Analyses of Jet-Buoyant Flow in a Multi-Compartment Containment using an Open-Source Solver

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ABSTRACT

Hydrogen mixing and distribution in a nuclear power plant containment during a postulated severe accident is a phenomenon with high safety relevance for current and advanced LWR. The OECD/NEA-SETH project was carried out to generate the experimental data on basic containment phenomena with the required instrumentation to assess CFD and LP codes.

In this paper, we analyzed the PANDA Test 16 of the OECD/NEA-SETH project by using containmentFOAM which is a tailored open-source CFD code package for containment analysis developed at Forschungszentrum Jülich (Germany) based on OpenFOAM®. The SETH Test 16 addressed steam-air mixture transport driven by jets and plumes in the multi-compartment PANDA facility (two vessels and interconnecting pipe) at Paul Scherrer Institut (Switzerland). Steam as a wall plume is injected with 0.040 kg/s and 140 ºC in Vessel 1 which is initially filled with dry air at 108 ºC. Steam-air mixtures are vented out from top of the Vessel 2. The system pressure is constant at 1.3 bar for the whole test duration (4000 s).

To simulate SETH Test 16, the *k*-ω SST turbulence model was adopted with GGDH (Generalized Gradient Diffusive Hypothesis) buoyancy turbulence model. The simulation represents the experimental phenomenology reasonably well. The trend for the calculated temperature distribution is similar to those of the experiments and only yields a slight discrepancy about 2.7 %. And the distribution of steam molar fraction is predicted well above the injection tube in Vessel 1. However, below the injection tube in Vessel 1 some discrepancies between the simulations and the experimental results were observed. It may be caused by the higher turbulent mass diffusivity in the physical model and the challenge of the mesh resolution in the middle region of the Vessel 1.

Keywords: Multi-compartment, Jet-plume flow, CFD, containmentFOAM, PANDA

I. INTRODUCTION

Phenomena such as mixture gases and distribution in a nuclear power plant containment during a postulated accident have high safety relevance. Because in the containment regions with high mass flow rates of steam may lead to damage equipment with safety functions due to pressurization and therefore challenging the containment's structural integrity [1]. Hydrogen mixing and distribution is driven by buoyant high-momentum jets or low-momentum plumes which could form in various geometrical configurations. For instance, free plumes could be produced by the gas (steam or steam/hydrogen) efflux from the break compartment in a larger containment room; wall plumes could be produced by low gas flows through aperture between compartments.

Safety analyses of a nuclear plant containment during postulated accident are carried out using advanced Lumped Parameter (LP) and Computational Fluid Dynamic (CFD) codes [2-8]. The computational modeling is improved taking into account the accumulated knowledge about containment phenomenology. Over the last years, the research community has devoted several international research projects to the hydrogen issues (e.g., distribution, mitigation, combustion) and experimental databases were created and extended for a variety of basic phenomena.

The OECD/NEA SETH project was selected for analyzing containment phenomena in this study. The PANDA experiments of the OECD/NEA SETH project (2001-2006) included three series of tests named wall plume, free plume, and horizontal jets [9]. The objective of OECD/NEA SETH project series was to investigate the basic flows with transport and mixing driven by jets and plumes in a large multi-compartment geometry consisting of two vessels connected by an interconnecting pipe (IP) [10]. Test results have been designed to provide database for basic assessment of CFD and advanced LP codes. Those demonstrated the physical mechanisms involved in the erosion process and the presence of complicated phenomena to be modelled for the validation of advanced LP and CFD codes [11].

Analytical activities of selected SETH PANDA experiments were performed with various codes, e.g., GASFLOW [11, 12], GOTHIC [13, 14], ASTEC [15], CFX-4.4, CFX-5.7, FLUENT 6.1.22, TONUS [16]. Those analytical activities provided contributions toward the assessment of strengths and drawbacks of different codes in analyzing the phenomena simulated in the PANDA tests. A number of simulation challenges were identified in relation to: gas transport and stratification for the case of high flow exit elevations; prediction of peak gas temperature (mainly in the near-wall plume test series); stratification disruption and erosion for the case of the three gas test; and condensation/condensate transport and re-evaporation phenomena.

The SETH Test 16, selected among those of the SETH series, represents one of the fundamental phenomena with simple geometry as a wall plume. The aim is to compare transient simulation results of gas-mixing behavior and interaction between steam and air in a multi-compartment with experimental results to analyze the governing parameters in these phenomena. This study would be a foundation for further studies on containment phenomena within the SETH series, encompassing complex geometries and various initial and boundary conditions with CFD. Furthermore, it constitutes a prominent step in conducting phenomenological analyses and breaking down dominant factors using containmentFOAM CFD, rather than simply predicting experimental outcomes.

In this paper we present the computational results using containmentFOAM (at the time of running the analysis based on OpenFOAM® v6) [17] of the PANDA Test 16 [18] carried out within the OECD/NEA SETH Project.

II. EXPERIMENTAL FACILITY AND TEST CONFIGURATION

II.A. Experiments of OECD/NEA SETH Test 16

PANDA is a large-scale, thermal-hydraulics facility that is operated for investigation related to LWR containment phenomena during postulated accidents [18]. An overview of investigations performed so far in PANDA facility is provided in the article [19].

