PRELIMINARY RESULTS OF A COMPARATIVE ASSESSMENT OF ATHLET-CD AND MELCOR BY SIMULATING THE EXPERIMENT PHEBUS FPT1

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ABSTRACT

System codes like MELCOR (**M**ethods for **E**stimation of **L**eakages and **Co**nsequences of **R**eleases) and ATHLET-CD (**A**nalysis of **Th**ermal hydraulics of **Le**aks and **T**ransients – **C**ore **D**egradation) are tools to simulate severe accidents in nuclear power plants, which enable estimations and predictions on the course of (hypothetical) accidents. These codes need continuous validation to ensure the quality of the results.
To support the validation and development progress of ATHLET-CD, in this work the code is used to simulate the in-pile experiment PHEBUS FPT1. Additionally, a MELCOR simulation is applied for comparison. The test was performed at IRSN (Institut de Radioprotection et de Sûreté Nucleaire) in France and was under research as International Standard Problem n°46 (ISP-46).
First simulation results mainly show similar trends concerning the main parameters of the experiment, in particular thermal hydraulics, fuel rod temperatures and hydrogen generation. Deviations between the simulation results are more clearly visible regarding phenomena, which depend partly on more different model assumptions and influencing variables, like degradation of material or the release of fission products.
Concluding, as far as the comparison is advanced, it can be stated that ATHLET-CD as well as MELCOR are able to simulate the experiment PHEBUS FPT1 basically with adequate accuracy. However, the results show specific deviations from the experiment which imply improvement potential of the codes.

KEYWORDS
ATHLET-CD, MELCOR, PHEBUS FPT1, code application & validation

1. INTRODUCTION

System codes like MELCOR (**M**ethods for **E**stimation of **L**eakages and **Co**nsequences of **R**eleases) and ATHLET-CD (**A**nalysis of **Th**ermal hydraulics of **Le**aks and **T**ransients – **C**ore **D**egradation) are tools to simulate and evaluate severe accidents in nuclear power plants and to enable estimations and predictions on the course of (hypothetical) accidents. These analyses provide necessary data concerning the behaviour of the plant's systems and parameters. Furthermore, they allow assessment of appropriate counter measures in order to stop or slow down the accident's progress. The global objective is to avoid or minimise further core damage and possible consequences to the environment meaning the release of radioactive fission products. Caused by the continuous improvement of the codes, new implemented models take phenomena into account, which were neglected or not modelled in detail before. These models and their interaction with existing ones will influence the results. Therefore, validations against experiments to ensure the simulation quality of the codes are needed.

To support the validation and development progress of ATHLET-CD, in this work the code is used to simulate the in-pile experiment PHEBUS FPT1. Additionally, a MELCOR simulation is performed for comparison.

In chapter two the PHEBUS test facility and the conduct of the FPT1 test is described. The modelling of the experiment in the system codes ATHLET-CD and MELCOR is presented in chapter three. Simulation results compared to each other and to experimental data are shown and discussed in chapter four. A summary and conclusions are given in chapter five. The results and conclusions presented in this work are preliminary since the work is not finished yet.

2. THE PHEBUS FPT1 EXPERIMENT

The PHEBUS FP (Fission Products) international experimental programme at the Research Centre in Cadarache in the South of France was conducted between 1988 and 2010. It was launched by the IRSN (under the former name IPSN – Institut de Protection et de Sûreté Nucléaire, Nuclear Protection and Safety Institute) in collaboration with the EC (European Commission) and EDF (Électricité de France). The cooperation in this programme included the United States of America, Canada, Japan, South Korea and Switzerland.

In total five experiments were performed in the frame of the PHEBUS FP programme. Table 1 lists the main characteristics of the different experiments [1].

Table I. Overview of PHEBUS FP experiments according to [1].

Test	Fuel rods	Bundle	Primary Circuit	Containment	Date
FPT0	20 new rods, 1 AIC control rod, 9 days pre-irradiated	Melt generation and FP release in steam rich environment	FP chemistry & residue material	Aerosol residue, iodine chemistry with pH 5 / 363 K sump	02/Dec./ 1993
FPT1	20 BR3[1)] rods – 23 GWd/tU 1 AIC control rod, 9 days pre-irradiated	As FPT0 with irradiated fuel	As FPT0	As FPT0	26/Jul./ 1996
FPT2	As FPT1 – 32 GWd/tU	As FPT1 in environment poor of steam, boric acid injection	As FPT1 in environment poor of steam and boric acid	pH 9 / 393 K evaporating sump	12/Oct./ 2000
FPT3	As FPT1, but with 1 B_4C control rod	As FPT2 with B_4C control rod instead of boric acid	As FPT2 with B_4C control rod instead of boric acid	pH-9 / 393 K evaporating sump, H_2 recombiners	18/Nov./ 2004
FPT4	EDF fuel – 38 GWd/tU in fragments, no re-irradiation	Weak volatile FP & actinoid release from UO_2/ZrO_2 debris bed until melting	Application of integral filters, post-test studies of samples		22/Jul./ 1999

[1)]: Belgian Reactor 3: Belgian PWR prototype, first criticality in 1962.

The programme's objective was to improve the knowledge of the phenomena occurring during a hypothetical severe nuclear accident involving a core meltdown in pressurised water reactors (PWR). "Global" or "integral" experiments were conducted. These are tests in which all the phenomena of a hypothetical accident were represented, starting with melting of a fuel bundle up to the release of fission products and structural material inside a simulated reactor pressure vessel. The aim is to reproduce the conditions that would occur in such an accident as close as possible. The PHEBUS FP experiments were so called "in-pile" tests e.g. the fuel rods were nuclear-powered in contrast to the electrical heating of "out-of-pile" experiments like the QUENCH experimental facility.
Furthermore the findings of the experiments were used to evaluate reactor simulation software which is applied to describe these phenomena in safety assessments.
The main components of the test facility are the primary circuit including the fuel rod bundle and a driver core with an autarkical cooling system. The maximum thermal power of the driver core is at 40 MW. However for the PHEBUS FP experiments it is limited to 23 MW. It is cooled by a forced water flow under ambient conditions.
Figure 1 shows the experimental setup schematically according to [2].

