VALIDATION OF CFD-MODELS FOR NATURAL CONVECTION, HEAT TRANSFER AND TURBULENCE PHENOMENA

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Abstract

Natural convection, heat transfer and turbulence phenomena play an important role for the distribution of steam and hydrogen in nuclear reactor containments in the case of a severe accident. In cooperation with other institutions the GRS adapts and validates the CFX code developed by ANSYS for containment applications. To simulate convection and turbulence phenomena in an accident scenario within nuclear reactor containments the simulation tools and models have to be validated with experimental data. For the validation of CFX two experiments performed at the THAI test facility were simulated (amongst others). The TH-18 experiment was designed for the validation of CFD models for turbulence. The TH-21 experiment was designed for the investigation of heat transfer and natural convection phenomena. The results of both simulations and the comparison to experimental data are presented in this paper. The simulation of the TH-18 experiment shows good results in the upper THAI vessel and not so good results in the lower vessel. The TH-21 simulation shows good results for the pressure and the temperature distribution and not so good results for the flow velocities.

1. INTRODUCTION

THAI is a downscaled containment facility operated at Becker Technologies GmbH, Eschborn, Germany, which was designed to perform experiments in the areas of nuclear reactor containment thermal hydraulics, hydrogen, and fission product (aerosol and iodine) transport and chemistry. The main component is a steel vessel with a height of 9.2 m and a diameter of 3.2 m (see figure 1).

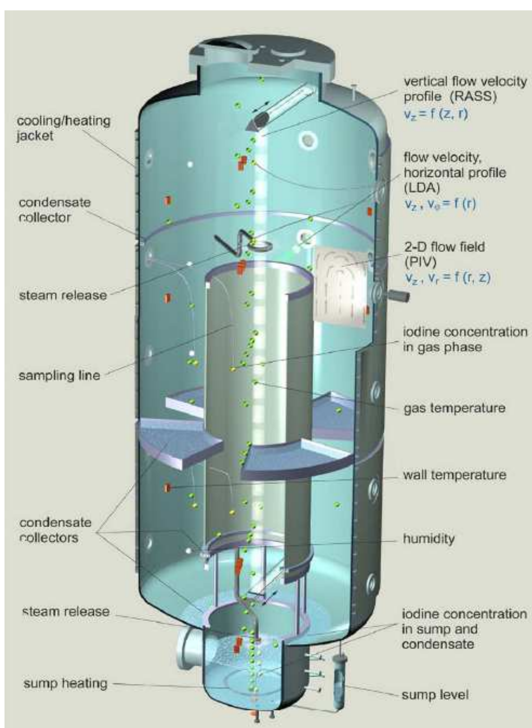

Fig. 1: The THAI test facility (Fischer, 2009)

The THAI program is performed by Becker Technologies GmbH, Eschborn, in close cooperation with AREVA NP GmbH, Erlangen and Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, Cologne. Experiments in the THAI facility began in 2000 under the sponsorship of the German Federal Ministry of Economics and Technology, following the traditions of German containment research in the large-scale facilities BMC (Battelle Model Containment) and HDR (Heissdampfreaktor) (Sonnenkalb/Poss 2009).
The THAI facility for nuclear reactor containment research is intended to conduct experiments in an intermediate scale between separate-effects (laboratory tests) and integral effects (large scale tests). The TH-18 and TH-21 experiments were simulated by using ANSYS CFX-11. Different CFD meshes were designed to analyze the mesh sensitivity. Different turbulence models were tested (K-epsilon, Shear-stress-turbulence and Reynolds-Stress-Model) and the simulation results were compared to experimental data.

2. VALIDATION OF CFD MODELS FOR TURBULENCE

2.1 Description of the CFX model for the TH-18 experiment

The TH-18 experiment was designed for the validation of CFD models for turbulence. In the inner cylinder of the THAI vessel a fan was installed which produces a circular flow field. At different positions in the THAI vessel the velocity of the flow field was measured by PIV (Particle Image Velocimetry) and LDA (Laser Doppler Anemometer). The experimental setup for the TH-18 experiment is shown in figure 2. On the left side is a schematic drawing which illustrates the inner cylinder, the condensate collectors and the fan. The condensate collectors have two different openings for the air flow. On the right side is a picture of the CFD mesh. A full 360° model of the THAI vessel with different numbers of elements was used. The fan was approximated by a mass flow at the fan outlet and a pressure boundary condition at the fan inlet. The mass flow at the outlet has a velocity profile which was gained by an experimental data fit. Table 1 shows the boundary conditions and models for the CFX simulation. The main aim was to study the influence of the turbulence model on the simulation of the flow velocities within the THAI vessel. Therefore different turbulence models (K-epsilon, SST, SGG) were used in the CFX simulations. In table 2 an overview of the performed calculations is given. This is only that part of all performed calculations which is discussed in this paper.

