
- Jon Birchley RELAP/SCDAPSIM
- LEI RELAP/SCDAPSIM

In comparison to the pre-test simulations the models of the participants were partially updated for the post-test analyses to predict the observed experimental behaviour correctly. Table II summarizes the used options by each participant while the ones for the pre-test analyses are given in [4,5]. The electrical resistance is in a small range for all simulations which means that the power in the heated zone of the bundle is approximately the same in all cases and the losses in the supply line are comparatively small. Also for the steam oxidation the models are comparable with only slight differences in the chosen correlation for the reaction rate. In contrast to the steam oxidation the assumption for the air ingress phase differs in the codes. ATHLET-CD includes a separate model for the reaction of oxygen and nitrogen from air. The re-oxidation of ZrN is not directly considered but by an accelerated oxidation depending on the thickness and porosity of the ZrN layer which leads to a high hydrogen release especially during reflooding. If steam and air are available, first the oxygen of the air is consumed and afterwards steam and nitrogen in parallel as it is observed in single effect tests at KIT. In SOCRAT both reactions of the air are considered, too. There is a model for oxygen diffusion which is enhanced depending on the ZrN molar fraction and an empirical model for the nitride formation depending on the nitrogen content in the gas. In the used RELAP/SCDAPSIM version nitride formation is not calculated at all in SCDAPSIM. Nitrogen is treated as a catalyst for the oxidation by both oxygen and steam. One can interpret that physically in terms of a small amount of nitriding occurring, even if there is no obvious uptake of nitrogen. RELAP/SCDAPSIM as well as SOCRAT do not model re-oxidation of ZrN. SCDAPSIM calculates the CR failure and movement of molten material within the rod, but does not model release of absorber and aerosol transport in the fluid, while the failure is predicted by all codes as function of temperature or Fe-Zr liquefaction. The cladding rupture is also considered in all codes which is mainly relevant for the burst of the pressurized fuel rod simulators.

Table II. Model options of the used codes for the post-test benchmark [6]

Code version	ATHLET-CD 3.1A	SCDAPSim/3.5da/psi		SOCRAT v2
User	GRS	Jon Birchley	LEI	IBRAE
Electrical resistance (mOhm/rod)	3.5	3.6	3.8	4.0
Steam Oxidation Correlation	Cathcart - Prater/Courtright	Leistikow/ Prater-Courtright	Leistikow-Schanz/Prater-Courtright	Cathcart-Pawel & Leistikov-Schanz / Prater/Courtright & Leistikov-Aly
Air Oxidation (or Oxygen) Correlation	NUREG2 (T<1180K) and NUREG1 (T>1450K) with interpolation inbetween	Utsuega-Hofmann/Urbanic Heidrick; FM reduction factor for low concentration	Utsuega-Hofmann/Urbanic-Heidrick for oxygen	Oxygen diffusion enhancement factor depending on ZrN molar fraction. Pure oxygen is treated as vapour except chemical heat.
Nitriding Correlation	Hollands	No nitriding. Birchley model for accelerated oxidation	No nitriding. Birchley model for accelerated oxidation	Empirical model depending on nitrogen content in gas mixture.
Possibility of nitrides re-oxidation	re-oxidation not modelled – consideration of porosity	no	no	no
Cladding failure criterion	max. strain 38 %	MATPRO ballooning burst	MATPRO ballooning burst	On temperature (T) if ZrO_2 layer thickness (d) less than prescribed value.
SIC degradation /release	release model not used	Candling of molten SIC when cladding and guide tube liquefied	Candling of molten SIC when cladding and guide tube liquefied	no
SIC failure criterion	1523 K	MATPRO Fe-Zr liquefaction	MATPRO Fe-Zr liquefaction	1450 K