Figure 1 is shown a 3D rendering of the PANDA facility with Vessel 1, Vessel 2 and interconnecting pipe. The total volume of vessels and pools is about 183.3 m^3 and the height of the facility is 8 *m*. The components are all made of stainless steel. The facility is thermally insulated with 200 *mm* of rock wool, and the heat loss characteristics for the individual vessels were experimentally determined.

In this paper, the comparison between simulation and experimental results is provided about gas mixture concentration and temperature in Vessel 1 and Vessel 2. In PANDA spatial and temporal distributions of the gas concentration were measured using sampling capillaries connected to two mass-spectrometers, while the gas temperature was measured using thermocouples at the same positions.

For the sensor used in this paper, the error for the gas concentration measurement is about 1.5 % and for the fluid and wall temperature measurements is about 0.7 ºC, for the pressure is 3.3 *kPa*.

The SETH experimental series have jets and plumes with various of configuration generated by an injection of steam/air or steam/helium/air mixtures in a volume initially uniformly filled with air or steam/air mixtures. Twenty-four tests of SETH cases have been performed in the large-scale PANDA facility. Among of these test cases, the SETH Test 16 have been selected for the analyses presented in this paper. Test 16 is characterized by a simple PANDA geometrical configuration and initial and boundary conditions. The Test 16 geometry consists of two vessels with steam injected in Vessel 1 and stratification and propagation throughout the IP and venting from top of the Vessel 2 as shown in Fig. 2. The vessel height and diameter are 8 *m* and 3.9 *m*, respectively. And diameter of IP is 0.928 *m*. The wall thickness is about 0.02 *m* except for the IP where it is 0.012 *m*. In addition, there has an injection nozzle located in low elevation (1.813 *m*) with diameter of nozzle 0.156 *m*. The flow conditions for two vessels are: Vessel 1 with a high momentum injecting steam and Vessel 2 with a very low momentum due to the flow from the IP.

II.B. Initial condition

The nominal and mean actual initial conditions in two vessels are given in Table I. The wall temperature was measured in 265° with vessel 1 and 97.5° with Vessel 2 over the elevation. And the fluid temperature where was measured at the center of the vessels according to the elevation has 107.508 °C almost same with nominal value (0.4% error). Temperature of the injected fluid with about 100 % of steam is set to 140 °C meaning of superheated steam (without condensation), which is measured at 0.20 *m* from the exit and center of the injection nozzle. And the mass flow rate of the injected steam is 0.040 *kg*/*s*. The pressure and steam injection flow rate and temperature are estimated over the whole test period approximately 4000 s.

Table I. Initial and boundary condition of SETH Test 16.

Initial condition		Nominal value	Mean actual value
Total pressure		1.3 bar	1.301 bar
Wall temperature		108 °C	108.171 °C
Fluid temperature		108 °C	107.508 °C
Molar fraction	**Air**	100 %	> 99 %
	Steam	0 %	< 1 %
Injected steam (Vessel 1)	**Temperature**	140 °C	139.7 °C
	Mass flow rate	0.040 kg/s	0.040 kg/s
Froude number		~ 2.9	~ 2.9

$$Fr = \frac{\rho_j u_j^2}{\left(\rho_m - \rho_j\right) g d_j} . \tag{1}$$

The fluid dynamic flow condition can be expressed by *Froude number* (*Fr*). It is a physical parameter that defined as relative force between inertia force ($\rho_j u_j^2$) and buoyancy force ($(\rho_m - \rho_j) g d_j$) as the dimensionless number. Where ρ_m is density of ambient and ρ_j is density of injected fluid. And d_j is diameter of injection tube, g is acceleration gravity and u_j is velocity at the injection nozzle.

When the *Fr* has a very high value, the flow is dominated by the inertia force, whereas in the vice versa case, the flow is dominated by the buoyancy force. *Fr* of 1 means that the buoyancy force is comparable to the inertia force. It can be expressed as

Based on the above equation, the *Fr* associated with the flow condition of Test 16 can be expected as 2.9 with jet-plume configuration. It means that the flow could be determined by dominating with inertia force (jet configuration) but not extremely.

III. NUMERICAL METHODOLOGY

The containmentFOAM CFD code was used to analyze the experimental results of the OECD/NEA SETH Test 16. The containmentFOAM package is a multi-physics toolbox based on OpenFOAM® (at the time of running the analysis version 6). It has been developed with the purpose of efficiently simulating transport processes inside confined domains for instance a nuclear reactor containment under postulated accident scenarios. FZJ (Forschungszentrum Jülich GmbH) leads the development activities of containmentFOAM [17]. Generally, the proposed baseline modeling approach for containment atmosphere mixing processes was adopted except for gas radiation modeling, which was neglected in this case. The baseline model is used to analyze and validate accidental flows in a nuclear reactor containment according to the fundamental models set over the last ten years [17].

