VALIDATION OF A SIMPLE CONDENSATION MODEL FOR SIMULATION OF GAS DISTRIBUTIONS IN CONTAINMENTS WITH CFX

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ABSTRACT

In cooperation with other institutions, GRS adapts and validates the CFX code developed by ANSYS for LWR containment applications. In a severe accident scenario in a LWR large amounts of steam and hydrogen are released into the containment at different locations. To simulate the main phenomena relevant for accident scenarios within LWR containments models, especially the ones provided to CFX by the users have to be validated. A simplified wall and bulk condensation model was implemented by GRS in CFX using USER-FORTRAN routines and has been validated by simulating several experiments where condensation processes are significant.

The main focus of this paper will be on the simulation of the experiments Panda4 and Panda4bis performed at the Paul Scherrer Institute. These experiments differ only in temperature boundary conditions; hence condensation occurred in Panda4bis only. For the simulation of the Panda4 experiment a grid sensitivity study was performed and the influence of the turbulence model and other parameters like turbulence intensity of the inflowing steam were investigated. CFX is able to simulate very well the flow pattern of the experiment with the counter current in the connecting pipe between the two Panda vessels and the steam distribution. The developed model for the wall and bulk condensation was validated by calculating the Panda4bis experiment using similar models as for Panda4. The influence of the mesh resolution near the vessel walls was investigated, because this is a critical parameter for the condensation model. Some model shortcomings lead to larger deviations from experimental data than in simulating Panda4, but in general the simulation results are satisfactory.

1. INTRODUCTION

In cooperation with other institutions GRS adapts and validates the CFX code developed by ANSYS for LWR containment applications. Thus for a correct prediction of the gas composition an accurate simulation of the wall and bulk condensation of steam is necessary as well. For containment application a modelling of the condensation with the multiphase approach, as implemented in ANSYS CFX, is too CPU-time consuming. Thus a simplified condensation model was implemented in CFX using USER-FORTRAN routines [Heitsch 2005]. The condensation model has been validated by simulating several experiments performed at different facilities. The main focus here will be on the CFX-11 simulation of the experiments Panda4 and Panda4bis performed at the Paul Scherrer Institute [Auban 2005], [Cachard 2006] in the framework of the PANDA SETH experimental program. This experimental program investigates jets and plumes generated by an injection of steam or steam/helium mixture and the resulting propagation of stratification fronts.

These experiments differ only in temperature boundary conditions; hence condensation occurred in Panda4bis only. The simulation of both experiments offers the opportunity to separate errors: errors of the condensation model from other model and numerical errors (e.g. turbulence model).

2. CONDENSATION MODEL

In the following chapter only a short overview of the condensation model will be given, a detailed model description can be found in [Heitsch 2005]. The condensation model consists of a model for bulk condensation and a model for wall condensation.

Bulk condensation occurs when the partial pressure of steam is greater than the saturated vapour pressure of water at the temperature of the gas mixture. When bulk condensation occurs the excess steam is removed from the gas mixture and a corresponding latent heat is released into the gas. In this simplified bulk condensation model the droplets produced are not considered any further. It is not possible to assume an instantaneous new equilibrium; instead the transition to this state has to be calculated. Thus additional source terms for the removed steam and for the released heat were implemented.

The wall condensation model determines the mass flux into the condensate film at the wall. The steam mol fraction at the interface is determined by the partial pressure of the vapour, assuming the vapour to be saturated at the interface temperature. The condensate film is not modelled in detail. Instead a correlation is used to determine the effective heat transfer coefficient through the film. The released heat due to the condensation process is taken into account by an additional temperature source term in the wall.

3. SIMULATION OF THE PANDA4 EXPERIMENT

3.1 Initial and boundary conditions

The experimental facility consists of two vessels (D1 and D2; height ~ 10.7 m; diameter ~ 4 m) connected by a pipe with a curvature of 110° (Fig. 1). Initially the vessels are filled with dry air. Steam flows through a horizontal pipe into the vessel D1 with a mass flow rate of about 50 g/s. In the upper part of the second vessel D2 is a valve, which is used to keep the pressure constant at 1.3 bar. The initial temperature is 108 °C and the temperature of the inflowing steam is 140 °C [Paladino 2006]. Under these conditions no condensation processes occur. The steam concentration is measured at different locations in the vessels and in the connecting pipe. The error of the measured molar fraction is assessed to be within +/- 1.5%. The time resolution of the measurements at most points is 10 to 15 concentration measurements during the whole experiment [Cachard 2006].