4.2. Simulation Results

The simulation results of the post-test are given in Table III and in Figure 6 to Figure 9 in comparison with the experimental values. For the pre-oxidation phase the overall predicted results are comparable for all simulations. The maximum temperatures are quite close at the end of pre-oxidation also for the subsequent intermediate cooldown which is necessary to avoid too strong oxidation reactions leading to a fast temperature increase during the air/steam mixture phase. All simulations show that reflooding causes a temperature escalation up to over 3000 K except for the SOCRAT calculation. Due to the fact that the measured boundary conditions were used for the calculations the main times are quite close for all simulations, only the quench phase differs in the predictions. Table III indicates that oxygen starvation is calculated in a quite small range, but for ATHLET-CD local starvation moves downwards to 150 mm leading to high oxygen consumption and temperature increase while in the other calculations the starvation front moves only to the middle bundle elevations. Corresponding to that the lowest elevation of absorber failure is much lower for ATHLET-CD.

Table III. Main events of the post-test simulations

Code version		ATHLET-CD 3.1A	SCDAPSim/3.5da/psi		SOCRAT v2
User		GRS	Jon Birchley	LEI	IBRAE
Total H_2 generation (g)	end of preoxidation	10.5	12.3	8.2	4.4
	end of reflood	151.0	202.7	263.7	232.0
Maximum T (K)	end of pre-ox (before cooldown)	1382	1416	1311	1258
	end of intermediate cooldown	1038	1071	908	939
	during reflood	(3000)	3069	3126	2230
Time (s)	of T_{max} at the end of air phase	12329	12329	12325	11666
	of T_{max} during reflood	12410	12434	12394	12304
	of final QUENCH	13450	12988	13000	15372
	onset of complete O_2 consumption	10400	10836	10306	10174
Lowest elevation	O_2 was complete consumed (mm)	150	650	550	550
	at time (s)	12300	11374	12200	10174
Lowest elevation	control rod failure (mm)	50	450	250	950
	at time (s)	12225	11450	9999	10452

The results of the post-test simulations show that the codes are in good agreement to the experiment during the pre-oxidation phase and the intermediate cooldown (Figure 6 and Figure 7), only SOCRAT underestimates the temperatures in the lower and middle bundle elevations. During the steam/air ingress phase the spreading of the predicted temperatures are wider for the simulations and also the deviation to the measured data increases. Due to the different models for the phenomena of air ingress and the priority of the reactions of oxygen, steam and nitrogen of the three used codes the behaviour is not similar, but in general the calculations show the capability of the codes to consider the phenomena. Furthermore, especially in the lower and middle elevations up to 750 mm the calculated qualitative behaviour of all codes represents the experimental observations. From the point of oxygen and steam starvation the temperatures spread due to the different stages of model implemented in the codes.

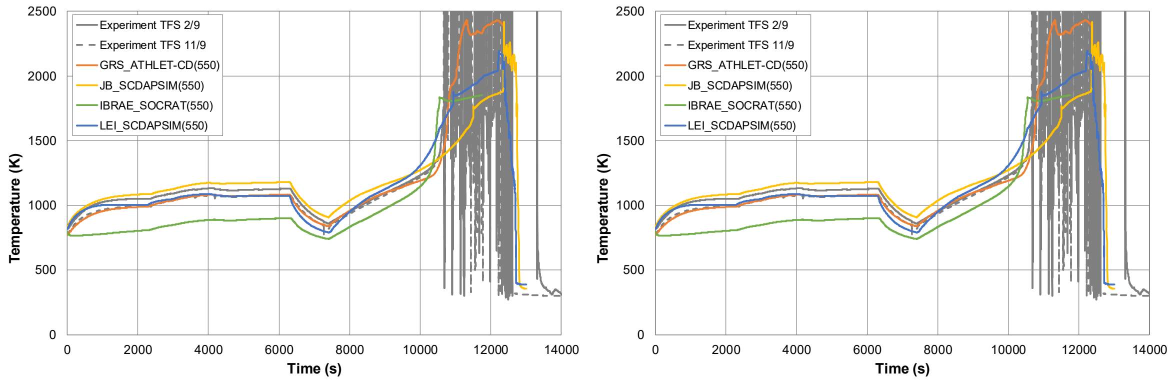

Figure 6, Measured and calculated cladding temperatures at 350 mm (left) and 550 mm (right)

