SIMULATION OF THE AIR INGRESS EXPERIMENT PARAMETER SF4 USING ATHLET-CD

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Abstract

The air ingress test PARAMETER SF4 was performed in July 2009 with the aim to investigate the behavior of a VVER bundle during reflooding after air ingress. Simulations are performed using the severe accident code ATHLET-CD. The results of the simulations show a good agreement in comparison to the experimental data during the pre-oxidation phase and in most bundle regions also during air ingress. The hydrogen generation is very close to the experimental data up to the beginning of quenching; afterwards the total amount of H_2 is underpredicted. Further improvement can be achieved by using a model to consider ZrN formation.

1. Introduction

In the case of postulated incidents or accidents in nuclear facilities air can be in contact with the cladding of the rods mainly in the following three cases [1]:

1. loss of coolant accident (late phase after reactor pressure vessel failure or in mid loop operation),
2. spent fuel pool accident or
3. spent fuel storage cask break.

In these cases zirconia and nitride formation can occur by the reaction of the cladding material zirconium with the two main components of air – oxygen and nitrogen. Both reactions are exothermal, but the exothermal heat of the zirconia formation is nearly three times higher than that of the nitride formation. At first zirconia formation will occur by water or steam, because of the affinity of metals like zirconium to react with oxygen. This process is estimated as the leading one. Afterwards in cases of local or global oxygen starvation the nitride formation can take place. The phenomenology of zirconia formation is mainly understood for zirconium based cladding material and implemented in severe accident codes.

The consideration of the nitride formation is necessary to calculate the physical behavior of the core completely and correctly in severe accident codes due to the impact on the cladding material and its further behavior in the case of a severe accident. Therefore, the knowledge of the phenomenology during nitride formation has to be improved. Detailed analyses of single effect tests show that two main phenomena have to be considered for nitride formation. On the one hand the reaction of pure nitrogen with zirconium is weak and mainly based on impurities of the metal in a binary system. On the other hand nitride formation increases in case of a ternary system of Zr-O-N, which might be the case for reactor applications. Therefore, the existing ZrO_2 layer on the metal has a dominant influence, since the nitrogen reacts with defects in the under-stoichiometric zirconia layer or under oxygen starvation conditions after breakaway and formed cracks at the phase boundary between Zr and ZrO_2 [2], [3].

2. PARAMETER SF4 Facility and Test Conduct

In the following subchapters the PARAMTER test facility is described and all data of the test conduct, considered in the simulation, are given.

2.1 PARAMETER Facility

The PARAMETER facility represents a part of a typical VVER core and consists mainly of 19 fuel rod simulators. This assembly was used for four tests within the SF test series which was performed to investigate the bundle behavior under different quenching conditions e. g. top and/or bottom flooding. The fourth test was performed as air ingress test, so that the facility had to be modified in comparison to the previous tests. The assembly of the bundle and the special features for air ingress are discussed in the following, because these components are substantial for the simulation using ATHLET-CD.

The bundle consists of 18 electrically heated fuel rod simulators which are arranged around one unheated central rod in a VVER typical triangular assembly (cp. Figure 1). The tantalum heater with a heated length of 1275 mm is surrounded by UO_2 pellets and a cladding which has an outer diameter of 12.75 mm and is made of the typical VVER material Zr1%Nb. The unheated central rod is instrumented with measurement devices and consists basically of a cladding. During air ingress the cladding is streamed with air from the bottom up to -120 mm below the beginning of the heated length (cp. Figure 1), where twelve holes are drilled and air can stream in the heated bundle to simulate the air ingress. The bundle is surrounded by a 1.2 mm thick shroud (outer diameter 69.7 mm) made of Zr1%Nb like the rod cladding. The shroud itself is isolated by an insulation of 23 mm ZrO_2. At the outer side of the shroud and its insulation a flow path called “Cooling jacket” is arranged which is streamed with cooling water during the test.

At the beginning of the test, the lower plenum (900 mm) is partial filled with water below the inlet pipes for steam and argon. The inlet for quench water is located nearly the bottom of the lower plenum [4], [5]. By the implementation of separating plates in the upper plenum the injected water and the exhausting gas/steam mixture cannot directly flow into the outlet pipe. This part can lead to an underestimation of the pressure drop, because the plates cannot be simulated exactly (cp. [5]).

