Simulation of an SBO Accident in a PWR with AC^2/ATHLET-CD with and without using ATF Cladding Material

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ABSTRACT

ATHLET-CD (Analysis of THermal-hydraulics of LEaks and Transients with Core Degradation), which is part of the system code package AC^2 (ATHLET, ATHLET-CD, COCOSYS), is designed to simulate the behaviour of a nuclear power plant during accident scenarios, including core damage progression as well as fission product and aerosol behaviour and lower plenum phenomena. The code system is being developed and improved by GRS. Previously, models and input decks were using standard, zirconium-based materials as cladding. These cladding materials have been used in nuclear reactors all over the world, despite their exothermic reaction with hot steam that can aggravate accident progression and produce easily combustible hydrogen. In order to eliminate or mitigate this drawback of the zirconium-based claddings new materials were developed. These so-called accident tolerant fuel/cladding (ATF/ATC) materials have much better oxidation characteristics during some or most accident conditions.

For predicting and analysing the impact of ATF on accident scenarios, AC^2/ATHLET-CD started improving and adapting the existing models and input decks for ATF materials. In this paper we show two calculations of accident progressions for a postulated SBO accident in a generic PWR. One calculation is performed with standard zirconium-based cladding, one with ATF (FeCrAl) cladding. The comparison of the two calculations will be presented and future development needs will be discussed.

1 INTRODUCTION

The safety of nuclear power plants has always been a paramount concern, motivating continuous efforts to improve and innovate safety measures. The emergence of Accident Tolerant Fuel (ATF) has brought new hope for enhancing reactor safety during severe accidents. ATF materials are designed to withstand more extreme conditions, compared to the currently used materials, reducing the rapid and exothermal reaction between hot steam and cladding material, thus also reducing the likelihood of fuel failure and the release of radioactive materials in case of an accident. As the nuclear industry seeks to implement ATF in existing and future reactors, rigorous evaluations of its effects become imperative. One powerful tool that enables us to explore the potential benefits and challenges of ATF is the use of severe accident codes, sophisticated computer simulations specifically designed to model and predict the behaviour of nuclear reactors under severe accident conditions.

GRS, developer of the severe accident code AC2/ATHLET-CD, is dedicated to follow the developments in the field of nuclear safety research and wants to provide for the AC^2/ATHLET-CD users the simulation capabilities to investigate accidents in reactors, where ATF materials are used. There are multiple ATF concepts currently under active investigation in the nuclear community. The most advanced concepts aim to enhance the accident tolerance capabilities of the cladding, either by coating the zirconium with chromium (Cr-coated Zr) or by using iron-aluminium-chromium (FeCrAl) as cladding material.

Recent model developments, therefore, focused on extending the current AC2/ATHLET-CD modelling basis with ATF specific models. GRS is implementing models for FeCrAl material, while RUB, an AC2/ATHLET-CD development partner of GRS, is aiming to allow the representation of Cr-coated zirconium in the simulations.

The ongoing developments in GRS are based and supported by international experiments with ATF materials (for example: Quench-19 [1]) and by international projects (for example: TCOFF-2, QUENCH-ATF). The developments reached a status, where a meaningful validation of the implemented models could have been started and the first investigative simulations on the effects of ATF on the accident scenario could have been carried out.

This paper summarizes the already achieved model developments towards FeCrAl material modelling in AC^2/ATHLET-CD, demonstrates some validation calculations of those models and presents two simulations of the same hypothetical accident scenario in a nuclear reactor, where one core consists of standard fuel elements and the other is using FeCrAl material. The effects of FeCrAl material on the simulation results are then shorty discussed, as well as further development needs and outlook are outlined.