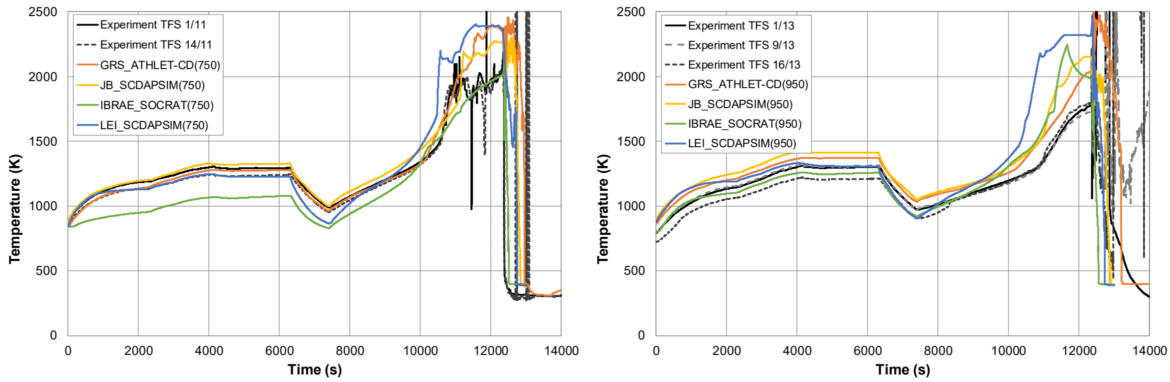

Figure 7, Measured and calculated cladding temperatures at 750 mm (left) and 950 mm (right)

The main objective of the test to ensure oxygen and steam starvation during the mixed steam/air phase is predicted by the codes (Figure 8). Especially for the oxygen consumption, which is due to the chemical process, the first and preferred reaction of the metallic Zr leading to total oxygen starvation at approximately 10700 s in the experiment is calculated in close agreement to the measured data by the codes. E.g., for ATHLET-CD 100 g of O_2 are consumed compared to 104 g measured in the experiment. The subsequent steam oxidation, which occurs in parallel to nitride formation, led to an almost total steam starvation at 11000 s in the test. This steam starvation is predicted by the codes roughly at the same time compared to the experiment, but SOCRAT and RELAP/SCDAPSIM of LEI calculates a faster and the other simulation with RELAP/SCDAPSIM a slower steam consumption, while ATHLET-CD is closest to the measured behaviour. Both codes ATHLET-CD and SOCRAT, which consider also nitrogen consumption leading to ZrN (with intermediated reaction stages), predict also nitrogen consumption (Figure 9), e.g., for ATHLET-CD 80 g of N_2 are consumed compared to 120 g in the experiment, which shows an underestimation although the mass flow rates at the outlet of the bundle is comparable. This could be an indicator for the very diffusive local processes during the steam/air phase, which may be clarified by the final post-test examination of the bundle.

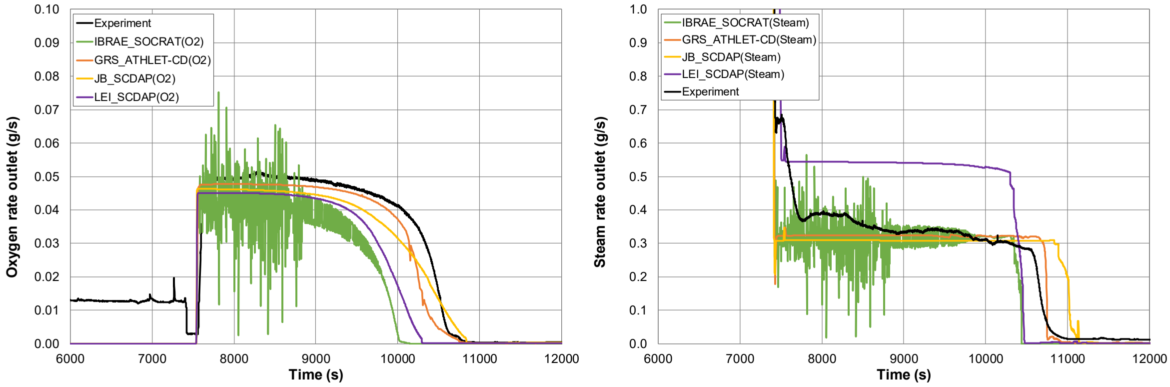

Figure 8, Measured and calculated oxygen (left) and steam flow rate (right) at the outlet

