Simulation of Atmosphere Mixing and Stratification in the ThAI Experimental Facility with a CFD Code

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ABSTRACT

The CFD code CFX4.4 was used to simulate an experiment in the ThAI facility, which was designed for investigation of thermal-hydraulic processes during a severe accident inside a Light Water Reactor containment. In the considered experiment, air was initially present in the vessel, and helium and steam were injected during different phases of the experiment at various mass flow rates and at different locations. In the performed work, the 1st and 2nd phase of the considered experiment were simulated. The main purpose was to reproduce the non-homogeneous temperature and species concentration distributions in the ThAI experimental facility.

A three-dimensional model of the ThAI vessel for the CFX4.4 code was developed. The flow in the simulation domain was modelled as single-phase. Steam condensation on vessel walls was modelled as a sink of mass and energy using a correlation that was originally developed for an integral approach. A simple model of bulk phase change was also included. The calculated time dependent data together with temperature, concentrations and velocity distributions at the end of each phase are compared to experimental results.

1 INTRODUCTION

During a severe accident in a Light Water Reactor nuclear power plant, large amounts of hydrogen would presumably be generated due to metal oxidation during core degradation and released into the containment. The integrity of the containment could be threatened due to hydrogen combustion. The prediction of hydrogen behaviour at severe accident conditions may help to develop adequate accident management procedures (Royl et al. [1],[2]). The main issue is to predict whether, due to atmosphere mixing and stratification, the local hydrogen concentration in certain parts of the containment may exceed flammability limits.

Lately, many investigations about the possible application of so-called Computational Fluid Dynamics (CFD) codes for this purpose have been started (see, for instance, the works of Andreani et al. [3], Blumenfeld et al. [4], Martin-Valdepenas and Jimenez [5], Rastogi [6], Siccama et al. [7]). CFD codes solve the transport mass, momentum and energy equations when a fluid system is modelled using local instantaneous description. Some codes, which also use local instantaneous description, have been developed specifically for this purpose (Choi et al. [8], Royl et al. [2], Sharma et al. [9]).
These investigations are complemented by adequate experiments. Recently, the following novel integral experimental facilities have been set up in Europe: TOSQAN, at the Institut de Radioprotection et de Sureté Nucléaire (IRSN) in Saclay, France (Brun et al. [10]), MISTRAS, at the Commissariat à l’ Énergie Atomique (CEA) in Saclay, France (Caron-Charles et al. [11]), ThAI, at Becker Technologies GmbH in Eschborn, Germany (Kanzleiter et al. [12], Fischer et al. [13],[14]). A multi-compartment experimental facility has also been set up in Korea (Lee and Park [15]).

These facilities are equipped with instrumentation, which allows measurement of local temperature, species concentration and velocities. Thus, the non-homogeneous structure and the flow patterns of the containment atmosphere may be observed, which enables a better understanding of mixing and stratification processes in the containment of an actual nuclear power plant. Besides, local experimental measurements may be used to assess the validity of simulations performed by CFD codes.

In the present work, the CFD code CFX4.4 was used to simulate an experiment in the ThAI facility, which was also proposed for the OECD/NEA International Standard Problem No.47 (ISP-47). The same code has already been used by other authors for similar simulations (Houkema et al. [16]). Also, analyses of similar experiments have already been carried out by other authors (Malet et al. [17]).

The main purpose of the simulation was to reproduce the non-homogeneous temperature, species concentration and velocity fields. The calculated time dependent data together with temperature, concentrations and velocity distributions at the end of each phase are compared to the experimental results.

2 THAI EXPERIMENT

The ThAI facility can be characterized as a coupled-effects test facility. It allows investigation of natural convection and atmospheric stratification, heat exchange between solid structures and vessel atmosphere, heat conduction in solid structures, as well as steam condensation on walls and in the atmosphere, and transport of condensed water [14]. The thermal-hydraulic behaviour is determined by the dominant physical phenomena: gas injection, steam condensation, heat transfer, and buoyant flow. The dynamics of thermal-hydraulic processes are transient and are being governed by the thermal inertia of the heat exchanging structures. That is also most likely true for reactor containment at accident conditions.