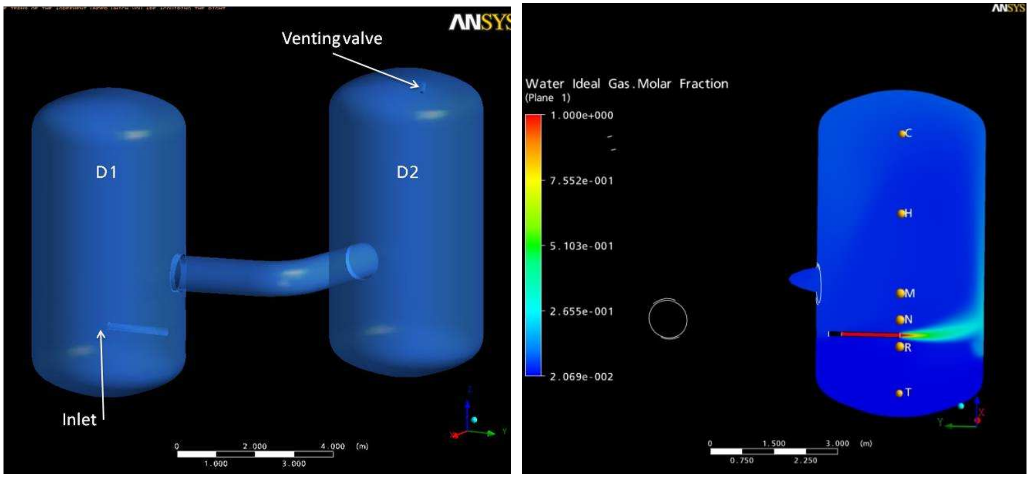

Fig. 1 Geometry of the experiments Panda4 and Panda4bis (left) and measurement points in vessel D1 (right)

3.2 Modelling with CFX

CFX-11 was used for the simulation of both Panda experiments. The turbulence was modelled by the SST model (Shear Stress Transport), which is a two-equation URANS (Unsteady Reynolds Averaged Navier-Stokes equations) turbulence model. Using the SST model the "automatic near-wall treatment" of CFX was applied. In this method CFX automatically switches from a low-Re formulation to wall functions based on the grid spacing provided by the user. The influence of the turbulence model is investigated and described in chapter 3.4. The mass flow and the temperature are defined at the inflow and a pressure boundary condition is chosen at the venting valve. At the inlet a medium turbulence level is assumed. Investigations performed show that the turbulence level assumed at the inlet has a minor effect on the flow in the Panda vessels, because the inlet is in the pipe.

The heat transfer in the walls is modelled by CFX, too, which is important for Panda4bis.

Air and steam are modeled as ideal gases and a kinematic diffusivity of 2.5-5 m^2/s for steam is assumed. A hybrid mesh is used for the simulation consisting of 190000 structured cells and 3000 unstructured cells. A grid sensitivity study (see chapter 3.3) shows that this discretisation is sufficiently fine enough. Adaptive time steps are used for all simulations; typical values are 0.5 s - 1 s. The standard numerical schemes were adopted for all simulations (advection scheme: "High resolution", transient scheme: "Second order").

3.3 Comparison with experimental data

The calculated steam concentration in vessel D1 is in good agreement with the measured values. Only in the lower part (T20, height 0.54 m) of the vessel larger deviations occur (Fig. 2). In this part the increase of the steam concentration is overestimated. At T20 a steam concentration of 20 % is measured after 1450 s, but in the simulation this concentration is already reached after 700 s. At other measurement points (R20-C20, height >1.7 m) the steam concentration is measured with a sufficient accuracy. After 4000 s the steam concentration is overestimated by 2 vol %, which corresponds to a relative error of 2-3 %. The deviation is only slightly higher than the measurement error, estimated by the experimenter to be +/- 1.5 %.

In the second vessel D2 the steam concentration is well predicted in the part above the connecting pipe. At M20 (height=3.02 m) the deviations are smaller than the measurement errors. At H20 and C20 the deviations of the steam concentrations are about 2 vol % after 4000 s, which is only slightly larger than the measurement accuracy.

Below the connecting pipe the delay in the mixing and the slower increase of the steam concentration is simulated qualitatively correct, but quantitatively larger deviations occur. The steam concentration at N20 (height = 2.376 m) is overpredicted and at T20 underpredicted. A too strong stratification is simulated in the lower part of the vessel D2.

CFX calculates the flow pattern with the counter current in the connecting pipe correctly (Fig. 3). The steam concentration in the connecting pipe is well predicted, the largest errors occur at TDD10. Even at this point the error is smaller than 4 vol %, which corresponds to a relative error of 5 %.

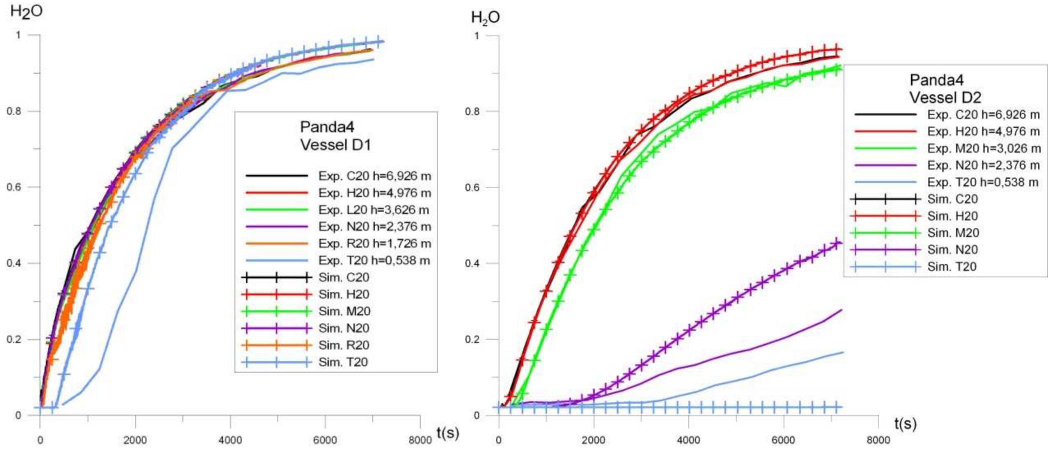

Fig. 2 Molar concentration of steam in the two vessels D1 (left) and D2 (right)

