

Numerical Domain Reduction in Containment Atmosphere Mixing Simulations

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ABSTRACT

Four experiments on mixing of stratified atmosphere, performed in the PANDA experimental facility with different jet injection velocities and atmosphere compositions, are simulated with the computational fluid dynamics code OpenFOAM. A 3D numerical model considering both vessels with interconnecting pipe is developed. Non-essential parts of the experimental facility, which do not contribute much to the mixing process, are identified according to experimental results. As the phenomena can be assumed to be axisymmetric, an axisymmetric 2D numerical model is proposed. Simulation results obtained with both numerical models are compared with experimental results and the effects of the use of smaller computational domain with axisymmetric boundary condition are studied.

1 INTRODUCTION

During a severe accident in a light water nuclear reactor, hydrogen combustion could threaten the integrity of the nuclear power plant (NPP) containment, which could lead to release of radioactive material into the environment. The study of hydrogen distribution in the containment is thus important to predict the occurrence of regions with high local gas concentrations and flammable mixture in order to effectively install mitigation systems in containments [1].

Various experiments are being performed to simulate atmosphere mixing occurring in NPP containment during severe accidents. During these experiments, a stratified atmosphere is first established and then homogenized using forced or natural convection. Experiments on mixing and homogenization of a stratified atmosphere are performed in containment experimental facilities of volumes between 10 m³ (small scale facilities) and 200 m³ (large scale facilities). Within the OECD project SETH-2 (2007-2010), experiments of erosion of a helium gas layer with a vertical jet were performed in the PANDA experimental facility at the Paul Scherrer Institute (PSI) in Villigen (Switzerland) [2].

A computational fluid dynamics (CFD) calculation of a single experiment performed in the PANDA facility can last up to one month, despite using parallel computing. Furthermore, to perform calculations with needed sensitivity analyses (effect of different numerical meshes, numerical schemes, boundary, and initial conditions) several calculations are needed. To reduce computational time, numerical domains used in calculations can be reduced. In our work, the suitability of reduction methods is studied on experiments performed in the PANDA experimental facility. First, parts of the experimental vessel, which do not contribute much to the mixing process, are identified according to experimental results and are not considered in the numerical model. In addition, these experiments are performed within the cylindrical vessel with injection taking place in the axis of the vessel. In such setup, axisymmetry can be assumed. Therefore, a simplified axisymmetric two-dimensional numerical model of the PANDA facility is developed. The results obtained with reduced models are compared to results obtained with the numerical model of the entire experimental facility and also to experimental results. Finally, the effects of reduced numerical domain are assessed and the suitability of the reduction is discussed.

2 PANDA EXPERIMENTAL FACILITY AND EXPERIMENTS

The PANDA experimental facility is designed to study physical phenomena during accidents in a system of containment vessels for different designs of nuclear reactors. The setup used in the ST1 experimental campaign for observation of interaction of low-momentum jet with a helium layer consists of two cylindrical vessels and an interconnecting pipe, with a total volume of 183 m³ (Figure 1). Each vessel has a height of 8.0 m and an external diameter of 4 m. The volume of a single vessel is 89.9 m³. The injection pipe located in the vertical axis of the cylindrical vessel has a diameter of 0.2 m. The injection pipe outlet is located 4.03 m below the vessel ceiling and 0.22 m above the interconnecting pipe, which serves as the outlet into the second vessel [3]. Figure 1 (b) shows sampling positions, from which results are compared.



Figure 1: Schematic of PANDA facility with initial conditions (a) and sampling positions (b) [2][3].

Before the tests, a 2 m thick layer of helium and steam was established in the upper part of one of the vessels. In the other parts of the vessels, only steam was present. as shown in Figure 1 (a). The volume fraction of helium in this layer differs depending on the case. The conditions of the four tests simulated in the present work are listed in Table 1. Figure 2 shows vertical distribution profiles of initial helium volume fraction. The initial atmosphere temperature and pressure were 108 °C and 1.3 bar, respectively. During the experiments, steam at a temperature of 140 °C was injected at a constant mass flow rate (Table 1).

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Test	Helium content	Jet velocity	Injection flow rate	Interaction Froude
	[vol. %]	[m/s]	[g/s]	number [-]
ST1_3	25	4.16	90	2.13
ST1_4	25	1.02	22	0.52
ST1_5	40	1.39	30	0.53
ST1_6	40	3.88	84	1.48

Table 1: Boundary and initial conditions for simulated tests [2].



Figure 2: Initial helium distribution for different initial concentrations [2].

3 SIMULATION MODEL

Numerical simulations are performed with the OpenFOAM CFD code, version 1606+ [4]. To simulate the transient mixing process, the Unsteady Reynolds Averaged Navier Stokes (URANS) approach is used. A pressure-implicit split-operator (PISO) algorithm was used to iteratively couple the flow equations. An adaptive time step is used, to sustain a Courant-Friedrichs-Lewy (CFL) number of less than 0.5. The convergence criterion within a time step is specified with maximum residual values listed in Table 2. Besides, to ensure an accurate calculation of the transient process, at least 3 iterations per time step are used.

Table 2: Maximum residual convergence criteria for individual quantities.

