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\textbf{ABSTRACT}

This paper describes the computational fluid dynamics (CFD) analysis and validation works from the previous experimental study on the natural convection driven by outer surface cooling in the presence of density stratification consisting of air and helium (as a mimic gas of hydrogen). The experiment was conducted in the Containment InteGral effects Measurement Apparatus (CIGMA) facility at Japan Atomic Energy Agency (JAEA). CIGMA vessel is a large cylindrical stainless steel with an inner diameter of the main cylindrical part 2.5 m and an overall height of 11 m. The mass fraction proportion of helium in the whole vessel was 11\% and the helium molar fraction at the top vessel was 48\%. Two experiments were performed and the numerical simulation was carried out to analyze the detailed effect of the cooling region on the cooling process and the motion of the helium stratification layer. First test was named CCLP30 or case 1 and second test was named CCPL34 or case 2. The main difference between case 1 and case 2 was the cooling area of case 1 was narrower than case 2. In case 1, cooling area was only located at the one-fourth of outer vessel. Whereas, in case 2, cooling area was located at one-half of outer vessel. The temporal and spatial evolution of the helium concentration and the gas temperature inside the containment vessel was predicted and validated against the experimental data. The results indicated that the numerical predictions fairly agreed with the experimental data. However, the predicted erosion rate showed discrepancies compare with the experimental data. The relative errors time required for the complete dissolution of the helium gas were within 15\%. In addition, two stratification behaviors that depend on the cooling location were presented and discussed. The CFD simulation confirmed that an upper head cooling caused two counter-rotating vortices in the helium-rich zone. Meanwhile, the upper half body cooling caused two counter-rotating vortices in the helium-poor zone. These findings are important to understand the mechanism of the density stratification process driven by natural convection in the containment vessel.

1. Introduction

The presence of hydrogen within the containment vessel is one of the main contributors to the containment early failure during a severe nuclear accident. The hydrogen released to the containment-free volume could mix or accumulate at different parts of the containment building. The combustion would occur inside the containment if the composition of the hydrogen–steam–air mixture lay within a specific limit. Aftermath, hydrogen generation, and other phenomena leading to overpressurization could threaten the containment integrity. Accordingly, understanding hydrogen behavior is crucial for planning and implementing effective accident management measures.

Several experimental and numerical studies on the nuclear containment thermohydraulic had been extensively performed to gain knowledge on the hydrogen transport inside the containment vessel (Karwat et al., 1999) (Studer et al., 2007) (OECD/Nea, 2007) (Malet et al. 2010) (Freitag et al., 2016) (S Kelm et al. 2019) (Abe et al., 2015) (Abe et al., 2018) (Ma et al., 2018) (Liu et al., 2021). The thermal-hydraulic processes in the containment atmosphere, particularly the stratification and mixing phenomena, are primarily governed by the density differences in the atmosphere. Hence, different research facilities have studied several international projects related to hydrogen stratification and mixing driven by natural convection. The natural convection of air-helium (substitute of the air-hydrogen gas) experiment (NATHCO) in the framework OECD/NEA-SETH2 project was conducted (OECD/NEA/CSNI 2012) in the MISTRA facility (CEA, France). The
main objective was to study the effects of natural convection generated by the heating up of the middle and upper condensers on the behavior of the helium cloud. The NATHCO test gradually heated condensers ranging from 100 to 130 °C, installed near the vessel wall, to heat the nearby gas and induce buoyant flow in the stagnant atmosphere. As a result, the natural convection enhanced the mixing process characterized by the gradual erosion of the stratification layer from the top, increasing the layer thickness. In the NATCHO test, the vessel was only heated to obtain a single effect on mixing. Therefore, complex mixing which would occur with condensation during a cooling phase could be avoided. A similar test on natural convection of helium-air, namely the TH22 test, was conducted in the THAI facility (Becker, Germany) under the German national project THAI-III (Gupta et al., 2015). The top part of the vessel was cooled, and the lower part was heated by cooling and heating jacket. In the TH22 test (see Fig. 1), an injection of light gas into the upper plenum of the vessel formed a stable stratification. Later, the natural convection enhanced the mixing process which characterized by gradual erosion of the stratification layer from the bottom with decreasing the layer thickness.