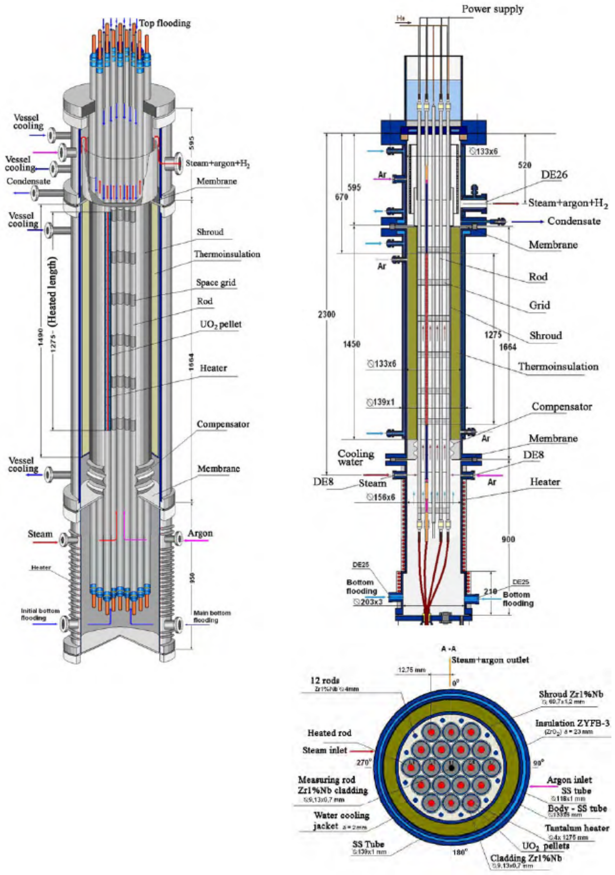

Figure 1 PARAMETER SF4 test section and bundle cross section.

All given lengths are related to the beginning of the heated length, which is set to 0 mm (cp. Figure 1).

2.2 SF4 Test Conduct

On the basis of pre-test calculations performed by different institutes the air ingress test SF4 was performed on the 21st July 2009 at LUCH research center in Podolsk, Russia. The test consists of following phases given in Figure 2 (cp. [4], [5], [6]):

1. Heat up of the bundle with an electrical power of 2 kW up to app. 500 °C. In this phase argon and steam are injected in the test section.
2. Stepwise increase of the power to reach app. 1200 °C in the hottest part of the bundle.
3. Pre-oxidation by steam for 6000 s at app. 1200 °C with an electrical power of 7.5 to 8 kW.
4. Intermediate cool down by decreasing the power to ~ 4 kW to attain app. 900 °C before the onset of air ingress. End of steam flow at 16022 s.
5. Beginning of air ingress (0.5 g/s) at 16035 s. Low flow rate to get oxygen starvation conditions which are necessary for nitride formation. Accelerated heat up by a stepwise increase of the power from 4 to 6 kW. End of air ingress at 17511 s.

6. At the temperature criterion of 1740 °C at 17412 s the electrical power is switched off and bottom flooding is initiated at 17434 s with a flow rate of 80 g/s which is reduced and increased again. Top injection of argon during quenching. A temperature escalation is observed at the beginning of the quench phase.