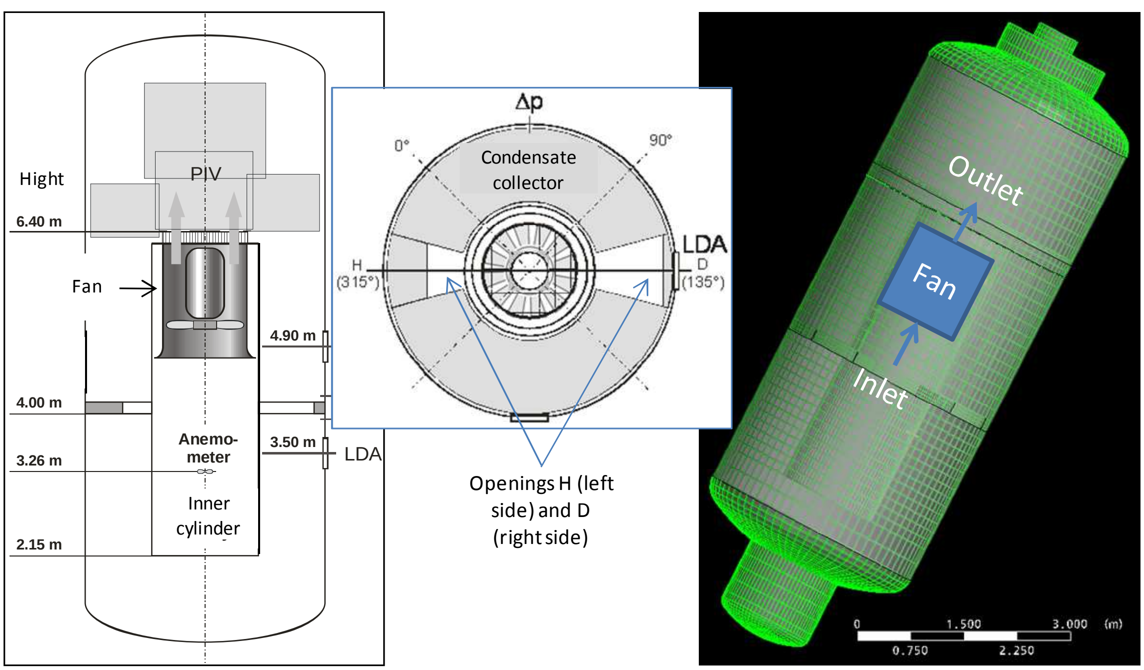

Fig. 2: THAI setup for TH-18
(Left and middle: Schematic drawings (Fischer, 2009), right: CFD mesh with fan inlet and outlet)

Table 1: Boundary conditions and models for the simulation

Boundary conditions	Configuration	Full 360° model		
	Mass flow at the fan outlet	4.46465 kg/s		
	Intensity of turbulence at the fan outlet	5 % (Best value in a sensitivity study)		
	Pressure difference at the fan inlet	1 Pa		
	Simulated time	1000 s		
Physical models	Turbulence	K-ε	SST	SSG Reynolds
	Buoyancy	Neglected		
Material description	Fluid model	Air ideal gas		
	Temperature	22 °C		
	Pressure	1 atm		
	Density	1.185 kg/m³		
Numerical parameters	Number of elements	166,437	1,188,800	
	Mesh type	Structured		
	Simulation type	Transient und isothermal		
	Convergence criteria	RMS < 0.0001		

Table 2: Overview of the performed calculations

ID number of the simulation	**Number of elements**	**Turbulence model**	**Flow profile at the fan outlet**	**Turbulence intensity at the fan outlet**
TH18_01	166.437	K-epsilon	Fit of experimental data	5 %
TH18_02	1.188.800	K-epsilon	Fit of experimental data	5 %
TH18_03	1.188.800	SST	Fit of experimental data	5 %
TH18_04	1.188.800	SSG Reynolds Stress	Fit of experimental data	5 %

2.2 Study of discretisation errors

To quantify the discretisation and model errors two characteristic values $F_{Discrete}$ and F_{Model} were calculated. The first of the following equations shows the calculation of the discretisation error and the second one the calculation of the model error:

$$\langle F_{Discrete} \rangle = \frac{\sum \left| v_{Coarse} - v_{Fine} \right|}{N_{Measure}} \tag{1}$$

$$\langle F_{Model} \rangle = \frac{\sum \left| v_{Model} - v_{Experiment} \right|}{N_{Measure}} \tag{2}$$

In equation (1) v_{Coarse} is the velocity calculated with a coarse (CFD-)mesh, v_{Fine} the velocity calculated with a fine mesh and $N_{Measure}$ is the number of (separately located) measurement points considered for the averaging procedure. In equation (2) v_{Model} is the simulated velocity and $v_{Experiment}$ is the experimental velocity value.

Figure 3 demonstrates the velocity field calculated in a CFX simulation. This distribution shows time dependent oscillations of the flow velocities. Because of this the CFX results were averaged over a certain time period.

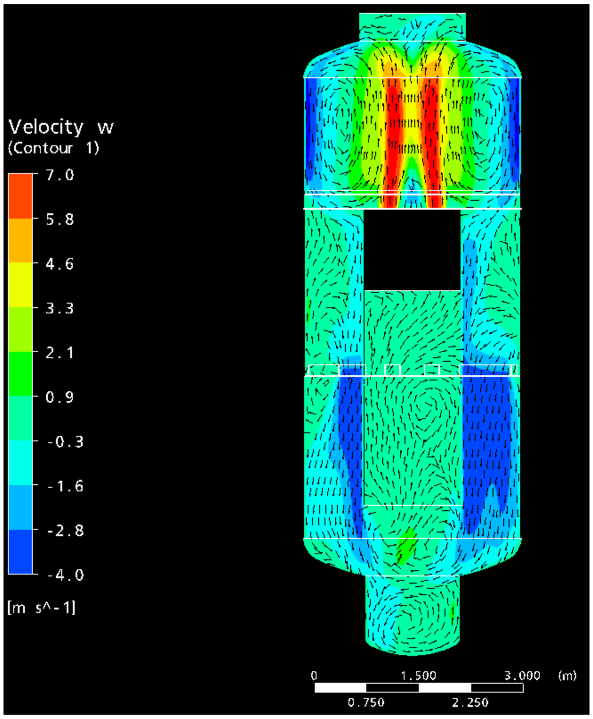

Fig. 3: Snapshot of the flow velocity field in the THAI facility, calculated with CFX

To analyze the influence of the mesh size two different simulations with different numbers of elements were performed (TH18_01 with 166,437 elements and TH18_02 with 1,188,800 elements). One result of these simulations is presented in figure 4. The diagram shows the vertical flow velocities plotted versus the THAI vessel radius at a height of 4.9 m above opening D (see figure 1). The error bars represent the time dependent oscillations of the flow velocities, assumedly induced by an instable flow field and small numerical errors. The results for the different meshes are similar, but not equal. Because of the still remaining differences of the results the mesh with 1,188,800 elements was used for the following turbulence model analysis.