III.A. Governing equations

The unsteady Reynolds Averaged Navier Stokes (U-RANS) approach was utilized for the gas mixture phase to solve conservation equation within a single phase. The governing equations are outlined in Eqs. (2) – (5). Eq. (2) presents the continuity equation which can be concurrently solved with *N-1* species equations (Eq. (3)). The diffusive mass flux ($\overrightarrow{J_k}$) is Fick's law, where Y_k denote the mass fraction of the species and $D_{k,j}$ represents the binary diffusivity adopted as a Fuller model. This model was illustrated in subsequent chapter.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{U} \right) = 0 \tag{2}$$

$$\frac{\partial \left(\rho Y_k \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} Y_k \right) = -\nabla \cdot \vec{J}_k \text{ where } \vec{J}_k = -\rho D_{k,j} \nabla Y_k \text{ and } \sum_{i=1}^{N} Y_k = 1 . \tag{3}$$

Equation (4) represents the momentum equation, where the viscous stress tensor (τ) is defined as follows: $\underline{\nu}$ represents the kinematic viscosity, ν_t stands for the turbulent eddy viscosity of the gas mixture, and δ presents the Kronecker delta. The *k-ω* Shear Stress Transport (SST) turbulence model was utilized to determine the turbulent eddy viscosity.

$$\frac{\partial \left(\rho \vec{U} \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} \otimes \vec{U} \right) = -\nabla p + \nabla \cdot \tau + \rho \vec{g} \text{ where } \tau = \rho \left(\nu + \nu_t \right) \left[\nabla \vec{U} + \left(\nabla \vec{U} \right)^T - \frac{2}{3} \delta \nabla \cdot \vec{U} \right]. \tag{4}$$

The total energy equation is shown in Eq. (5). The left-hand side includes the temporal and convection terms of total enthalpy energy ($h_{tot} = h + K$) and $K = |U|^2/2$. In the right-hand side, the second term may be the dominated term among those of terms which corresponds to the enthalpy transport from net heat flux due to conduction and mass diffusion ($\overrightarrow{\dot{q}''}$). The third term related to viscous dissipation is neglected due to the low-speed flows. The fourth term indicate the work due to the buoyancy force in the momentum equation. The fifth term is the volumetric source term due to radiation heat transfer, but in this study it does not consider. The heat flux term could be transformed to Eq. (6) according to $\lambda_{eff} = \lambda + \lambda_t$ and $\alpha_{eff} = \lambda_{eff}/(\rho/c_p)$. Where λ_{eff} is the conductive heat flux consisted of molecular (λ) and turbulent (λ_t) according to Fourier's law and α_{eff} is the thermal diffusivity based on the conductive heat flux. More detailed explanation can be found in [17].

$$\frac{\partial \left(\rho h \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} h \right) + \frac{\partial \left(\rho K \right)}{\partial t} + \nabla \cdot \left(\rho \vec{U} K \right) = \frac{\partial p}{\partial t} - \nabla \cdot \vec{\dot{q}''} + \nabla \cdot \left(\vec{U} \cdot \tau \right) + \vec{U} \cdot \left(\rho \vec{g} \right) - \nabla \cdot \overrightarrow{\dot{q}''_{rad}} \tag{5}$$

$$\text{where } \vec{\dot{q}''} = -\lambda_{eff} \nabla T + \sum_{k=1}^{N} \overrightarrow{J_k} h_k .$$

$$\vec{\dot{q}''} = \rho \alpha_{eff} \nabla h + \sum_{k=1}^{N} \rho \left(\alpha_{eff} - D_{k,j} \right) h_k \nabla Y_k \tag{6}$$

III.B. Physical models

The *k-ω* SST turbulence transport model, which incorporates a buoyancy term is illustrated in Eqs. (7) and (8). Here, *k* denotes turbulent kinetic energy, *P* represents turbulence production. And β^*, σ_k, γ, β, σ_ω, $\sigma_{\omega 2}$, a_1, γ_1, C_3 refer to modeling coefficients. Additionally, ω signifies turbulence dissipation rate, μ and μ_t represent fluid and turbulent dynamic viscosities, respectively. $P_{k,b}$ stands for turbulence production owing to buoyancy. And F_1, F_2 represent blending functions of modelling coefficients. And $P_{\omega,b}$ denotes turbulence dissipation caused by buoyancy, and *S* is the strain invariant.

$$\frac{\partial(\rho k)}{\partial t} + \nabla \cdot \left(\rho \vec{U} k\right) = P - \beta^* \omega k + \nabla \cdot \left[\left(\mu + \sigma_k \mu_t\right) \nabla k\right] + P_{k,b} \text{ and} \tag{7}$$

$$\frac{\partial(\rho\omega)}{\partial t} + \nabla \cdot \left(\rho \vec{U} \omega\right) = \frac{\gamma}{\nu_t} P - \beta \rho \omega^2 + \nabla \cdot \left[\left(\mu + \sigma_\omega \mu_t\right) \nabla \omega\right] + 2\left(1 - F_1\right) \frac{\rho \sigma_{\omega 2}}{\omega} \nabla k \cdot \nabla \omega + P_{\omega,b} \tag{8}$$

$$\text{where } P = min\left(\overline{\overline{\tau}} \nabla \vec{U}, 10\beta^* \omega k\right), \ \mu_t = \frac{\rho a_1 k}{max\left(a_1 \omega, SF_2\right)} \text{ and } P_{\omega,b} = \frac{\rho}{\mu_t}\left[\left(\gamma_1 + 1\right) C_3 \cdot max\left(P_{k,b}, 0\right) - P_{k,b}\right] \tag{10}$$

In several studies, GGDH (Generalized Gradient Diffusion Hypothesis), and SGDH (Simple Gradient Diffusion Hypothesis) as a buoyancy turbulence model may be considered. We have selected to model the buoyancy turbulence production and dissipation term by means of the GGDH. Because it takes accounts not only the density gradient in gravity direction but also the cross-stream density gradients. In contrast, the SGDH model tends to underpredict the spread rate in vertical thermal plumes and overpredict the spread rate in horizontally stable-stratified flows [20]. The turbulence production term ($P_{k,b}$) can be replaced with GGDH buoyancy turbulence term. Reynolds stresses are modeled using Boussinesq approximation as following as

