VALIDATION OF CFD-CODES FOR NATURAL CONVECTION AND CONDENSATION PHENOMENA IN CONTAINMENTS WITH GERMAN THAI-EXPERIMENTS

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ABSTRACT

In the case of a severe accident in a PWR the flammability of the hydrogen/steam/air-mixture and the resulting pressure loads in the case of combustion are mainly influenced by the local and global distribution of these gases within the PWR containment. A reliable prediction of gas distribution in case of a severe accedent is necessary for the development of mitigation strategies.

CFD codes have in principal the capability to predict local gas concentrations and distribution processes within NPP containments, but validation is needed to ensure that the implemented models are able to simulate all relevant phenomena (gas mixing, build-up and erosion of stabile light gas layers, steam condensation processes, …) expected under accident conditions.

Relevant thermal-hydraulic phenomena within the containment are represented with increasing complexity by the German THAI experiments TH-21 (natural convection), TH-22 (natural convection and dissolution of a light gas cloud) and TH-24 (natural convection, steam cloud dissolution and condensation processes) which were performed by Becker Technologies (Germany). All experiments are used by the German Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH for the verification and validation of Ansys CFX in projects sponsored by the German Federal Ministry of Economics and Technology (BMWi).

This paper is mainly focused on the validation of Ansys CFX with the last experiment TH-24 in the series, while only some general conclusions from the earlier analyses of TH-21 and TH-22 are presented. In this last experiment a natural convection was induced by heating and cooling of different parts of the outer THAI vessel wall. A steam-stratification was built up by injecting steam at a higher elevation in the THAI vessel. This steam stratification was afterwards dissolved by the natural convection flow.

This experiment was simulated with Ansys CFX-14.5, applying the SST (Shear Stress Transport) turbulence model and additional wall- and volume-condensation models. Mesh sensitivity studies were performed to ensure compliance with the CFD best-practice-guidelines. The results show that the CFX simulation is able to predict the gas concentrations and the temperature distribution in the THAI vessel in good agreement with experimental data. Good agreement between CFX simulations and experimental results were also found for the earlier experiments TH-21 and TH-22.

KEYWORDS
Thermal hydraulics, CFD, Natural convection, Condensation, RANS turbulence modelling

1. INTRODUCTION

1.1 Objectives of THAI TH-21 to TH-24 Test Series

The THAI TH-24 experiment is part of a test series for code validation which has an increasing complexity (Figure 1). In the test series natural convection flow was the main subject while in the TH-24 experiment the dissolution of an upper steam layer by natural convection was investigated. The THAI vessel is made out of stainless steel. It has a volume of about 60 m³ and a height of about 9 m. Parts of the vessel wall could separately being cooled or heated with oil. This differential heating induces a natural convection flow within the THAI vessel.
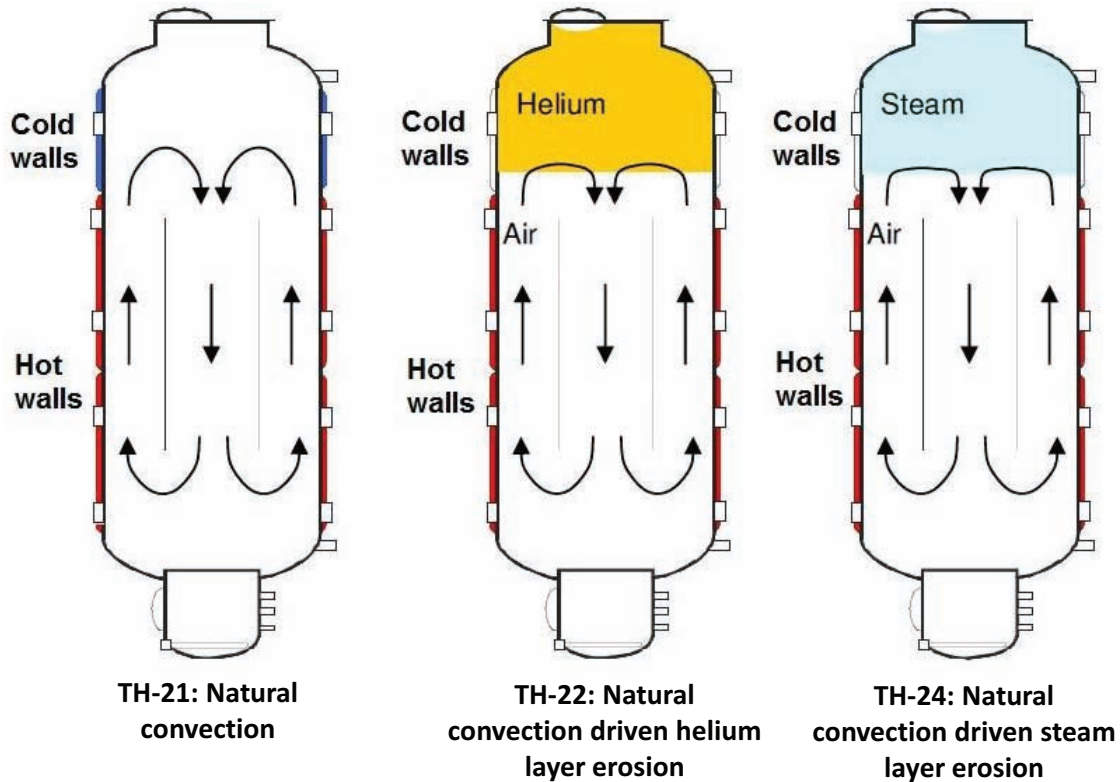

Figure 1. The THAI experimental test series (Image by: Becker Technologies GmbH).