2 AC^2/ATHLET-CD

The system code system AC^2 is primarily developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) and consists of three major modules: ATHLET, ATHLET-CD and COCOSYS. The three modules are dedicated to simulating different stages of a nuclear accident:

- ATHLET covers all the relevant processes during a design basis accident inside the reactor cooling circuit. Core degradation effects are not taken into account, fission product release and transport processes are not considered. The program can simulate the response of the plant safety system via a user-dependent instrumentation control.
- ATHLET-CD uses as basis the original ATHLET input for the calculation of the thermodynamic phenomena and extends the models of ATHLET to be able to calculate processes during a severe accident: phenomena related to oxidation and deformation, as well as core degradation including fission product release and transport inside the cooling circuit.
- COCOSYS simulates the main phenomena in the containment from operational to severe accident conditions. If not used in stand-alone mode COCOSYS receives the thermohydraulic, melt and fission product data from ATHLET/ATHLET-CD.

Coupling all these modules the user can simulate the whole extent of a nuclear accident. However, the user can also use the modules individually. This paper focuses on in-vessel phenomena, therefore only ATHLET/ATHLET-CD was used. ATHLET-CD was developed for standard materials; this means that multiple models assumed that the cladding is made out of zirconium and the fuel consists of UO_2. In order to be able to simulate systems using ATF material, the existing modelling basis had to be reviewed and extended, to allow other correlations, constants and material properties, not just zirconium.

The next chapter will summarize the modelling changes and improvements that made it possible for ATHLET-CD to simulate accidents of nuclear reactors that are using FeCrAl material.

2.1 Model changes in AC^2/ATHLET-CD for ATF material

In order to allow the users to simulate FeCrAl material in the core, the following changes in the source code and in the input deck are required:

1. Change of material properties
2. Change of oxidation kinetics
3. Change of material interactions

1, There were no source code modifications required to change the material properties of the cladding, as the code reads the appropriate values defined by the user from the input deck. Nonetheless, users have to be aware that the parameters for FeCrAl and oxidized FeCrAl have to be provided in the input deck.

2, The largest effort was put into extending the modelling capabilities of ATHLET-CD regarding oxidation. In ATHLET-CD the oxidation rate (of all materials) is determined by a parabolic law that was derived from the analytical solution of the diffusion equation:

$$dW^2 = K * dt \longrightarrow \frac{dW}{dt} = \frac{K}{2W} \tag{1}$$

Where:

- W: m_{ox} / (surface area) in [g/cm^2]
- m_{ox}: mass of the resulting oxidized material
- K: reaction rate in [g^2/cm^{4}s]
- dt: time step [s].

The reaction rate is determined by the following Arrhenius equation:

$$K = A * e^{\frac{-B}{R*T}} * g(p_s) \tag{2}$$

Where:

- R: gas constant [8.314 J/molK]
- T: cladding temperature [K]
- g(p_s): reduction factor to consider steam starvation [$0 \leq g(p_s) \leq 1$]
- A, B: material specific rate constants

The oxidation rate also determines the rate of heat generation from oxidation and the resulting hydrogen generation, each specific for the interacting materials. For zirconium, a lot of correlations exists for different temperature regimes [2]. For FeCrAl, new correlations had to be implemented. Recent single effect tests performed by KIT, presented at TopFuel 2021 [3], lead to the implementation of the following correlations to determine the oxidation rate:

$$K = \begin{cases} 9.62 \times 10^{-12} [g^2/cm^4 s], & T \leq 1473\,K \\ A_B\, exp\left(\frac{-E_B}{RT}\right), & 1473 < T < 1648\,K \\ A_{Fe}\, exp\left(\frac{-E_{Fe}}{RT}\right), & T \geq 1648\,K \end{cases} \tag{3}$$

Where:

- The first two regimes assume oxidation of aluminium
- The third regime assumes oxidation of iron
- R: gas constant [8.314 J/molK], T: cladding temperature [K]
- A_B, E_B: material specific rate constants, A_B=3*10^9 [g^2/cm^{4}s], E_B=594354 [J/mol]
- A_{Fe}, E_{Fe}: material specific rate constants, A_{Fe}=2.4*10^6 [g^2/cm^{4}s], E_{Fe}=352513 [J/mol]

A 50 K transition range was also implemented between the regimes, to limit the abrupt changes in the correlations, however, as the correlations in different regimes deliver significantly different results, the built in transition regime does not have a large effect, as visible in the validation results shown in the next chapter. The contribution of the second equation is very small in the temperature regimes below 1470 K and increases very rapidly from T = 1473 K.