Dry tests (steam was not considered) on NATCHO and TH22 showed how important the role of natural convection on the erosion of density stratification layer. However, no systematic investigation has focused on the difference in mixing modes by natural convection. Therefore (Abe et al., 2022), performed experimental series on the natural convection in the presence of density stratification consisting of a non-condensable gas mixture in the Containment InteGral effects Measurement Apparatus (CIGMA) facility at Japan Atomic Energy Agency (JAEA), Japan. The aim was to gain insights into the mixing mechanism of density stratification driven by outer surface cooling. They (Abe et al., 2022) concluded that the relative location between the outer surface cooling and stratification layer determines the stratification behavior. The stratification behavior was classified into two types: dissolution and breakup. The stratification dissolution occurred when the cooling region was narrower than the stratification layer thickness. It was characterized by expanding the stratified Helium gas layer to the lower part while decreasing the concentration. The stratification erosion occurred when the cooling region was wider than the stratification layer thickness. It was characterized by eroding the stratified helium gas layer from the bottom with decreasing the layer thickness. Even though the stratification dissolution and erosion could be classified based on the temporal and spatial profile of temperature and helium molar fraction, the detailed information on the three-dimensional flow dynamic inside the vessel could not be obtained due to the experimental limitations. In this regard, Computational Fluid Dynamics (CFD) is a handy tool for better understanding the turbulent transport and mixing of hydrogen and other gases in nuclear containment vessels.

We need to consider the computational cost and time when simulating a large-scale facility like a nuclear containment vessel. In this particular case, the most thorough approach for simulating buoyant turbulent flows is based on the Reynolds-Averaged Navier-Stokes (RANS) equations. However, the accuracy of the RANS simulations strongly depends on the computational settings (Wang et al., 2021). Previous studies had shown the important impact of the grid size, turbulence models, boundary conditions, and conjugate heat transfer model when simulating natural convection inside the containment vessel (Visser et al., 2012; S.; S Kelm et al. 2019; Hamdani et al., 2020; Vijaya Kumar et al., 2020; Ishigaki et al., 2021).

In the RANS model, the turbulent scalar fluxes are estimated by assuming the Standard Gradient Diffusion Hypothesis (SGDH) (Pope 2000) (Rossi and Iacarino 2009) (Gualtieri et al., 2017). The assumption of the SGDH requires the estimation of the turbulent Schmidt number, $Sc_t$ and turbulent Prandtl number, $Pr_t$. Additionally (Mohr-Bahar et al. 2012), found that the eddy diffusivity needed to be reduced by increasing $Sc_t$ with dependence on Richardson number to model the experimental data correctly. Our previous study (Abe et al., 2018, 2020) demonstrated that the dynamic $Sc_t$ model provided better agreements with the experimental data on the stratification breakup behavior by a vertical jet. Therefore, it is suggested to implement the dynamic $Sc_t$ in the RANS model to increase the numerical accuracy in modeling stratification and mixing phenomena driven by natural convection inside the containment vessel.

In the present study, we performed the unsteady RANS simulation with the conjugate heat transfer and dynamic turbulent Schmidt number model to simulate natural convection driven by outer surface cooling. The main objective is to understand the flow dynamics during the transient stratification and helium mixing process. The numerical simulation was carried out using the open-source CFD package OpenFOAM®. Recently OpenFOAM® has been widely used for CFD simulation on nuclear power system (He et al., 2021) (He et al., 2022) (Liu et al., 2021). The natural convection behaviors were analyzed and validated with the experimental data. Furthermore, binary gas helium-air mixing characteristics were evaluated based on helium gas concentration and its temperature distributions. In addition, the present numerical simulation was compared with the “containmentFoam” solver, which is currently developed at Forschungszentrum Jülich, Germany (Stephan Kelm et al., 2021) (Kampili et al., 2021a) (Vijaya Kumar et al., 2021). The “containmentFoam” solver comprises a complete multi-species transport solver and additional models for containment thermohydraulic in the frame of accident scenarios.

The outline of present study is as follows: section 2 describes the CIGMA experimental facility, measurement instrumentation, and experimental procedure on the natural convection at the CIGMA vessel. Section 3 introduces the numerical modelling, governing equations, computational mesh, and followed by initial and boundary conditions. Section 4 presents results and discussion, and finally concluding remarks is presented in section 5.