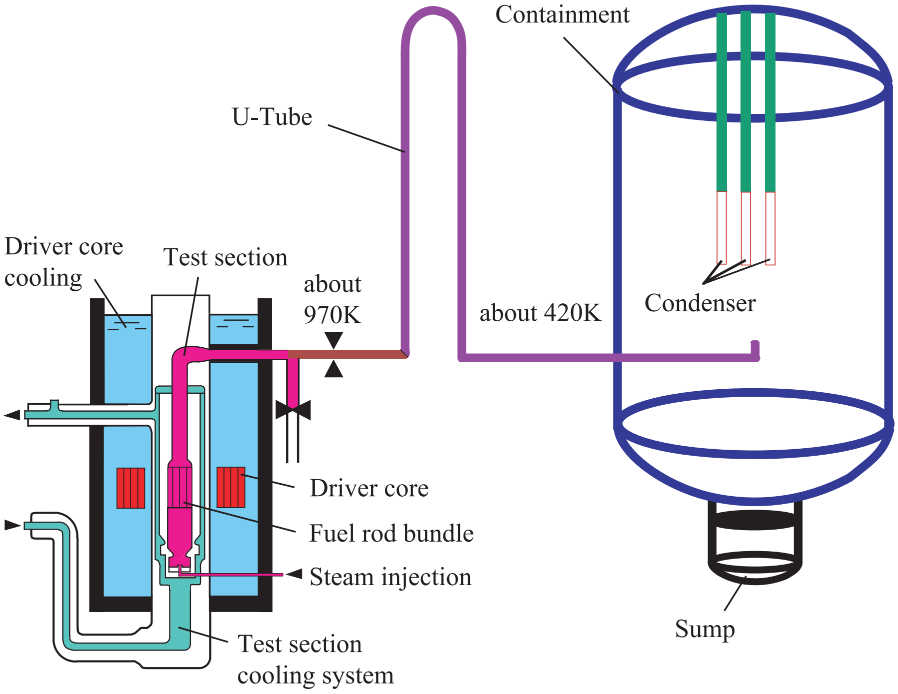

Figure 1. PHEBUS FP schematic side view according to [2].

The test section including the fuel rod bundle is positioned concentrically inside the driver core and is separated by a pressure-resistant structure. A separate cooling system is connected to the test section. This cooling circuit is a pressurised water loop (PWL) and carries the water at about 438 K and approx. 2.5 MPa. At a system pressure of 0.2 MPa in the primary circuit, steam is generated by heating up the cooling water of the primary circuit by the hot water of the test section's cooling system. This steam is injected into the bundle, where it heats up further and flows through the 4.5 m long vertical part of the test section afterwards, which represents the upper plenum. Subsequently it enters the 9 m long horizontal part of the test section – the "hot leg" –, whose pipe walls are electrically heated at 973 K. This temperature ensures minimisation of fission product deposition caused by condensation at the walls. A steam generator simulator consisting of an upside down U-tube guarantees the heat transfer to the secondary system and cools down the medium. Before the cooling medium finally enters the simulated containment, it passes the 4 m long horizontal “cold leg”. The containment is represented by a tank of 10 m³ volume, which is scaled by the factor 1:5000.

The bundle has an active length of about 1,000 mm and a total height of 1,100 mm. The fuel rods are arranged lattice-like and the spacing is 12.6 mm. In FPT1, a PWR typical AIC (Silver-Indium-Cadmium) control rod is positioned in the centre of the bundle and surrounded by a Zircaloy (Zry-4) guide tube. A thermally insulated structure – e.g. the shroud – is surrounding the bundle. The shroud is connected to the bundle by four stiffeners.

The positioning of the measuring instruments is important for the modelling, respectively for the comparison of the simulation results against experimental data. Thermocouples (TCW and TC, see Figure 2) are installed at different locations to record temperatures of the bundle and of the shroud. The following Figure 2 shows the axial and radial positions of the installed thermocouples [2].

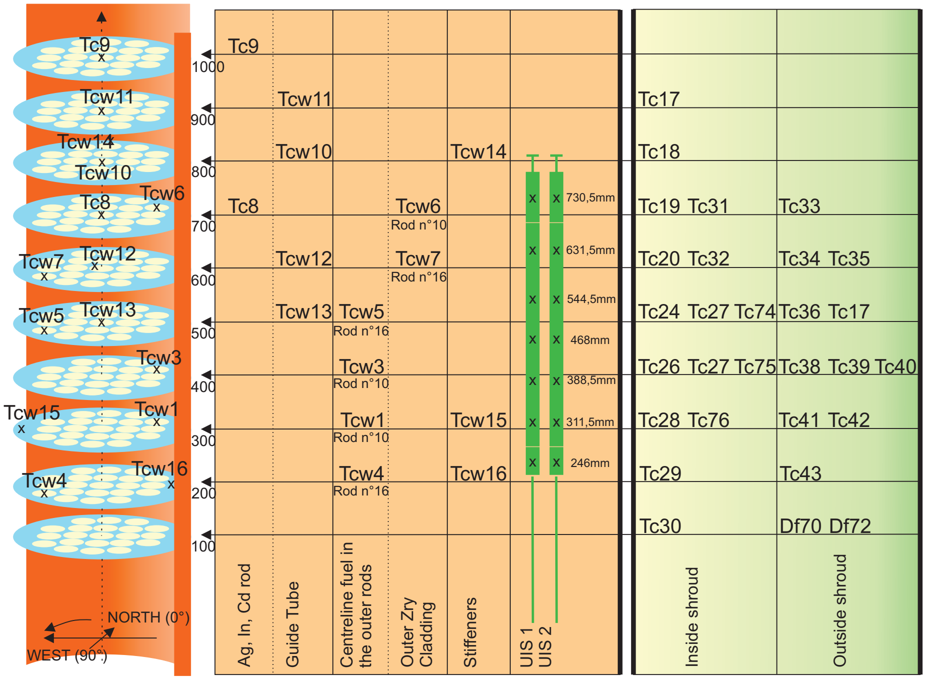

Figure 2. PHEBUS FPT1 thermocouple overview [2].