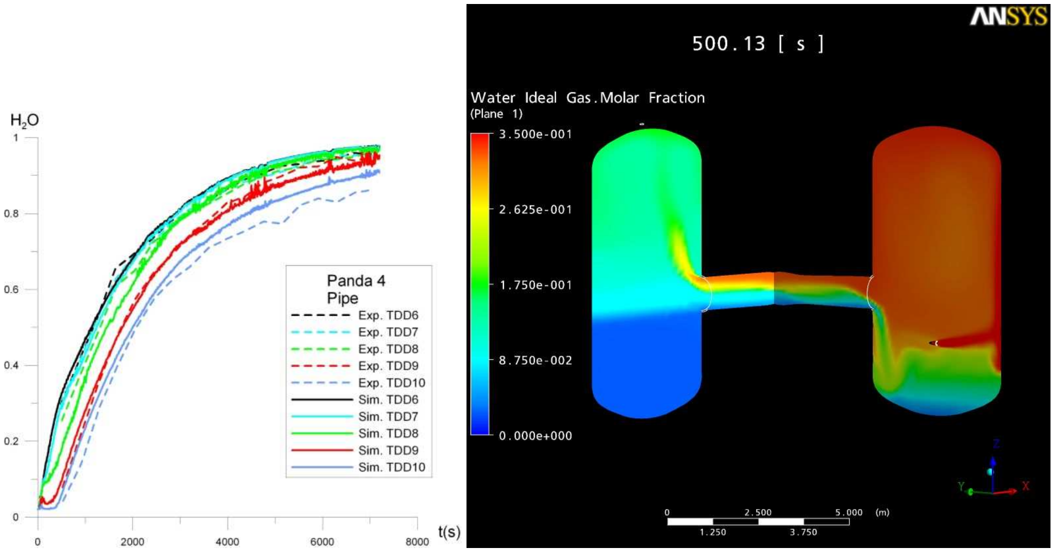

Fig. 3 Left: Steam concentration in the connecting pipe
Right: Steam concentration in the two vessels after 500 s

3.4 Grid dependency study

In order to investigate the influence of the mesh a simulation is performed with a finer grid. The standard mesh consists of 193000 elements, the finer mesh of 608000 elements. This corresponds more or less to a refinement factor of 1.5 in each dimension.

At most measurement points no significant grid dependency can be observed (Fig. 4). Only at measurement point T20 in vessel D1 and at measurement point M20 a grid dependency can be observed, but the differences due to the discretisation are small compared to the differences in the experiment. Due to the high CPU-time needed (47 CPU days with a mesh of 193000 elements for 7200 s simulation time and 90 CPU days with a mesh of 60800 elements for 3400 s simulation time) no further mesh refinement was performed.

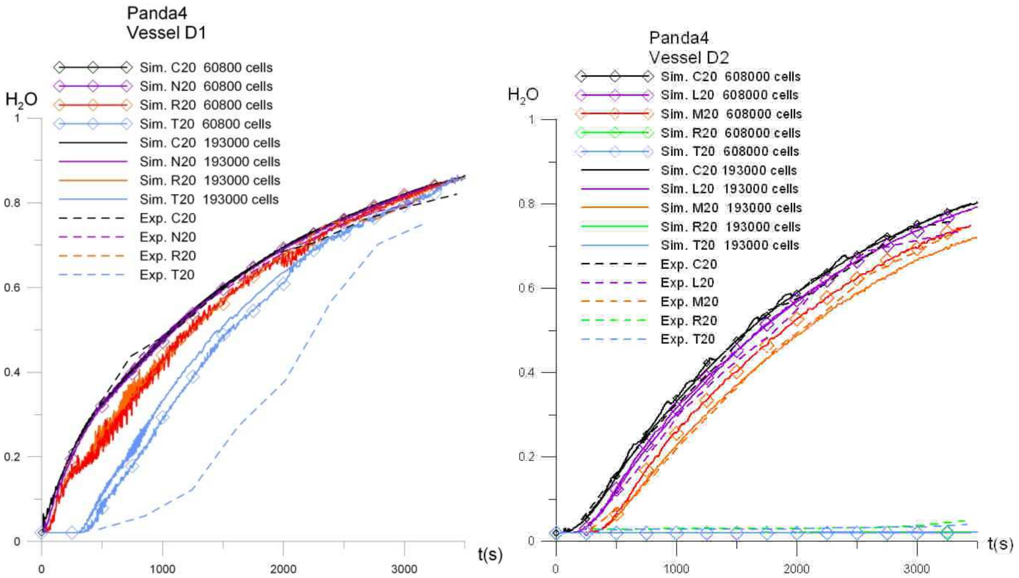

Fig. 4 Influence of mesh refining on the steam concentration; vessel D1 (left) and D2 (right)