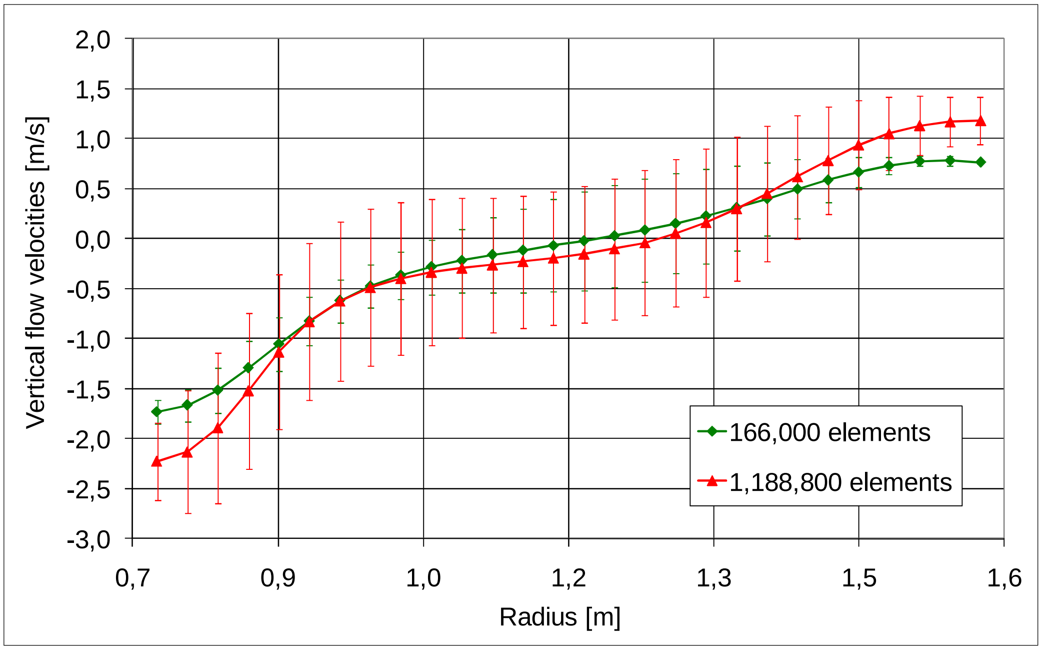

Fig. 4: Vertical flow velocity at 4.9 m and 135° (simulations TH18_01 and TH18_02)

2.3 Influence of the turbulence model

To study the influence of the turbulence model on the simulation results three simulations with different turbulence models were performed. These were TH18_02 with the K-epsilon turbulence model, TH18_03 with the SST turbulence model and TH18_04 with the SSG Reynolds stress model. In figure 5 the vertical flow velocities for the different turbulence models are plotted against the radius at a height of 4.9 m above opening D. This figure shows the best results for the SSG model compared to the experimental results.

Figure 6 demonstrates the influence of the turbulence model on the simulation error at different measurement positions within the THAI vessel. It shows similar errors for the different turbulence models. The smallest error has the SSG Reynolds Stress model. It has an overall model error of 1.08 m/s when all values at different measurement points are averaged (see also table 3).

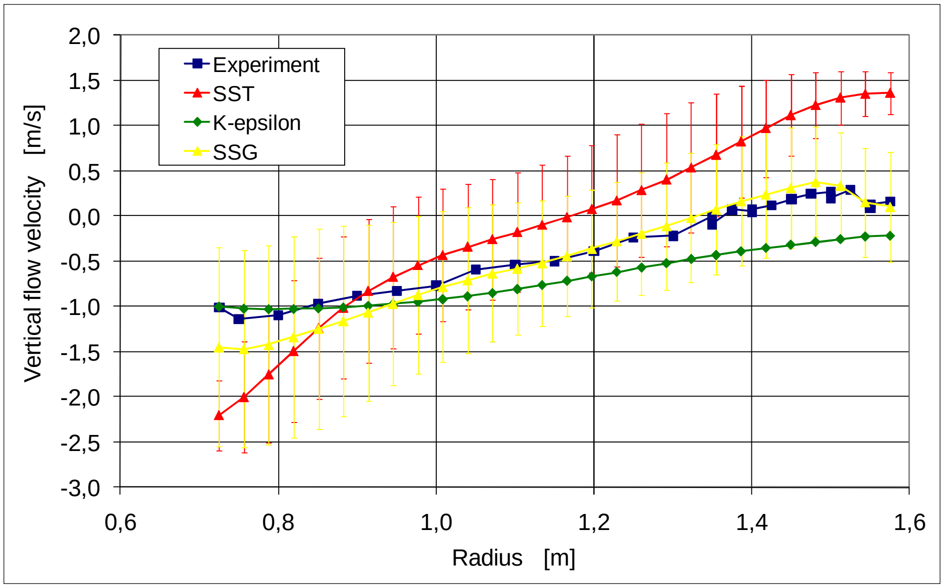

Fig. 5: Vertical flow velocity at 4.9 m and 135 ° (simulations TH18_02, TH18_03 and TH18_04)