The experiment FPT1 can be divided into four main phases:

- Calibration phase (0 s – 7900 s)
- Oxidation phase (7900 s – 14580 s) including the pre-oxidation (7900 s – 11060 s) and the main oxidation (11060 s – 14580 s)
- Heat-up phase (14580 s – 17039 s)
- Cool down phase (17039 s – 18660 s)

The bundle power and the injected steam mass flow are depicted in Figure 3. Additionally the four different phases of the experiment are indicated.

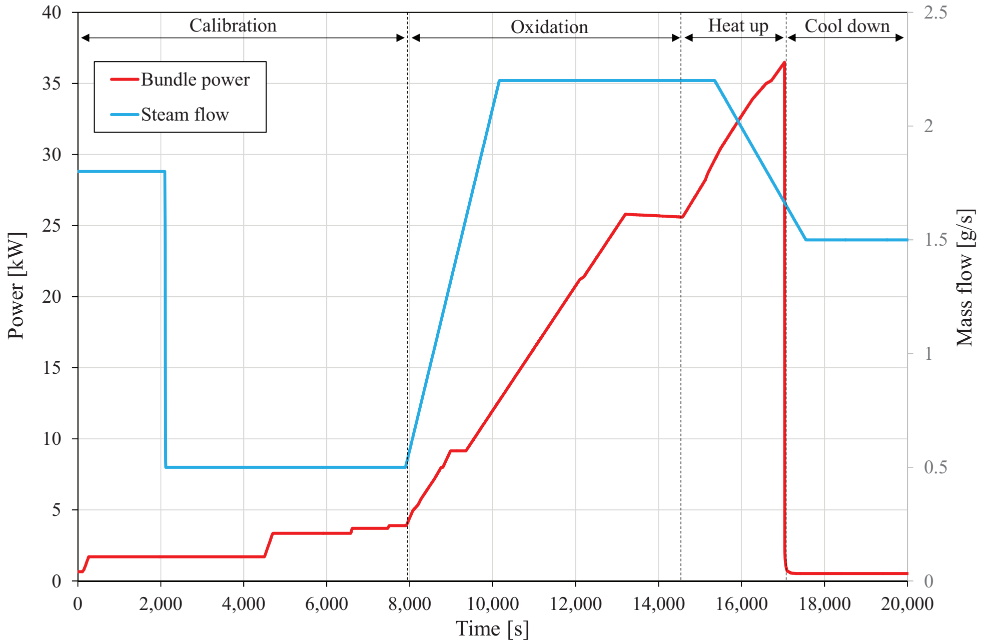

Figure 3. PHEBUS FPT1 bundle power and steam mass flow.

After these four phases further investigations of the fission product deposits in the primary cooling circuit and the containment were performed in the experiment. These analyses are not considered in this work. Further information of the PHEBUS FPT1 experiment may be found in the final report [2]. This test was also under research as International Standard Problem n°46 (ISP-46) [3].

3. MODELLING IN ATHLET-CD AND MELCOR

The severe accident analysis code ATHLET-CD is developed by the German Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH. GRS is the central expert organisation in the field of nuclear safety and radioactive waste management in Germany.
MELCOR, a fully integrated, engineering-level computer code is developed by Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (U.S.NRC).
For the simulation of the experiment PHEBUS FPT1 in this work, the version 3.0A of ATHLET-CD and version 2.1.6342 (official build, base code version 2.1 SEP-06-2014) of MELCOR are used. Both codes are one-dimensional and base on the so-called "lumped parameter" concept. Using this method, a facility is divided into defined control volumes (CV) for which variables like the gas and sump temperatures, the pressure as well as the flow velocities are calculated. Inside a CV, these variables are considered constant. MELCOR and ATHLET-CD are able to simulate the main characteristics of accidents in nuclear power plants, which involve:

- thermal-hydraulic response in the reactor coolant system,
- core heat-up and degradation,
- radionuclide release and transport,
- hydrogen generation and transport,
- heat structure response
- and the impact of engineered safety features on thermal-hydraulic and radionuclide behaviour

In contrast to ATHLET-CD, MELCOR is not limited to the simulation of cooling circuits (like the primary and the secondary cooling loop in a PWR). It is moreover able to calculate processes in the reactor cavity, in the containment and in confinement buildings. Furthermore, the simulation of hydrogen combustions, of melt ejection phenomena and of core-concrete interactions (CCI) is covered by MELCOR.
A schematic diagram of the modelling in both codes is depicted in Figure 4.