3, Due to high temperatures and contact of different materials, material interactions can occur. The implemented models for interaction between zirconium and different materials are not valid anymore, if the cladding is made out of FeCrAl material. Many of the possible interactions with FeCrAl are still under active theoretical and experimental investigation, therefore, no specific model was added yet to ATHLET-CD. However, the standard models for zirconium interactions were disabled, if the cladding material is FeCrAl. This topic will be in the focus of upcoming developments.

3 VALIDATION

Before using the development version of AC^2/ATLHET-CD for analysing the effects of FeCrAl material in the core on the accident evolution, the newly implemented models, correlations and approaches had to be validated. The QUENCH-19 experiment provided data for the validation.

3.1 QUENCH-19 Facility/Experiment

“The QUENCH-19 bundle experiment was conducted at KIT on 29th August 2018. It was performed in cooperation with the Oak Ridge National Laboratory (ORNL) and was supported by the KIT program NUSAFE. The test objective was the comparison of FeCrAl and ZIRLOTM claddings under similar configuration and similar boundary conditions as the previous QUENCH-15 experiment [4]. Different to QUENCH-15, the new test QUENCH-19 had FeCrAl (Y) claddings and 4 FeCrAl (Y) spacer grids as well as 8 KANTHAL APM corner rods and a KANTHAL APM shroud. For both tests the PWR-typical bundle consisted of 24 heated rods and 8 corner rods inside a shroud, which was insulated by ZrO_2 fiber and surrounded by an Inconel cooling jacket. Inspite of very similar boundary conditions there was a significant difference in the bundle heat-up, a temperature excursion in QUENCH-19 experiment was not observed. The total hydrogen release during the whole test was 9.2 g compared to 47.6 g in the QUENCH-15 test with a much shorter period of high electrical power [1].

3.2 Simulation of QUENCH-19 Experiment with AC^2/ATHLET-CD

The simulation of the QUENCH-19 experiment was performed using a slightly modified version of the input deck of the QUENCH-15 experiment, described in detail in [4]. The modifications included specific boundary condition changes compared to the QUENCH-15 experiment and the required material properties changes that were described in section 2.1. Due to the constraints of this paper, only the most important figures and findings are going to be presented here, to demonstrate the validity of the implemented changes.

Napaka! Vira sklicevanja ni bilo mogoče najti. shows the evolution of the cladding temperature of the innermost fuel rod, at the top of the test section, at elevation of 1050 mm. The measured temperatures at the start of the experiment can be reproduced in the simulations very well, but an approximately 50 K overprediction of the cladding temperature can be observed, beginning at around the start of the pre-oxidation phase, lasting up until the quenching. The amount of overprediction of temperatures is smaller in lower regions. Overall, qualitatively, the evolution of temperatures in the bundle can be simulated. The observed quantitative differences are to be further investigated, but the most likely explanation of the overestimation is the combination of the following points:

- Uncertainty of the temperature measurements (± 0.01*T) ~ ± 10-15 K [1].
- Uncertainties in the input deck.
- ATHLET-CD simulates cladding surface temperatures, the thermocouples were not simulated. In reality, there is a non-ideal contact between the surface of the cladding and the thermocouples. This could lead to lower measured temperatures.
- Inaccuracy of the simulation/models.

The temperature evolution is directly related to the oxidation of the cladding material. ATF materials react with the hot ambient vapour in a similar way to zirconium-based cladding, only the reaction rates and thresholds are different. This exothermic reaction produces heat and hydrogen, which affects the heating of the fuel. The accumulated mass of produced hydrogen is shown in Figure 2.

The initial hydrogen production observed in the experiment, which was slow and gradual, could not be replicated in the ATHLET-CD simulation. Percentual differences between the measured and simulated values are significant in this region. However, the hydrogen production rate remains extremely low until around 1480 K. Therefore, the precise depiction of the low-temperature regime is not crucial. Nonetheless, the constant parameters derived for the low-temperature part of equation (3) require further adjustments.