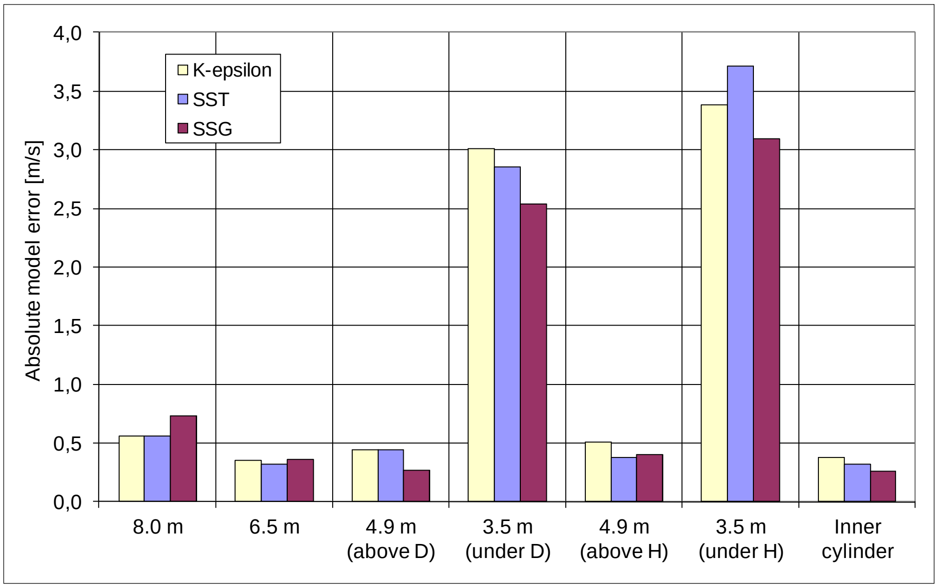

Fig. 6: Influence of the turbulence model on the model error F_{Model} (see also equation 2)

Table 3: Influence of the turbulence model on the model error

Turbulence model	Averaged model error F_{Model}
K-epsilon	1.23 m/s
SST	1.23 m/s
SSG Reynolds Stress	1.08 m/s

3. INVESTIGATION OF HEAT TRANSFER AND NATURAL CONVECTION PHENOMENA

3.1 Description of the CFX model for the TH-21 experiment

The TH-21 experiment was designed for the investigation of heat transfer and natural convection phenomena. Pressure, temperature and flow velocity were measured at different positions within the vessel. The geometry for the TH-21 simulation is a quarter of the THAI vessel (figure 7). This simplification is possible because of the experimental symmetry. Within the facility only the inner cylinder and the condensate collectors were installed for this experiment. Three CFD meshes with different numbers of elements were designed. Two of these meshes are without the vessel wall structures; one mesh is with explicit modeling of the vessel wall. For the turbulence modeling the k-epsilon model was used. More geometrical data and starting conditions can be found in table 4.

To investigate heat transfer and natural convection phenomena the walls of the THAI vessel were differentially heated. The lower vessel wall was heated up to 120 °C and the upper vessel wall was cooled down to 46 °C (outside wall temperatures, see figure 7). This differential heating induced a natural convection process within the THAI vessel (see figure 8). The experiment has two phases: Phase 1 (0 h < t < 7.5 h) is the heat up phase; Phase 2 (7.5 h < t < 10.3 h) is a quasi-stationary phase. The time dependent boundary conditions for the simulation are shown in table 5.

Table 6 shows three different calculations which were performed for this study. From the comparison of these different calculations information about the mesh discretisation error and about the influence of the wall structure model on the simulation results was gained. In the next chapter the analysis of the discretisation errors is shown.

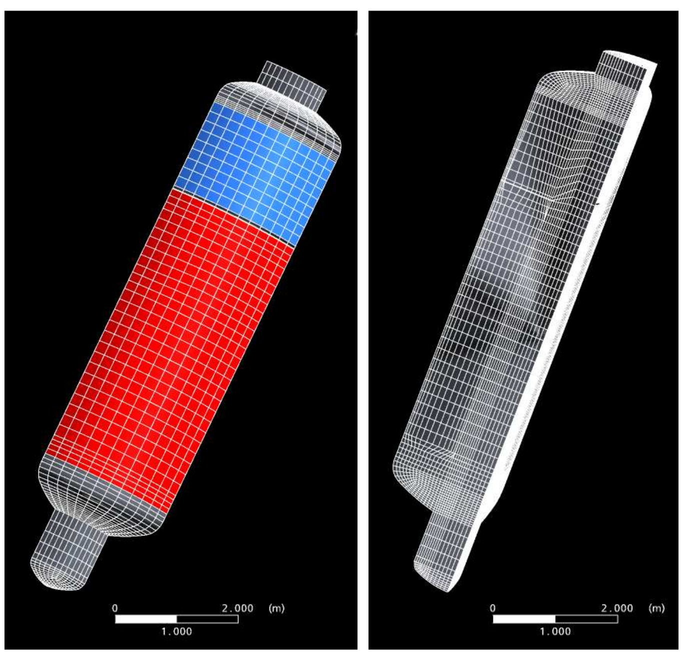

Fig. 7: Geometry model for the TH-21 simulation; Heating jacket (red) und cooling jacket (blue)