The THAI experiments TH-21 and TH-22 were successfully simulated by the GRS with Ansys CFX. The temperatures, flow velocities (Figure 2) and helium concentrations (Figure 3) were found in good agreement to experimental data. It was found that the temperature boundary conditions and the heat transfer in the steel walls must be modelled very accurately because the simulation results are very sensitive to it. Different parameter variations (turbulence model, mesh discretization, convergence criterion, …) were performed to found an optimal set of numerical parameters. These numerical parameters were afterwards used for the simulation of the TH-24 experiment (Table 1), which has condensation processes as an additional phenomenon. More details about the TH-21 and TH-22 simulations could be found in [4].
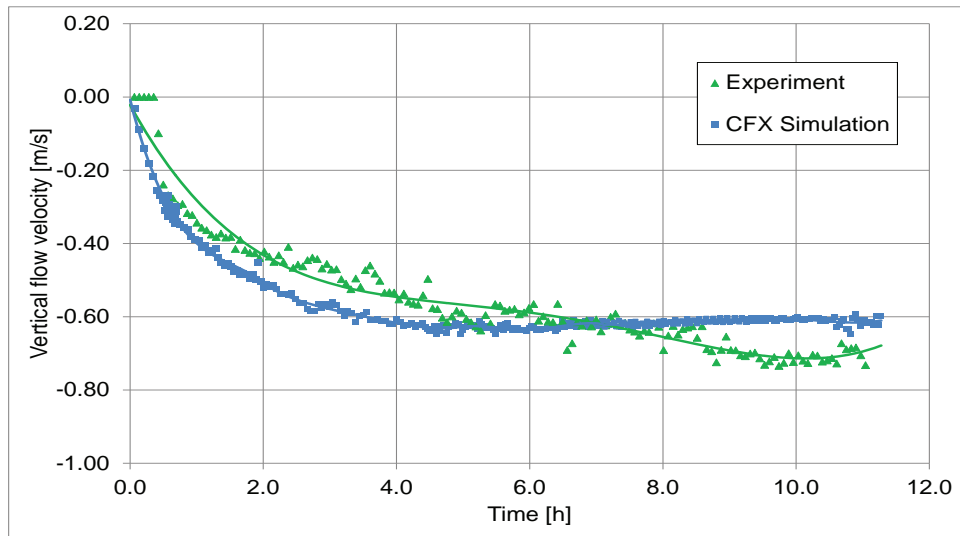
Figure 2. TH-21 experiment: Comparison of simulated and experimental vertical flow velocity in the inner cylinder (5.3 m height).
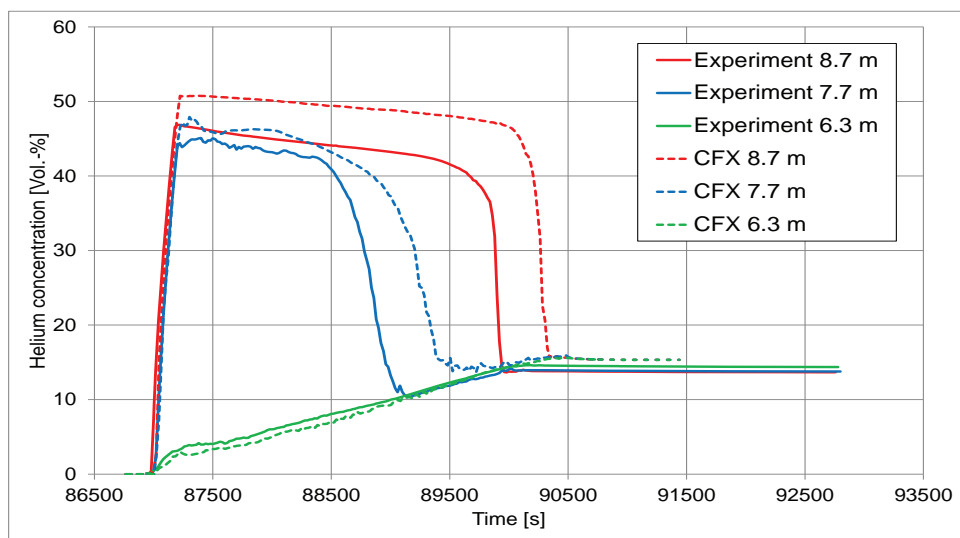

Figure 3. TH-22 experiment: Comparison of simulated and experimental helium concentrations.

1.2 TH-24: Experimental Setup

Figure 4 shows the configuration of the TH-24 experiment. At the beginning of the experiment the THAI-vessel was filled with air. It has a cooled wall in the upper part (blue) and a heated wall in the lower part (red). The heated wall has a temperature of about 100 °C and the cooled wall a temperature of about 60 °C. This differential heating leads to a natural convection flow. After the heat up phase steam was injected in the upper part of the vessel at an elevation of 6.8 m. At first it builds up a stable stratification which was afterwards dissolved by the natural convection process. Bulk and wall condensation also has influence on the local steam concentrations. The steam concentrations, the temperature and pressure were measured at different positions within the THAI vessel.
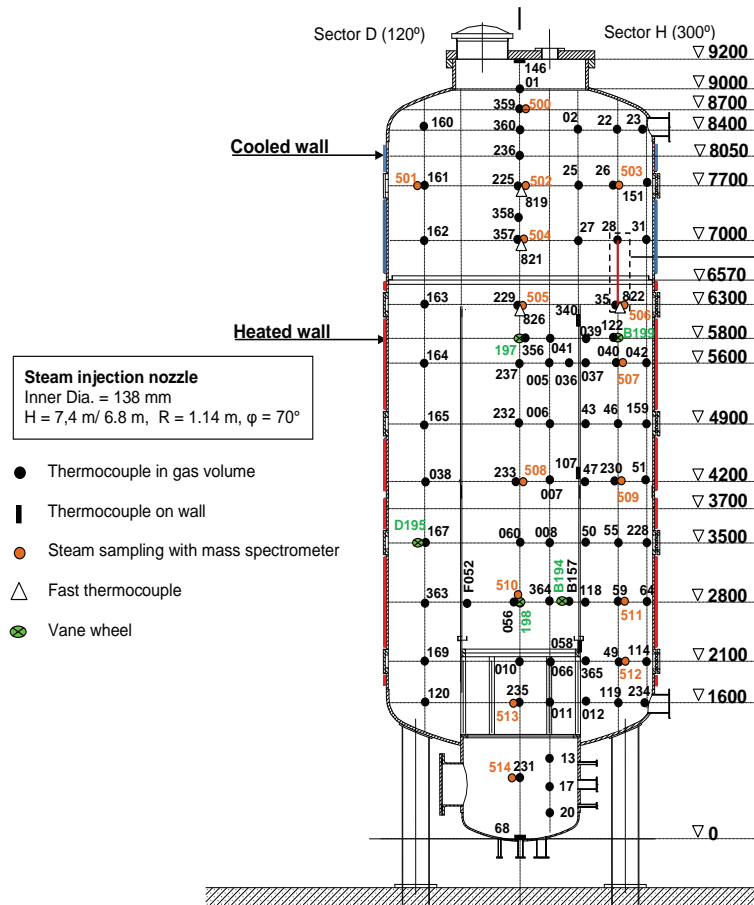
Figure 4. Configuration of the THAI TH-24 experiment (Image by [1]).