GGDH model

$$P_{k,b} = -\frac{3}{2} \frac{\mu_t}{\sigma_t \rho k}\left[g \cdot \left(\overline{u_j' u_k'} \cdot \nabla \rho\right)\right] \tag{11}$$

$$\text{where } -\overline{u_j' u_k'} = \nu_t \left(\frac{\partial U_j}{\partial x_k} + \frac{\partial U_k}{\partial x_j}\right) - \frac{2}{3} k \delta_{jk} \ .$$

The Fuller model, depicted in Eq. (12), is used to drive mass diffusivity, considering the pressure and temperature dependent binary diffusivity of the species *k* in species *j*. Where *M* and *V* represent molar mass and diffusion volume of species *k* and *j*, respectively.

$$D_{k,j} = \frac{0.00143 T^{1.75} \left(\frac{1}{M_k} + \frac{1}{M_j}\right)^{\frac{1}{2}}}{p\left[\left(\sum V_k\right)^{\frac{1}{3}} + \left(\sum V_j\right)^{\frac{1}{3}}\right]^2} \tag{12}$$

Wilke's mixture model was chosen to define mixture gas transport properties (φ_m). The properties of mixed fluid, such as c_p, μ, κ can be calculated with Eq. (13), where A_{jk} represents the inter-collisional parameter, as follows,

$$\varphi_m = \sum_j \frac{Y_j \varphi_j}{\sum_k Y_k A_{jk}} \text{ where } A_{jk} = \frac{\left[1 + \left(\mu_j / \mu_k\right)^{0.5} \left(M_k / M_j\right)^{0.25}\right]}{\sqrt{8\left(M_j / M_k\right)}}. \tag{13}$$

III.C. Numerical description

Figure 3 illustrated the mesh grid of SETH Test 16 with front and top view created using ICEM CFD. The cell type was 3D hexahedron with quadrilateral surfaces and the total number of the cells was 1,564,014. As shown in right side of Fig. 3, the vent is located in the top and center of the Vessel 2 and it has a square plane with size of 0.25 *m* by 0.25 *m*. In the actual PANDA facility, the shape of the vent is a tube with an inner diameter of 105.3 *mm* (outer 114.3 *mm*). This tube protruded approximately 70 *mm* into the interior of the Vessel 2. To avoid significant skew near the vent line of the mesh, the square plane was set as a simple configuration. Eventually, there was no effect on the phenomena such as reverse flow. It is expected that the phenomena are more complex in Vessel 1 and IP than that of Vessel 2. Therefore, we have used more refined grids for Vessel 1 and IP, while less refined grids were used in Vessel 2.

In the region below the injection elevation and up to the middle region in the Vessel 1, we refined the meshes due to the interaction of the injected plume with the complex flow from the IP. Simultaneously, it was kept to requirement regarding non-orthogonality and aspect ratio at the interface between the wall injection and vessel part and IP and vessel part [21]. On the other hand, in the Vessel 2, it was set as less refined meshes as the flow pattern and physical phenomena were less complex, resulting in fewer discrepancies between simulation and experimental results.

This mesh quality could be treated to be optimized according to the criteria of mesh quality; maximum skewness < 20, non-orthogonality < 65°, maximum aspect ratio < 60 (max. skewness ~ 2.30, max. non-orthogonality ~ 64.45, max. aspect ratio ~ 52.69) [21].

The numerical schemes for the present work for the discretization are second order accurate; temporal is Crank-Nicolson, convection is Gaussian linear upwind, Gradient and Laplacian are set to Gaussian linear upwind.

In general, OpenFOAM and containmentFOAM specifically, employ a segregated approach to solve the governing equations via the PIMPLE algorithm. Conjugate heat transfer (CHT) between the vessel wall and fluid part was taken into consideration. The time step is selected to uphold a mean CFL ≤ 1, while allowing a local maximum CFL ≤ 10 is tolerated if outer loop convergence is satisfied [17]. For the specific explanation are demonstrated in the publication of Kelm *et al*. [17].

The initial temperature of the center and wall of the vessel in the calculation was set as follows with the experimental initial conditions of Vessel 1 and 2 (except for the IP). The temperature variation in the center of Vessel 1 and 2 are 106.22 ℃ - 109.32 ℃ and 105.12 ℃ - 108.07 ℃, respectively (from the bottom of the vessel 0.5 *m* - 7.5 *m*). The temperature variation in the wall of Vessels 1 and 2 are 106.64 ℃ - 108.91 ℃ and 106.68 ℃ - 108.15 ℃, respectively (from the bottom of the vessel 1.8 *m* - 7.8 *m*). Additionally, as a boundary conditions the heat losses from the wall (1.455 W/m^2K) was taken into account the data measured in the PANDA characterization tests for the heat losses [22].

IV. RESULTS AND DISCUSSION

IV.A. Basic phenomena

In terms of phenomena evolution, Vessel 1 can be divided into three regions. These three regions were derived from the tendency of steam molar fraction and temperature of both computational and experimental results. Resultingly, the interpretation associated with the flow behavior such as velocity vector and temperature distribution could be helpful to what to focus on as shown in Fig. 4.