2. Natural convection experiments in the CIGMA vessel (CCPL30 and CCPL34 test)

2.1. CIGMA facility in JAEA

The outline of the CIGMA vessel and its instruments is shown in Fig. 2 and Table 1. CIGMA vessel is a large cylindrical stainless steel with an inner diameter of the main cylindrical part 2.5 m and an overall height of 11 m. The vessel’s volume is approximately 48 m³. The main characteristic of the CIGMA is the vessel wall equipped with an external cooling system, i.e., upper pool, middle jacket, and lower jacket. The radial gap between the outer wall and cooling jackets is 50 mm. The coolant medium is subcooled water, and it can be injected independently in three different cooling locations. The whole vessel is thermally isolated using rock-wool mats covered by reinforced wire mesh to avoid significant heat loss. The temperature and pressure boundary of the containment vessel can withstand up to 300 °C and 1.5 MPa. The test section of CIGMA has many thermocouples (TCs), i.e., 650 TCs and

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**Fig. 1.** Natural convection tests were conducted in the THAI facility.
The vessel wall is equipped with three independent cooling systems, i.e., one upper pool and two jackets over the height.

The natural convection inside the CIGMA vessel is mainly induced by outer surface cooling on the vessel wall. Fig. 3 shows the comparison of natural convection conducted in the THAI and CIGMA facility. Two experiments, i.e., CCPL30 (case 1) and CCPL34 (case 2) were carried out to study the effect of the cooling region on helium transport and mixing. TH22 is similar to the CCPL34 (case 2), where the cooling area is wider than the thickness of the helium stratification layer. In the CIGMA facility, the subcooled water is used as a cooling medium, and helium gas is adopted as a substitute hydrogen gas for safety reasons. Accordingly, it was confirmed that experiments on containment atmosphere flow dynamics using helium instead of hydrogen could provide meaningful data for identifying flow phenomena and code validation (Gupta et al., 2015).

The CIGMA vessel was preheated with superheated steam injection, and later steam was replaced with heated air after preheating process was completed. Then, the mixture of air helium gases was injected through a nozzle located at the upper vessel. Thus, the air/helium stratified conditions have been achieved inside the test vessel before injecting subcooled water in the upper pool and water jacket. A helium region occupies the region EL > 6 m, and in the transition region between 6 m < EL < 8 m, the gradient of helium molar fraction is steep. The description of each test is shown in Table 2.

The upper pool and middle jacket are used as a cooling method in CCPL30, whereas the upper pool, middle and lower jackets are used as a cooling method in CCPL34. Hence, the cooling region is narrower than the stratification layer thickness in CCPL30. While, in CCPL34, the cooling area is wider than the stratification layer thickness. Henceforth, the CCPL30 test is case 1, and CCPL34 is case 2.

### 3. CFD analysis method

CFD analysis was performed to reproduce the experimental results based on the experimental data on CCPL30 (case 1) and CCPL34 (case 2). The present simulation was carried out using conjugate heat transfer solvers “chtMultiRegionFoam” in OpenFOAM-6 and a tailored solver “containmentFoam” in OpenFOAM-6. Both solvers are based on unsteady Reynolds-averaged Navier-Stokes equations, total energy equation (non-unity Lewis number formulation), and transport equation for species mass fraction. uRANS model is selected because it does not require a high-resolution mesh compared to large eddy simulation (LES) and direct numerical simulation (DNS) model. Therefore, it is less computational expensive when simulating a long-time transient calculation of gas mixing and processes inside the containment vessel.

Turbulence modeling in “chtMultiRegionFoam” and “containmentFoam” is based on the two-equation eddy viscosity turbulence model. Based on the previous publications and validations (S Kelm et al., 2016) (Ishigaki et al., 2020) for a more detailed description of the CIGMA facility.

### 2.2. Natural convection in CIGMA facility

The size of the CIGMA vessel is large enough to establish stratification atmosphere conditions and a natural convection flow by water cooling at the wall’s outer surface. A similar TH22 test was performed in the CIGMA facility to investigate the mixing process of light gas induced by natural convection in a large cylindrical vessel. In the CIGMA facility, capillary tubes (CTs), i.e., 100 CTs to measure the temperature and gas concentration. The thermocouples are K-type, and they are arrayed like a grid. A thermocouple is used to measure both gas and wall temperature. The positions of the thermocouples and capillary tubes are indicated by small dots, as shown in Fig. 2.

**Fig. 2.** 2D cross-sectional view of CIGMA vessel and its sensor point location. The left figure is XZ-plane at Y = 0 m, and the right figure is XY-plane at Z = 5 m.