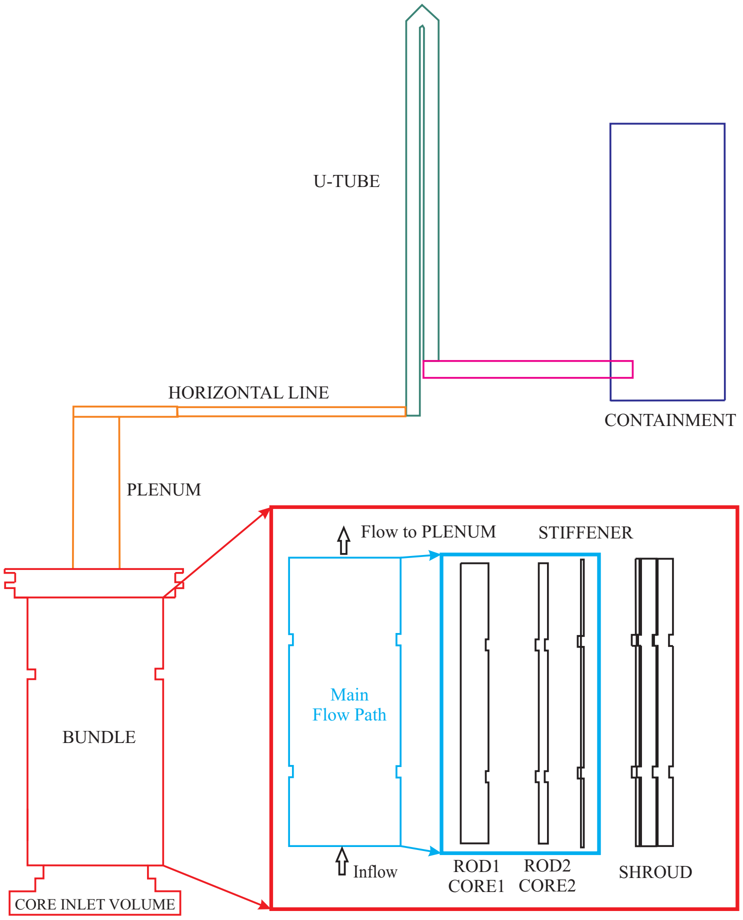

Figure 4. Schematic diagram of the PHEBUS FPT1 modelling in ATHLET-CD and MELCOR.

Key component of the modelling is the main fluid channel “BUNDLE” containing the bundle in which the steam is injected (see Figure 1). At the top, the “PLENUM” is vertically connected to the bundle. As listed in Table 1, the fuel rod bundle consists of 21 rods containing 20 fuel rods from the Belgian Reactor 3 and one AIC control rod in the centre. To consider differences for instance in the temperature distribution, the rods are radially subdivided into two rings as shown in Figure 4. Each ring is placed in the main flow path (see Figure 4). According to the lattice-like bundle configuration, the model consists of nine fuel rods in the outer ring called “ROD2” (ATHLET-CD), respectively “CORE2” (MELCOR) as well as eight fuel rods and the central control rod in the inner ring named “ROD1”, respectively “CORE1”. The modelled fuel rods are defined as “HEAT” (ATHLET-CD) respectively as “COR” (MELCOR) objects in order to consider structure failure and melting of cladding as well as fuel including relocation of molten material. The shroud, surrounding the bundle, as well as the stiffeners are implemented as heat conducting objects (in ATHLET-CD), respectively as heat structures (in MELCOR). In contrast to the fuel rods, these components cannot fail or melt due to the specific implementations of the models used in the codes. The inner side of the shroud is connected to the "BUNDLE" which is the main flow path (see Figure 4).

In ATHLET-CD, the Zry-4 oxidation in steam atmosphere is considered by the correlations according to "Leistikow and Prater / Courtright" (oxidation model 3). Correlations of "Urbanic-Heidrich" are used in MELCOR to describe the oxidation of Zry-4 in steam atmosphere. Both models are Arrhenius based and depend mainly different coefficients. The temperature is the main influencing factor. Further details concerning the oxidation models may be found in the users' manuals of ATHLET-CD and MELCOR [4, 5].

Initial and boundary conditions like heating power and steam flow (compare Figure 1), etc. are implemented in the input decks of the codes according to the experiment recordings. Further information concerning these data may be found in the FPT1 final report [2].

4. RESULTS

The results of the simulations compared to the experimental measurements will be presented and discussed in the following chapter.

4.1. Temperatures

Temperatures of the fuel rods at a bundle height of 700 mm are illustrated in Figure 5.

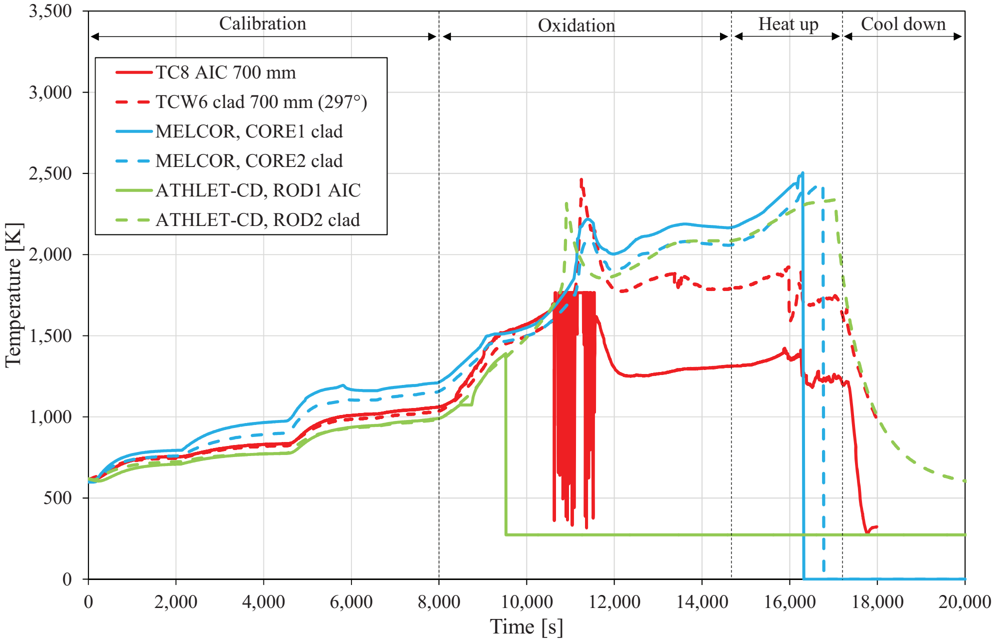

Figure 5. Measured and simulated temperatures at 700 mm bundle height.