In the upper region of the vessel, the flow is dominated by significant turbulent flow induced by having high momentum due to the superheated steam injection. The middle region of the vessel has somewhat complicated by a boundary region with stratification from the bottom of the vessel and injected flow on the wall. In addition, it is characterized by the coexistence of high velocity from injection nozzle and low velocity from the IP. In the bottom region of the vessel, this region has low momentum flow region and effective stratification because the flow is dominated by molecular diffusivity. These three regions show in Fig. 4.

IV.B. Mesh dependency

We have two cases of mesh grids which are coarse and refined mesh. The description of the later one was explained in the section of ‘III.C. Numerical description’. The number of coarse mesh is 1,474,630. The most different thing is the mesh density in the middle region of the vessel as shown in Fig. 5. In the calculations, there appears to be a deviation in the steam molar fraction between (a) and (b) located below the injection nozzle. In other words, a denser mesh tends to be closer to the experimental results. This means that the middle and bottom regions require a higher density mesh than any other region even they have reasonable mesh quality. It is the one of the findings. Subsequently, the analysis of the calculation results is based on the refined mesh (b) due to its more suitable mesh grid compared to the coarse mesh (a) when compared against the experimental results.

IV.C. Steam molar fraction distribution

Figure 6 illustrates the steam molar fraction according to height of the Vessel 1 at each time step comparing with experiments and calculations using containmentFOAM. For the experimental results, the steam molar fraction steeply increases from the bottom of the vessel to about 2 *m*, which is comparable with the elevation of the wall-plume exit in Vessel 1 (e.g., 1.813 *m* elevation, Fig. 2). On the other hand, in the upper region of the vessel the steam molar fraction indicates constant value. This tendency of the steam molar fraction according to height presents similarity in all the considered time steps (Those of experimental results can also be confirmed in the results [23].). The injected superheated steam accumulates in the upper region of the Vessel 1 because the molecular weight of steam (~18.02 *g*/*mol*) is lighter than that of air (~28.87 *g*/*mol*) and therefore the steam plume has the buoyant. Subsequently, highly concentrated steam accumulates at the top of Vessel 1, then propagates through the top of the IP to Vessel 2 driven by buoyancy and diffusion. As a result, the steam molar fraction steeply decreases in the lower region of Vessel 1 without accumulating.

The comparisons between calculations and experiments indicate in Vessel 1 a reasonable prediction of the steam molar fraction above the elevation of steam plume injection (i.e., from 1.813 *m* up to 8.0 *m* elevations). In the region below (i.e., below 1.813 *m*) the calculated steam molar is higher than the experiment. We can explain the calculations of over-predictions from two different perspectives.

From a phenomenological perspective, the over-prediction of steam molar fraction with the calculations can be due to a significant mixing in the lower region of Vessel 1 that hinders the formation of a stable steam/air stratification front. In other words, the gas mixing seems to be created by the turbulent mixing compared to the experimental results. Besides, with respect to the other phenomenological perspective higher mass diffusivity could be one of the reasons.

From a numerical perspective, according to the 'mesh dependency' the mesh density of the bottom region of the vessel can be attributed to one of the reasons for the over-prediction. Regarding this point of view, further work with even more refined mesh would be needed.

Moreover, the low steam concentration in the experiments can also be affected by spurious condensations in the lower region of Vessel 1 due to the heat transfer to Vessel 3 which is at room temperature. Meanwhile, the experimental results show that the steam concentration is more fluctuating over the time with the height oscillating trajectory of the injected fluid plume. Fig. 7 was provided to see the order of magnitude of oscillating flow pattern according to the time. Experimental data were modified with Bézier curve [24], and the definition of the normalization is as follows (14).

$$\text{Normalized steam molar fraction} = \frac{x - x_{\min}}{x_{\max} - x_{\min}}, \ \text{Normalized temperature} = \frac{T - T_{\min}}{T_{\max} - T_{\min}} \tag{14}$$

It should be pointed out that the repeatability of oscillating patterns was observed twice in the same test (Test 16.1 and Test 16.2) [23]. Additionally, similar observations were made during the SETH Test 9 experiment [14].

Although this oscillating pattern is not evident in the calculations, the velocity vector of Vessel 1 in Fig. 8 suggests its possible influence. Fig. 8 illustrates velocity vectors at approximately 800 *s*, 2400 *s* and 3200 *s* in Vessel 1. At the initial time (t = 800 s), the flow orientation is upward toward the top of the vessel, but it gradually shifts towards the IP side of the vessel due to a weakening of the buoyancy force.

However, the large single anti-clockwise circulation has appeared in the top of the vessel as increasing the time (2400 *s* and 3200 *s*) since the angle of the injected fluid decreased owing to the reducing buoyancy force. The buoyancy force of the injected steam has been weakened due to filling a large amount of steam in the ambient initially with only air as shown in Fig. 9. The reason for the oscillation pattern with a steam molar fraction over the elevation can be due to the anti-clockwise circulation flow pattern in the upper region of the vessel. It seems that this crossed stream flow based on the centerline makes the zigzag measurement of the steam molar fraction.

Figure 10 shows contour fields together with the measured value of steam molar fraction with Vessel 1, Vessel 2, and IP.

In case of Vessel 2, it can be observed that the trend of steam molar fraction according to the height is similar to that of Vessel 1 as shown in Fig. 10. The inflowing fluid from IP flows upward and release up to the upper region of Vessel 2. While, in the lower region of Vessel 2 the values of the steam molar fraction indicate close to 0 for all the time steps. In other words, it seems effective stratification in Vessel 2 owing to low velocity of the highly concentrated steam flowing from IP. The calculations were reasonably predicted and quite comparable with the experimental results.

