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Validation of the AC^2 Codes ATHLET and ATHLET-CD

Verification and validation are basic quality assurance elements in code development and essential for code release. Therefore, the codes of AC^2 (ATHLET – ATHLET-CD – COCOSYS) are tested on separate effect tests, integral tests as well as plant scenarios to verify and validate the models after new implementation or updates. The verification assures that the models are implemented and working correctly while the validation checks if the models predict the right phenomena and combined with other models and modules. The selected experiments are summarized in GRS's validation matrices, which in turn are based on the CSNI validation matrices derived from OECD/WGAMA task groups as well as current activities on experimental test campaigns. For ATHLET several test series are used to cover a wide range of phenomena which can occur in PWR, BWR and VVER. Additionally, plant transients are considered for German LWR. The ATHLET-CD validation matrix contains experiments covering most phenomena which can occur during a severe accident. But due to the interaction of several effects even in small scale experiments mainly integral experimental campaigns are used for the validation. Over the last decades the validation of the AC^2 codeds ATHLET and ATHLET-CD has reached a high degree of fulfilment of GRS's validation matrices over all code versions. Innovative and advanced reactor concepts come with new or newly relevant phenomena, which AC^2 needs to provide models for. Extending the validation base of AC^2 for these models is one challenge for further code validation efforts besides the on-going update of the validation basis to recent code versions.

Validierung der AC^2-Programme ATHLET und ATHLET-CD. *Verifikation und Validierung sind wesentliche Elemente der Qualitätssicherung in der Programmentwicklung und -freigabe. Die Programme (ATHLET – ATHLET-CD – COCOSYS) des Programmsystems AC^2 werden hierbei für Einzeleffekttests, Integraltests sowie Anlagenszenarien angewendet, um die Modelle nach ihrer Implementierung oder Weiterentwicklung zu verifizieren und bzw. das Programm(system) zu validieren. Dabei stellt die Verifikation sicher, dass ein Modell korrekt implementiert wurde und arbeitet, während die Validierung überprüft, ob das richtige Modell implementiert wurde sowie das Zusammenwirken mit anderen Modellen. Die ausgewählten Experimente sind in den GRS-Validierungsmatrizen zusammengefasst, die einerseits auf den CSNI-Validierungsmatrizen basieren, die von verschiedenen OECD/WGAMA-Arbeitsgruppen erstellt wurden, sowie sich andererseits an aktuellen Versuchsprogrammen orientieren. Für ATHLET wurden solche Versuchsprogramme ausgewählt, wo möglichst viele Phänomene untersucht werden, die in DWR, SWR oder WWER auftreten können. Zusätzlich werden Transienten für deutsche LWR betrachtet. Die ATHLET-CD-Validierungsmatrix berücksichtigt Experimente, die weitestgehend die Phänomene beinhalten, die in Unfallsequenzen auftreten können. Aufgrund des meist zeitgleichen Zusammenwirkens von Phänomenen sogar in kleinskaligen Versuchsanordnungen, werden im Wesentlichen Integraltests für die Validierung herangezogen. Über alle Programmversionen gesehen hat der Validierungsstand der Programme ATHLET und ATHLET-CD in den letzten Dekaden einen hohen Erfüllungsgrad der GRS-Validierungsmatrizen erreicht. Für innovative und fortschrittliche Reaktorkonzepte kommen allerdings neue Phänomene hinzu, wofür Modelle in AC^2 bereitgestellt werden müssen. Die Erweiterung der Validierungsbasis von AC^2 für diese Modelle stellt neben der Aktualisierung der vorhandenen Validierungsmatrizen eine Herausforderung für die zukünftige Validierungsarbeiten dar.*

1 Introduction and motivation

Computer codes like the codes ATHLET – ATHLET-CD and COCOSYS of the GRS code package AC^2 aim to simulate the system behaviour of nuclear power plants as realistic as possible ("best estimate"). These computer codes are used to investigate

- incidents and accidents of different scenarios and their consequences,
- the effectiveness of emergency procedures.

The process carried out by comparing code predictions with experimental measurements or measurements in a reactor plant (if available) is called validation. A code or code model is considered validated when sufficient testing has been performed to ensure an acceptable level of predictive accuracy over the range of conditions for which the code may be applied. Accuracy is a measure of the difference between measured and calculated quantities taking into account uncertainties and biases in both. Bias is a measure, usually expressed statistically, of the systematic difference between a true mean value and a predicted or measured mean. Uncertainty is a measure of the scatter in experimental or predicted data. The acceptable level of accuracy is judgmental and will vary depending on the specific problem or question to be addressed by the code. The procedure for specifying, qualitatively or quantitatively, the accuracy of code predictions is also called code assessment. The international literature often distinguishes between the terms "validation" and "verification". A mathematical model, or the corresponding computer code, is verified if it is demonstrated that the code behaves as intended, i.e. that it is a proper mathematical representation of the conceptual model, and that the equations are correctly encoded and solved. Verification may include the demonstration of convergence of the calculated results during a process of reduction of time steps and the size of the nodes of simulation. Also, the comparison of selected results with exact mathematical solutions and with the results obtained by similar codes may fall under the term verification. In this context, the comparison with measured values is not part of the verification process, it is rather a validation task. The term verification, however, is often used synonymously with validation and qualification. Especially in the past, the term verification was used in the frame of the ATHLET code validation work, including comparisons between calculations and measurements. [1, 2].