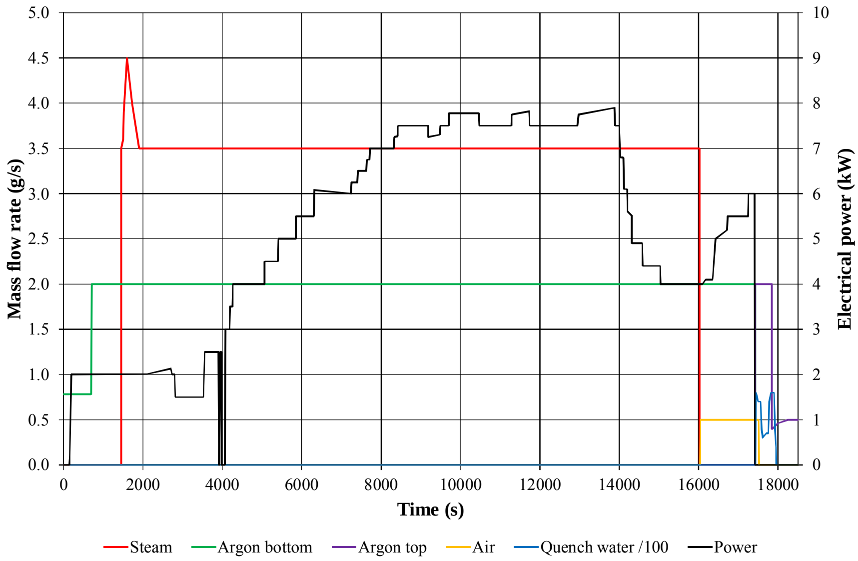

Figure 2 Boundary conditions of PARAMETER SF4.

3. Numerical Modeling

The used severe accident code ATHLET-CD (Analysis of THermal-hydraulics of LEaks and Transients – Core Degradation) as well as the modeling of the air ingress in ATHLET-CD is briefly described in the following subchapter. Additionally, the nodalization of the test section is given.

3.1 ATHLET-CD code description

The ATHLET-CD code has been developed and validated for accidents resulting in major core damage. The development and integration of models in ATHLET-CD is done by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) in close co-operation with the Institut für Kernenergetik und Energiesysteme (IKE), of the University of Stuttgart. By the models for the formation and movement of metallic and ceramic melts in the core area and the thermal behavior of particle beds, as well as for the release of fission products and aerosols in the core area and their transport and deposition in the cooling circuit, the application range of the computer code has been extended significantly. This is demonstrated by successful post calculations of bundle and integral experiments or the TMI-2 accident and the incident at Paks-2. Full plant simulations can be performed by coupling ATHLET-CD with the containment code COCOSYS. The ATHLET-CD structure is modular, both to provide a variety of models for the simulation and to provide an optimum basis for further development. For a comprehensive simulation of the thermal-fluid dynamics in the nuclear steam supply system, the ATHLET system code has fully been integrated [7].

3.2 Modeling of air ingress in ATHLET-CD

The current released version ATHLET-CD 2.2A1 contains a model for considering the oxidation of Zr alloys by oxygen of air, but no model to calculate nitride formation by nitrogen of air, because as discussed above nitrogen is handled as an inert gas like in other severe accident codes, too. The model for air oxidation is quite similar as for the oxidation by steam, but the heat of this exothermal chemical process is nearly two times higher, because no dissociation of water or steam is necessary. The reaction in air starts with parabolic kinetics given by the following equation for the formation of zirconia using m' as mass of oxidized zirconium per surface area in kg/m^2 and a reaction rate R_i as function of temperature [8]:

$$dm'/dt = R_i\,(T)\,/\,m'. \qquad (1)$$

At an oxide layer thickness which is defined by input data (standard value 0.25 mm) a transfer to linear kinetics is made. This has the effect that a further increase of oxide mass is not considered on the right side of equation (1) to simulate the effects of cracking and breakaway observed in experiments [8].

The reaction rate R_i which is needed for the solution of equation (1) is described by an Arrhenius type equation:

$$R_i = A_i \cdot e\,(-E_i / T) \cdot g(p_{O2}) \cdot F_{lim,O2}, \qquad (2)$$

where i selects the empirical correlation with A_i and E_i (cp. Figure 3). $g(p_{O2})$ is a function of the oxygen partial pressure to consider oxygen starvation. $F_{lim,O2}$ is an input value which could be used as a preliminary compensation for the up to now unavailable nitride formation model or to consider geometric effects, since the empirical values are mainly determined for rod geometries [8].