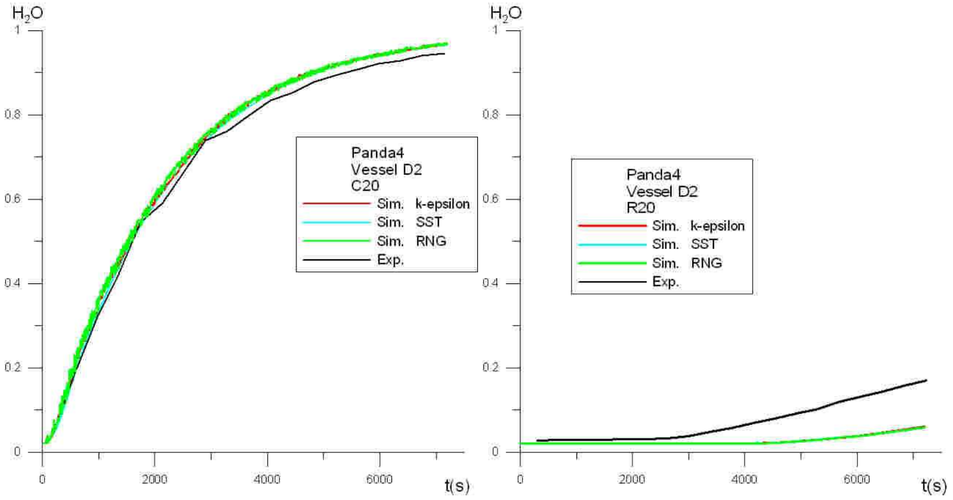

Fig. 5 Influence of turbulence model on the steam concentration in vessel D2

3.5 Influence of turbulence model

In order to investigate the influence of the turbulence model, simulations with different turbulence models (SST, k-ε, RNG-k- ε, and SSG-Reynold-Stress) were performed. Due to numerical instabilities the simulation with the SSG-Reynold-Stress model stopped after ~246 s. Thus this simulation will not be taken into account for the comparisons.

The simulation results show very similar steam distributions at all measurement points (Fig. 5). The discrepancies in the lower part of the vessel D2 (point R20) are similar in all tested turbulence models. It has to be considered that the SST, the k- ε and the RNG- k-ε model are all URANS turbulence models describing the turbulence by two equations. Therefore they have common limitations, for example they cannot take into account the anisotropy of turbulence.

3.6 Conclusions

The Panda4 experiment was successfully simulated with CFX-11. For the most part of the facility the calculated steam concentrations are in good agreement with the measured values, but in the lower part (below the connecting pipe) of the vessel D2 larger deviations occur. A grid dependency study shows that with a mesh consisting of 193000 cells a satisfying accuracy can be achieved. Different 2-equation URANS turbulence models (SST, k-ε, RNG-k-ε) lead to similar steam concentrations.

4. Simulation of the Panda4bis Experiment - Validation of the Steam Condensation Model

4.1 Initial and boundary conditions

The geometry of the Panda4bis experiment is similar to the Panda4 experiment (Fig. 1). The main differences are the initial temperature and the temperature of the inflowing steam. The initial temperature of the dry air in the facility and the steel walls is 76 °C [Zboray 2006]. Steam is released with an average mass flow of 54.16 g/s and a temperature of 107.8 °C into the vessel D1, which is only slightly higher than the saturation temperature of steam at 1.3 bar. Due to these conditions condensation occurs in this experiment and has a major influence on the steam concentration.

4.2 Comparison with experimental data

When comparing the steam concentration it has to be taken into account that the experimental time resolution of the concentration measurement is quite coarse. Typically 10 to 15 measurements were performed at each location during the first 5000 s. At some points even less than 10 measurements were performed. Due to this coarse time resolution fast changes in the steam concentration cannot be measured. Yet, when comparing temperatures this problem does not occur because the time resolution of the temperature measurements is much higher (~Δt 2 s).

In the simulation the steam concentration in vessel D1 increases up to 45 vol % in the first 1000 s (Fig. 6). After 1000 s there is a slower increase due to condensation processes. After 6000 s a steam concentration is reached of about 80 vol %. This corresponds qualitatively with the measured concentration, but in the experiment the concentration is 5 vol % to 10 vol % lower. The steam concentration is relatively homogeneous distributed, but in the experiment higher fluctuations are measured between the different locations. In the upper part of the vessel no distinct stratification can be found (C20-L20). In the simulation no significant regional distinctions were found in this area.

In the lower part of the vessel the increase of the steam concentration is delayed. During the whole experiment a lower steam concentration is measured in this area. This weak stratification is predicted in the simulation, too, but the absolute value of the steam concentration is overpredicted.