2 Overview on validation activities for ATHLET and ATHLET-CD version 3.2

The AC^2 codes ATHLET and ATHLET-CD for the simulation of normal operation conditions, anticipated operational occurrences, design basis accidents, and severe accidents thermal-hydraulics as well as core degradation up to late phase and fission product behaviour are validated against different test series and plant fault sequences within the current validation project RS1548. The systematic validation of the AC^2 codes is based on a well-balanced set of integral and separate effects tests [2, 3] mainly derived from the CSNI validation matrices. Furthermore, a very useful part of the validation is the participation in International Standard Problems (ISPs) or other International Benchmark activities under the auspices of, e. g., OECD/NEA or the SARNET network of excellence. Among several others, the validation of ATHLET includes test series of the facilities Batelle, BETHSY, LOFT, LOBI, ROSA/LSTF, PKL, PACTEL, PSB, UPTF, and ATLAS. Also, GRS participated with ATHLET in eleven ISPs. Additionally, operational transients of Western LWR, particularly German ones, are used for the code validation. Similarly, the ATHLET-CD validation [3] makes use of experimental campaigns in the facilities CORA, QUENCH, LIVE, PHEBUS, PARAMETER, STORM as well as the accident in TMI-2. This is complemented by participation in six ISPs and several additional benchmarks. Furthermore, the code system AC^2 was applied to simulate the sequences of the Fukushima Daiichi accident in the frame of the OECD/NEA projects BSAF and BSAF-2. In general, GRS participates in several international programmes like the OECD NEA projects PKL, ATLAS, SFP, BETMI and dedicated task and working groups of the OECD/NEA and the IAEA. Finally, the validation of ATHLET and ATHLET-CD strongly benefits from active users, both at GRS and in national and international partner organisations like, e. g., in Germany Ruhr-Universität Bochum, IKE Stuttgart and HZDR or the Russian Kurchatov Institute and SEC NRS, and their feedback from applications of ATHLET and ATHLET-CD to numerous reactor designs and fault and accident sequences.

The intensive validation of the codes ATHLET and ATHLET-CD (including previous code versions) over more than 30 years leads to a high degree of fulfilment compared to the internal validation matrices in terms of tests simulated successfully at least once. Referring to the ATHLET and ATHLET-CD specific validation matrices derived from CSNI matrices and recent test series used the degree of fulfilment is the following:

- ATHLET
  - 70 % of the 80 SET,
  - 76 % of the PWR experiments,
  - 100 % of the BWR experiments and
  - 90 % of the WWER experiments.
- ATHLET-CD
  - 70 % of the 66 validation experiments.

Future activities are foreseen to update the GRS validation matrices for ATHLET and ATHLET-CD with respect to single effect tests as well as integral tests and to establish a continuous validation procedure for all these cases to validate the current code version.

For the current version 3.2 of the codes ATHLET and ATHLET-CD, several tests have been calculated for the first time or have been re-calculated to compare the results with experimental data and, if applicable, the results of previous code versions to evaluate the code predictability and model improvements. The following test series were chosen so as to use as much models as possible and especially investigate the interaction of models and modules:

- ATHLET
  - ATLAS: APR-1400 model in the volumetric scale 1:288
  - PKL: German Konvoi PWR model in the scale 1:145
  - ROCOM: Rossendorf Coolant Mixing Model to investigate mixing phenomena in the RPV
  - UPTF: Upper Plenum Test Facility: Full-scale simulation of the primary system of Siemens KWU PWR
  - EASY: Integral INKA test facility test series
  - NOKO: Emergency condenser test rig
  - KASOLA: Karlsruhe Sodium Loop
  - NACIE-UP: Liquid metal natural circulation test with Argon flow
  - MHTGR: Gas cooled reactor: Investigation of the compressor model
- ATHLET-CD
  - CORA(-SWR): BWR tests with core degradation
  - QUENCH-11/16: QUENCH tests with boil-off/air ingress and reflooding
  - PARAMETER-SF2/3: Core degradation tests with top and top/bottom flooding
  - PHEBUS FPT1/3: Core degradation test with AIC/B4C absorber, fission product release and transport
  - LIVE-10/-11: Molten pool experiment with salt melt, with external cooling by water or steam
  - LOFT LP-FP-2: Core degradation test with reflooding as well as fission product release and transport
  - TMI-2: Three Mile Island Unit-2
  - BWR: Postulated SBO in a generic BWR
  - PWR: Postulated 250 cm^2 break in cold leg and SBO with AM, coupled with the containment code COCOSYS
  - WWER-SFP: Postulated SBO in a generic SFP of a WWER-1000

In general, the improved version ATHLET(-CD) 3.2 shows good agreement to the experimental data and better results than previous code versions or at least the same quality of results. The validation demonstrated that improvements of several code and model weaknesses identified based on user feedbacks from prior versions are effective. Minor points for improvement could be identified especially in the field of interfacial friction modelling. The re-calculation with the revised version of ATHLET(-CD) 3.2 further improved the results compared to the measured data.

3 Selected validation results of the codes ATHLET and ATHLET-CD

The results of one simulation for each of the in-vessel codes of AC^2 are described and discussed in the following chapter. For ATHLET the simulation of the ROCOM experiment 2.1, investigating mixing in the downcomer and lower plenum performed in the OECD project PKL-2, was chosen to show the improvement of the results in comparison to the measurement and to the previous release version ATHLET 3.1A Patch 4. The same comparison is done for ATHLET-CD simulation of the in-pile experiment Phébus FPT-3, which was subject of a benchmark in the frame of the NoE SARNET.

3.1 ROCOM 2.1

The four-loop integral test facility ROCOM replicates at a scale of 1:5 the cold legs, the downcomer (DC) and the lower plenum (LP) of the primary circuit of a German KONVOI-type PWR. The linear scaling factor of 1:5 corresponds to a volume ratio of 1:125 between the ROCOM facility and the primary coolant circuit of the original PWR. Each of the loops includes a pump to adjust the coolant mass flow. The test facility was constructed to provide a validation basis focusing on mixing processes for multidimensional computer codes, such as CFD and system codes [4, 5].