1.3 Geometry, Boundary Conditions and Numerical Parameters for the CFX Simulation

Figure 5 shows the CFD mesh which was designed for the simulation of the TH-24 experiment. It is a structured grid with 2 613 840 elements. The upper part (where the steam cloud builds up and is dissolved afterwards) is more refined than the lower part. A second coarser mesh with 639 058 elements was also generated for a mesh sensitivity study which will be discussed in the next section.

The models and the numerical parameters for the CFX simulation are shown in Table 1. For the turbulence modelling the Shear Stress Transport (SST) model is used. This turbulence model had shown good results in further experimental simulations (TH-21, TH-22 and other experiments). The k-epsilon model had shown similar results. The Reynolds Stress turbulence model often seems to be numerical instable. For the wall condensation the Ansys wall condensation model of CFX (Version 14.5.7) is used. For the bulk condensation a model developed by GRS is used. This model reduces the steam fraction until the saturation equilibrium is reached. The generated fog is neglected in this model. A model that can handle the fog is under development at the moment. First results show only a minor influence of the model on simulation results for the TH-24 experiment. But further validation is necessary for a general conclusion. Thermal radiation was simulated with the discrete transfer model. The absorption coefficient for steam was calculated with a correlation by Schack [3] which describes the pressure and temperature dependence of this coefficient. The resulting steam absorption coefficients were in the range of 0.9 – 1.1 m^{-1}.

Table 2 shows the initial and boundary conditions for the CFX-simulation. The heat-up phase of the TH-24 experiment was simulated with a steady state simulation. The steam distribution phase of this experiment was simulated with a transient simulation.
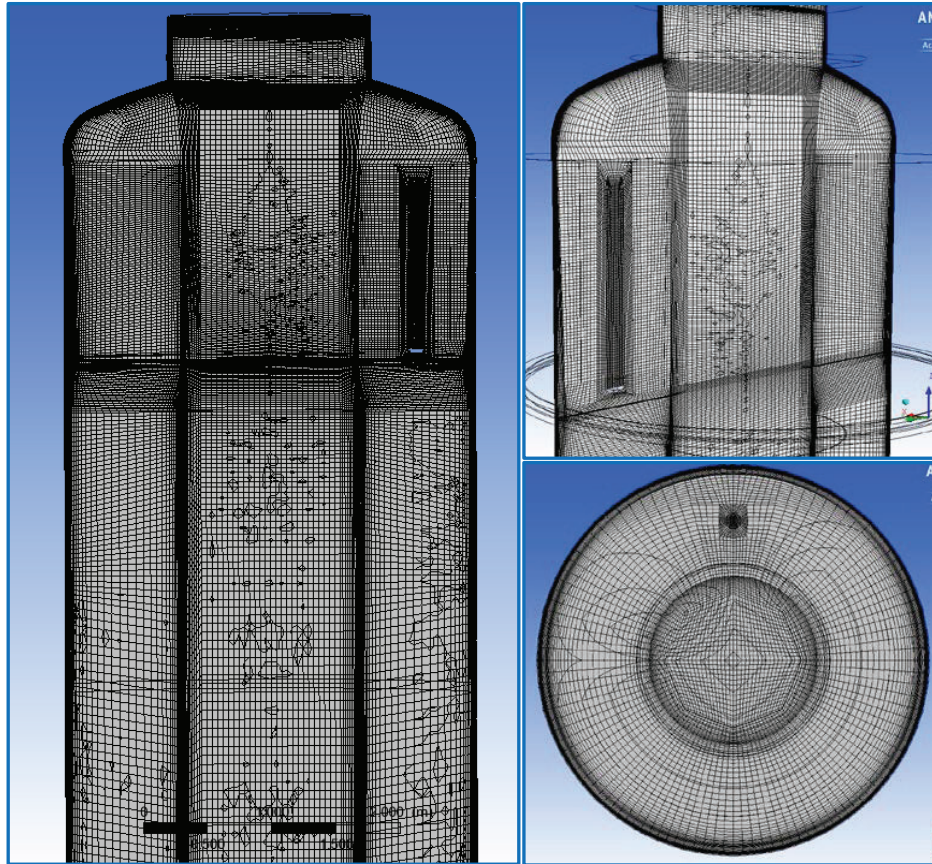
Figure 5. CFD-Mesh of the THAI vessel (2.6 Mio elements).