The reproduction of the temperature is in good agreement to the experimental data with both codes until middle of the oxidation phase. After that point in time (about 12,000 s), the simulations start to overestimate the measured temperature. During the ATHLET-CD simulation, the absorber material fails and relocates at ca. 1,400 K at about 9,600 s. The corresponding thermocouple of the absorber material fails at approximately 1,750 K at around 11,000 s. That the thermocouple is still functioning at this temperature cannot be interpreted as a sign for still intact AIC material, since the melting temperature of AIC is around 1075 K according to [5]. In MELCOR it was not possible to readout the temperature of the absorber material.

The following Figure 6 shows the temperatures at a bundle elevation of 500 mm. ATHLET-CD provides good agreement to the experiment until the end of the oxidation phase. The recorded value of thermocouple TCW13 is questionable from approx. 11,500 s on. MELCOR starts to underestimate both, the experimental data and the ATHLET-CD results from the beginning of the oxidation phase on.

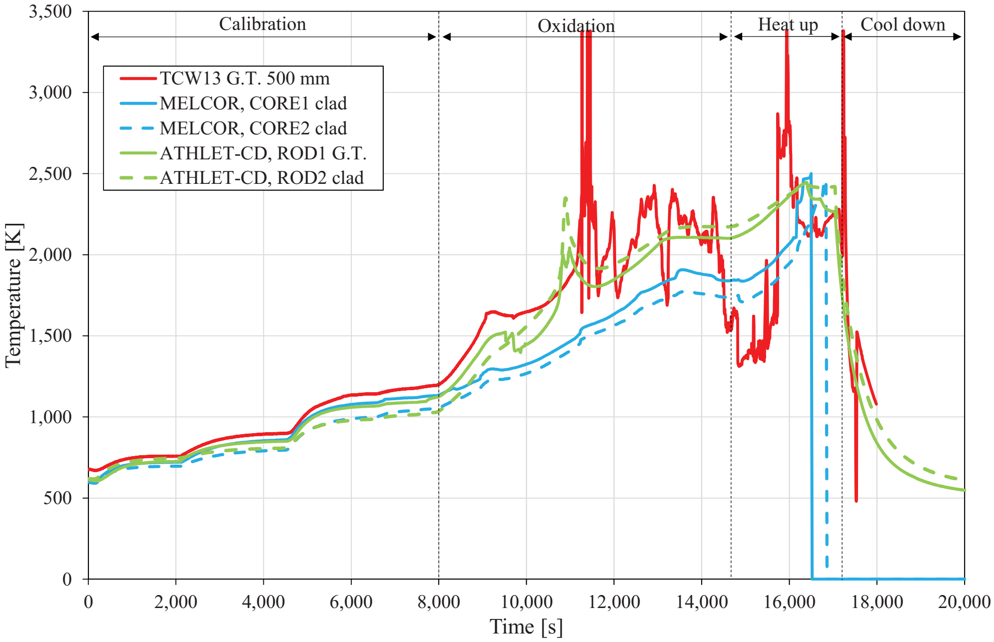

Figure 6. Measured and simulated temperatures at 500 mm bundle height.

MELCOR calculates significantly lower temperatures at a bundle height of 400 mm compared to ATHLET-CD and to measured values, as shown in Figure 7. In general it is observable that the lower the considered bundle elevation is the higher are the deviations of the MELCOR simulation. The results of ATHLET-CD are in good agreement to the experiment until the end of the oxidation phase. From this point of time on a further comparison of the temperatures is difficult since the recordings from TCW3 are questionable due to the assumed thermocouple defect implied by the fast drop of approx. 700 K in the last third of the oxidation phase.

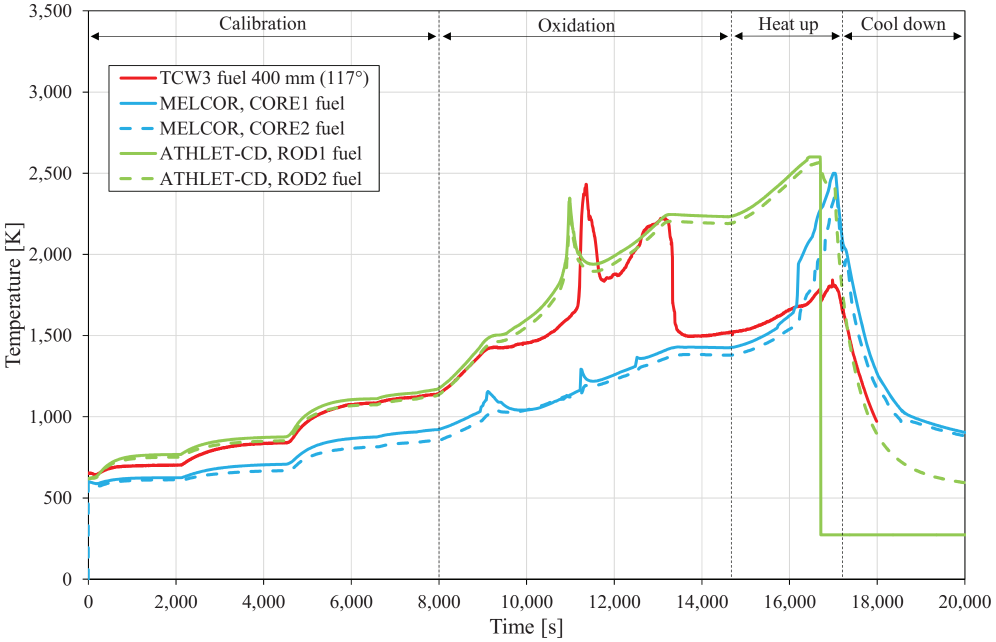

Figure 7. Measured and simulated temperatures at 400 mm bundle height.

4.2. Hydrogen Release

The measured and simulated released mass of hydrogen is depicted in Figure 8.