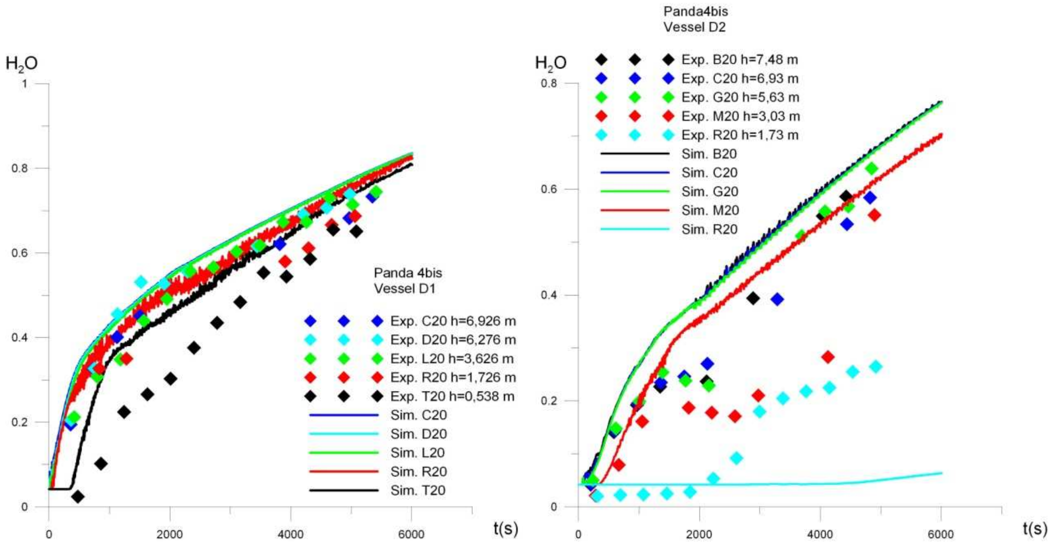

Fig. 6 Steam concentration in vessel D1 (left) and D2 (right)

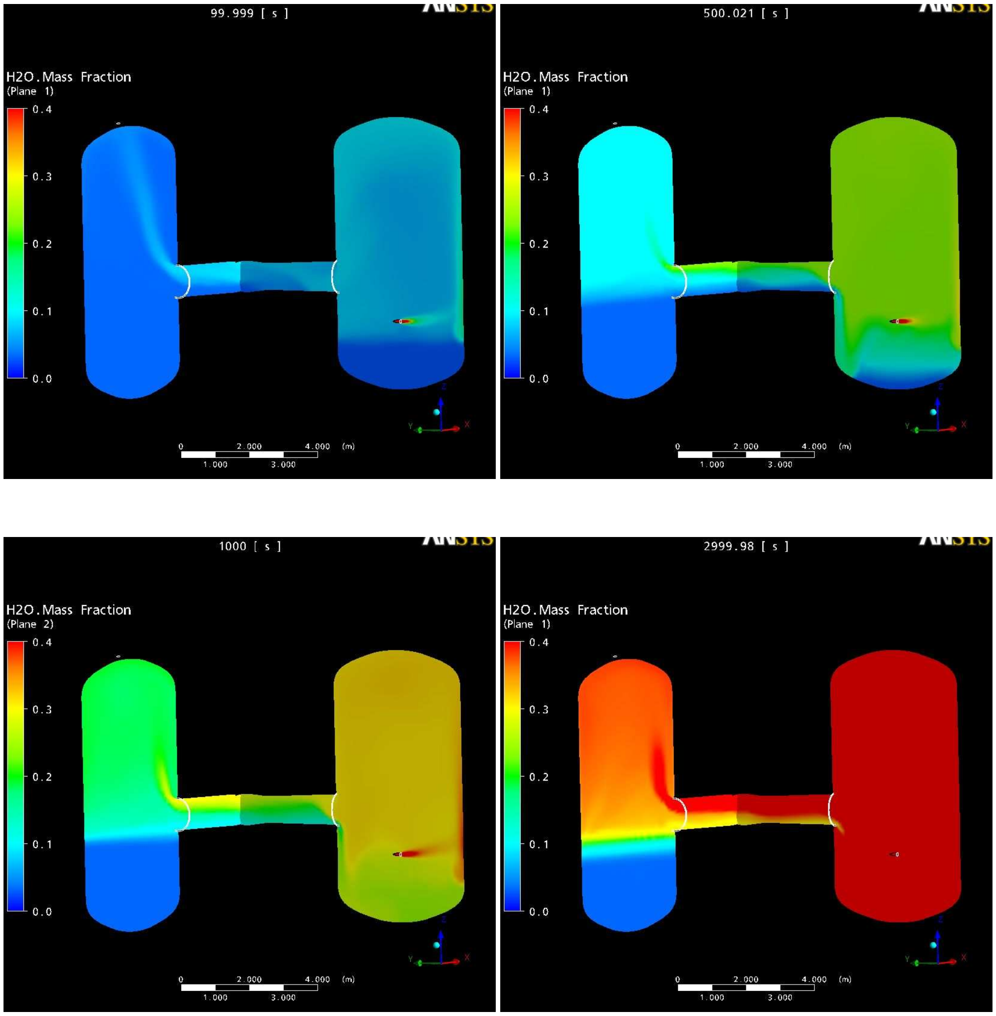

Fig. 7 Steam distribution in the Panda vessels after 100 s, 500 s, 1000 s and 3000 s

Hot gas with a high steam concentration accumulates in vessel D1 above the connecting pipe (Fig. **7**). The gas flows into vessel D2 through the upper part of the pipe. Through the lower part of the pipe cold gas with a low steam content flows back into D1. Due to its higher density the cold gas sinks down to the bottom of D1. This flow pattern is observed during the whole experiment und is well predicted by the simulation. In the upper part of vessel D2 an increase of the steam concentration is measured during the whole experiment (B2-G2). This increase is predicted in the simulation, too, but as in D1 the concentration is overpredicted by 5 vol % to 10 vol %.