Table 1. Models and numerical parameters for the CFX simulation.

Experiment	TH-24.3 (THAI-Facility)
Number of elements	Mesh 1: 639 058 elements Mesh 2: 2 613 840 elements
Advection scheme	High resolution [5]
Time differencing scheme	Second Order Backward Euler (Implicit)
Materials	Ansys material database: Air ideal Gas, H2ORKv
Turbulence model	Shear Stress Transport (SST)
Diffusion coefficient	Correlation by Fuller [2]
Thermal radiation model	Discrete Transfer / Gray Number of rays: 64 Absorption steam: Correlation by Schack [3]
Bulk condensation model	GRS-Model [4]
Wall condensation model	Ansys-Model
Convergence criterion	RMS-Residuum < 0.0001 or Max-Res. < 0.001
CFX-Version	14.5.7

Table 2. Initial and boundary conditions for the CFX simulation.

	Heat transfer coeff. [W/m²K]	Outside Temperature [°C]
Heated wall	45	100
Cooled wall	48.5	57.3
Electrical heater up	-	102
Electrical heater down	-	105
Initial conditions at t = 0	Begin of steam injection, calculated by a steady state simulation	
Steam injection	0 s – 400 s: ~35 g/s with 110 °C 400 s – 2 500 s: 1 – 4 g/s	

2. DISCUSSION OF THE CFX-SIMULATION RESULTS

2.1 Results of the Base Case Analyses

Figure 6 shows the build-up and dissolution of the steam layer in the upper part of the THAI vessel. The greatest amount of the steam was injected in the time range between 0 s and 400 s (pictures 1 to 3 in Figure 6). After 400 s the dissolution of the steam layer begins. This dissolution was induced by the differential heating/cooling of the outer vessel walls. At t = 2 000 s the complete steam layer was almost homogeneously dissolved (picture 5 in Figure 6).
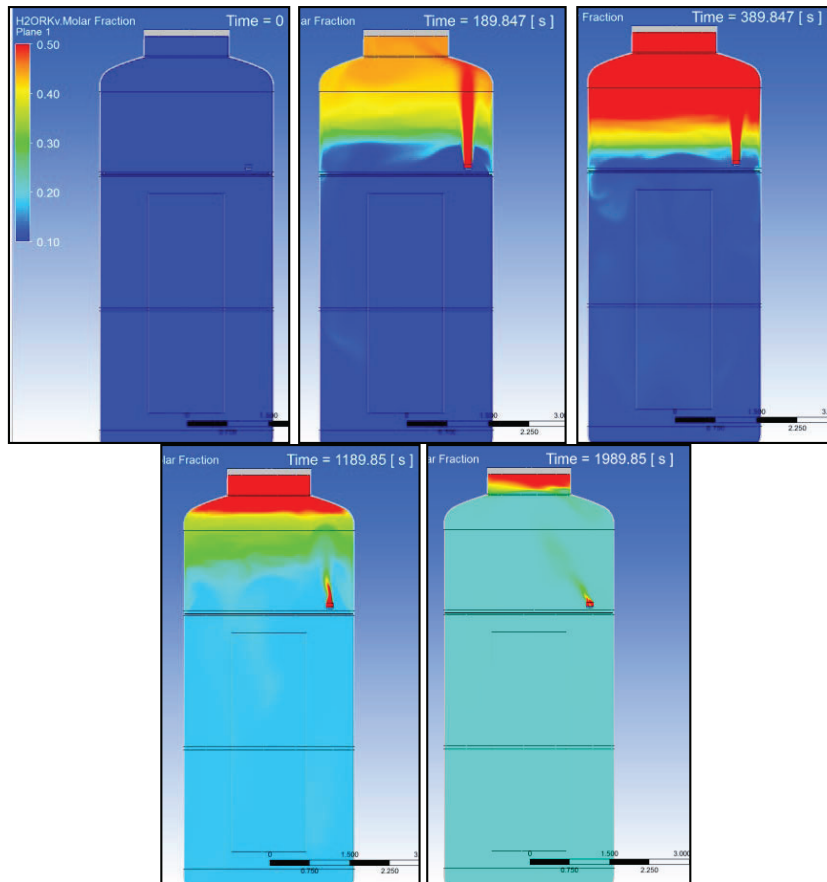

Figure 6. Build-up and dissolution of the steam layer (calculated with 2.6 million elements).

2.2 Mesh Sensitivity Study

Two different simulations were performed to analyze the influence of the mesh discretization on the simulation results. One simulation uses a coarse mesh (639 058 elements) and the other one a fine mesh (2 613 840 elements). Both meshes are compared in Figure 7.
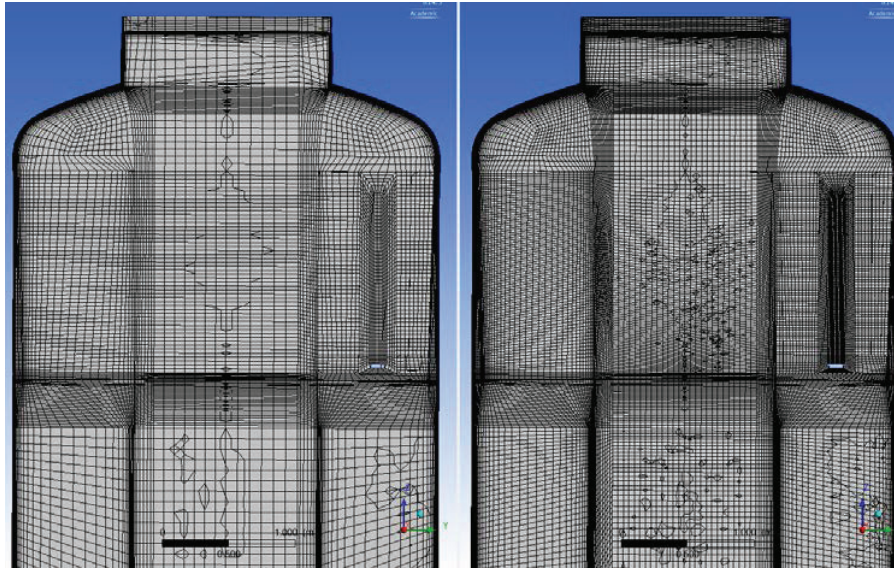

Figure 7. Left: Coarse Mesh (639 058 elements), Right: Fine Mesh (2 613 840 elements).