2.1 Vessel Geometry

The main component of the facility is a cylindrical steel vessel of 9.2 m height and 3.2 m diameter, with a total volume of 60 m³ (Figure 1). At the lower end, a sump compartment is attached. The vessel space is subdivided by an open inner cylinder with an internal diameter of 1.38 m and a horizontal separation plane in the annular region with vent openings. The separation plane consists of 4 equally spaced condensate collecting trays that span from the inner cylinder wall to the vessel wall. Each tray is covering 60° circumference (Figure 2). The outer cylindrical wall has oil cooling / heating jackets subdivided in three vertical sections. Vessel walls and internal structures are all made of steel of thickness from 15 to 130 mm. The outer edge of the vessel including cooling/heating jackets is thermally insulated by a 12 cm layer of rock wool and covered by 1 mm thick aluminium.
2.2 ISP-47 Experiment

Initially, air with about 70% humidity was present in the vessel. The vessel structures temperature, atmosphere temperature and surrounding temperature was 22 °C, while the atmosphere pressure was 1 bar. The experiment was divided into 3 phases, with gas injections at 3 different locations and a last (4th) phase with no gas injection. During the 1st phase of the experiment which lasted from 0 to 2700 s, helium at 20 °C was injected into the vessel with a mass flow rate of 0.59 g/s together with a small amount of steam (0.16 g/s). Later, during the 2nd phase of the experiment, from 2700 to 4700 s, steam at 111 °C was injected into the vessel with a mass flow rate of 35 g/s. Steam condensed on the cold structures of the ThAI vessel. Helium and steam were injected upwards during these phases in the upper part of the ThAI vessel. During the 3rd phase, steam at 111 °C was injected in the lower part of the vessel in the horizontal direction with a flow rate of 35 g/s from 4700 to 5700 s. The last (4th) phase lasted from 5700 to 7700 s without any injection of gases. The injection locations in cylindrical coordinates and the injection tube internal diameters are given in Table 1.

Table 1: Injection locations and injection tube diameters.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Vertical elevation m</th>
<th>Radius m</th>
<th>Azimuthal position °</th>
<th>Injection tube diameter mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.8</td>
<td>1.15</td>
<td>135</td>
<td>28.5</td>
</tr>
<tr>
<td>2</td>
<td>5.0</td>
<td>1.15</td>
<td>315</td>
<td>44.3</td>
</tr>
<tr>
<td>3</td>
<td>1.8</td>
<td>1.28</td>
<td>315</td>
<td>138</td>
</tr>
</tbody>
</table>

3 COMPUTATIONAL MODELLING

3.1 Input Model

The CFX 4.4 code is a general purpose CFD commercial code, which has been first developed by AEA Technology (UK) and is now being developed by ANSYS Inc. The code...
solves the conservation equations for mass, momentum and energy together with their initial and boundary conditions. The software uses the finite volume method for the numerical solution of these equations.

For the simulation of the ThAI ISP-47 experiment, a 3-dimensional grid was developed, covering only one half of the vessel. This is possible due to the assumption of symmetry relative to the vertical plane crossing the injection locations. The numerical grid consists of 44 cells in vertical direction, 22 cells in radial direction and 17 cells in azimuthal direction. All heat structures (steel, mineral wool, oil, aluminium, trays, and inner cylinder walls) are modelled as 1-cell thick layers of conducting solid.

The air-steam, air-steam-helium and air-steam-helium-fog atmospheres were treated as homogenous mixtures with air as the carrier fluid. The calculation of the mixture properties is described in the CFX manual (AEA [18]). The following options were prescribed in the CFX command file:

- compressible flow,
- turbulent flow (standard k-ε model with wall functions),
- buoyant flow (C₃ constant of k-ε model set to 1.0),
- no-slip condition at the vessel wall.

The default options of the CFX4.4 code that correspond to these physical models were applied. The convective heat transfer between the vessel atmosphere and the heat structures was calculated by the CFX code.

On the outside wall of the vessel, a uniform boundary condition of 22 °C and the heat transfer coefficient from walls to surroundings of 0.0001 W/m²K were set. Inlets were treated as mass flow boundaries on faces of a single cell with face area corresponding to the specified inlet area. The values of mass flow rates and injection temperatures were taken from experimental data.

3.2 Wall Condensation Model

As the modelling of wall steam condensation is not included in the CFX4.4 code, it had to be implemented in a user-defined subroutine. Due to the coarse grid and wall function approximation of the boundary layer flow in the k-ε model, Fick’s law of diffusion could not be used to determine the wall condensation mass flow. Instead, a correlation had to be used. We decided to use a simple, but well known Uchida correlation [19], which was basically developed for the description of condensation on an integral scale. In our work, we replaced bulk variables with variables from cells contiguous to the walls where condensation takes place. In each cell, when the steam pressure was higher than the steam saturation pressure at the wall temperature, the mass sink was calculated from the Uchida correlation:

\[ m^0 = C_U \left( \frac{\rho_{\text{steam}}}{\rho_{\text{air}}} \right)^{0.8} \cdot A \cdot (T_{\text{cell}} - T_{\text{wall}}) / h_{lg} , \]