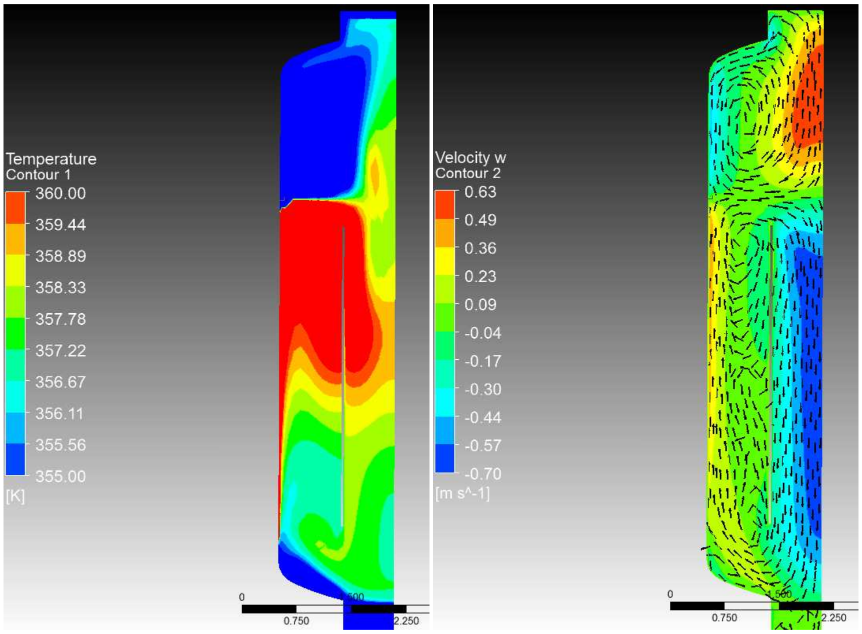

Fig. 8: Temperature distribution (left) and velocity distribution (right) for t = 11.3 h

Table 4: Geometrical data and starting conditions for the CFX simulation

Meshes without wall structures	24,192 elements (per quarter)	74,173 elements (per quarter)
Mesh with wall structures	24,854 elements + 19,006 steel elements = 43,860 elements (per quarter)	
Turbulence model	K-epsilon	
Boundary conditions	Symmetric at the two cutting planes	
Convergence criteria	RMS < 0.0001	
Simulation time	40,600 s = 11.3 h	

Table 5: Time dependent boundary conditions

Temperature of the upper cooling jacket		**Temperature of the lower heating jacket**	
Time [s]	**Temperature [°C]**	**Time [s]**	**Temperature [°C]**
0	12.97	0	13.00
3380	14.06	5500	53.06
5500	16.02	9600	77.02
9600	21.02	16200	102.25
21380	36.02	21380	113.96
28800	42.41	27600	121.61
40600	46.22	30500	120.22
		40600	120.82

Table 6: Overview of the performed calculations

ID number of the simulation	**Number of elements**	**Wall structure modeling**
TH21_01	24,192 per quarter	Without structures
TH21_02	74,173 per quarter	Without structures
TH21_03	43,860 per quarter (24,854 fluid + 19,006 steel)	With structures

3.2 Study of discretisation errors

To study the influence of the discretisation errors on the simulation results two different calculations with 24,192 fluid elements and 74,173 fluid elements were performed (TH21_01 and TH21_02). Figure 9 shows that the influence of the discretisation on the calculated pressure is very small. In phase 2 (t > 7.5 h) the difference between the two calculations averages 0,004 bar. This was calculated with equation (2) using pressure values instead of velocities. Similar observations could be found for temperature values and for vertical flow velocities. The median difference for the temperature values is 0.3 °C and for the vertical flow velocities 0.01 m/s. It could be stated that the performed calculations are nearly independent from the mesh size for this number of elements.

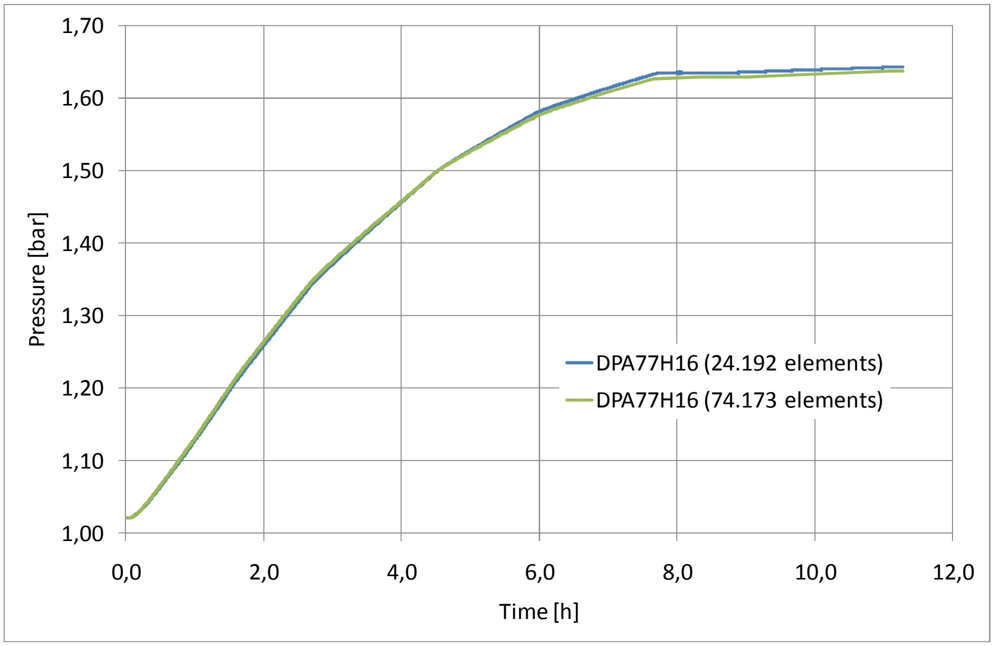

Fig. 9: Influence of the discretisation on the calculated pressure
(simulations TH21_01 and TH_21_02)

Table 7: Influence of the mesh discretisation on pressure temperature and vertical flow velocities

Calculated value	**Absolute discretisation error**
Pressure	0.004 bar
Temperature	0.3 °C
Vertical flow velocity	0.01 m/s

3.3 Influence of the wall structures

To study the influence of the wall modeling in CFX simulations with and without the steel wall of the THAI vessel were performed (TH21_01 and TH21_03). Figure 10 shows the pressure history calculated in these two simulations. It shows a clear lower pressure for the simulation with explicit modeling of the vessel walls (TH21_03). The reason for this is the effect of the walls which store a large part of the energy. The effect is so big that it could not be neglected in the simulations. A similar effect could be observed for the temperature development. The temperatures were clearly lower in the simulation with the steel vessel walls. Because of this the simulation with vessel walls is used for the comparison to experimental data.