Figure 8 shows the influence of the mesh discretization on the simulated steam distribution within the THAI-vessel. In general there is a good qualitative agreement between both simulations, but in detail there are some differences. All measurement points show that the coarser mesh leads to a slower dissolution of the steam cloud. The absolute magnitude of the steam concentration is in good agreement for all measurement points. One exception is the point at 7.00 m. This is a region with strong concentration and velocity gradients in the flow field. Because of that it is very sensitive to the mesh discretization.

Figure 9 shows the influence of the mesh discretization on the temperature for one measurement point at 7.7 m height. Here again in general a good agreement of both simulations is visible. The influence of the mesh discretization on the calculated temperatures is similar for other measurement points (not shown here).

The influence of the mesh discretization on the absolute pressure in the THAI-vessel is shown in Figure 10. There is again a good qualitative agreement between both simulations. The pressure is slightly lower for the coarser mesh. The comparison shows that for the analyzed region between 0.6 million and 2.6 million elements no final mesh independence was reached. The next step would be to perform an analysis with about 10 million elements. But for the moment the computational costs are too big. The following simulations were performed with the fine mesh with 2.6 million elements.
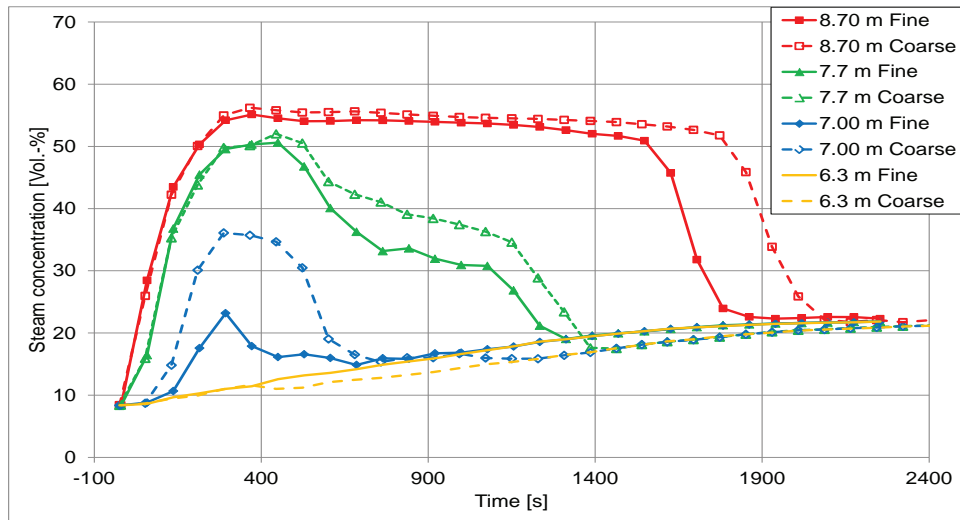
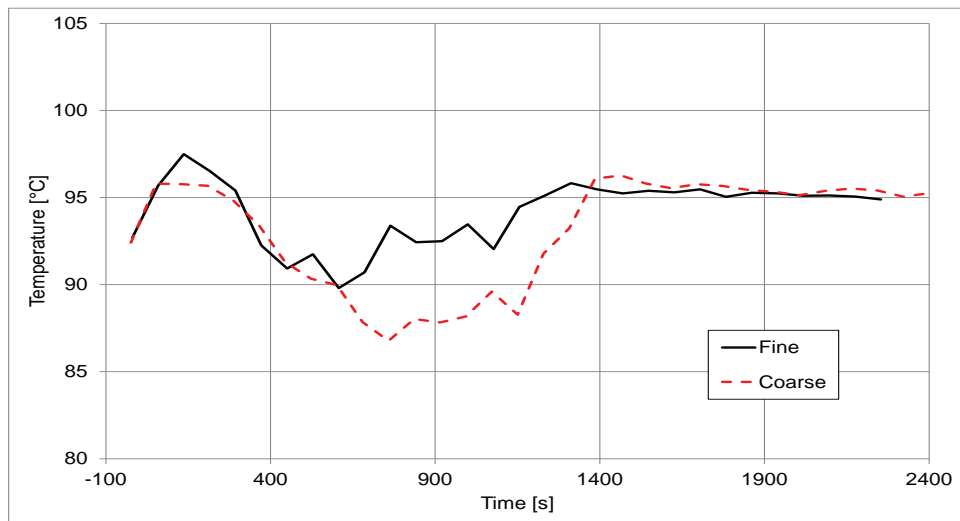**Figure 8. Influence of the mesh discretization on the steam distribution.**