When the cladding temperatures reach 1473 K a very sharp change in the oxidation characteristics can be observed, hydrogen generation increases rapidly. The increase in the hydrogen production happens earlier in the simulation than in the experiment. This can be attributed to the fact that there is an overall overprediction in the temperatures, therefore the critical threshold temperatures are reached sooner, leading to a larger hydrogen generation sooner. The transition from the low hydrogen generation rate to the high generation rate is not depicted qualitatively. The lower end of validity of the second part of equation (3) needs further improvements, as the rates are increasing extremely rapidly in that region. At the end of the calculation there is an overprediction of the total produced hydrogen mass by about 30% (~3g). The difference to the measured values is relatively large, however, this is the current state of the art [5]. In order to further improve the accuracy of the models experimental and theoretical research on ATF behaviour under BDBA conditions has to continue. Further improvements are expected when the international projects on this topic (for example: QUENCH-ATF [6], IAEA ATF-TS [7] and TCOFF-2 [8]) are finished.

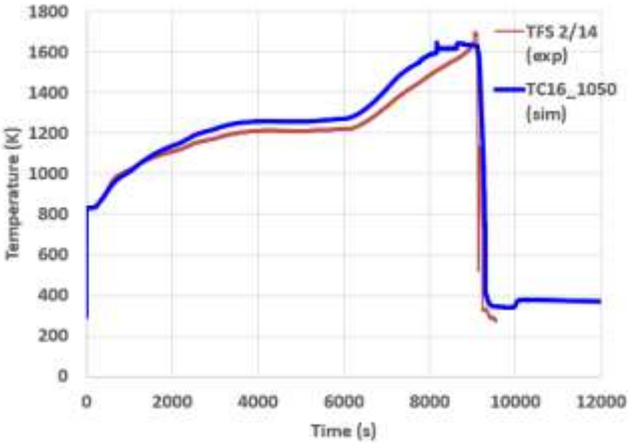

Figure 1: Temperature evolution of cladding in QUENCH-19 at elevation 1050 mm in experiment (blue) and in red (simulated)

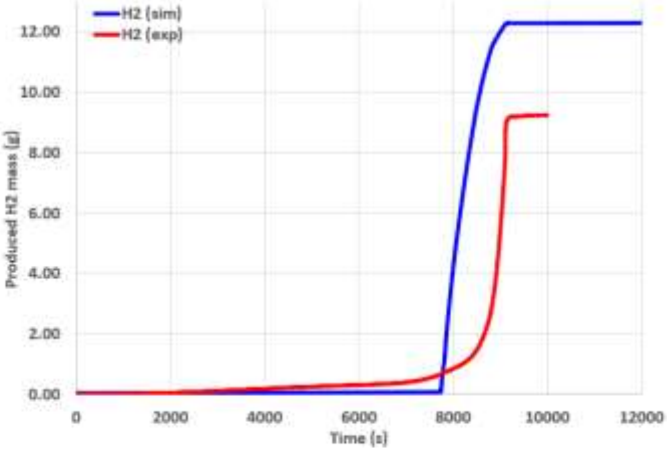

Figure 2: Temperature evolution of cladding in QUENCH-19 at elevation 1050 mm in experiment (blue) and in red (simulated)

Despite the above-mentioned inaccuracies of the simulation, ATHLET-CD can take the effects of ATF on the accident evolution into account. Without the newly implemented ATF-specific models the simulation of QUENCH-19 experiment would have resulted in much larger temperature escalations (max temperature ~2000 K) and much larger hydrogen production (~50 g), like in QUENCH-15 experiment [4].

These acceptable and plausible validation results lead us to use ATHLET-CD to investigate the effects of ATF on the accident evolution of a PWR during a postulated accident.