3.1.1 Description of the ROCOM experiment 2.1

In general, the ROCOM experiments are carried out with water at atmospheric pressure and room temperature. The impact of the temperature difference between the primary coolant and the emergency core coolant is represented through a density difference by means of adding sugar solution. The mixing behaviour is measured exploiting the local electrical conductivity of the fluid. Additives such as salt or brine tracer are used to mark the denser (i. e. colder) water and subsequently study its distribution within the system. This is monitored by specially designed electrical conductivity Wire Mesh Sensors (WMS) which provide high-resolution measurements of the tracer concentration both in space and time. WMS are installed at the RPV inlets, at two concentrical layers close to the inner and outer DC wall, stretched along nearly the entire length of the DC, and at the Core Inlet (CI). Figure 1 shows the RPV model of the ROCOM facility and the locations of the installed WMS. The geometry of the core and the upper plenum is simplified within the ROCOM facility and considered only by means of its hydraulic resistance. The core contains 193 rods counterparts simulating the 193 fuel assemblies of the KONVOI reactor. The DC wire mesh sensors are subdivided into 64 azimuthal and 29 (outer sensor) or 15 (inner sensor) axial measuring planes [5].

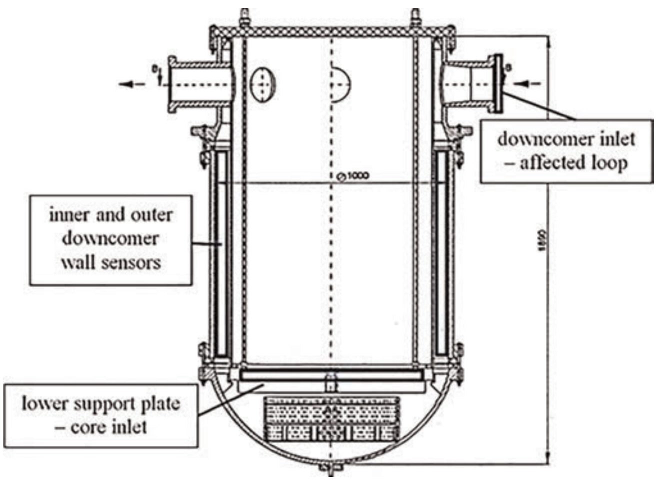

Fig. 1. RPV of the ROCOM facility with the installed WMS [4]

The ROCOM experiment 2.1 was carried out as a counterpart test in the frame of the OECD PKL-2 project, dedicated to the fast cool-down transient induced by a main steam line break. The experiment scenario can be divided in two main phases. The first phase starts immediately after the main steam line break on the secondary side, resulting in an increase of the heat transfer due to the enhanced evaporation in one Steam Generator (SG) following the pressure decrease. As a result, the corresponding primary loop is strongly affected. This first phase lasts until the entire fluid inventory of the affected SG evaporates. The first phase is also called the cool-down phase of the primary coolant. The second phase is characterized by the activation of the Emergency Core Cooling (ECC) system, which injects cold and highly borated water into the cold legs. The over-cooling phase can, for example, trigger a re-criticality process due to boron dilution while the ECC injection in the second phase can lead to a pressurized thermal shock (PTS) phenomenon.

The ROCOM experiment 2.1 was dedicated to the over-cooling phase. Constant Boundary Conditions (BC) of the quasi-stationary experiment were fixed based on the results of the experiment G3.1 performed previously in the PKL facility. The leak was postulated in the steam line of the steam generator of loop 1. The over-cooled fluid with increased density was therefore modelled in this loop. The needed amount of sugar was diluted into the RPV injected water to achieve the density difference measured during the PKL experiment. Loop 1 was plugged behind the main coolant pump. The fluid mass flow rate with the appropriate density ("over-cooled fluid") was directly pushed into the cold leg of the Affected Loop (AL), between the main pump and the DC inlet. The injected water mass was consistently discharged from the corresponding hot leg during the experiment. In the other three loops the fluid was circulated with the main coolant pumps.

3.1.2 Results of the simulation of ROCOM 2.1

For the system analysis code simulation of the ROCOM experiment 2.1 the DC region of the RPV consisted of 16 azimuthal distributed control volumes (CV) and an axial nodalization of twelve CV. The core was divided into 33 parallel hydraulic channels arranged in two rings around the central channel. Each channel has an axial resolution of five computational cells. A schematic drawing of the sixteen azimuthal DC CV and the 33 core channels together with the indication of the broken loop is presented in Fig. 2. The complex set-up of the lower core plate was considered in the ATHLET model of the ROCOM facility. The lower plenum below the core was split into the same number of channels, while the curved shape of the lower plenum calotte was modelled with 16 curved channels continuing the DC channels.

Two different modelling approaches have been used for the computer simulation of the LP of the ROCOM test facility. Within the first approach so called branch-objects have been used for the modelling of the LP region of the RPV. This method corresponds to the typical lumped parameter system code nodalization. In the second approach pipe components have been employed instead. The first model employed the classical (one-dimensional) description of the flow in the LP of the RPV, while the second model employed the three-dimensional model equations in cylindrical coordinates in the same region [5].