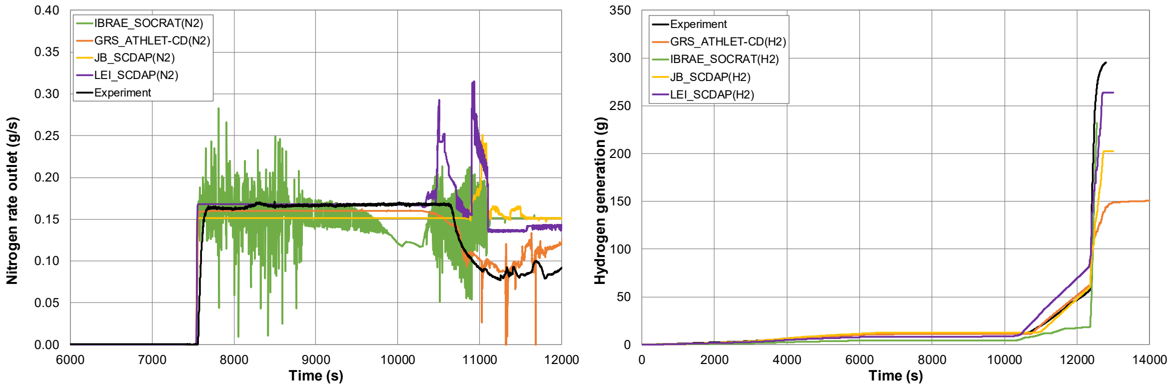

Figure 9, Measured and calculated nitrogen flow rate at the outlet (left) and hydrogen generation (right)

In general, the calculations show the capability of the codes to predict steam and air oxidation (notably nitride formation) in parallel, which lead to a more or less developed H_2 generation in that phase (Figure 9). Both RELAP/SCDAPSIM simulations as well as ATHLET-CD show a comparable behaviour to the measurement, while SOCRAT underestimates the H_2 production during the mixed steam/air phase. All codes underestimate the hydrogen generation more or less distinctive (cp. Figure 9 and Table III), but for the quantification of the hydrogen generation by each component the post-test examinations have to be finalized. Afterwards, the comparison and evaluation of the simulations can be done, because not all components of the experiment are modelled, e.g. in previous test the outer side oxidation of the shroud led to significant H_2 production after shroud failure, but this is not considered in all numerical models.

5. CONCLUSIONS

The pre- and post-test simulations supported the experiment QUENCH-18 performed at KIT in 2017 by the set-up and approval of the initial and boundary conditions also by parameter studies as well as by the prediction of the bundle behaviour. In general, the pre-test simulations show a good agreement to the observed data until the boundary conditions were changed in the experiment due to aerosol reasons. The post-test calculations performed with ATHLET-CD, RELAP/SCAPSIM and SOCRAT predict in general a good agreement to the measured values. Due to different stages of modelling of the phenomena during the mixed steam/air ingress phase the behaviour differs in that phase but represent qualitatively the measured temperatures. Nevertheless, the main objective of the experiment to ensure oxygen and steam starvation are fulfilled by the calculations in close agreement to the test. Nitrogen consumption, which can occur in parallel to steam oxidation after oxygen consumption, is predicted by the codes which have a dedicated nitride formation model (ATHLET-CD and SOCRAT). During the mixed phase the steam oxidation led to H_2 generation which is predicted by the codes. The hydrogen production during the subsequent flooding is underestimated by all codes, which could be explained by the different level of detail of the modelling or the considered models. For the concluding comparison and evaluation of the simulation results for the whole test sequence the post-test examinations are needed, which will be done in the future also to identify further potential for model improvement.

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