4 HYPOTHETICAL ACCIDENT SCENARIOS IN A GENERIC PWR

Now that ATHLET-CD is equipped with the initial modelling capabilities to simulate severe accidents in nuclear reactors using ATF materials, it is possible and necessary to assess the benefits and potential drawbacks of ATF materials on the evolution of the accident. This is one of the main goals also of the OECD-NEA TCOFF-2 project [8]. A series of calculations with different postulated scenarios were and are going to be performed on generic reactors to achieve this goal. Each scenario is calculated twice, once with standard cladding material and once with ATF cladding material. Comparing these two calculations can provide information about the usefulness of the ATF materials. In this paper, we present the comparison of the simulations of two postulated SBO+SB LOCA scenarios in a generic PWR, with and without ATF materials, respectively.

The total thermal power of the simulated reactor is 3.78 GW, it has four coolant loops, the leak is defined in the cold leg of the loop with the pressurizer. Postulated area of the leak is 0.025 m^2. The leak and the loss of power are initiated at t = 10 s, after that no operator action is modelled. The simulation is stopped after the reactor vessel failed.

4.1 Simulation of an SBO Scenario with/without FeCrAl material

The combination of the complete loss of power (SBO) and break in the cold leg leads to rapid depressurization. At t = 468 s the hydro accumulators start to inject water into the primary circuit and are emptied in 200 s. At this time, the core is still flooded, which is the reason why the fuel temperatures are still falling and remain more or less constant up until t = 2500 s (left side of Figure 3). In both simulations the core temperatures start to rise at around t = 2500 s, as the water level sinks, and the fuel rods start to get uncovered. There is a slight difference in the start of the temperature increase. This can be attributed to the differences in the material properties, most notably, FeCrAl has a larger heat capacity than zirconium. The temperature increase remains linear in case of the reactor with ATF material, as the power from oxidation is not very dominant. The fuel temperatures with zirconium cladding start to escalate due to oxidation from around t = 3000 s. This leads to a growing difference between the temperatures in the two simulations (left of Figure 3). The presented node reaches its failure temperature and relocates at t = 4000 s in case of zirconium cladding and at around t = 4800 s in case of ATF cladding. In this case, ATHLET-CD turns off the node and sets the fuel temperatures to zero. Note, that the left side of Figure 3 shows the fuel temperature, not the cladding temperature, that is why they have identical melting points. The differences in the oxidation powers can be seen in the right side of Figure 3. There are orders of magnitude differences in the released energy during oxidation, this causes the growing temperature differences in the core. However, the amount of hydrogen generated during the oxidation process does not differ that much (Figure 4). That is, because the energy release during iron oxidation is much less than the energy release during aluminium or zirconium oxidation, but still produces hydrogen. The accident in case of the reactor with ATF cladding produces around 150 kg less hydrogen. In both calculations there are two significant hydrogen production phases, followed by two slower increases, respectively. The first ramp is the initial oxidation, when the cladding temperatures reach the threshold for an extensive oxidation. This leads to core degradation, melt relocations occur and blockages are formed. As a result, steam starvation limits the oxidation, causing only a minor further increase in the hydrogen production. At t = 4050 s (Zr case) and at t = 5000 s (ATF case), the lower grid plate fails, and the accumulated melt relocates to the lower plenum. This opens up the previously formed blockages and the relocated hot melt evaporates the water in the lower plenum, providing sufficient steam for further oxidation in the core. This causes the second ramp in the hydrogen production, followed again by a much lower, steam starved oxidation period. At t = 4990 s the reactor vessel fails in case with zirconium cladding and at t = 6500 s the reactor vessel fails in case with ATF cladding. At the latter time both simulations were stopped. Based on this first investigative and comparative calculations the following preliminary conclusions can be drawn: oxidation of FeCrAl cladding produces significantly less power, thus slowing down the accident progression, but without any operator action, the core still melts. In the analysed scenario the delay of melting is around 800 seconds, and the delay for vessel failure is about 1500 s. This is the extra grace period the operators get as a benefit, if the core consists of cladding with FeCrAl material. The amount of hydrogen produced is less than in case of zirconium, although it is still considerably large.