**Table 1**

<table>
<thead>
<tr>
<th>CIGMA vessel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1.5 MPa</td>
</tr>
<tr>
<td>Wall temperature</td>
<td>300 °C</td>
</tr>
<tr>
<td>Injection temperature</td>
<td>700 °C</td>
</tr>
<tr>
<td>Fluid medium</td>
<td>Air, steam, helium, water</td>
</tr>
<tr>
<td>Steam generator power</td>
<td>200 kW</td>
</tr>
<tr>
<td>Height</td>
<td>11.2 m</td>
</tr>
<tr>
<td>Diameter</td>
<td>2.5 m</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>25 mm</td>
</tr>
<tr>
<td>Volume</td>
<td>48 m³</td>
</tr>
<tr>
<td>External cooling system</td>
<td>Upper pool, middle jacket, lower jacket</td>
</tr>
<tr>
<td>Internal cooling system</td>
<td>Spray nozzle in the top vessel</td>
</tr>
</tbody>
</table>

**Fig. 3.** Comparison of natural convection tests on THAI and CIGMA facility.
2019) (A. Hamdani et al., 2019) (Vijaya Kumar et al., 2020) (Stephan Kelm et al., 2021). The baseline model was employed in the present simulation, including production and dissipation terms for buoyancy turbulence based on SGDH. In addition, k-ω SST turbulence model can be used at the low-Reynolds number model without the need for extra damping functions.

The low-Reynolds number model is mainly adopted when simulating a natural convection flow in the enclosed domain. A previous study on the natural convection flow in a square cavity by Henkes et al. (Henkes et al., 1991) showed that the low-Reynolds number models could predict reasonably close to the experiment. In contrast, the high-Reynolds number model overpredicted the wall-heat transfer and the wall-shear stress. The overprediction was mainly due to using the logarithmic wall function in the boundary layer. However, the wall functions were initially derived and experimentally verified for forced convection flows. Therefore, the wall functions cannot be used in natural convection flows as they will incur significant errors in predicting wall heat flux and shear stress values (Vijaya Kumar et al., 2020).

The multi-species transport in both solvers is based on the Wilke mixture for transport properties. Transport properties and specific heat capacity are temperature dependent. The binary diffusion coefficient is mixture for transport properties. Transport properties and specific heat capacity are temperature dependent. The multi-species transport in both solvers is based on the Wilke mixture for transport properties. Transport properties and specific heat capacity are temperature dependent. The binary diffusion coefficient is described by polynomials of 2nd order, fitted to the JANAF table data (VDI heat atlas data, 2010).

The transport equation for mass fraction of species \( Y_k \) can be written as:

\[
\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot (\mathbf{D} \nabla Y_k) + \sum_{j=1}^{N} \frac{\partial}{\partial x_j} \left( \rho \frac{D_{ij}}{M_j} \frac{\partial Y_k}{\partial x_j} \right)
\]

Where \( \rho \) is density, \( \mathbf{u} \) is velocity vector, \( D_{ij} \) is the molecular diffusivity of the mass fraction of species \( k \) in the mixture.

### Table 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>contentamoinFoam</th>
<th>chtMultiRegionFoam</th>
</tr>
</thead>
<tbody>
<tr>
<td>OpenFOAM® version</td>
<td>OpenFOAM-6</td>
<td>OpenFOAM-9</td>
</tr>
<tr>
<td>Turbulent Schmidt number (Sc)</td>
<td>Constant Sc = 1</td>
<td>Dynamic Sc as function of local Richardson number</td>
</tr>
<tr>
<td>Specific heat capacity (cp)</td>
<td>temperature dependent</td>
<td>temperature dependent</td>
</tr>
<tr>
<td>Dynamic viscosity (( \mu ))</td>
<td>polynomials of 4th order, fitted to the NIST Chemistry Webbook and VDI heat data table</td>
<td>polynomials of 4th order, fitted to the NIST Chemistry Webbook and the JANAF table</td>
</tr>
<tr>
<td>Thermal conductivity (( \lambda ))</td>
<td>polynomials of 2nd order, which were fitted to the NIST Chemistry Webbook data</td>
<td>Eucken correlation</td>
</tr>
</tbody>
</table>

### 3.1. Governing equations

In the compressible flows, density variations due to temperature or pressure variations can be significant, and consequently, these enter into the conservation equations when considering their averaged forms. The Reynolds-averaged equations for continuity, momentum, mass transport, and energy are described below. The bracket \( \langle \ \rangle \) denotes Reynolds-averaging operation, and the angle bracket \( < > \) is expressed the Favre density averaging.