There exists a counter current flow in the IP. In the upper part of the IP, the high concentration steam flows into the Vessel 2 while in the lower part of the IP, the low concentration steam flows into Vessel 1, and is directed to the bottom of Vessel 1 with very low velocity. The flow with a low steam concentration could impact the stratification break at the bottom of Vessel 1, resulting in chaotic behavior in the steam molar fraction. This is illustrated by the white arrow near the IP of Vessel 1 in Fig. 10.

The evolution of steam molar fraction in the PANDA multi-compartment configuration can be summarized as follows: in Vessel 1 there is the combined effect of flow created by the injected plume from the wall nozzle and the flow through the IP which is located on the opposite side of the plume injection nozzle; in Vessel 2, the flow patterns are driven only by the flow through the IP. Therefore, the overall flow pattern evolution has a more complex behavior in Vessel 1 with respect to Vessel 2.

IV.D. Gas-mixture temperature distribution

Figure 11 indicates the comparison between experiments and calculations for the gas mixture temperature according to the Vessel 1 height and radial distance at selected times. In Fig. 11 (a), for both experiment and calculation results, the temperature increased until the height of the lower bound for IP, and the peak temperature could be observed between 2 *m* and 4 *m* elevations. The profiles with the temperature peaks at these elevations are since the jet flow exit elevation is at about 1.8 *m*. It should be noted that the height of the peak temperature decreased as increasing the time steps. This is caused the buoyancy force getting weaker according to the time likewise that of steam molar fraction as shown in Fig. 9. Above the IP (e.g. above 5 *m*), the temperature remains relatively constant.

One of the prominent observations, it is shown that the noticeable difference in the distribution of steam molar fraction and temperature over time. Specifically, the distribution of steam molar fraction exhibited significant variance with respect to the height of the vessel over time, whereas the temperature remained constant over time. Based on this finding, we concluded that there is a notable deviation in the magnitude of turbulent diffusivity between the steam molar fraction and temperature.

It should be noted that the calculated temperature is in general higher than that of experimental results. The maximum temperature difference was about 3°C, which corresponds to a maximum relative difference of about 2.7 %.

The over-prediction of the gas mixture temperature at all elevations can be attributed to two factors: temperature measurement and phenomenological effects. Firstly, the temperature measurement errors range from approximately 0.7 °C to 1.16 °C, which is within the tolerance of a K-type thermocouple [22]. Considering these thermocouple errors, the maximum temperature over-prediction of about 3 °C could be partially explained within the range of thermocouple error. Secondly, another contributing factor could be a combination of dynamic effects, including turbulent mixing, gas thermal radiation, heat exchange with walls and gases etc. These dynamic effects can contribute to discrepancies between predicted and observed temperatures.

The over-prediction of the gas mixture temperature cannot solely be attributed to the single effect from the interaction between the gas mixture and flow behavior. The variation in deviation between compartments can be attributed to various influences. This demonstrates the need for variable effect testing and validation confirmation of modelling.

In Fig. 11 (b), the temperature distribution was observed over the transverse direction at each time step in Vessel 1. The location showing the maximum temperature moved to the right side of the Vessel 1. It is due to the buoyancy force of the plume becomes a decrease as it fills with a large of amount of steam in Vessel 1. As discussed above, the values of temperature still have a discrepancy of about 2 °C.

Figure 12 indicates the temperature distribution in Vessel 2 and IP according to height. The range of temperature of experiments through the elevation of Vessel 2 is about from 104 °C to 108 °C (Fig. 12 (a)). The maximum temperature where can be found in the upper region of Vessel 2 seems to have decreased more than those of Vessel 1 with same as the initial condition like with 108 °C. Obviously, this may be due to the venting in the upper part of the vessel. According to the result of the comparison of the experiments and calculation, the maximum relative difference between both cases is about 2 %. Meanwhile, in case of the IP temperature, the maximum relative difference is about 3.7 % as shown as Fig. 12 (b). The reason why the relative difference is larger than Vessel 2 is due to the heat loss. This heat loss is caused by a larger surface to volume ratio and thinner walls than the rest of the vessels.

IV.E. Analysis of turbulent mass diffusivity

As demonstrated in the preceding section, it could be figured out that there has been an apparently different behavior of steam molar fraction and temperature as demonstrated by the experiments in Vessel 1. To obtain a clear comparison with steam molar fraction (Steam MF) and temperature, it is shown that the normalization with steam molar fraction and temperature according to the height has been plotted in Fig. 13 with the results of experiments and calculations. The experimental data have been modified with Bézier curve [24] and the definition of the normalization is given in Eq. (14).

Analyzing the comparison between steam molar fraction and temperature distributions, there are two remarkable observations. In the case of the experiments, it can be found that the peak value pattern appeared in the middle of the vessel only in the temperature behavior but not in the steam molar fraction. While, in the case of the calculation, the peak value pattern can be found in both parameters. It means that the behavior of mass and thermal diffusions should be different. In addition, it would be analyzed that the mass diffusion is well dispersed vertically more than thermal diffusion. It can be judged that it should be treated as corrected with thermal and mass diffusion in the calculation.