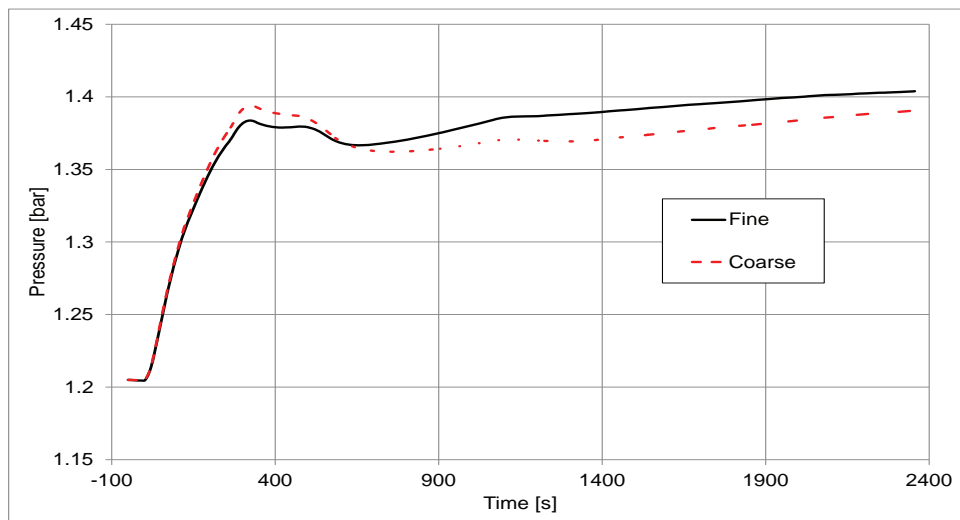**Figure 9. Influence of the mesh discretization on the temperature (at 7.7 m height).**

Figure 10. Influence of the mesh discretization on the pressure distribution.

2.3 Comparison of Simulation Results with Experimental Data

A comparison of experimental and simulated steam concentrations is presented in Figure 11. It shows a good agreement for the most measurement points. The biggest difference is at a height of 7.00 m (blue lines). Again – this is the region with the strong concentration and velocity gradients in the flow field. Therefore, the simulation results are very sensitive to small changes in the setup (mesh discretization, convergence criterion, …).

The simulated time for the complete dissolution of the steam cloud at about 1 800 s is in good agreement with the experimental data. This is the most important result of this CFX validation. The absolute magnitude of the steam concentration after the dissolution of the steam cloud is too low in the simulation. Possible reasons for the remaining differences between simulation results and experiment could be:

- Simplifications of the inlet tube geometry. This could lead to differences in the primary steam distribution, the condensation rates and the pressure development.
- The neglect of effects like re-evaporation of fog and wall condensate in this simulation.

In Figure 12 the experimental and simulated temperature for one measurement point is presented. The agreement is good. The calculated temperature is slightly too high. This result is the same for other temperature measurement points (not shown here).

Comparing the absolute pressure, a difference of about 0.1 bar between simulation and experiment could be seen (Figure 13). Again – possible reasons for this could be the neglect of re-evaporation of fog and wall condensate in the simulation or simplifications of the inlet tube geometry.

Additional measurement was performed for the vertical flow velocity. One measurement point was in the inner cylinder at 5.3 m height. Here a good agreement between simulation results and experimental data is reached (Figure 14).
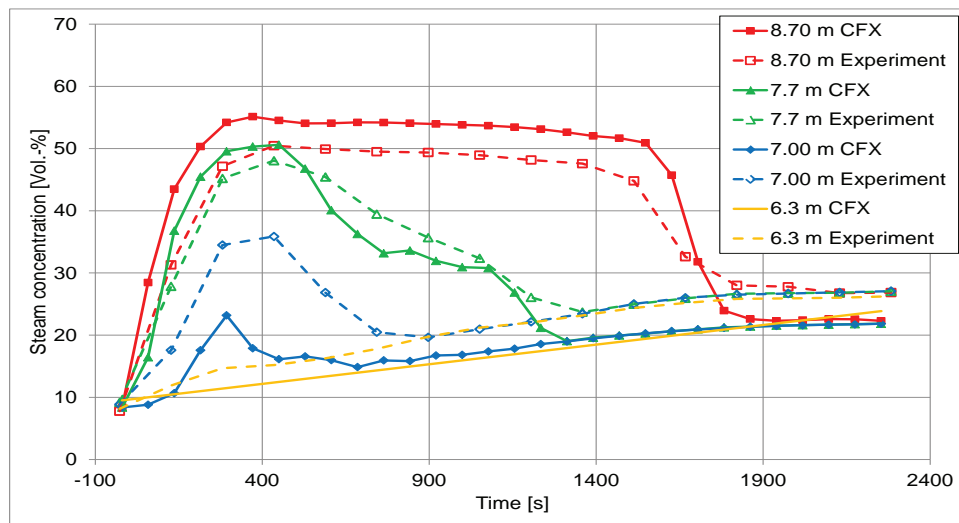

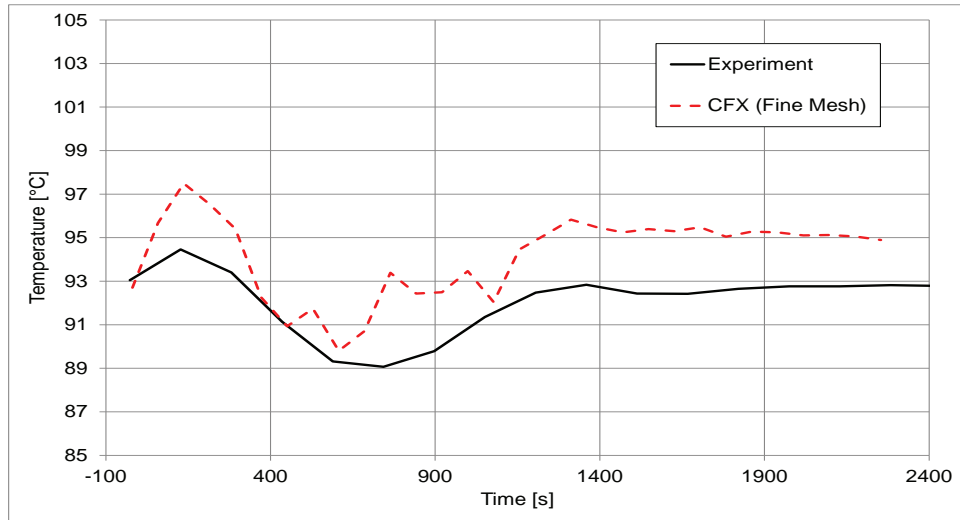**Figure 11. Comparison of experimental and simulated steam concentrations.**