Enthalpy, velocity, turbulence	10-7
Pressure, gas species mass fraction	10-6
Radiation	10-5

In simulations, a second-order accurate finite volume discretization scheme with secondorder accurate interpolation scheme is used. The temporal term is discretized using a first-order implicit differencing scheme.

3.1 Computational mesh and boundary conditions

A 3D numerical model considering both vessels with interconnecting pipe was developed, as shown in Figure 3 (a). The mesh in the first vessel, where the helium was initially present, was refined above the inlet, in the mixing region.

During the experiments, the temperature in the interconnecting pipe was increasing linearly. Furthermore, despite the vessel being non-symmetrical due to the interconnecting pipe on one side, the helium molar fractions measured at two opposite locations inside the vessel were equal. On the other hand, there is a 1°C difference between the temperatures measured at

two opposite sides of the injection pipe, but in positions above the inlet no asymmetry can be observed [2]. Thus, it is assumed, that the backflow from the second vessel does not contribute much to the mixing process in the first vessel, where the helium is present from the beginning. Also, it can be observed in the experimental results that the part of the vessel below the injection does not contribute much to the mixing process. Namely, the temperature in the lowest measuring positions up to z = 3.676 m increases by only 2 °C and the increase of helium volume fraction at z = 0.538 m is less than 1 vol.% [2].

As the phenomena can be assumed to be axisymmetric, an axisymmetric 2D numerical model in the shape of a 5° wedge was also created. Furthermore, as previously discussed, only the part of the vessel above the inlet is considered, as shown in Figure 3 (b). The inlet is prescribed on the bottom inner side of the domain, as shown in Figure 3 (b). The rest of the bottom patch is prescribed as outlet; other patches is prescribed as walls.



Figure 3: 3D numerical domain (left) and axisymmetric 2D numerical domain (right).

Wall functions are prescribed on walls for turbulence quantities and the no-slip boundary condition was prescribed for velocity. From the experimental results, it was observed that during the experiment the wall temperature is, on the average, constant and a constant wall temperature is prescribed in the simulations.

Time-varying mass flow rates and temperature values at the inlet were prescribed as measured in the experiments. The injection pipes inside the numerical domains are used only as a flow obstruction, with the inlet prescribed at the pipe end. However, additional separate simulations of the flow inside injection pipes are performed to obtain fully developed flow conditions according to the case. These fully developed velocity, turbulence and temperature profiles are then prescribed at the pipe outlet in atmosphere mixing simulations.

The total number of mesh cells (N), the edge lengths (Δ) of the smallest and largest cells, the diameter of the refinement region above the injection pipe (D), the calculated maximal nondimensional wall distance (y^+) at the end of the transient, and the aspect ratio (AR) are listed in Table 3. Although the 3D meshes seem much coarser than 2D meshes, the cells in the mixing region have similar size. To reduce the computational time in larger computational domain, the coarser mesh was used in non-essential parts away from the injection.

Mesh	Ν	Δ [cm]	D [m]	y_{max}^+	AR
2D	128,018	0.75	/	1.95	1.95
3D	11,293,927	1-8	1.4	88.7	1

Table 3: Parameters of numerical meshes: total number of mesh cells, cell size, refinement region diameter, calculated maximal non-dimensional wall distance, max aspect ratio.

4 RESULTS AND DISCUSSION

Figure 4 shows time-dependent helium volume fractions at several locations directly above the injection. The results obtained with the 3D numerical model and the 2D simplified model are compared to experimental values. Despite a smaller computational domain, no major discrepancies can be observed between the calculations. When compared to the experiment, the start of the erosion of the helium rich layer and the helium concentration seem predicted well in all measuring positions in all considered experiments.

Figure 5 shows time-dependent atmosphere temperatures at different locations directly above the injection pipe. The results obtained with the 3D numerical model and the results obtained with the 2D axisymmetric model are compared to experimental values. Some minor discrepancies (2°C at most) can be observed in the temperature values given by the 3D and 2D numerical model. Nonetheless, when compared to experimental values, temperatures obtained in simulations are reasonably well predicted. Temperatures between the jet and the wall, at x = 1.43 m or x = 1.69 m, in the ST1_4 case are shown in Figure 6 as an example. The temperatures away from the rising jet are well predicted in the lowest sampling position (z = 4.98 m). At higher positions, the maximal temperature value is overpredicted, but nevertheless final values are the same as measured in the experiment.

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Figure 4: Helium volume fractions above injection (x = 0 m) at different elevations with different injection flow rates.

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Figure 5: Atmosphere temperatures above injection (x = 0 m) at different elevations with different injection flow rates



Figure 6: Atmosphere temperatures at different off-centre radial positions and elevations in ST1_4 case.

5 CONCLUSIONS

The results of four experiments on mixing of stratified atmosphere, performed in the PANDA experimental facility with different jet injection velocities and atmosphere compositions, are used to validate a proposed modelling based on description on the local instantaneous scale. Non-essential parts of the experimental facility, which do not contribute much to the mixing process, are identified according to experimental results. The use of axisymmetric two-dimensional numerical domains appears to be an efficient way to reduce the computational time without any major effects on simulations results. The CFD code is able to correctly reproduce the mixing process and the homogenization of stratified atmosphere.

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