Through a perspective of the turbulent mass diffusivity (D_t), it has deeply related to the turbulent Schmidt number (Sc_t). Thus, it was performed to simulate varying the Sc_t with reducing the D_t (as resulting the Sc_t would be increased.). The reason why the D_t should be decreased is caused by over-predicted with the results of the comparison. In general, the value of Sc_t could be varied from 0.2 to 1.7 under condition of the turbulent flow phenomena with numerical analytical studies [25-28]. In this case, Sc_t was chosen with 1.0 to figure out the impact of Sc_t into the behaviors of steam molar fraction and temperature in Fig. 14.

Figure 14 (a) shows the comparison of the steam molar fraction between experiments and calculations which were resulted by $Sc_t = 0.9$ and 1.0 at $t = 2400$ s as a representative case. The value of $Sc_t = 1.0$ where is the peak steam molar fraction in the middle of the vessel has narrower than that of $Sc_t = 0.9$. Besides, the steam molar fraction indicates a bit smaller than the results of $Sc_t = 0.9$ in the lower of the vessel. In other words, the results of the lower Sc_t seems to close value with experimental results.

As can be seen from Fig. 14 (a), the temperature distribution has changed slightly, particularly in the middle and bottom of the vessel. This is caused by the steam distribution.

To sum up with this comparison, the turbulent mass diffusivity may be associated with the behavior of the steam molar fraction and temperature along with the mesh sensitivity. Thus, it could be known that there is needed to be implemented how to prove and improve analysis of these model as simulating further cases.

V. CONCLUSIONS

In this study, we conducted an analysis of experiment SETH Test 16 with containmentFOAM CFD, which is based on OpenFOAM® (currently v6) and is developed further for the analyses of nuclear power plant containment phenomena.

The experiment SETH Test 16 was carried out in the large-scale-multi-compartment PANDA facility as part of the OECD/NEA SETH project. It can be addressed "basic phenomena" in the containment, focusing on the steam and air mixture with plumes and jets, postulated to be released in a dry containment under a design basic accident like LOCA. The SETH PANDA experiments were defined (*i.e.* test procedures, test initial and boundary conditions, instrumentation) in such way to enhance their suitability for the assessment and validation of CFD codes. The phenomena of interest for the analyses in Test 16 are: the evolution of plume pattern in an environment with variance of buoyancy during the experiment, air-steam transport in a multi-compartment containment, mixing and stratification, etc.

We have used the k-ω SST turbulent model including buoyancy turbulence production and dissipation. We have performed sensitivity studies for turbulent mass diffusivity and mesh studies. In particular, we have improved the mesh resolution in the middle of the region of PANDA Vessel 1 where the experimental phenomena appear to be more complex.

The variables which have been compared (between computational analyses and experiments) are the evolution of gas-mixture temperature and steam molar fraction over the height of the Vessel 1 and Vessel 2 and interconnecting pipe and radial distances. Based on the results of experiments and calculations, it has been determined that the area can be divided into three regions: the upper region dominated by high momentum and turbulence mixing, the middle region where complications arise from the injected steam and induced flow from the IP, and the bottom region characterized by low momentum.

It can be concluded that the computational analyses of Test 16 are in reasonable agreement with the experimental results in most of the vessel regions. The gas mixture temperature is over-predicted about 2 %, which might be caused by a tolerance of the thermocouples and other dynamic effects.

An over-prediction of steam molar fraction is observed in the lower region of Vessel 1 (*i.e.* below the elevation of 1.8 *m* where is the level of the steam injection nozzle). The over-prediction can be caused by three reasons namely: higher turbulent mass diffusivity in the physical model than in the experiment; mesh resolution in the middle and bottom region of Vessel 1, *i.e.* where the steam-air stratification interface is observed in the experiment, and some spurious condensation taking place in the bottom of Vessel 1 (in the simulation uniform heat losses were assumed in Vessel 1).

As future studies we will analyze other SETH PANDA experiments, where the jet/plumes have different momentum and also configurations where the jet/plumes exit are at higher elevations, *e.g.* above the elevation of the IP. The foreseen analyses should provide further insight on the mesh and physical models needs to analyze basic phenomena such as large-scale plume/jets with safety relevance, in a containment, using containmentFOAM.