In the simulation a layer with a low steam concentration is predicted in the lower part of vessel D2. This layer dissolves slowly in the calculation. In the experiment much higher steam concentrations are measured. The reason for the large discrepancies is, that in the experiment condensate is generated in the upper part of the vessel and transported into the lower part [Cachard 2006]. There some of it evaporates and steam is generated. Due to model limitations condensate is not modelled and thus no evaporation processes can be simulated. An improvement of the simulation results for this part of the vessel is only possible if the condensation model will be improved (modelling of condensate) and evaporation processes will be taken into account.

The evaporation process may also be the reason for the increase of massflow through the venting valve between 2000 s - 4000 s.

The steam is flowing through a several meter long pipe into the vessel D1. A part of the pipe lies in vessel D1. It can be assumed that this part of the pipe has initially the same temperature as the gas and the walls of the Panda facility (76 °C). Thus condensation and heat losses appear. Therefore it has to be expected that less steam with a lower temperature is flowing into vessel D1 than the measured 64 g/s in the first period of the experiment.

Simulations, which have taken into account the condensation in the pipe, failed due to numerical instabilities. Numerical instabilities may be the result of the fact that the wall condensation model was developed for condensation, if non-condensing gas components are existent. Thus condensation and the heat losses were neglected in the simulation. This will lead to an overestimation of the inflowing steam and can explain the overprediction of the massflow at the venting valve in the first 750 s. An overprediction of the massflow into D1 would correspond to the overprediction of the steam concentration in D1 and the upper part of D2.

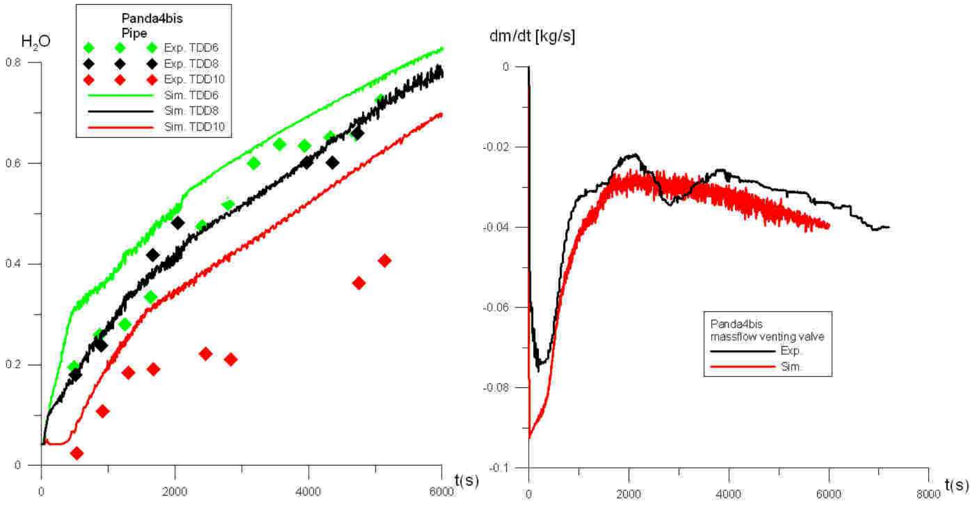

Fig. 8 Steam concentration in the connecting pipe (left)
and massflow through venting valve (right)

After 750 s the simulated massflow through the venting valve is in satisfactory agreement with the measurement, after 3000 s the massflow tends to be overpredicted. The deviations at 2500 s might be explained through the neglection of evaporation in the simulation.

The temperature development is well predicted in vessel D1 and in the upper part of D2 (Fig. 9 D1C20, D1L20, D2C20). The slower temperature increase in D1 at the beginning was not predicted. An explanation for this might be the neglection of the influence of the inlet pipe. There is a satisfactory agreement later on between experiment and simulation, but there is a moderate overestimation of the temperature increase. After 6000 s the temperature is overpredicted by 2 to 3 K. At the bottom of D2 (Fig. 9, D2S20) the temperature decreases due to evaporation in the experiment. Due to the already mentioned model limitation, this cannot be simulated.

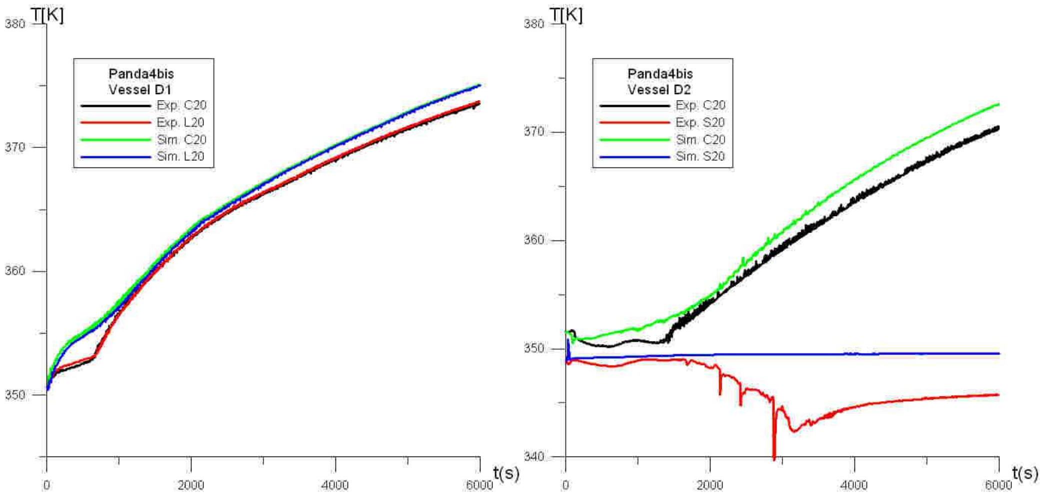

Fig. 9 Temperature at different measurement points in vessel D1 (left) and D2 (right)