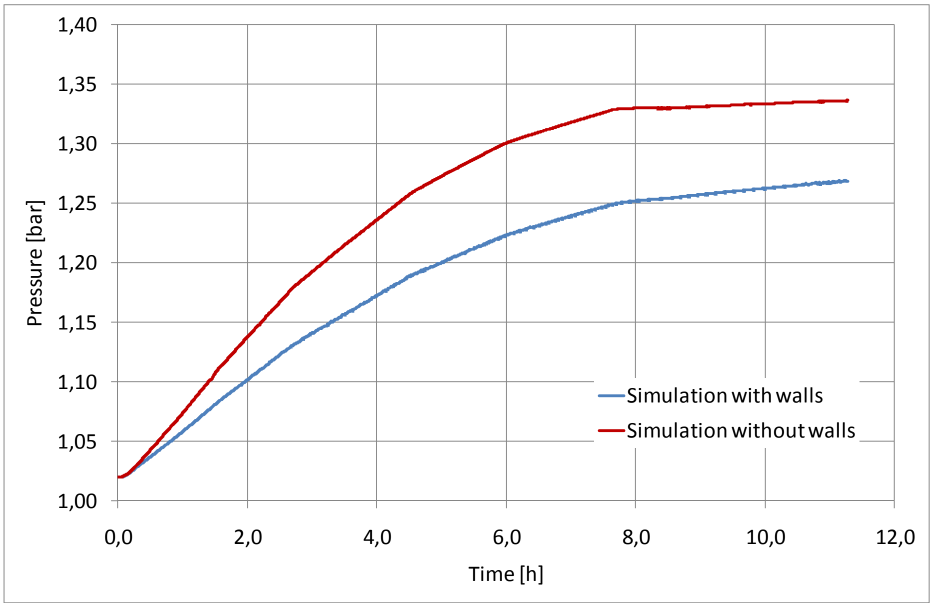

Fig. 10: Influence of the wall structures on the pressure development
(simulations TH21_01 and TH21_03)

3.4 Comparison to experimental data

Figure 11 shows the calculated pressure development (TH21_03) and compares it to the experimental data. The calculated pressure values are a little above the experimental values. The median pressure for the time range 10.3 h < t < 11.3 h is 1.266±0.001 bar. The error of ±0.001 bar demonstrates the standard deviation of the pressure values. The experimental value for this time interval is 1.239±0.001 bar. So there is a difference of 0.027 bar in this time range, which is rather small. One reason for the still remaining difference between the calculation and the experimental data could be the non-perfect isolation of the THAI vessel in the experiment. The heat conduction to the outer atmosphere leads to a lower pressure in the experiment. This effect was neglected in the simulation because the experimental heat loss could not be quantified.

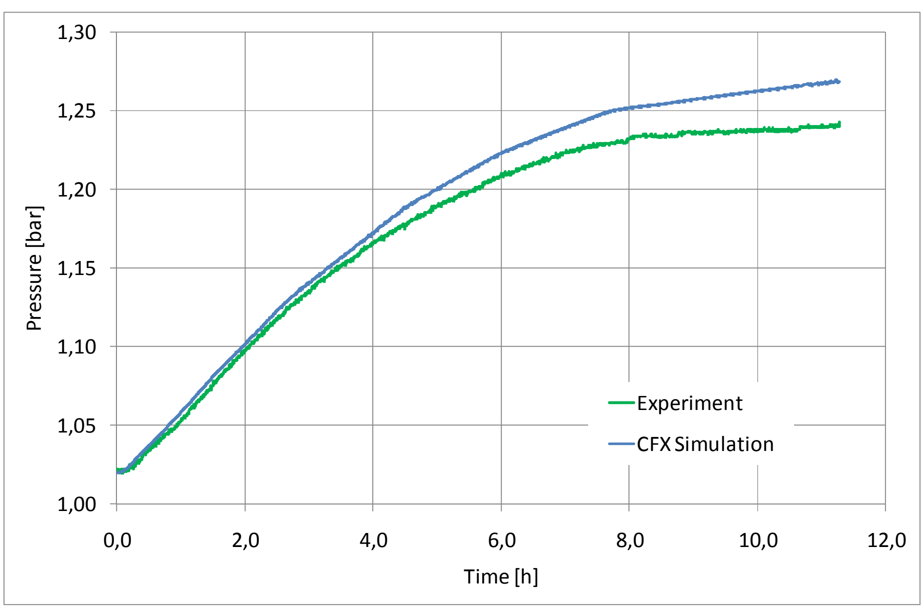

Fig. 11: Pressure history in the THAI vessel for gauge DPA77H16 (simulation TH21_3)

Figure 12 shows the temperature history in the THAI vessel for one gauge (DTF84H11). The temperature rise is similar to the pressure development. The comparison of the simulated temperatures and the experimental data show that they are in good agreement. In Figure 13 the median temperatures for all gauges and for t > 10.3 h are presented and are compared to experimental data. The error bars represent the time dependent temperature oscillations. The median difference between calculated values and measurements is 4.0 °C (calculated with equation (2)). The positions of the gauges can be found in table 8.