The comparison of the simulation results against the experimental data was performed in a two-step approach. First a qualitative comparison was performed. During this step, the multidimensional flow model applied to the improved nodalization in the LP region showed good overall prediction of the flow distribution both in the DC region, after the activation of the emergency core cooling system, and at the CI. The formation and shape of the denser coolant plume in the DC could be simulated satisfactorily, although the overall calculation results were slightly impaired by a temperature stratification in the lower part of the DC region towards the end of the investigated transient, which was not observed in the experiment (Fig. 3). Only the three-dimensional LP model was able to reproduce a coolant temperature distribution across the CI with a low temperature bulk in the central core region, thus highlighting the improved nodalization compared to the previous one-dimensional description of the LP. In the second step of the validation process a comparison against temperature trends at key locations in the RPV was performed. These included the upper and the lower part of the DC, three core channels neighbouring the affected loop, three core channels diagonally across the affected loop and the central core channel. Additionally, a comparison against the average core inlet temperature was performed. Again, the three-dimensional LP model outperformed the standard one-dimensional approach [2, 5].

The comparison of both code versions ATHLET 3.1A Patch 4 and ATHLET 3.2 show almost no significant deviations of the main results (Fig. 4). In general, the simulations show good qualitative agreement to the experiment with

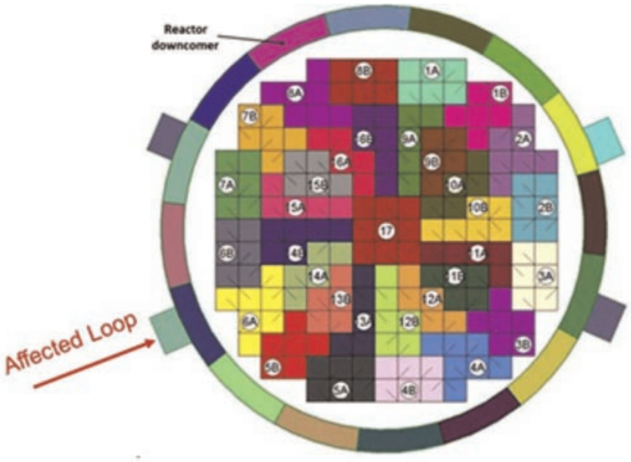

Fig. 2. Schematic drawing of the ATHLET sixteen azimuthal CV representation of the DC and the thirty-three core channels (1A – 17) [5]

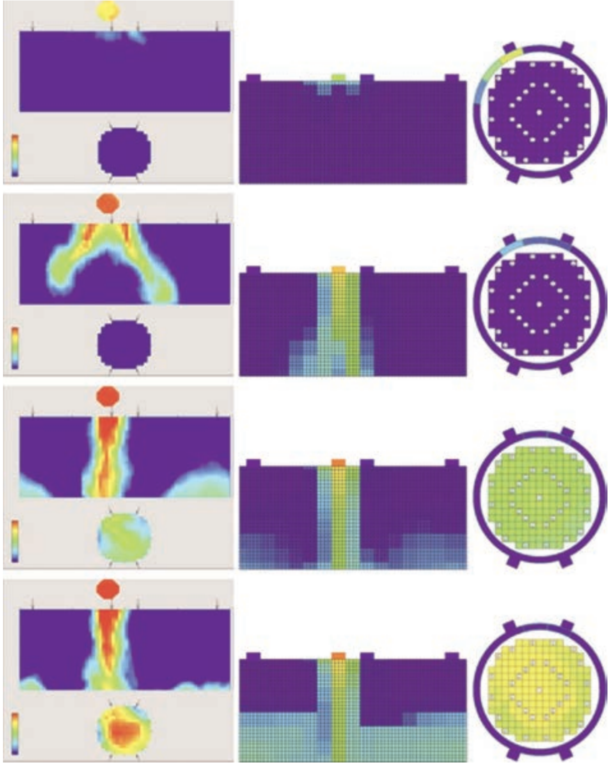

Fig. 3. Comparison of the temperature fields derived from measured data (left) and simulated data in the DC (mid) and at the CI (right) at temporal key points of the experiment (12.4 s, 18.4 s, 37.9 s and 149.5 s) [2]

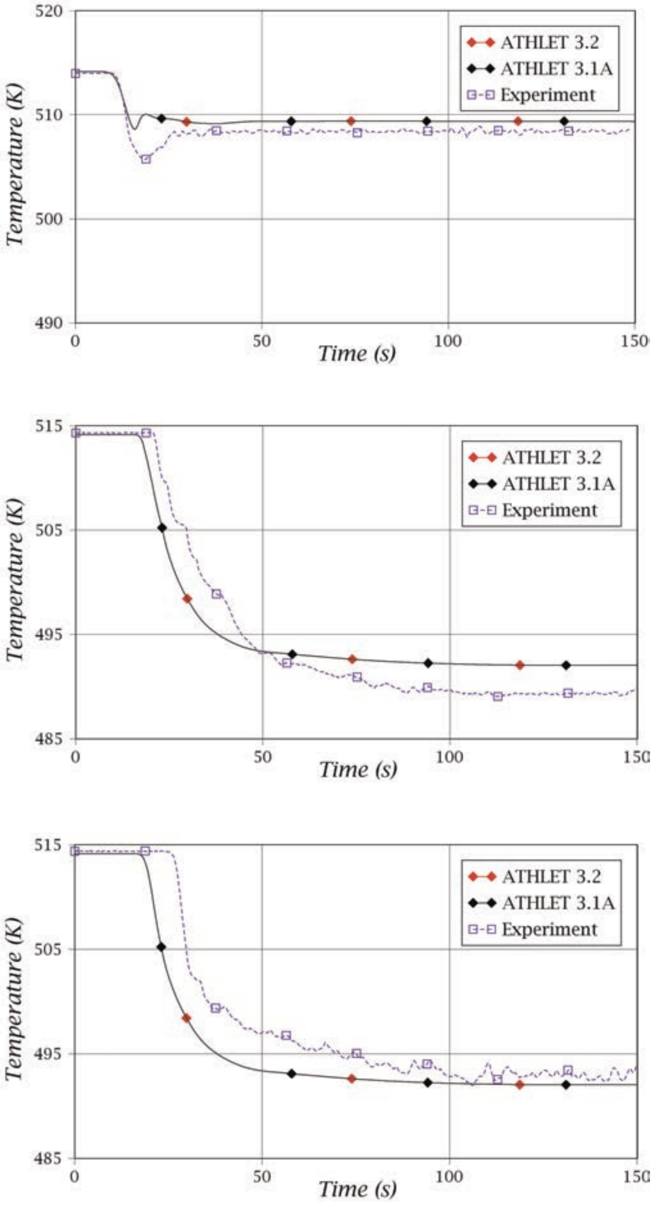

Fig. 4. Measured and calculated temperatures in the DC (top), core inlet (middle) and affected loop (bottom) [3]