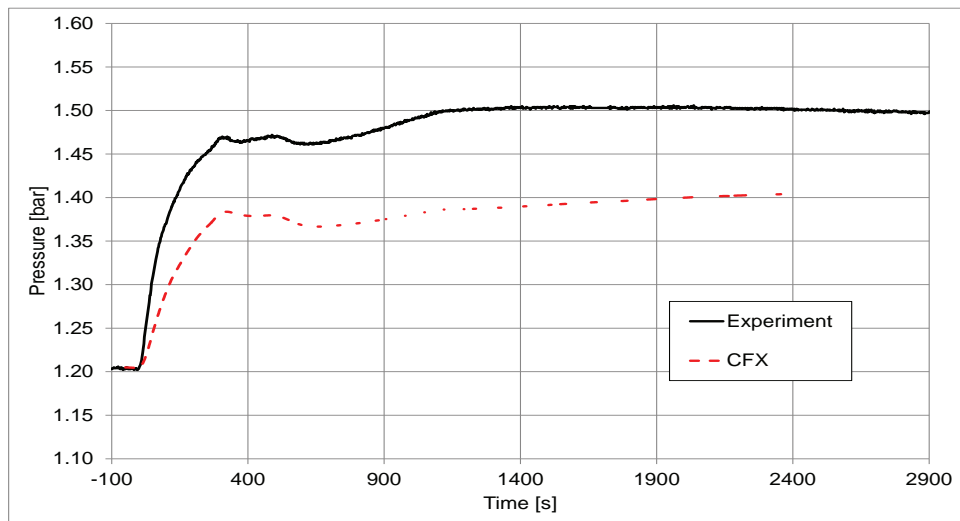**Figure 12. Comparison of experimental and simulated temperature (at 7.7 m height).**

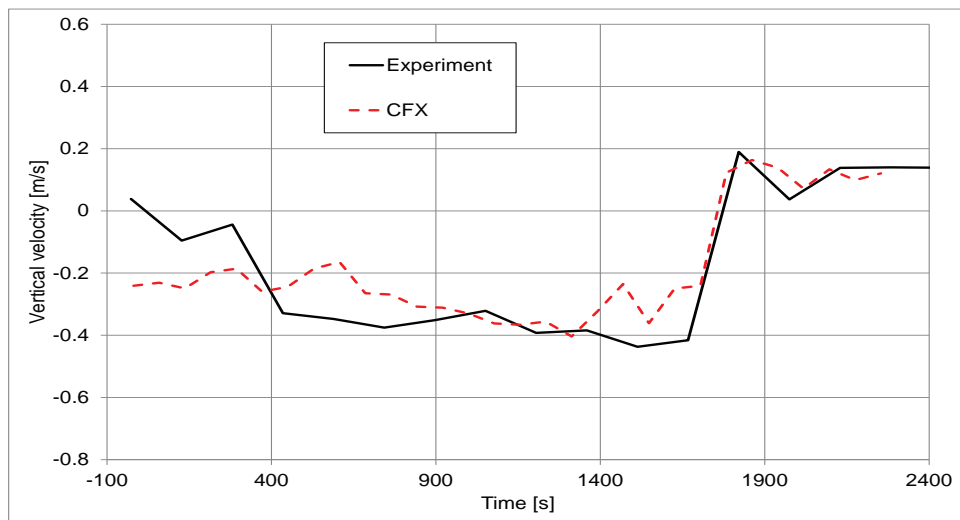**Figure 13. Experimental und simulated pressure development.**

Figure 14. Experimental and simulated vertical flow velocity (at 5.3 m height).

2.4 Effect of the Convergence Criterion

Two different simulations were performed to study the effect of the convergence criterion on simulation results, one simulation with the criterion RMS-Residuum < 1.0E-4 and the other simulation with the stronger criterion Maximum-Residuum < 1.0E-3. Both simulations are compared in Figure 15 to Figure 17. The simulation with the stronger criterion ends at about 1 320 s as the calculation was too CPU-time consuming.

Figure 15 shows a small influence of the convergence criterion on all steam concentrations despite of the concentration at 7.7 m height. A higher steam concentration for the calculation with the stronger convergence criterion (Max.-Res < 1.0E-3) can be seen there.

In Figure 16 the effect of the convergence criterion on the temperature (at 7.7 m height) is shown. There are some differences between both simulations, but the absolute magnitude of the temperature is similar.

Figure 17shows that the stronger convergence criterion leads to a higher pressure, which fits better to the experimental results. Thus the stronger criterion and the more accurate simulation of the convection flow could explain a part of the pressure difference between the simulation with the weaker criterion and the experimental results.
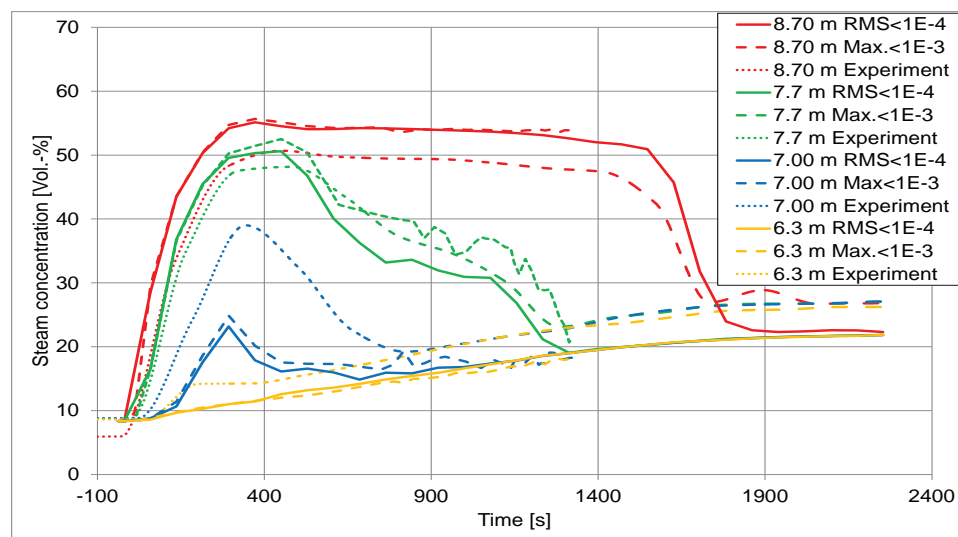