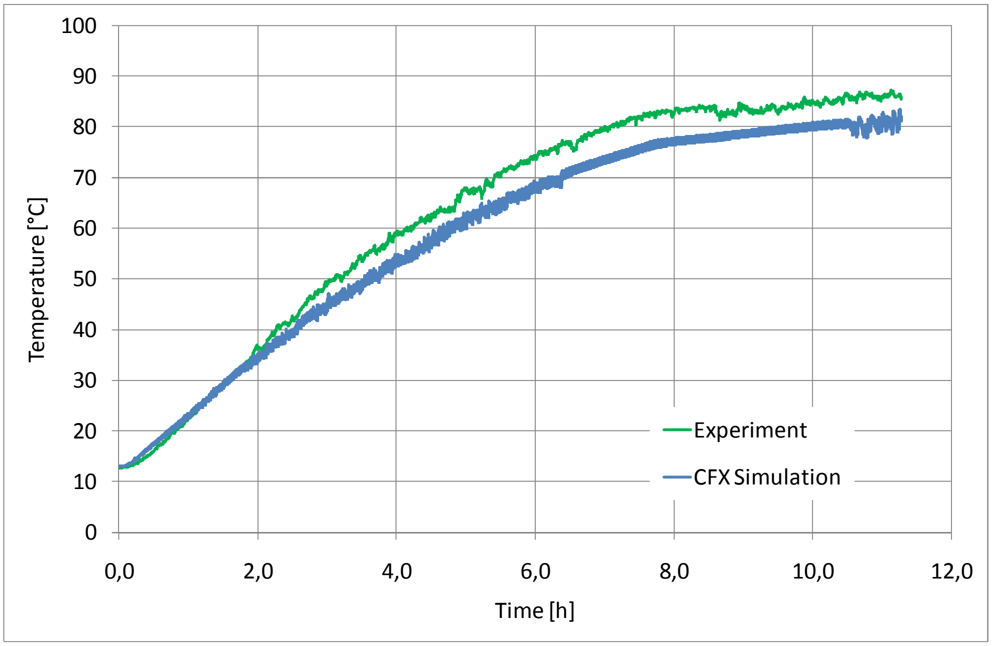

Fig. 12: Temperature history in the THAI vessel at gauge DTF84H11 (simulation TH21_03)

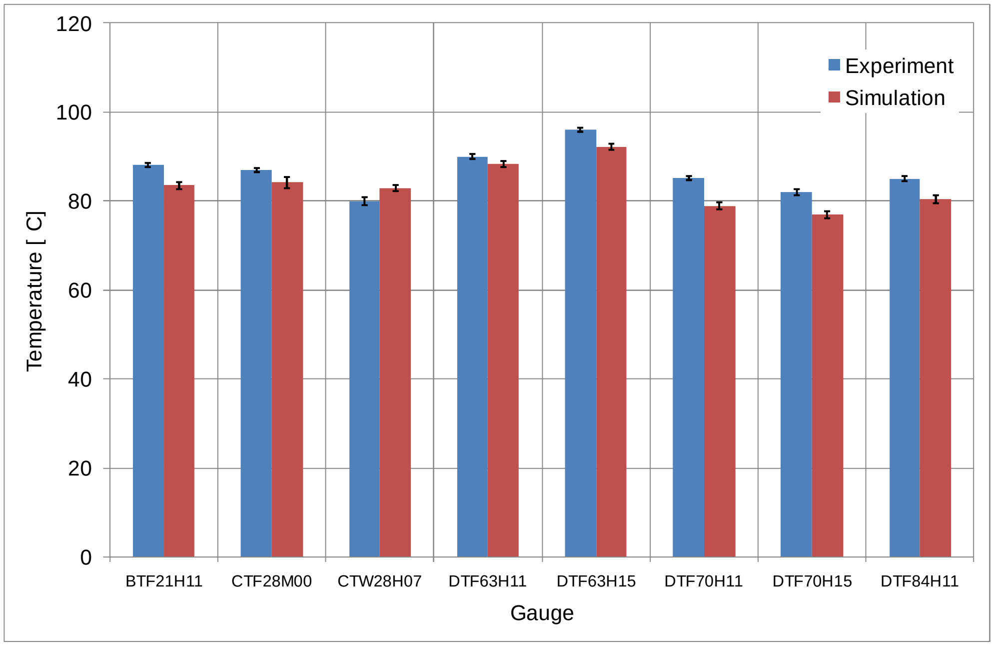

Fig. 13: Calculated and measured median temperatures for t > 10.3 h at different gauges (simulation TH21_03)

Table 8: Position of the temperature gauges

Gauge	**BTF21H11**	**CTF28M00**	**CTW28H07**	**DTF63H11**
Height	2.10 m	2.80 m	2.80 m	6.30 m
Radius	1.14 m	0.00 m	0.70 m	1.14 m
Gauge	**DTF63H15**	**DTF70H11**	**DTF70H15**	**DTF84H11**
Height	6.30 m	7.00 m	7.00 m	8.40 m
Radius	1.53 m	1.14 m	1.53 m	1.14 m

The vertical flow velocity for gauge CVT58M00 (located in the inner cylinder) is presented in figure 14 and shows a good qualitative agreement with the calculated data. Figure 15 shows the median vertical velocities in phase 2 (t > 7.5 h) for all three velocity gauges. The error bars represent the time dependent velocity oscillations. The calculated data is compared to the experimental data. The differences to the experimental data are bigger for the two other gauges than it is for gauge CVT58M00. The average difference between simulation and experiments is 0.23 m/s.