some minor quantitative deviations. Only for the temperatures at the core inlet the trend changes from a predicted overestimation to an underestimation of app. 3–5 K.

The comparison of two simulations with ATHLET 3.2 by application of the 3D model and the 1D modelling with parallel channels indicates that the results in the downcomer can be slightly better predicted with the 3D model, but overall the differences between the models are small. Additionally, portability tests on different platforms beside Windows systems show no differences of the results for ROCOM 2.1. In general, the CPU time does not increase significantly by application of the 3D model due to its already lumped parameter approach with a quite rough mesh.

3.2 Phébus FPT-3

The purpose of the Phébus FP (Fission Product) research program, conducted by IRSN and CEA in Cadarache, was to improve the understanding of phenomena occurring during a severe accident in light water reactors and to validate computer software used to simulate them. The test matrix comprises five in-pile experiments, which have been carried out between 1993 and 2004

3.2.1 Description of the experiment Phébus FPT-3

The final test, FPT3, performed in November 2004, studied the impact of a boron carbide control rod on fuel degradation, fission product transport/deposition in the circuit and behaviour in the containment, using irradiated fuel (24.5 GWd/tU), and featuring a steam-poor period as in FPT-2 [6]. The test facility represents a 900 MWe PWR at the scale of 1:5000. It comprises of the test core (surrounded by a driver core to produce thermal neutrons), the circuit with hot leg, steam generator and cold leg as well as the containment (Fig. 5). The test bundle consists of 20 Zircaloy-clad fuel rods, out of which 18 are previously irradiated. In the central position a boron carbide (B_4C) control rod can be found.

Before the transient test phase, a re-irradiation phase was carried out for obtaining a representative bundle fission product inventory by re-creating short lived fission products. This phase was followed by a transition phase, after which the experimental phase was performed starting with the bundle degradation phase and followed by a long-term phase for investigation of phenomena in the containment. The core degradation phase can be divided into six phases: the calibration phase (till 7920 s) followed by the pre-oxidation (7920 s–8640 s) and the oxidation (8640 s–11100 s), the P4 power plateau (11100 s–15420 s), the heat-up phase (15420 s–17370 s), and finally the cool-down (starting at 17370 s).

3.2.2 Simulation Results of Phébus FPT-3

The simulation was performed with ATHLET-CD 3.1A Patch 4 and ATHLET-CD 3.2. Details about the used nodalization and modelling options can be found in [7]. For all intents and purposes, there is nearly no difference between the simulated temperatures within the core region for the two versions. Details are discussed in detail in the validation report of ATHLET-CD [8]. The small deviations are negligible throughout the whole simulation. Therefore, the following discussion focuses on ATHLET-CD 3.2 results.

Fuel and clad temperatures are both well predicted. The qualitative progression of the heat up is very well captured, and the simulated values are generally in a good agreement with the measurements. The amount of molten mass in the experiments were about ~1.6 kg, which is slightly overestimated by the calculated value of about ~1.8 kg. The majority of the hydrogen production takes place during the first oxidation period (~9800 s–~10900 s), and only a fraction of the whole produced amount is obtained during the second oxidation phase (~16000 s–~17000 s). This qualitative characteristic is well captured by the simulations. For the ATLET-CD 3.2 version slightly more hydrogen is produced (105 g or 52 mol), but the code still somewhat underestimates the measured value of 60 ± 3 mol [6].