A first approach is formulated to consider also nitride formation, which is used in the simulations to identify the direct and indirect impact of nitride formation as well (cp. Chapter 4). The numerical approach differs from the ones of oxidation, but it was necessary to formulate a general equation depending only on temperature ranges. The mass gain is formulated as a function of the reaction rate, a time depending value and the free surface for the reaction [3]:

$$\Delta m = R_i\,(T) \cdot t^{n_i} \cdot A_{rod}. \qquad (3)$$

The reaction rate is also expressed as an Arrhenius function as in equation (2) including comparable parameters for nitrogen:

$$R_i = A_i \cdot e\,(-E_i / T) \cdot g(p_{N2}) \cdot F_{lim,N2.} \qquad (4)$$

By using the method of least squares the parameters for the empirical correlations (A_i, E_i and n_i) are determined on the basis of single effect tests performed at KIT (formely: Forschungszentrum

Karlsruhe), Germany (cp. [2], [3]). For the determination of the parameters it is also necessary to distinguish between cladding which is pre-oxidized or not, but due to the fact that cladding is nearly always pre-oxidized in reactor applications only this case is shown in Figure 3.

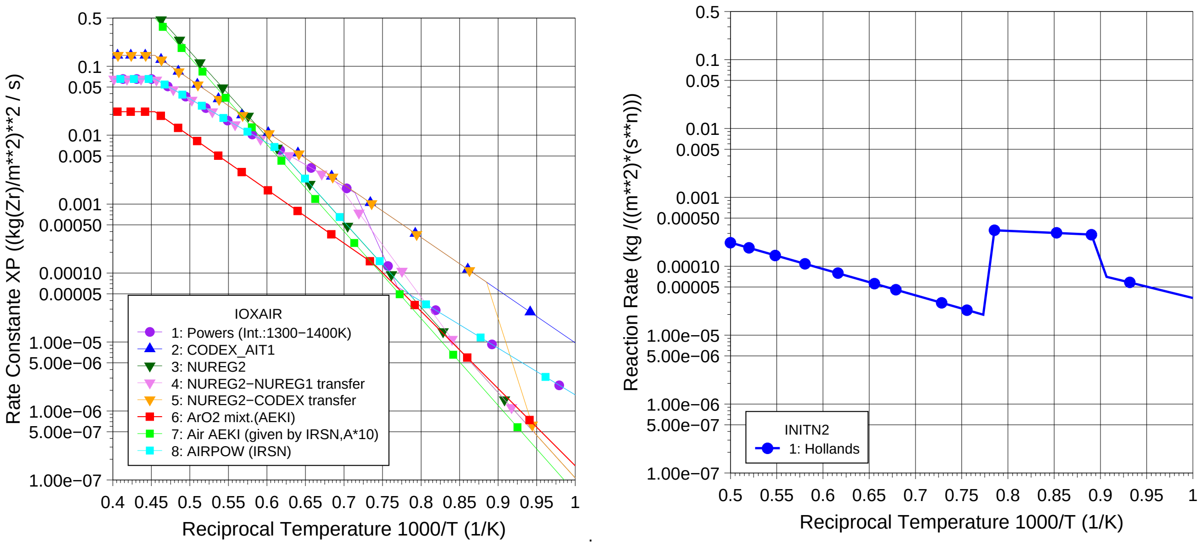

Figure 3 Reaction constant of oxidation and reaction rate of nitride formation.

3.3 Nodalization of the test section

For the simulation of the test only the test section itself is considered and all peripheral components and flows are implemented as initial or boundary conditions [9].

The bundle is modeled as three rings representing one unheated central fuel rod simulator (ROD1), six heated fuel rod simulators (ROD2) and twelve fuel rod simulators (ROD3), which are axial divided into 21 nodes (Figure 4). The part of the electrical molybdenum heaters contains 14 nodes and the upper copper electrode is not considered in the simulation. The flow path through the bundle is divided into two regions, CORE2 which is connected with the RODs and CORE3 which is connected with the twelve corner rods made of Zr1%Nb, too (cp. Figure 1). Both flow regions are connected by cross connections. Inside two cells above the SHROUD the cross connections have high friction coefficients to simulate internals of the facility. The outer vessel region is coupled with the outlet pipe OUTPIPE which has a time depending volume at its end to simulate the condenser.

The inlet flow of air, which is inserted via the unheated rod, is modeled as separate external fills for O_2 and N_2 on the same level like the fills for steam and argon, while the inlet for the quench water is located at the bottom (cp. Figure 4).