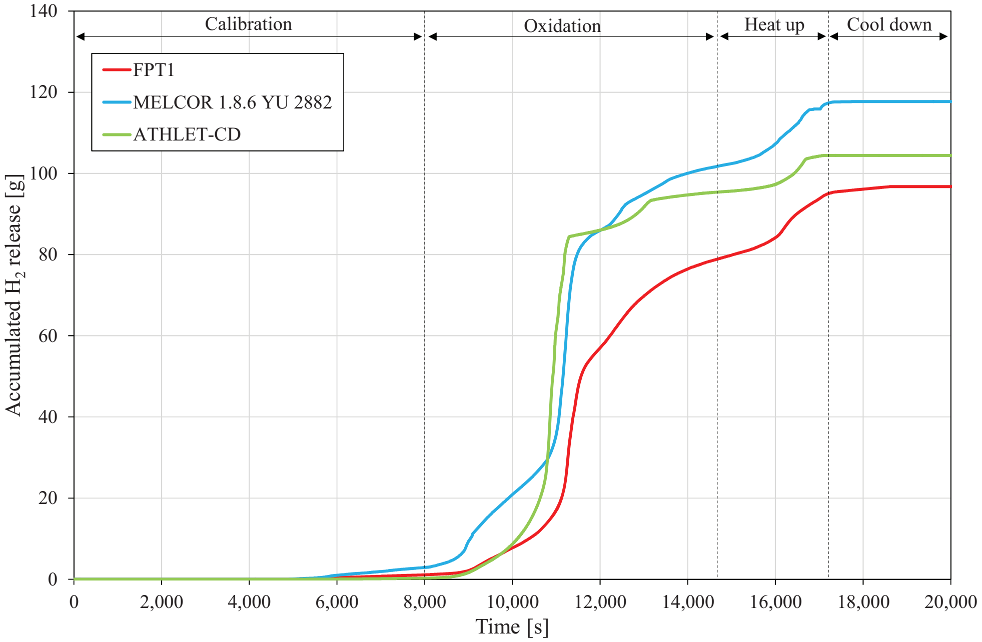

Figure 8. Measured and simulated accumulated hydrogen release.

It shows the general overestimation of both simulations compared to the experimental data. MELCOR provides the highest total hydrogen release with about 114 g H_2 and therefore approx. 10 g more H_2 compared to the ATHLET-CD value of about 104 g. Thus, MELCOR overestimates the experiment by around 17 g H_2. This corresponds to a relative deviation of 17.5 % for MELCOR and 7.2 % for ATHLET-CD compared to the recorded value.

The ATHLET-CD results show an increase which is too strong in the first half of the oxidation phase. Subsequently, there is a short period in which the amount stays almost constant. This does not agree with the experiment. The qualitative progress of the hydrogen release is calculated in better agreement to the experimental conduct by MELCOR. Nevertheless, using MELCOR the hydrogen release starts earlier than in the experiment and the gradient is too steep until about 11,500 s.

4.3. Degradation of Core Material

The following Figure 9 shows the relative value of intact Zry-4 material in the bundle. Concerning this parameter there is no continuously recorded measurement available, so that only the simulation results are compared in this section.

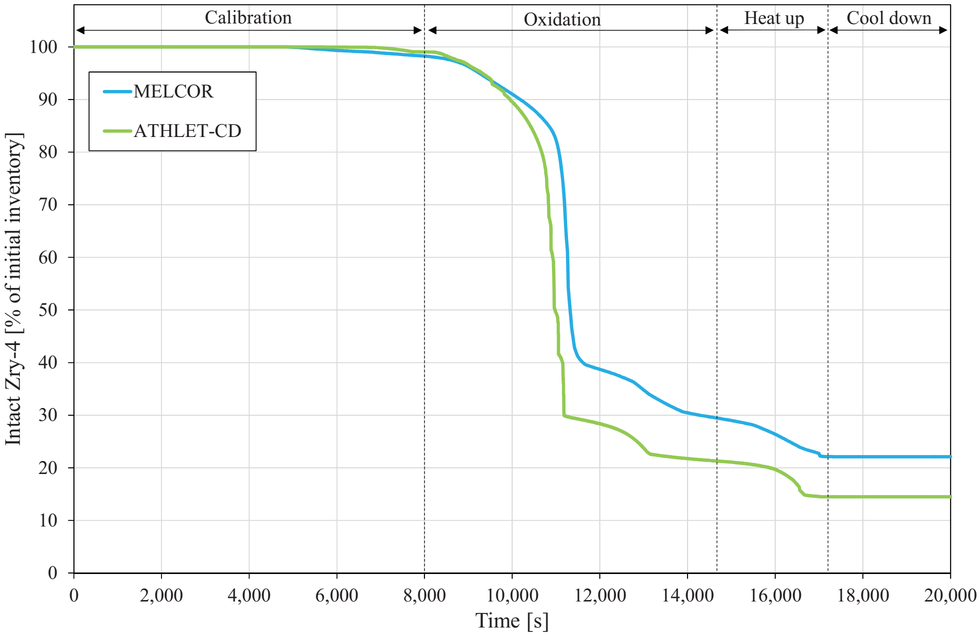

Figure 9. Simulated intact Zry-4 cladding material.

The graph in Figure 9 shows a similar behaviour of the MELCOR and the ATHLET-CD simulation concerning the final value of still intact Zry-4 material as well as the progress of the Zry-4 degradation process. Differences between the results of the codes become visible during the oxidation phase. After about half of this phase there is a major decrease in the intact Zry-4 mass in both codes caused by the high temperatures (see section 4.1). In ATHLET-CD the degradation process is slightly faster simulated resulting in a lower amount of remaining intact Zircaloy. Until the end of the experiment this deviation decreases constantly but stays visible. Between about 14.54 % (ATHLET-CD) and ca. 22.1 % (MELCOR) of the initial Zry-4 material in the bundle are still intact at the end of the simulations.