#### 3.1.1. Continuity equation

The continuity equation for a compressible fluid under unsteady conditions is written as:

\[
\frac{\partial (\rho \mathbf{u}_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_i \mathbf{u}_i) = 0
\]

(1)

Where \( \rho \) is density, \( \mathbf{u}_i \) denote the distance and flow velocity in the \( i \)-direction. No additional source term in Eq. (1).

#### 3.1.2. Momentum equation

The momentum equation can be written as:

\[
\frac{\partial (\rho \mathbf{u}_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_i \mathbf{u}_i) = \nabla \cdot \mathbf{S} + \rho \mathbf{F}_i
\]

(2)

Where \( \rho \) is pressure, \( \delta_{ij} \) is Knocker delta, and \( \mathbf{u}_i \) \( \mathbf{u}_j \) denote the velocity fluctuation in the \( i \)- and \( j \)-direction.

#### 3.1.3. Transport equation for species (\( k \))

The composition of a mixture is usually represented in terms of the constituent mass fractions. The mass fraction of species \( k \), \( Y_k \) is a ratio of the mass of species \( k \) and the total mixture mass:

\[
Y_k = \frac{\rho_k}{\rho_{\text{total}}}
\]

(3)

where \( k = 1, 2, \ldots, N \) and \( N \) is the number of total species. In the present study, the working gas is binary mixing of helium and air. Therefore, the sum of helium and air mass fractions must be unity:

\[
\sum_{k=1}^{N} Y_k = \sum_{k=1}^{N} \frac{\rho_k}{\rho_{\text{total}}} = 1
\]

(4)

The gas is to be assumed as a perfect gas, meaning that pressure \( p \), density \( \rho \), and temperature \( T \) are related using the ideal gas equation of state

\[
p = \rho R T \sum_{k=1}^{N} Y_k M_k
\]

(5)

\( R \) is the universal gas constant, and \( M_k \) is the molar mass of the \( k \)-th species.

The transport equation for \( Y_k \) can be written as:

\[
\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot \left( \mathbf{D} \nabla Y_k \right) + \sum_{j=1}^{N} \frac{\partial}{\partial x_j} \left( \rho \frac{D_{ij}}{M_j} \frac{\partial Y_k}{\partial x_j} \right)
\]

(6)

\( Y_k \) is the mass fraction of gas species \( k \) and \( D_k \) is the molecular diffusivity of the mass fraction of species \( k \) in the mixture.

#### 3.1.4. Energy equation

The energy equation is written in terms of the mixture enthalpy. Thus, the energy flux is the sum of a heat diffusion by Fourier’s law and species diffusion given by Fick’s law.
3.2. Turbulence modeling

In the present model, the turbulent Prandtl number $Pr_t$ is assumed to be equal to turbulent Schmidt number $Sc_t$. Consequently, $D_t = u_t$ and the second term in the RHS Eq. (10) vanishes, only the first term or laminar part remains.

3.2. Turbulence modeling

The $k$-$\omega$ shear stress transport (SST) model of Menter (2009) combines the $k$-$\varepsilon$ and $k$-$\omega$ model. This model activates the standard $k$-$\varepsilon$ model in the fully turbulent region far from the wall and the $k$-$\omega$ in the near-wall region. The implementation of the $k$-$\omega$ SST model in OpenFOAM® for compressible flow is given by

$$\frac{\partial(p\rho k)}{\partial t} + \frac{\partial(p\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \nu_t \frac{\partial k}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \frac{\sigma_k}{\omega} \frac{\partial \omega}{\partial x_i} \right] + G_k + \frac{\partial}{\partial x_i} \left[ \frac{\sigma_k}{\omega} \frac{\partial \omega}{\partial x_i} \right] + G_w$$

(13)

$$\frac{\partial(p\rho \omega)}{\partial t} + \frac{\partial(p\rho u_i \omega)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \nu_t \frac{\partial \omega}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] + \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] + G_k$$

(14)

Where $\nu_t$, $\alpha_t$, $D_t$ and $\delta_t$ are turbulent/eddy viscosity, turbulent thermal diffusivity, and turbulent mass diffusivity.

$$D_t = \frac{\nu_t}{Sc_t}$$

(11)

$$\alpha_t = \frac{\nu_t}{Pr_t}$$

(12)

Turbulent/eddy viscosity $\nu_t$ is calculated with the formulation according to $k$-$\omega$ SST turbulence model as described in the following section. In the present model, the turbulent Prandtl number $Pr_t$ was assumed to be equal to turbulent Schmidt number $Sc_t$. Consequently, $D_t = u_t$ and the second term in the RHS Eq. (10) vanishes, only the first term or laminar part remains.