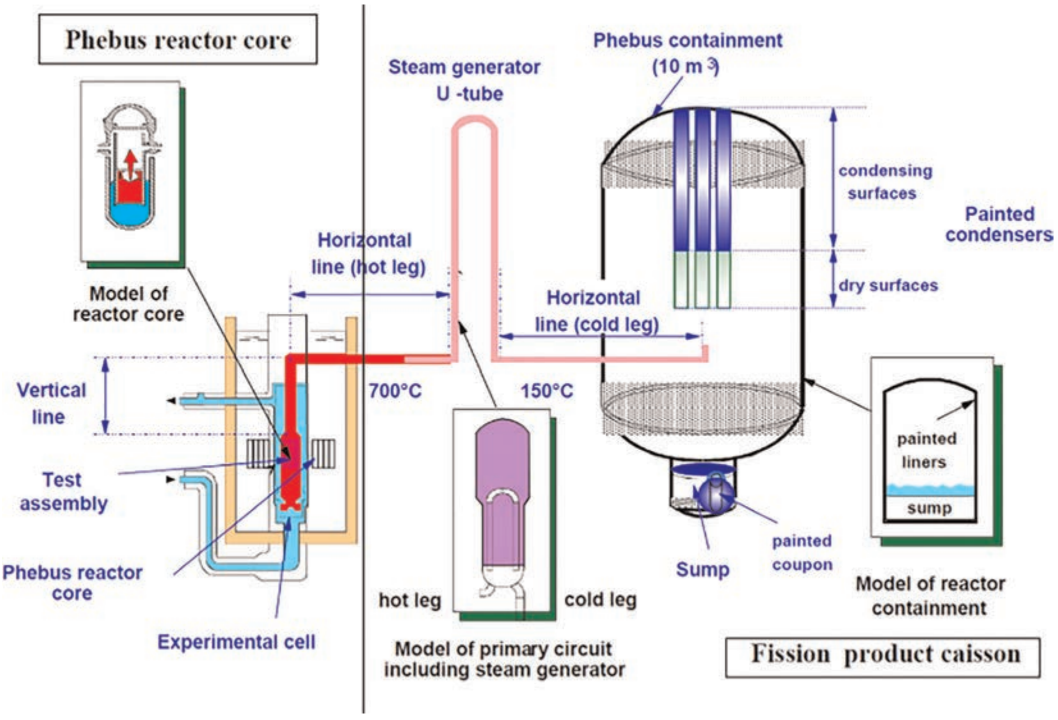

Fig. 5. Phébus experimental facility [6]

Both code versions predict very similar results for the release fraction of fission products from the core. While there are some deviations, e. g. with regard to release dynamics, which is overestimated, the total amount of noble gases such as xenon and the total amount of iodine are predicted quite well. Regarding cesium, the release is overestimated compared to measurements, but qualitatively the release is well captured. Generally, the simulation results are acceptable in comparison to the experiments.

The fission product release into the containment is calculated with the modules SOPHAEROS (ATHLET-CD 3.1A Patch 4) and SAFT (ATHLET-CD 3.2). In case of the noble gases both versions predict almost the same values, which are in good agreement with the experiment. Generally, ATHLET-CD 3.2 (SAFT) predicts a higher deposition in the circuit and consequently a lower release into the containment. As can be seen in Fig. 6, this leads to a better prediction of the measured values compared to version 3.1A Patch 4. The only exception is tin, for which a higher release is calculated with ATHLET-CD 3.2 increasing the overestimation of the experimental value. Generally, the model captures the qualitative evolution of the release vector well, while to some extent overestimating the actual values.

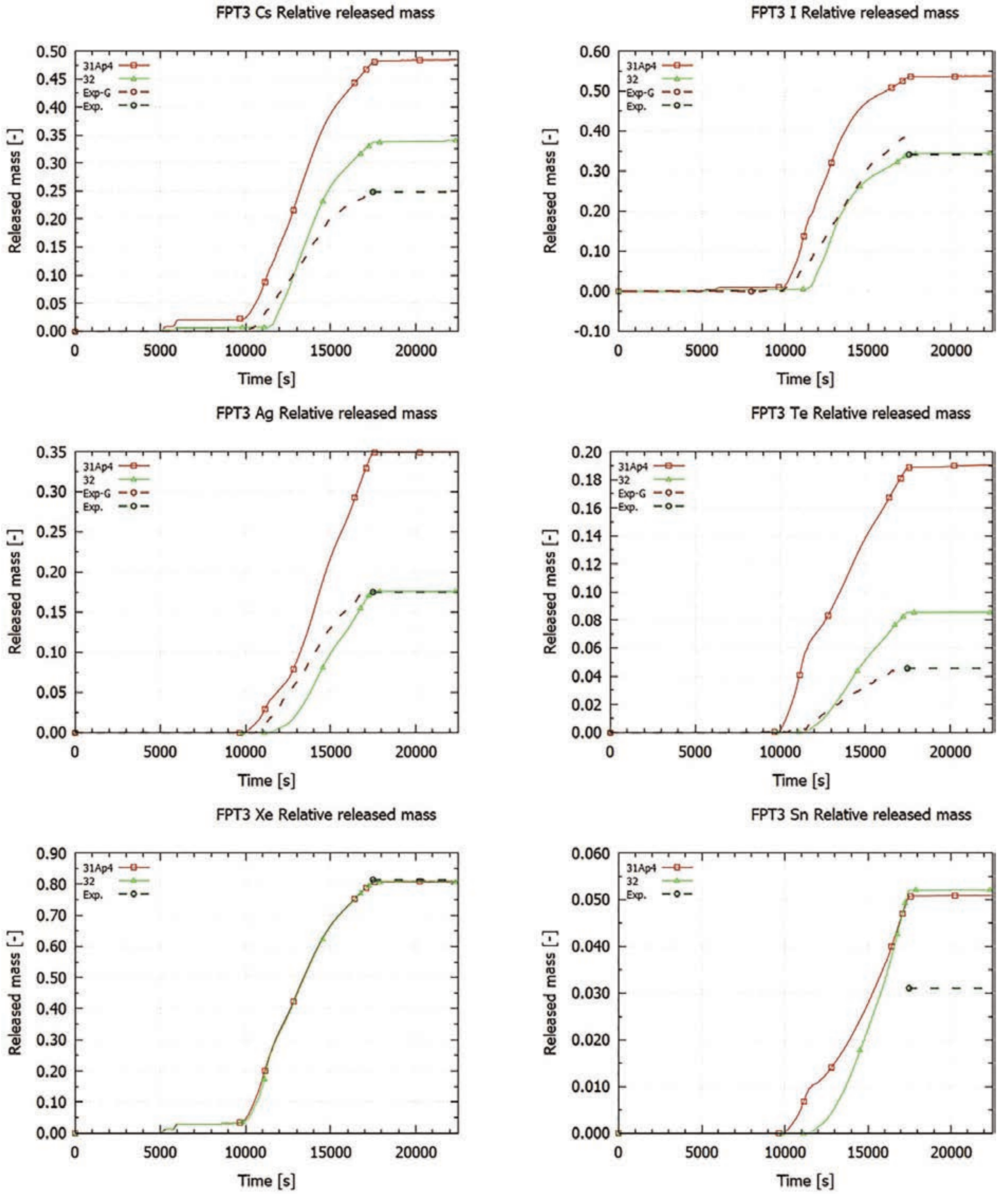

Fig. 6. Phébus FPT3: Relative released mass into the containment

It is of high importance in what chemical form iodine enters the containment. Contrary to previous tests, where iodine was almost entirely injected in an aerosol form, in case of the FPT-3 test 87.7 % of the released iodine into the containment was in gaseous form and only to a lesser extent in an aerosol form (12.3 %). This behaviour was not well captured by the ATHLET-CD 3.1A Patch 4 version, which predicted about 67 % of aerosol, and only 33 % gaseous iodine to enter the containment. The new version delivers a better result but still only about half of the iodine entering the containment has been predicted to be in gaseous form.