In contrast to the Zry-4 degradation, the UO_2 degradation is very differently simulated, as presented in Figure 10. MELCOR calculates about 65 % still intact UO_2 at the end of the simulation and thus significantly more degraded fuel compared to the ATHLET-CD result of about 83 % degraded UO_2. The exact reason for this is not evaluated yet, as the temperatures are simulated to be high enough to cause melting of UO_2 with both codes.
In the MELCOR simulation the UO_2 degradation starts approximately two thirds of the heat-up phase. Contrary to that, the UO_2 degradation starts early in the oxidation phase using ATHLET-CD. The gradient is significantly lower. Compared to the experimental post-test analysis of about 4.6 kg relocated UO_2, ATHLET-CD underestimates the fuel degradation significantly in this experiment.

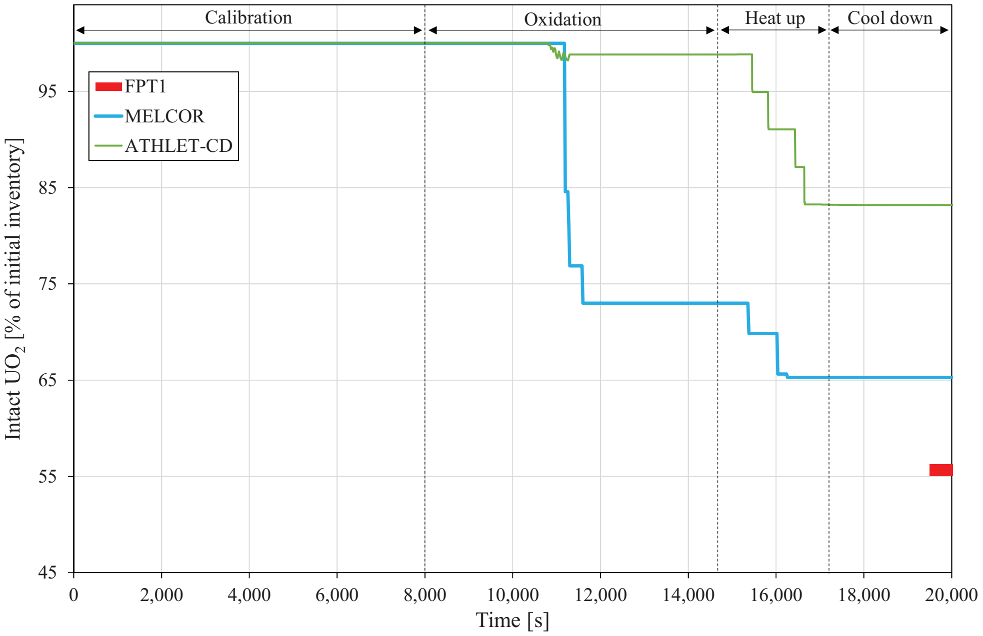

Figure 10. Intact UO_2 mass in the experiment and the simulations.

4.4. Fission Product Release

The severe degradation of the fuel rod bundle enables fission product release into the primary circuit. Measured and simulated total released amounts of selected elements are listed in the following Table II. These are relative values referred to the initial inventory of the experiment, which may be found in the final report of the experiment [2].

Table I. Measured and simulated relative fission product release

Fission Product	**FPT1**	**MELCOR**	**ATHLET-CD**
Xe (Xenon)	76,60 %	89.7 %	81.8 %
Cs (Caesium)	84,00 %	79.2 %	81.7 %
Te (Tellurium)	83,00 %	79.5 %	52.9 %

Fission Product	FPT1	MELCOR	ATHLET-CD
Ag (Silver, Cont. Rod)	15,00 %	2.2 %	3.8 %
Mo (Molybdenum)	56.0 %	54.2 %	70.3 %
Ba (Barium)	1.0 %	0.3 %	8.4 %
Ru (Ruthenium)	1.2 %	1.4 %	0.9 %

The following two figures (Figure 11 and Figure 12) show exemplarily the release progression of Cs as a volatile and Ba as a nonvolatile fission product. Figure 11 shows a similar reproduction of the experimental Cs release in good agreement by both codes. In contrast, Figure 12 illustrates a very different simulation behaviour concerning the Ba release. Furthermore, both simulations differ clearly from the measured Ba release. This shows exemplarily the dependence of the simulation results on specific fission product species. Additionally, this implies that there is no general assessment possible concerning the simulation quality of fission product release. In fact, the reproduction of experimental recordings by the simulation depends on the specific release model used for the considered fission product. Additionally, processes like oxidation and other chemical interactions, which are very difficult to model in detail, can affect the release behaviour of fission products.

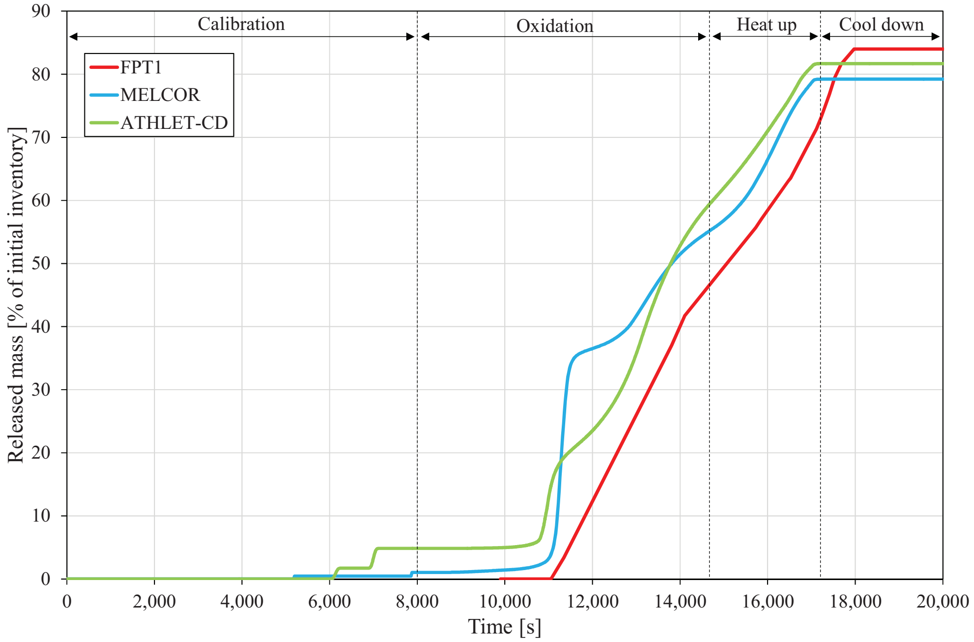

Figure 11. Measured and calculated Cs release.