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(13)

$$\frac{\partial(p\rho \omega)}{\partial t} + \frac{\partial(p\rho u_i \omega)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \nu_t \frac{\partial \omega}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] + \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] - \frac{\partial}{\partial x_i} \left[ \frac{\sigma_\omega}{\nu_t} \frac{\partial \nu_t}{\partial x_i} \right] + G_k$$

(14)

$\rho$ is density, $\nu_t = \mu_t/\rho$ is the turbulent/eddy kinematic viscosity, and it is calculated as follow

$$\nu_t = \frac{\alpha_k}{\max(\alpha_k \omega, SF_C)}; \quad S = \sqrt{2S^2 + S^2}$$

(15)

$$P_t = \frac{\partial u_i}{\partial x_i}; \quad \alpha_t = \min(P_t, 10k_B^2 \rho \omega)$$

(16)

$$\tau_0 = \nu_t \left( 2S^2 - \frac{\partial u_i}{\partial x_i} \right) - \frac{2}{3} \rhoWalk through the steps of the derivation and the application of the $k$-$\omega$ SST turbulence model in OpenFOAM® for compressible flow.
From the dynamic viscosity \( \mu \), the specific gas constant \( R \), and the specific heat capacity at constant volume \( C_v \), the thermal conductivity \( \lambda \) is determined using modified Eucken correlation (Poling, Prausnitz, and O'Connell 2001).

\[
\frac{\lambda M}{\mu C_v} = 1.32 + \frac{1.77}{R}
\]  
(30)

The transport properties of the gas mixture \( \eta_m \), i.e., dynamic viscosity and thermal conductivity, are defined using Wilke’s mixture model (Wilke 1950), which is based on kinetic gas theory.

\[
\eta_m = \sum_{i=1}^{N} \eta_i \left( 1 + \frac{1}{R_i} \right)^{\phi_{ij}}
\]  
(31)

Where \( \eta_i \) is the mole fraction of a component in the mixture and \( \phi_{ij} \) is the dimensionless constant defined as follow

\[
\phi_{ij} = \left[ \left( 1 + \frac{\nu_i}{\nu_j} \right)^{\frac{1}{2}} \right] \left[ \frac{4 \nu_i}{(4\sqrt{2})} \right]^{\frac{1}{2}}
\]  
(32)

The specific enthalpy \( h_m \) and heat capacity \( c_{p,m} \) is obtained with a mass-weighted summation of the species mass fraction \( Y_i \), i.e.,

\[
h_m = \sum Y_i h_i \quad \text{and} \quad c_{p,m} = \sum Y_i c_{p,i}
\]  
(33)

The binary diffusion coefficient of the species pair A-B is calculated according to (Fuller et al. 1969).

\[
D_{AB} = \frac{10^{-3}T^{7/6} (1/M_A + 1/M_B)^{1/2}}{p \left( \left( \sum \nu_i \right)^{1/2} + \left( \sum \nu_j \right)^{1/2} \right)^{2}}
\]  
(34)

Where \( \nu_i \) is diffusion volume. Diffusion volume for air and helium gas is given in Table 4.