Both models predict similar deposition for iodine and cesium, but the new version simulates a higher deposition at the beginning of the hot leg (in the curvature region) and in the cold leg (Fig. 6). The predicted evolution of other elements is similar. A quantitative analysis of the deposition (where measurements are available) shows the following: While the version ATHLET-CD 3.1A Patch 4 achieves a better agreement with experimental data in the hot and cold legs, in the steam generator, where the majority of the deposition takes place, experimental values are better predicted with the new model in version ATHLET-CD 3.2. As can be also seen in Fig. 7, the better prediction of the deposition in the steam generator as well as a generally higher deposition along the length of the circuit lead to a lower release into the containment, which is in a better agreement with the experiment.

4 Application of ATHLET and ATHLET-CD on recent experiments

4.1 Application of ATHLET

The code ATHLET is currently applied for simulation of experiments of the OECD/NEA projects PKL4 (complementary to the German PKL IIIi project) and ATLAS-2. In both test series the behaviour of the primary circuit is investigated under different accident conditions like small and intermediate leaks. Therefore, accident management procedures as well as passive safety systems are considered in order to evaluate the effectiveness of such measures or systems for assuring core cooling during these scenarios. For both test series pre- and post-test simulations are being performed to predict the plant behaviour and to evaluate the simulation results in comparison to experimental data as well as to the results of other advanced system codes. Initial results show that ATHLET generally predicts most of the phenomena of these sequences in good agreement to the experiment with some smaller deviations for some aspects of the experimental results.

Additionally, ATHLET is applied on integral and single effect tests dealing with passive safety systems like in the INKA test facility (Framatome, Germany), the PERSEO test facility (ENEA, Italy) or the COSMEA facility (HZDR, Germany). Results will be presented separately.

4.2 Application of ATHLET-CD

The code ATHLET-CD is currently applied for two experiments of the QUENCH test series performed at KIT. On the one hand pre-test simulations were performed for the next test QUENCH-20, which will be the first experiment considering BWR configuration in comparison to the previous PWR test configurations in the QUENCH facility [9]. The results of the simulations will also be used for the set-up of the test conduct. On the other hand pre- and post-test simulations were performed for QUENCH-19, which was performed in 2018 as the first test with accident tolerant fuel (ATF) claddings [10]. ATF are investigated to get longer grace times for accident management measures due to inhibition or preclusion of the exothermic Zr-steam reaction that escalates core heat-up with degradation for conventional Zr-cladding fuels. Different to QUENCH-15 as reference test, the new test QUENCH-19 had FeCrAl claddings and 4 FeCrAl 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. Due to a lack of information on material properties and oxidation behaviour of FeCrAl cladding, for the pre-test simulations some assumptions were necessary. To predict the range of the possible bundle behaviour two scenarios were investigated using the same boundary conditions like in QUENCH-15 with Zirlo claddings: One without oxidation and another with oxidation by application of the strongest Zry oxidation (Cathcart/Prater-Courtright) under consideration of ZrO_2 properties instead of FeCrAl oxides. The results show a plausible behaviour of the temperature evolution with maximum temperatures below the melting point of FeCrAl (no oxidation: 1350 °C, with oxidation: 1475 °C) and no escalation during quenching, not like