Conspicuous is in these graphs that in the experiment the release of both species starts approximately at the same time. In contrast to this, the simulation codes calculate a significantly earlier start of the Cs release. Concerning Ba the simulated begin of release is distinctly closer to the data of the FPT1 experiment. An additional reason for this could eventually be found in partly overestimated temperatures at higher bundle elevations.

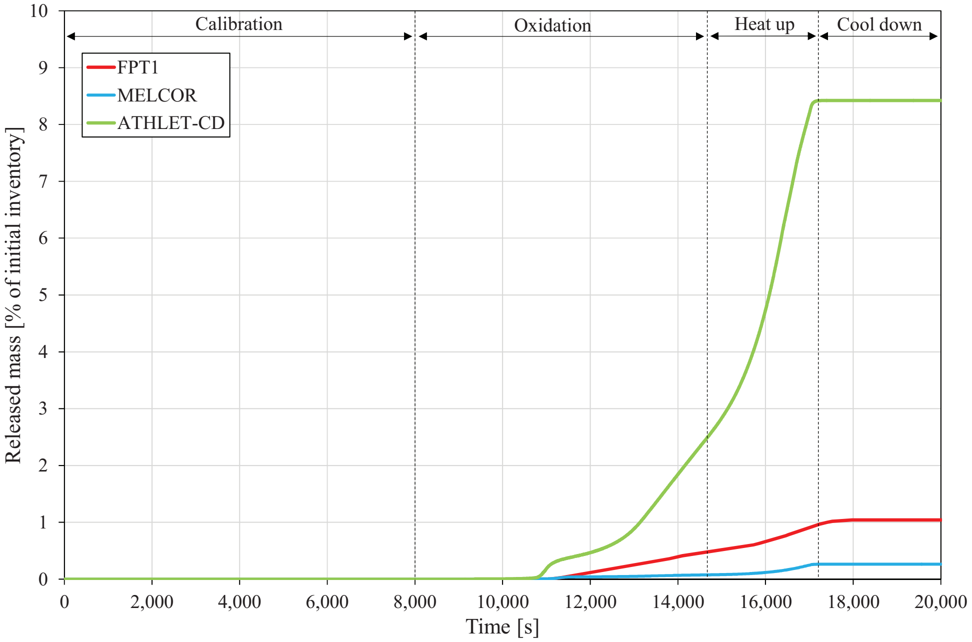

Figure 12. Measured and calculated Ba release.

5. CONCLUSIONS

Simulations of PHEBUS FPT1 are performed using ATHLET-CD 3.0A and MELCOR 2.1.6342.
At lower bundle heights (below approx. 500 mm) significant differences between the simulation results are visible. MELCOR calculates lower temperatures in this bundle region compared to the experimental values and to ATHLET-CD results. This might be caused by still existing differences in the modelling between the MELCOR and the ATHLET-CD input deck. These have to be analysed further.
The total released hydrogen mass is overestimated in both codes. One reason for this behaviour might be partly overestimated temperatures in the simulations. The exact evaluation though is difficult at higher temperatures due to thermocouple defects and the therefore questionable readings.
The degradation of Zry-4 material of the claddings is similarly reproduced by the applied codes. In contrast to this, the deviations concerning the calculation of the UO_2 degradation are distinct. ATHLET-CD simulates significantly less degraded UO_2 than MELCOR. Furthermore the deviation of the ATHLET-CD result compared to experimental data is substantial.
Comparing the relative fission product release, it may be observed that the codes calculate very similar results for some species (e.g. Cs Ru, Xe), which are in good agreement to the experimental values. However, there are different elements (e.g. Ba) for which the simulated results differ between the used codes as well as from recorded data. On the one hand, these results are highly influenced by other boundary parameters (e.g. temperature), which can already be differently calculated by each code and also deviate from the measured values. On the other hand, these results are influenced even more by how the fission products are treated internally in the code and how the corresponding models are implemented and adapted to fit the characteristics of the different codes.
As far as the evaluation is advanced, it can be stated in general that MELCOR as well as ATHLET-CD show qualitatively reasonable results most of the time. Nevertheless, to decrease the deviations in comparison to the experiment further, the used input decks might still be improved and extended to describe the PHEBUS FPT1 experiment more detailed. On the other hand there are phenomena (e.g. interaction of the fuel with the cladding and other material, dissolution of material) involved in the

PHEBUS FPT1 experiment, which cannot be reproduced entirely by the codes so far. The oxidation of specific elements and its compounds as well as other chemical interactions may cause a change in the volatileness of the fission products. This greatly influences the release behaviour of fission products. Concerning the core degradation there are several interactions between different materials (Zircaloy, UO_2, Stainless Steel, Inconel, AIC, etc.) in different states which affect for example the melting behaviour. Exemplarily the dissolution of UO_2 by solid or liquid Zircaloy can be stated, which leads to liquefied uranium significantly below the melting point of UO_2. There are approaches implemented in the codes to cover those interactions. Nevertheless, potential lacks in the modelling of these and other phenomena – caused by the complex processes and insufficient experimental data – can lead to deviations of the calculated results compared to experimental data.

ACKNOWLEDGMENTS

This work is funded by the German Federal Ministry of Economic Affairs and Energy under grant number 1501465 on the basis of a decision by the German Bundestag.

The simulations were performed with the codes ATHLET-CD developed by GRS and MELCOR developed by SNL. The Authors thank these institutions for providing access to the codes and technical support.

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