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REFERENCES

1. B.R. Sehgal, *Nuclear Safety in Light Water Reactors*, First Edition, Academic Press, ISBN 978-0-12-388446-6 (2012).
2. G. Yadigaroglu, M. Andreani, J. Dreier, P. Coddington, "Trends and needs in experimentation and numerical simulation for LWR safety," *Nucl. Eng. Des.* **221**, pp. 205-223 (2003).
3. M. Scheuerer *et al.*, "Evaluation of computational fluid dynamic methods for reactor safety analysis (ECORA)," *Nucl. Eng. Des.* **235** (2-4), pp. 359-368 (2005).
4. A. Bentaib *et al*., "Containment thermal hydraulic simulations with an LP-CFD approach: qualification matrix of the TONUS code," *Proceedings of the 14th International Conference on Nuclear Engineering (ICONE 14)*, Miami, FL, USA, 2006, pp. 489-499.
5. J. Malet, E. Porcheron, J. Vandel, "OECD International Standard Problem ISP-47 on containment thermal-hydraulics-Conclusions of the TOSQAN part," *Nucl. Eng. Des.* **240** (10), pp. 3209-3220 (2010).
6. M. Houkema, N.B. Siccama, S.W. Willemsen, E.M.J. Komen, "CFD analyses of steam and hydrogen distribution in a nuclear power plant," *Proceedings of the 10th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-10)*, Seoul, Korea 2003.
7. M. Houkema, N.B. Siccama, J.A. Lycklama à Nijeholt, E.M.J. Komen, "Validation of the CFX4 CFD code for containment thermal-hydraulics," *Nucl. Eng. Des.* **238**, pp. 590-599 (2008).
8. S. Kudriakov, F. Dabbene, E. Studer, A. Beccantini, J. P. Magnaud, H. Paillère, A. Bentaib, A. Bleyer, J. Malet, E. Porcheron, C. Caroli, "The TONUS CFD code for hydrogen risk analysis: Physical models, numerical schemes and validation matrix," *Nucl. Eng. Des.* **238** (3), pp. 551-565 (2008).
9. D. Paladino, M. Andreani, R. Zboray, and J. Dreier, "Toward a CFD-grade database addressing LWR containment phenomena," *Nucl. Eng. Des.* **253**, pp. 331-342 (2012).
10. F. de Cachard, D. Paladino, R. Zboray, M. Andreani, M. Huggenberger (Ed.), OECD-SETH Project Large-scale Experimental Investigation of Gas Mixing and Stratification in LWR Containments (2007) PSI Internal Report TM-42-07-04; ALPHA-07-18-A.
11. P. Royl, J.R. Travis, W. Breitung, "GASFLOW validation with steam/helium distribution in a multi room test facility (PANDA SETH Test 25)," *Proceeding of the Annual Meeting on nuclear Technology*, Hamburg, Germany, May 27–29 2008.
12. P. Royl, K. Jongtae, K. Sang-Baik, "GASFLOW Validation with PANDA Tests from the OECD SETH Benchmark covering steam/air and steam/helium/air mixtures," *Science and Technology of Nuclear Installations*, Article ID 759878 2009.
13. M. Andreani, D. Paladino, "Simulation of gas mixing and transport in a multi-compartment geometry using the GOTHIC containment code and relatively coarse meshes," *Nucl. Eng. Des.* **240** (6), pp. 1506-1527 (2010).
14. M. Andreani, D. Paladino, T. George, "Simulation of basic gas mixing tests with condensation in the PANDA facility using the GOTHIC code," *Nucl. Eng. Des.*, **240,** pp. 1528-1547 (2010).
15. A. Bentaib, A. Bleyer, S. Schwarz, "ASTEC validation on PANDA SETH," *Proceeding of the 13th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-13)*, Kanazawa City, Ishikawa Prefecture, Japan 2009.

16. M. Andreani, K. Haller, M. Heitsch, B.Hemström, I. Karppinen, J. Macek, J. Schmid, H. Paillere, I. Toth, "A benchmark exercise on the use of CFD codes for containment issues using best practice guidelines: A computational challenge," *Nucl. Eng. Des.* **238** (3), pp. 502-513 (2008).
17. S. Kelm, M. Kampili, X. Liu, A. George, D. Schumacher, C. Druska, S. Struth, A. Kuhr, L. Ramacher, H.J. Allelein, K.A. Prakash, G.V. Kumar, "The Tailored CFD Package 'containmentFOAM' for Analysis of Containment Atmosphere Mixing, H_2/CO Mitigation and Aerosal Transport," *Fluids* **6** (3) 100 (2021).
18. J. Dreier, M. Huggenberger, C. Aubert, T. Bandurski, O. Fischer, J. Healzer, S. Lomperski, H.-J. Strassberger, G. Varadi, G. Yadigaroglu, "The PANDA facility and first results," *Kerntechnik* **61,** pp. 214-222 (1996).
19. D. Paladino, R. Kapulla, S. Paranjape, S. Suter, C. Hug, M.S. Chae, M. Andreani, "PANDA Experimental Database and Further Needs for Containment Analyses," *Nucl. Eng. Des.*, **404** 112173 (2023).
20. A. Shabbir, D.B. Taulbee, "Evaluation of turbulence models for predicting buoyant flows". J. of Heat Transfer. **112** (4) pp. 945–951 (1990).
21. ANSYS Meshing User's Guide, Release 13.0 November 2010, 101-117.
22. OECD/SETH Large-scale investigation of gas mixing and stratification-PANDA Test Facility Description and Geometrical Data, Paul Scherrer Institut (PSI), Switzerland, p. 15, 21st January 2005.
23. O. Auban, R. Zboray, D. Paladino, "Investigation of large-scale gas mixing and stratification phenomena related to LWR containment studies in the PANDA facility," *Nucl. Eng. Des.* **237** (4), pp. 409-419 (2007).
24. Mortenson, E. Michael (1999). Mathematics for Computer Graphics Applications. Industrial Press Inc. p. 264.
25. A.N. Colli, J.M. Bisang, "A CFD study with analytical and experimental validation of laminar and turbulent mass-transfer in electrochemical reactors," *J. Electrochem. Soc.*, **165** (2) pp. E81-E88 (2018)
26. B. Lin, K. Shiono, Numerical modelling of solute transport in compound channel flows *J. Hydraul. Res.*, **33** (6) (1995), pp. 773-788
27. Y. Tominaga, T. Stathopoulos, "Turbulent Schmidt numbers for CFD analysis with various types of flow field," *Atmos. Environ.*, **41** (37) pp. 8091-8099 (2007).
28. C. Gualtieri, A. Angeloudis, F. Bombardelli, S. Jha, T. Stoesser, "On the values for the turbulent Schmidt number in environmental flows," *Fluids*, **2** (2) p. 17 (2017).