The surrounding shroud and its insulation are simulated as heat conducting structures in the same manner like the six grid spacers. The inner side of the SHROUD as well as the GRIDs can be oxidized by steam and air. The outer wall of the thin shroud cannot react, because it is part of one structure (SHROUD) including the insulation and has no free surface for oxidation.

The outer cooling gap is modeled by the flow path JACKETTUBE and the heat conduction structure H-JACTUBE as outer wall. Energy exchange due to radiation is simulated between RODs and SHROUD as well as between SHROUD and H-JACTUBE.

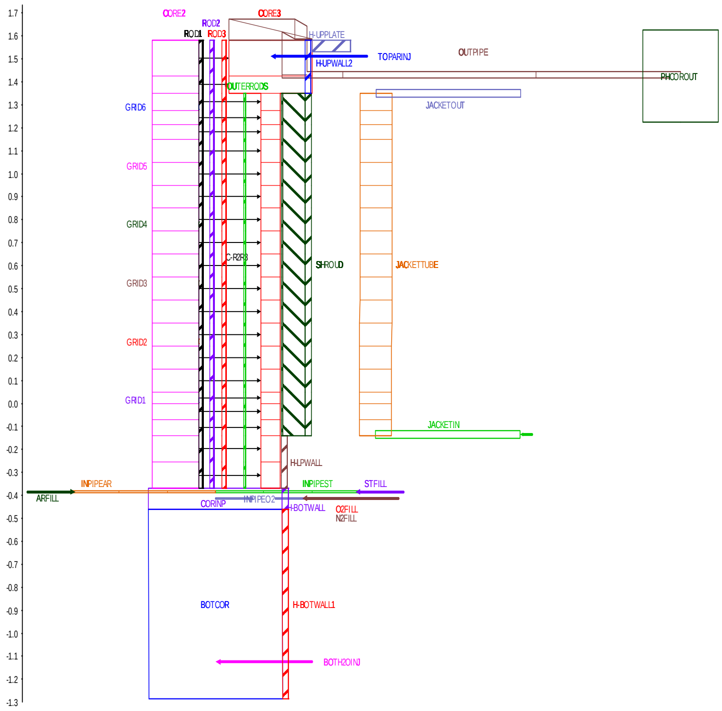

Figure 4 Nodalization of PARAMETER SF4 in ATHLET-CD [9].

4. Simulation results

The results of the simulations will be discussed in the following chapter focussing on the temperature behavior, the oxygen consumption and the hydrogen generation. Therefore, three different simulations are considered: a reference calculation, one with a lower candling velocity and one using a model for ZrN formation. Mainly the results of the reference calculation are discussed; the results of the other simulations are given for comparison.

4.1 Temperature behavior

The temperatures of the first three phases until the end of pre-oxidation are simulated by ATHLET-CD in good agreement to the experimental data and the maximum plateau temperature of app. 1155 °C is calculated at 1250 mm as in the test (1235 °C), but slightly underestimated.

At the beginning of the air ingress the simulated temperatures are also in good agreement to the experiment until app. 17000 s before a too fast heat up rate is calculated for all heights up to 900 mm (cp. Figure 5 and Figure 6). The chosen correlation, which represents the lowest reaction rate for the oxidation within ATHLET-CD, leads to an overestimation of the oxidation and the corresponding temperature escalation from that point of time when oxygen starvation occurs in the upper heights. Due to that, the temperature escalation moves downwards and the critical temperature of 1740 °C for power switch off and the subsequent bottom flooding is reached at 500 mm, which tallies with the experiment. Different to the experiment the beginning of the flooding is not controlled by the temperature but by the measured point of time (17412 respectively 17434 s) to be able to compare the bundle behavior during reflooding. This leads to an app. 210 °C too high maximum temperatures at the initiating of flooding. Although the reaction rate of the shroud is reduced due to geometric reasons the temperatures are calculated in good agreement up to 17000 s, but before start of reflooding the temperatures are higher than the corresponding cladding temperatures.