4.3 Influence of the grid resolution near walls

The simulation of Panda4 shows, that a grid of 193000 cells is sufficient to simulate the flow field at similar steam injection rates. From previous studies it is known, that the grid size near the walls has a large influence on the simulated wall condensation. Therefore in this grid sensitivity study only the grid size near the walls is refined (Fig. 10). In the grid used by default the size of the first cell in the gas is about $\Delta x \sim 5$ cm. In the next refinement step Δx was reduced to 1 cm. The finest mesh resolution has a $\Delta x \sim 1$ mm. It has to be mentioned that Δx might differ at edges or in some areas with curvature. The surface temperature is a significant parameter for wall condensation, therefore the heat transfer in the walls is modelled, too. The cell size in the steel walls is about 5 mm.

The investigation shows that there is only a minor grid influence (Fig. 12, Fig. 13). The steam concentration and the temperature at the measurement points and the massflow through the venting valve differ only slightly, refining the grid near the walls (Fig. 10, Fig. 11). The mesh resolution has a large influence on the computational power needed (Table 1). Beside the increase of the number of mesh cells, a refinement of the grid near the walls can lead to a reduction of the time step size, which can be used to achieve a converge solution. In the simulation with $\Delta x \sim 5$ cm and $\Delta x \sim 1$ cm a time step size of 0.1 s could be used, but for the finest grid ($\Delta x \sim$ 1 mm) the time step size has to be reduced to 0.025 s.