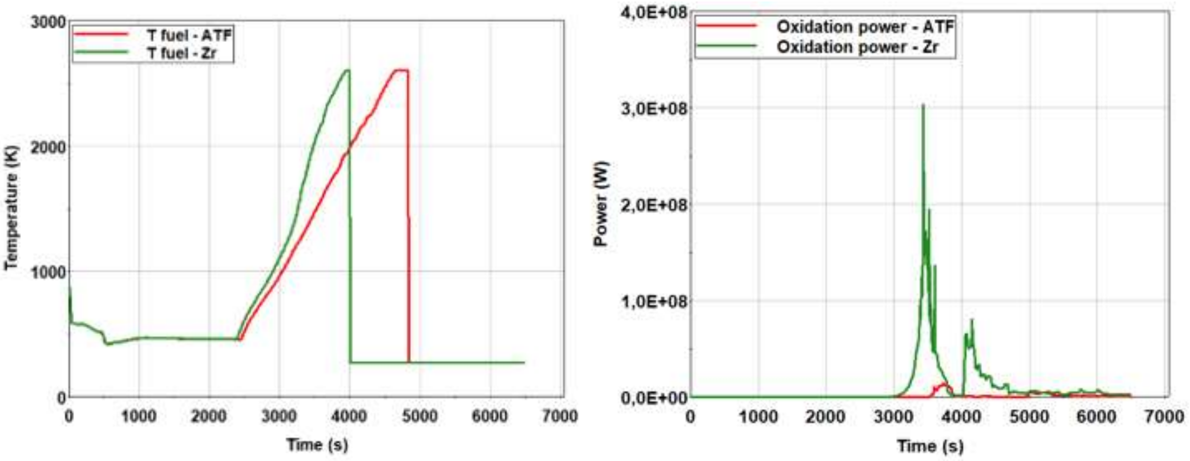

Figure 3: Evolution of the cladding temperatures at upper part (Node 17 out of 20) of the core (left), evolution of the oxidation power in the whole core(right)

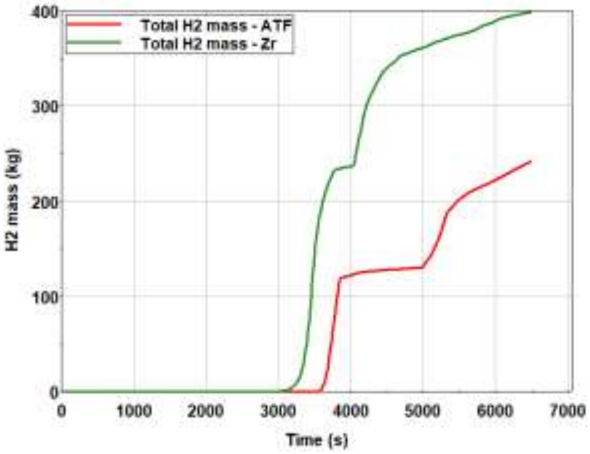

Figure 4: Evolution of the accumulated generated hydrogen mass

Note, that these extra time windows may vary widely with different designs and accident scenarios. This is why additional calculations are planned in the future. Also, it is important to highlight that material interactions with FeCrAl were completely ignored in this calculation, that most likely has an effect at least on the melting of materials and later probably at the phenomena in the lower plenum. Finally, the accuracy of the already implemented models for oxidation can also be further improved.

5 CONCLUSIONS AND OUTLOOK

In order to be able to simulate accident scenarios in nuclear reactors that are loaded with ATF, changes in the model basis of ATHLET-CD were implemented. The extended and new models were tested on the QUENCH-19 experiment. As they provided sufficiently accurate results, investigative calculations were performed on a generic PWR. A postulated accident was simulated with ATHLET-CD, once with and once without ATF material in the core. The effects of ATF material on the accident progression was analysed and was concluded that the usage of ATF material in the analysed scenario and design provides some benefits to the operators by giving them small amount of extra time budget for accident management, but the severity and extent of the accident is almost unchanged. Further model developments are needed, as well as additional simulations need to be performed in order to assess the efficacy of ATF under severe accident conditions.

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