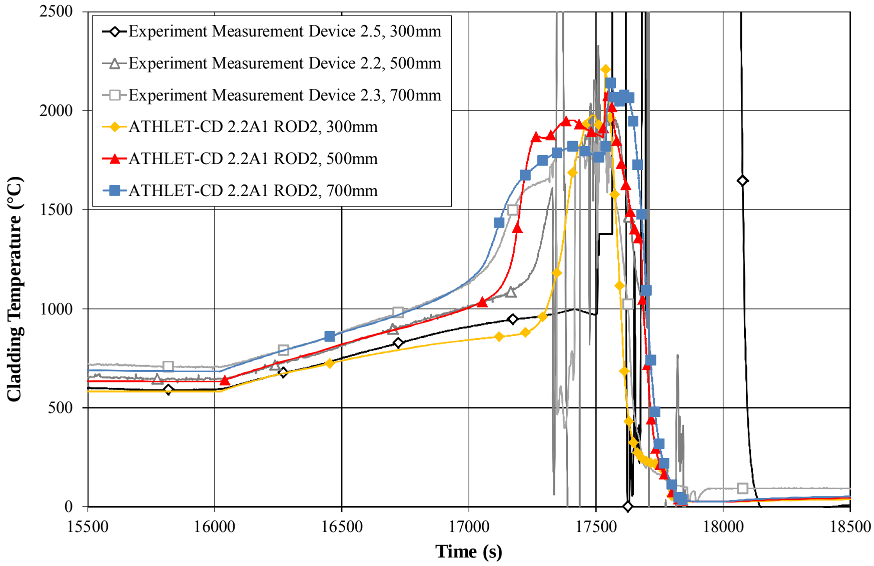

Figure 5 Measured and calculated bundle temperatures (300 to 700 mm).

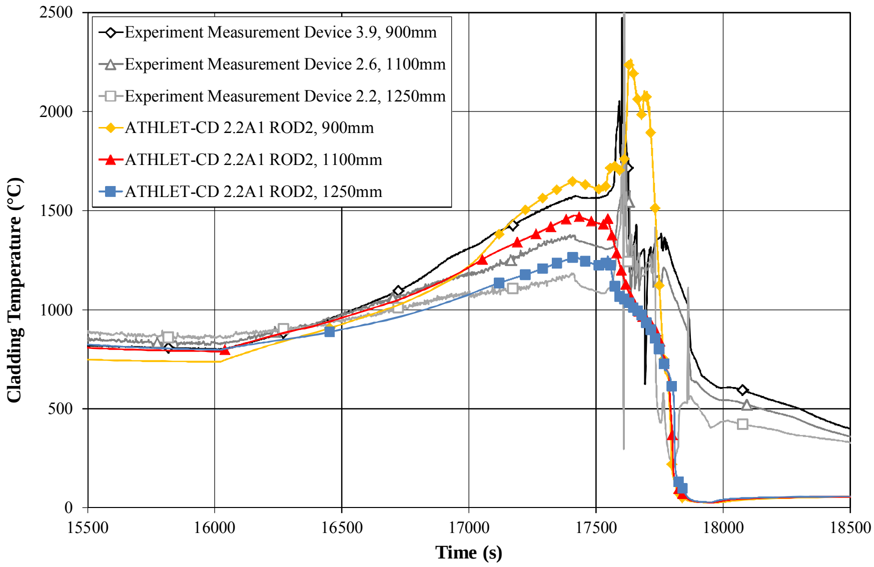

Figure 6 Measured and calculated bundle temperatures (900 to 1250 mm).

In the bundle region above 300 mm a further heat up can be observed after the beginning of quenching leading to a temperature escalation up to more than 2000 °C between 300 mm and 900 mm. A maximum temperature of app. 2320 °C is calculated. Reasons are the exothermal oxidation processes of the still ongoing air ingress and the quench water injection as well as high temperatures at the beginning of the reflood acting as a trigger for the oxidation rates. The measured temperatures up to 900 mm are calculated in a quite good agreement by ATHLET-CD during the first phase of quenching. The subsequent slow cool down of the experiment is not simulated, because of the relocation downwards to 200 mm (500 mm in the experiment) the propagation of the quenchfront is calculated faster and, thus, the cool down. In general, the relocation into lower bundle regions is calculated too fast in comparison to the experiment leading to a lower hydrogen production during the quench phase.