where \( C_U \) is an adjustable parameter, \( h_{lg} \) denotes the latent heat of phase change and \( A \) the area of the cell face at the condensation surface. Physical quantities in eq. (1) are evaluated at the cell centre. The corresponding enthalpy sink due to condensation is calculated as:

\[ h^0 = m^0 \cdot \left( C_{p,\text{ste}} T_{\text{cell}} - C_{p,\text{air}} T_{\text{ref}} \right) , \]

where \( T_{\text{ref}} \) denotes the reference temperature, defined in the CFX4.4 command file. As the mass and enthalpy sinks depend on values of physical quantities, which are evaluated at the cell centre, the modelling of condensation depends on the size of cells contiguous to the condensation surface. Thus, the value of the coefficient \( C_U \) in eq. (1) is valid only for a given
cell size. In this simulation, cells contiguous to the wall were 2 cm wide and the value of 360 \( W/m^2K \) was used for the constant \( C_U \). The flow of the liquid film on the walls was not taken into account.

### 3.3 Bulk Condensation / Evaporation and Rain-Out Models

A simple mechanistic bulk condensation and evaporation model was also incorporated into the code. In our simulation, fog was treated as a gas, but its effects on compressibility parameters were neglected. When the steam pressure \( P_{ste} \) in a cell was higher than the steam saturation pressure at the cell gas temperature \( P_{sat} \), then the bulk condensation rate (i.e. fog creation rate) was calculated from the following equation:

\[
m^0_B = \frac{(P_{ste} - P_{sat}) \cdot V_{cell}}{(R_{steam} \cdot T_{gas}) / \Delta t_{step}} \cdot C_B . \tag{3}
\]

In the case that fog was present in the cell and the steam pressure \( P_{ste} \) was lower than the steam saturation pressure \( P_{sat} \) at cell gas temperature, the bulk evaporation rate was calculated from the following equation:

\[
m^0_E = \frac{(P_{ste} - P_{sat}) \cdot V_{cell}}{(R_{steam} \cdot T_{gas}) / \Delta t_{step}} \cdot C_B . \tag{4}
\]

The corresponding enthalpy source due to release of latent heat is determined from the following equation:

\[
h^0_B = m^0_B \cdot h_{fg}(T_{gas}) \quad \text{or} \quad h^0_E = m^0_E \cdot h_{fg}(T_{gas}) . \tag{5}
\]

In case when the fog density was higher than 30 g/m\(^3\), the fog was removed from the cell at a rate:

\[
m^0_R = \frac{(m_{fog} - 0.03 \, \text{kg/m}^3 \cdot V_{cell})}{\Delta t_{step}} \cdot C_B \tag{6}
\]

with a corresponding enthalpy sink of

\[
h^0 = m^0 \cdot (C_{p,fog}T_{cell} - C_{p,air}T_{ref}) . \tag{7}
\]

In equations (3), (4) and (6), \( C_B \) is an adjustable coefficient and acts as a relaxation parameter. \( C_B \) was assigned a constant value of 0.1.

### 4 COMPARISON OF EXPERIMENTAL AND SIMULATION RESULTS

#### 4.1 Transient Data

During the 1st phase (0-2700 s), helium was injected upwards in the upper part of the annulus. Because helium is lighter than air, it accumulated in the upper part of the vessel. During the 2nd phase, steam was injected upwards, in the upper part of the annulus, on the opposite side of the annulus than helium. Hot steam flowed upwards from the injection location to walls in the upper parts of the vessel and then flowed downwards on the opposite side of the vessel. Some of the steam condensed in contact with colder walls.

Figure 3 shows the measured and calculated pressure in the ThAI vessel during phases 1 and 2. The calculated pressure during the first part of the 2nd phase is somewhat over-
predicted, while during the last part it is somewhat under-predicted. These discrepancies could be attributed to phase-change models.

Figure 4 shows the simulated and measured temperatures at 4 different locations in the vessel: in the upper and lower plenum (above and below the inner cylinder) and in the upper and lower part of the annulus (between the inner cylinder and the outer vessel wall). The simulated temperatures show similar behaviour as was observed during experiment, except that the temperature in the upper annulus is quite higher than the measured one.

Figure 5 shows the simulated and measured helium volume fractions. The agreement is good, except for the simulated helium volume fractions in the upper plenum, which shows significantly higher values from the beginning of the 2nd phase compared to the measured helium volume fraction in that region, which is increasing slowly during the 2nd phase.

Figure 6 shows the measured and simulated steam volume fractions in the upper plenum above the cylinder. The predicted values show the same trend but are somewhat higher than the measured values during the 2nd phase.

A plausible explanation for the discrepancies indicated on Figures 4, 5 and 6 could be that the simulation predicted higher mixing and convective flow rates in the indicated regions of the vessel than flow rates that were observed during the experiment.