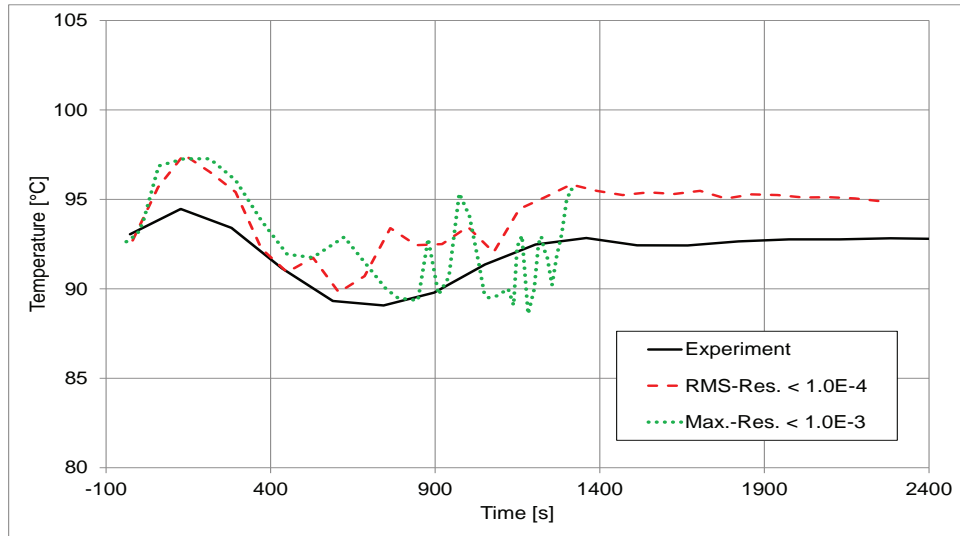**Figure 15. Effect of the convergence criterion on the steam distribution.**

Figure 16. Effect of the convergence criterion on the temperature (at 7.7 m height).
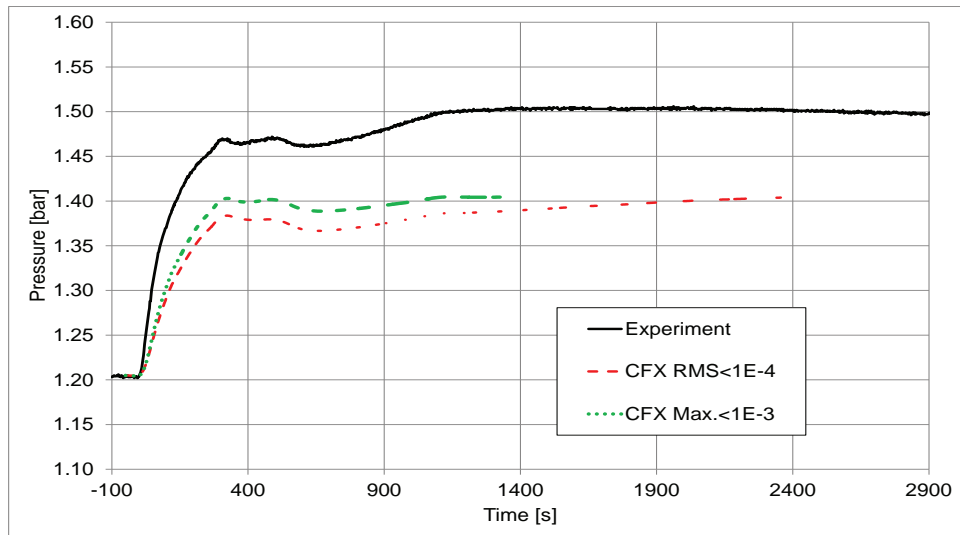

Figure 17. Influence of the convergence criterion on the pressure development.

3. CONCLUSIONS

The TH-24 experiment in the German THAI facility was simulated with Ansys CFX to validate the ability of the CFD code for the simulation of gas distribution, convection and condensation in open containment rooms. Previous simulations of the THAI experiments TH-21 and TH-22 were used to find an optimal set of numerical parameters (turbulence model, mesh discretization, …). For the TH-24 experiment a mesh sensitivity study and a parameter study for the convergence criterion were performed. No final mesh independence was found for the CFD mesh up to 2.6 million elements. But the differences to the coarser mesh with about 0.6 million elements were small.

CFX shows good agreement with experimental results for the build-up and dissolution of the upper steam layer. The time for the complete dissolution of the steam layer was in good agreement to experimental data. Also for the simulated temperatures and for the flow velocities a good agreement to experimental data was found. Only the simulated pressure was too low in comparison to experimental data. Possible reasons for this under-prediction of the pressure could be the neglect of effects like re-evaporation of fog and wall condensate or simplifications of the inlet tube geometry. This will be analyzed in future work.

ACKNOWLEDGEMENTS

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