The results of an alternative simulation using a slower melt rivulet candling velocity of 2 mm/s (5 mm/s in the reference calculation) show that the cool down is calculated slower and the relocation stops at 500 mm with the formation of a blockage, but the bundle cannot be fully cooled down and the simulation stopped.

4.2 Oxygen consumption

One main goal of the test PARAMETER SF4 was the investigation of the influence of nitride formation during air ingress and the subsequent flooding. Afterwards, the formed ZrN phases can be re-oxidized by steam or air and lead to further weakening of the cladding which can cause an accelerated failure. For the formation of ZrN oxygen starvation conditions have to occur locally or in total. In Figure 7 it can be observed that generally oxygen starvation conditions occur in the experiment as soon as no injected O_2 reaches the outlet of the test section at 17100 s. The reference simulation shows a delay of app. 100 s and oxygen starvation is also not simulated as sharp as in the experiment. Detailed analyses of the results show that oxygen starvation conditions are firstly reached at the top of the test section and move downwards. At 17200 s the program specific limit for oxygen starvation is calculated above 600 mm and nitride formation could occur, but cannot be calculated, because ZrN formation is not yet implemented in the released version ATHLET-CD 2.2A1.

In an alternative simulation using a first model to consider nitride formation the delay of oxygen consumption no longer exists in the simulation and the calculated point of oxygen starvation agrees with the experiment (cp. “ATHLET-CD 2.2A1_N2” in Figure 7), but because of further interactions between the different processes during air ingress the temperatures increase rapidly and their maximum moves downwards leading to a strong overestimation in the lowest heated parts.

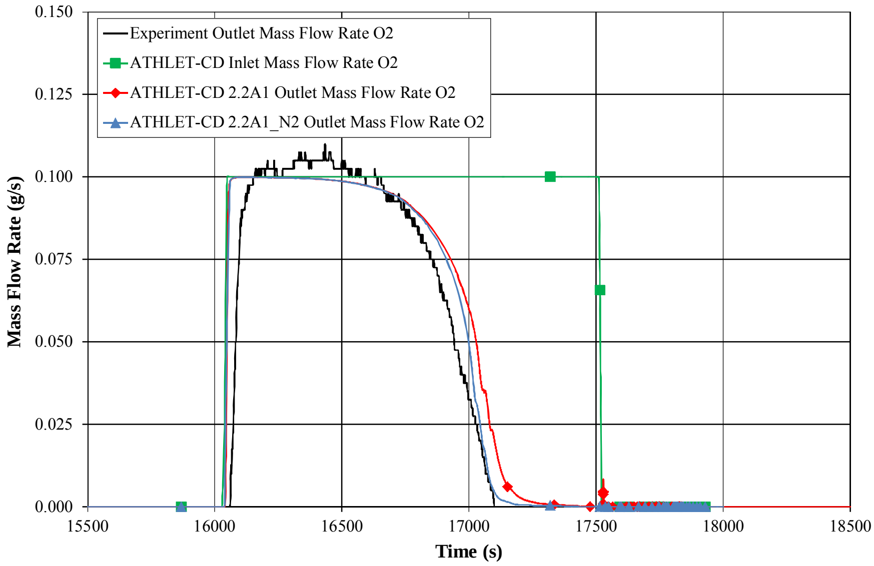

Figure 7 Measured and calculated oxygen mass flow rates.

4.3 Hydrogen generation

The released mass of hydrogen as a product of the exothermal Zr-H_2O reaction depends mainly on the Zr alloy and for each alloy several correlations were developed. In ATHLET-CD there are four main correlations implemented, one specific for Zr1%Nb, but comparable to other tests and codes this so called "Sokolov" correlation underestimates the H_2 generation, so that the correlation of "Cathcart/Prater-Courtright" is used to simulate the H_2 production more realistic during the pre-oxidation phase. In this phase the experimental value of app. 21 g is simulated in very good agreement to the experiment and corresponds to the thermal behavior as well [9].