4.2 Vertical Profiles at End of 1st Phase

Figure 7 shows the measured and simulated vertical profiles of the helium volume fraction at the axis of the vessel and in the annulus of the vessel at the end of the 1st phase ($t = 2700$ s). Both simulated profiles show that all helium is located in the upper part of the vessel.
Compared to measured data, the simulated profile in the annulus shows somewhat higher helium volume fraction in the upper part of the vessel.

Figure 7: Measured and simulated vertical profiles of helium volume fraction at the end of 1\textsuperscript{st} phase of ThAI experiment.

### 4.3 Vertical Profiles at End of 2\textsuperscript{nd} Phase

Figures 8 and 9 show the simulated and measured vertical profiles of helium volume fractions. In both figures, the experimental data were measured at the end of the 2\textsuperscript{nd} phase ($t = 4700$ s). The simulated vertical profiles are shown at 4200 s (Figure 8) and at the end of 2\textsuperscript{nd} phase (Figure 9). As can be seen, the simulated vertical profiles of helium volume fractions at 4200 s correspond well to the measured data. The simulation data from the end of the 2\textsuperscript{nd} phase shows that some helium transport occurred from the upper part to the lower part of the vessel at the end of the 2\textsuperscript{nd} phase, which resulted in lower helium content in the upper part of the vessel and higher helium content in the lower part of the vessel.

Figures 10 and 11 show the simulated and measured vertical profiles of temperatures. In both figures, experimental data were measured at the end of the 2\textsuperscript{nd} phase ($t = 4700$ s). The simulated vertical profiles are shown at 4200 s (Figure 10) and at the end of the 2\textsuperscript{nd} phase (Figure 11). As can be seen on both figures, the simulated vertical profiles of temperatures correspond well to measured data. The transition from lower to higher temperatures in the vertical direction of the vessel occurs at a somewhat lower elevation than was observed during the experiment.

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4.4 Analysis

The computation of first two phases of the ThAI ISP-47 experiment was very time consuming, lasting about 3 weeks on 3 MHz Pentium-IV processor with 512 Mb RAM. In order to reduce the simulation time to a reasonable level, we had to reduce the convergence criteria from $0.5 \times 10^{-3}$ to $0.5 \times 10^{-2}$ kg/s, which resulted in changes of the air mass in the vessel of approximately 5% during the entire simulation. The time step varied between 0.05 s to 0.2 s.

There are three issues that need to be addressed before analysing the simulation results. The first issue is the quality and resolution of the computational grid used for the simulation. The average computational cell dimension is about 20 cm. Due to long computational times, we were not able to perform grid independence test by refining the grid.

The second issue is concerned with the use of the standard k-ε model of turbulence together with wall functions. Due to low gas velocities in most of the ThAI vessel, the non-dimensional distance from the wall $y+$ in the cells contiguous to the wall was predominantly less than 11.25, which is the lower bound for the use of the log-law wall functions. The quality of the used computational grid and the standard k-ε model of turbulence have perhaps prevented a better agreement of the simulation with the experimental data.

The third issue is the wall condensation modelling. There are many correlations that predict the wall condensation rate and the Uchida’s correlation is one of the simplest. But as our simulations show, the correlation used together with the simplified bulk condensation and evaporation models gives reasonable results.

The simulation results of the 1st phase revealed nothing unexpected: due to helium injection, there was a gradual increase of pressure and temperature. The predicted helium distribution in the vessel agrees well with the measured non-uniform distribution.

The simulation of the 2nd phase replicated the experimental data adequately, but there were also some discrepancies. The calculated temperature in the upper part of the annulus (Figure 3) is considerably higher than the measured temperature at that location. The calculated helium volume fractions in the upper annulus (Figure 4) show a different behaviour than was observed during the experiment. A possible explanation is that the simulated flow pattern in the vessel was somewhat different than during the experiment.
5 CONCLUSIONS

The first two phases of the ISP-47 experiment on containment atmosphere mixing and stratification at accident conditions in a nuclear power plant containment, performed in the ThAI experimental facility, were simulated with the CFD code CFX4.4. A three-dimensional model of the ThAI facility was developed, and steam wall condensation, bulk condensation and bulk evaporation models were implemented in the CFD code.

Calculated time-dependent data, temperatures and species concentration distributions at the end of two simulated phases were compared to experimental measurements. Although grid quality and turbulence modelling were limited due to long computational times and the use of simple phase-change models, the simulations with the CFX4.4 code agree reasonably well with the measured data and adequately reproduce the measured temperatures and the helium and steam non-homogenous distributions at the end of both phases.

Despite some discrepancies, the general agreement between experimental and calculated results shows that the proposed approach is adequate and that it could be, with further improvements, applied to similar problems.

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