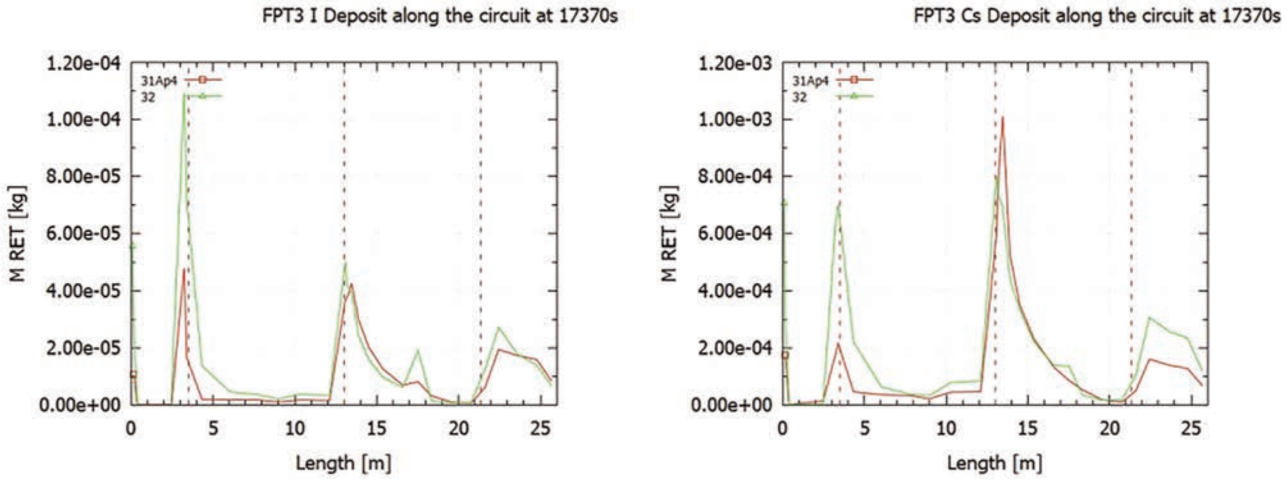

Fig. 7. Deposition of Cs and I in the cooling circuit

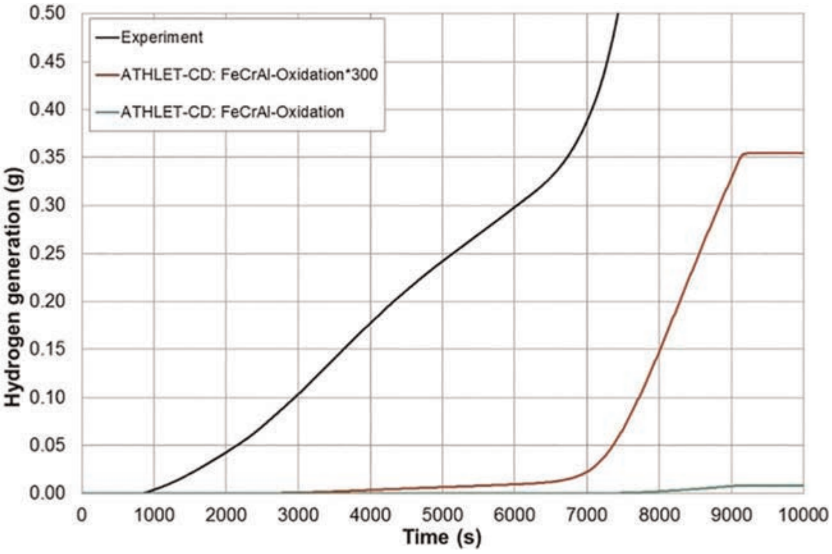

Fig. 8. Measured and calculated hydrogen generation of QUENCH-19

in QUENCH-15, where temperatures above 2000 °C occurred. For the post-test simulations an oxidation correlation for KANTHAL APMT was available and also a second approach derived from an OECD/NEA report. Both approaches were implemented in an internal version of ATHLET-CD. Compared to Zry oxidation both approaches are orders of magnitude lower in terms of reaction kinetics for hydrogen production. However, they are only valid for one single cladding composition (Al). Additionally, it was assumed that due to the bundle heat-up conditions only Al_2O_3 was formed by oxidation and no other oxides. Thus, deviations are to be expected.

The results of the post-test simulations show that ATHLET-CD can predict the thermal behaviour of the experiment in good agreement to the measured values, especially along the heated length. Compared to the observed radial temperature profile of up to 200–300 °C in the experiment ATHLET-CD calculates only a maximum of app. 50 °C. The maximum temperature was measured at 850 mm, while it is calculated at 950 mm with an underestimation of app. 50 °C. Both oxidation approaches for FeCrAl strongly underestimate the measured H_2 generation of app. 9 g (Fig. 8). For a detailed evaluation of the calculated hydrogen generation the post-test examination of the bundle is necessary to know which components contribute to the total value. Nevertheless, the oxidation modelling for FeCrAl will be improved.

5 Conclusions and outlook

The results of the validation simulations show that the AC^2 2019 codes ATHLET 3.2 and ATHLET-CD 3.2 can be successfully applied for

- Thermal-hydraulics of LWR Gen II, III and IV,
- Core degradation,
- Fission product release and transport as well as
- Late phase phenomena

by application on selected experiments and plants. Successful simulations of challenging integral test ROCOM 2.1, Phébus FPT-3 and QUENCH-19 underline the capability of the AC^2 code codes ATHLET and ATHLET-CD and the interaction of a wide range of code models.

From this work, some points for further model improvement have been identified, e. g. specific to ATF, and these will be pursued in the ongoing development of the AC^2 codes ATHLET and ATHLET-CD. Results from other work on the application on passive systems which are part of Generation III+ reactor concepts and Small Modular Reactors (SMR) show that potential for model improvement exist for heat transfer mechanisms of such systems. This is another train of future development work which will be subject to the ongoing validation of the AC^2 [11, 12]

While overall the coverage of the validation matrices is good, several validation calculations were performed with outdated code versions. GRS strives to redo important validation cases with the recent release versions. This will also include the (re-) calculation of single effect tests. Furthermore, the validation basis of each code as well as the interaction of all three codes of AC^2 need to be extended, e. g. by application of coupled ATHLET(-CD)/COCOSYS scenarios from the initial event up to behaviour in the containment and possibly the release of source term to the environment. Participation in international activities, especially OECD/NEA activities and EC sponsored projects, offer the possibility to evaluate the capabilities of AC^2 in comparison to experiments and especially to other advanced code systems is an essential task of the validation process. As this substantial validation program needs a lot of work, GRS is partnering up with other interested organisations like Ruhr-Universität Bochum, IKE Stuttgart or HZDR to share validation work.

Finally, for increasing effectiveness of validation efforts, to keep results up to date and make them easily available for feedback during code development, GRS is increasing its use of the continuous integration platform Jenkins for verification and validation tasks for AC^2 [13]. This will be one focus of the next validation cycle at GRS.

Supported by:

Federal Ministry
for Economic Affairs
and Energy

on the basis of a decision
by the German Bundestag

Acknowledgements

This work was supported by the German Federal Ministry of Economic Affairs and Energy (BMWi) based on a decision of the German Bundestag.

(Received on 30 July 2019)

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Bibliography
DOI 10.3139/124.190069
KERNTECHNIK
84 (2019) 5; page 397–405
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ISSN 0932-3902