During quenching the hydrogen generation increases very fast in the experiment up to 107 g in total while 86 g were produced in this phase. In the reference simulation totally only 76.6 g H_2 were released corresponding to 72 % of the total experimental mass. The largest fraction results from the RODs (53 g), while the hydrogen generation by melt oxidation is negligible (cp. Figure 8). A reason for the underestimation is the too fast relocation leading to a lower blockage compared to the experiment and the flooding water can penetrate the bundle quicker. Another one could be the fact that the outer side of the shroud cannot oxidize, which might have an impact in the experiment, because the bundle as well as the shroud were degraded and surfaces for oxidation occurred. Furthermore, a general underestimation of melt oxidation can be observed using ATHLET-CD.

In both alternative simulations the hydrogen generation is simulated in a better agreement to the experiment. The simulation using the lower candling velocity shows that 91 g H_2 are produced, representing 85 % of the experimental mass. Furthermore, the hydrogen release by oxidation of melt is 0.9 g, because more melt is available, but this ratio is still quite small in comparison to the total value and to the strong degree of degradation in the experiment. Using the model for the ZrN formation, which leads to higher temperatures at the beginning of the quench phase, the hydrogen production results totally in 99.6 g, representing 93 % of the total amount. Especially, the H_2 generation by melt oxidation increases up to 5.2 g because of the high degree of relocation in the lower heated part of the bundle including blockage formation. In all cases it can be assumed that the hydrogen production by melt oxidation is underestimated, caused by the very strong core degradation which is not simulated completely.

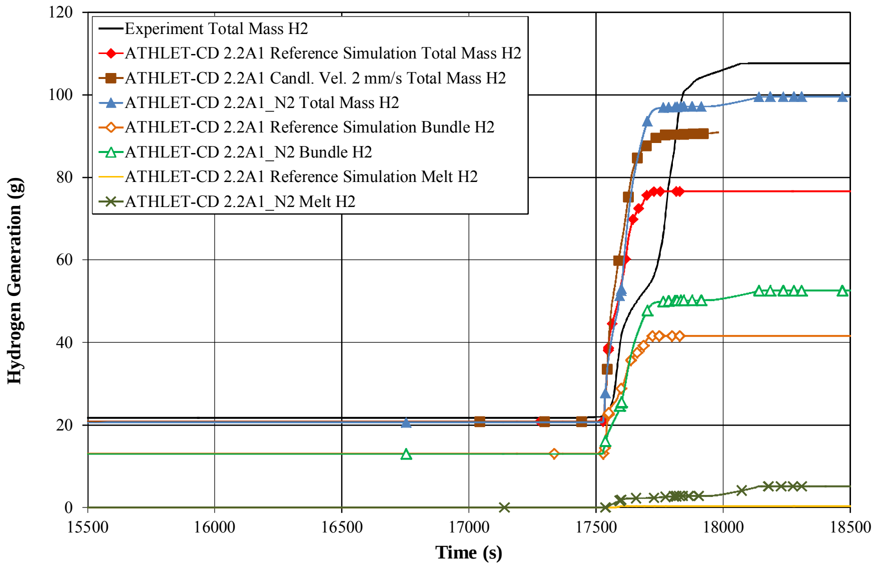

Figure 8 Measured and calculated hydrogen production.

5. Conclusion

The post-test simulation of the air ingress test PARAMETER SF4 using ATHLET-CD 2.2A1 shows that the measured physical bundle behavior can be simulated in very good agreement by the code up to the middle of the air ingress period. Although local oxygen starvation is calculated the temperatures increase because of a too high oxidation rate. In the subsequent flooding the temperatures rise again due to the exothermal oxidation, but decrease too fast afterwards, because the calculated relocation leads to a lower blockage of the bundle and therefore to a faster propagation of the quenchfront and the coolability. The hydrogen generation is simulated in good agreement to the experiment until the beginning of flooding, but during this phase the experimental mass is underestimated. The results of this simulation could be improved using more realistic input values for Zr melt temperatures and by implementing a new model to consider nitride formation during air ingress. First calculations considering the nitride model show an improvement of the results. The model and its input parameters will be further developed and validated.

Acknowledgement

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6. References

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