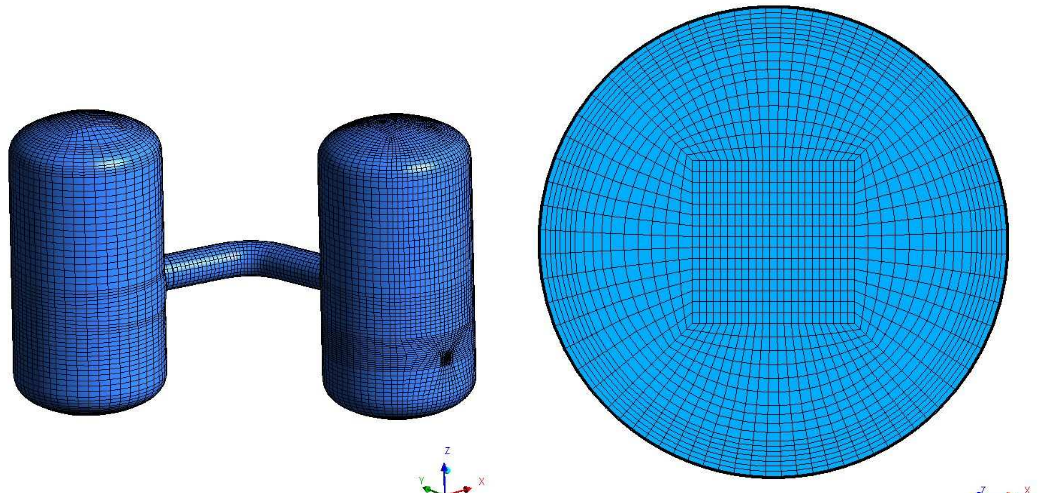

Fig. 10 CFD mesh used for grid dependency study. Right: Δx~ 5cm

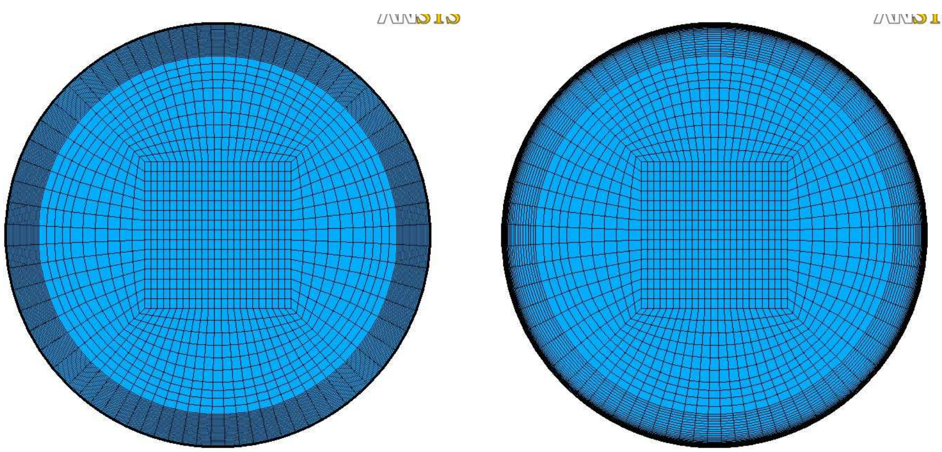

Fig. 11 CFD mesh used for grid dependency study. Left: Δx~ 1 cm Right: Δx~ 1

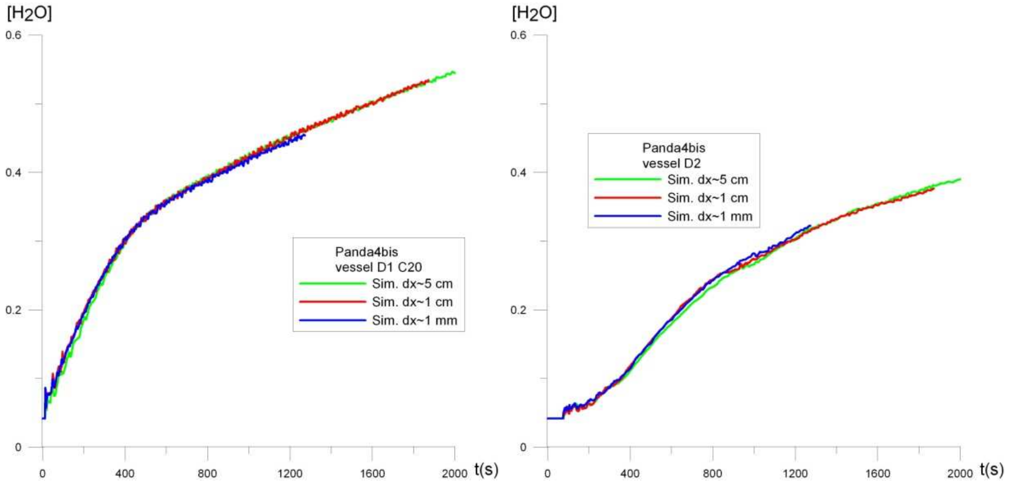

Fig. 12 Steam concentration using different grid resolutions near walls; vessel D1 (left) and D2 (right)

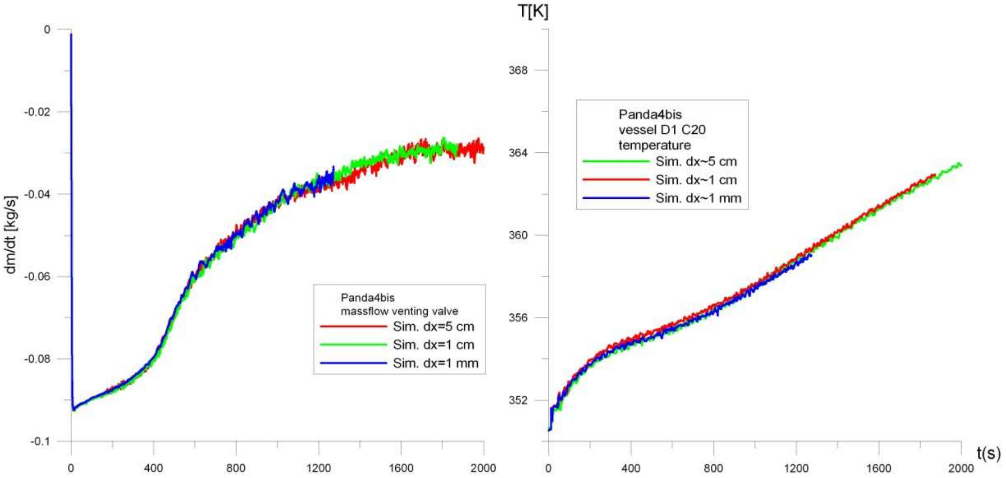

Fig. 13 Massflow through venting pipe and temperature using different grid resolutions near walls; vessel D1 (left) and D2 (right)

Table 1 CPU time needed for 1000 s problem time on a linux cluster with 4 CPUs

Mesh	CPU time
Δx~ 5 cm	64 h
Δx~ 1 cm	157 h
Δx~ 1 mm	582 h

5. SUMMARY

The experiments Panda4 and Panda4bis performed at the Paul Scherrer Institute were simulated with CFX-11. These experiments differ only in temperature boundary conditions; hence condensation occurred in Panda4bis only. The simulation of both experiments offers the opportunity to separate errors of the condensation model from numerical and other model errors (e.g. turbulence model). The simulated steam distribution is in good agreement with experimental data. CFX is able to simulate the flow pattern of the experiment with the counter current in the connecting pipe between the two Panda vessels.

A model for the wall and bulk condensation was validated by calculating the Panda4bis experiment, all other models were as for Panda4. The simulated steam concentration and the temperature in vessel D1 and in the upper part of D2 are in satisfactory agreement with the experiment, but for the lower part of D2 larger deviations occur due to the neglection of condensate and evaporation. Thus a reasonable enhancement of the condensation model would be an additional model for the transport of the condensate.

REFERENCES

Heitsch, M., Schramm, B.
Hydrogen Management for the VVER-440/213 Containment, Hungary, HU2002/000-632-04-01, GRS 2005, Final Report

Auban, O., Paladino, D. and Zboray, R.
OECD/SETH PANDA Test Facility Description and Geometrical Data, PSI 2005

de Cachard, F., Paladino, D., Zboray, R., Andreani, M.
Large-Scale Experimental Investigation of Gas Mixing and Stratification in LWR Containments, PSI 2006, Final Report

Paladino, D., et al
PANDA Test4bis-1 Quick-Look Report, Paul Scherrer Institut, 2006

Zboray, R., et al
PANDA Test 4bis-1 Quick-Look Report, Paul Scherrer Institut, 2006