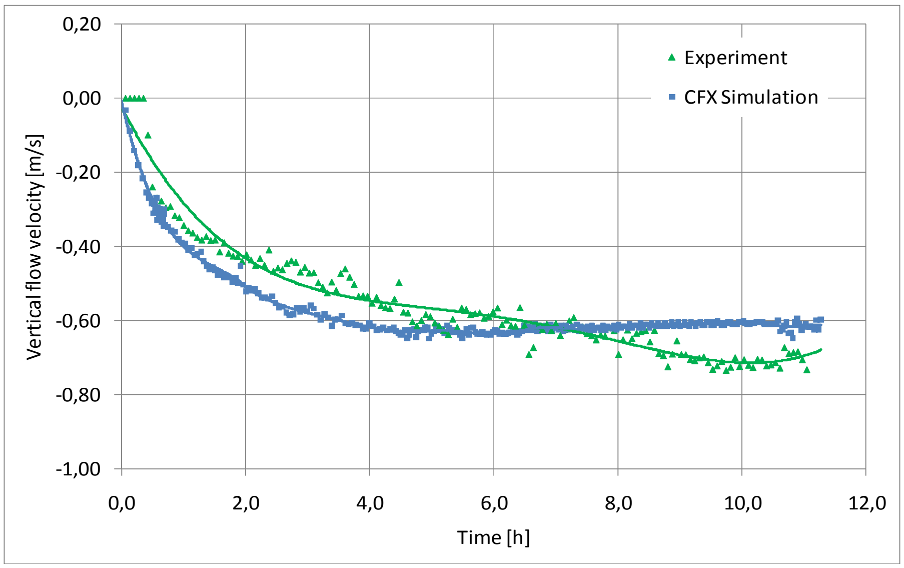

Fig. 14: Vertical flow velocities at gauge CVT58M00 (simulation TH21_03)

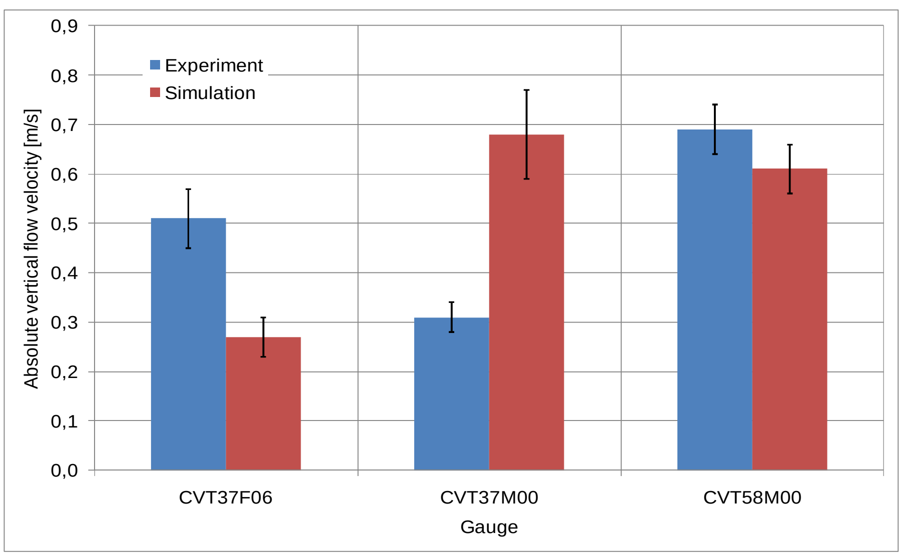

Fig. 15: Calculated and measured vertical flow velocities in phase 2 (t > 7.5 h) (simulation TH21_03)

4. CONCLUSIONS

The possibilities of the THAI facility to investigate coupled effects phenomena have been demonstrated by means of two different experimental setups, related to the fields of containment thermal hydraulics and their use for CFD code validation. THAI is best suited for experiments which cannot be conducted in small-scale laboratory vessels. THAI tests are characterized by situations where spatial inhomogeneous distributions and related transport processes are involved, like heat and mass transfer, boundary layers between atmosphere and structural or water pool surfaces, natural convection, and aerosol sedimentation. The larger scale of the THAI vessel makes it possible to investigate accident phenomena in an atmosphere under natural convection which could not be established in a small lab apparatus. The intensity of natural convection at the geometric scale of a nuclear reactor containment is considerably larger than in THAI, but such scale-up is accomplished by means of code simulation. In this sense, THAI takes a specific position in the model development/validation chain, different from lab-scale tests.

For the validation of CFX several of the numerous experiments performed at the THAI test facility in the last 10 years since the start of the operation were simulated, two of them are described in the paper (TH-18 and TH-21). In conclusion a good agreement of simulation results and experimental data was found in general. For the phenomena of natural convection, heat transfer and turbulence the following guidelines could be derived from this analysis:

- Discretisation / number of elements in TH 18/21: The calculated local flow velocities show a high sensitivity on the number of elements, the local temperatures have a medium sensitivity and the calculated pressure is not very sensible to the number of elements. The calculated pressure in TH-21 seems to be already grid independent for 24,000 elements per quarter (1,600 elements/m³). Due to the higher velocities and gradients in TH-18 a grid dependency is still existent for a much more fine mesh of 1,200,000 elements (20,000 elements/m³).
- Turbulence modeling: The best results in TH-18 were achieved with the SSG Reynolds Stress model. But the CPU-time needed is much higher than for the other two turbulence models tested (SGG/K-epsilon: Factor 13, SGG/SST: Factor 7).
- Modeling of wall structures: The modeling of the steel wall structures shows a significant influence on the calculated pressure and temperatures for TH-21, because of its effect as a heat-storage especially during the transient heat up phase. It is not possible to neglect the wall structures to save computing time.
- Flow profile at the inlet: For the TH-18 simulation also the flow profile and the turbulence intensity at the inlet (the fan outlet) were varied (not demonstrated in this paper) and they show a big influence on the simulation results. These effects should not be neglected for an accurate simulation.

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