### 3.4. Dynamic modeling for the turbulent schmidt number \( Sc_t \)

The turbulent Schmidt number \( Sc_t \) is generally set to the constant value of less than unity. Some ocean and atmosphere engineering researchers suggest that \( Sc_t \) increases with the increasing stratification strength. The stratification strength is characterized by the gradient Richardson number \( Ri_t \).

\[
Ri_t = \frac{N^2}{S^2}
\]  
(35)

Where \( N \) is stratification/Brunt–Väisälä frequency and \( S \) is the mean shear rate. \( N \) and \( S \) are defined as follows

\[
N = \sqrt{-\frac{g}{\rho} \frac{\partial \rho}{\partial z}} \quad S = \sqrt{\frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)}
\]  
(36)

The coefficient \( - (g/\rho) \partial \rho/\partial z \) is either positive or negative when the fluid with the greater densities is below the lesser densities \( (d\rho/dz < 0) \), accordingly the \( N \) is positive (stable stratified). The present model applied formulation proposed by (Venayagamoorthy and Stretch 2010) for \( Sc_t \) as follows:

\[
Sc_t = Sc_{t0} \exp \left( - \frac{Ri_t}{Sc_{t0}C_1 + \frac{Ri_t}{C_2}} \right)
\]  
(37)

Where \( Sc_{t0} \) is the turbulent Schmidt number under the neutral condition usually set to less than unity. Here, \( C_1 = 1/3 \), \( C_2 = 1/4 \) and \( Sc_{t0} = 0.85 \). The Venayagamoorthy and Stretch model is used in the present model because the functions shown agreement with experimental data and numerical results fairly well (Li 2018).

In our previous study, the formulation of Venayagamoorthy and Stretch with the threshold value of \( 20 \) was applied on the MISTRA HM1-1 test (Abe et al., 2018) and VIMES test (Abe et al., 2020). The numerical results predicted well the breakup behavior of the density stratification. Therefore, the same threshold value on the dynamic modeling of \( Sc_t \) is used in the present study, and it is defined as follows

\[
Sc_t = \max \left[ Sc_{t0,\min} \left( Sc_{t0} \exp \left( - \frac{Ri_t}{Sc_{t0}C_1 + \frac{Ri_t}{C_2}} \right) \right) 20 \right]
\]  
(38)

### 3.5. Computational mesh

3D CAD modeling software ANSYS® SpaceClaim was used to create a 3D CIGMA vessel. Later, the 3D CAD model was imported to the ANSYS® meshing tool for creating a high-quality hexahedral mesh. However, the ANSYS® mesh needs to be converted to the format that OpenFOAM® uses. Hence, the meshes were converted into OpenFOAM® mesh format using mesh conversion utilities.

Fig. 4 shows that the vessel wall and its flange are modeled as solid domain, and the mixture air-helium is modeled as the fluid domain. The
solid domain is colored in grey, and the fluid domain is colored in yellow. The computational domains were completely discretized by hexahedral mesh. However, the internal structures such as an injection nozzle and rods supporting instrumentation were not modeled due to complex geometry.

Two different computational meshes were constructed to study the effect of grid resolution on the wall. All meshes were only built for low Reynolds number turbulence models ($y^+ < 1$), therefore the boundary layer close to the wall was fully resolved. The grid convergence for a low Reynolds number was performed on two grids by keeping the near-wall resolution to $y^+ < 1$. The radial and vertical sizes of the solid cell region for both base and fine mesh are 5 mm and 75 mm. A separate test was carried out to determine how many layers were needed in the solid region. It was confirmed that a radial size equal to 5 mm could accurately predict the heat conduction in the solid region/wall. The detail of each grid model is presented in Fig. 5 and Table 5.

### 3.6. Initial and boundary conditions

The fluid inside the containment vessel is air and helium, and they are initially assumed to be quiescent. The initial distributions of the temperature and helium molar fraction of case 1 and case 2 are depicted in Figs. 6 and 7, respectively. The initial value of both temperature and helium molar fractions is derived from the experimental data interpolation. It should be noted that the internal structures such as an injection nozzle and rods supporting instrumentation were not modeled in the present simulation.

The initial internal fluid and solid temperature are assumed to be equal, as shown in Fig. 6b–c. All contour fields in the present paper are plotted using a python package named turbulucid developed by T. Mukha (2018). The initial fluid and solid temperature are given by temperature sensors located 0.9 m away from the center axis. The molar fraction data are provided by concentration sensors located at the center axis. The profile depended only on the height, and it was reproducible from test to test. Hence, radial distributions of temperature and helium molar fractions were not observed in Fig. 6b–c and Fig. 7b–c. Moreover, as shown in Figs. 6a and 7a, the initial distribution of case 1 is similar to case 2.

Fig. 8 shows the wall temperature boundary conditions at the outer wall of the vessel. The boundary condition at the wall was divided into 18 faces, and it was distinguished by a different color, as shown in Fig. 8a. The temperature value on the outer walls was specified in the present CFD simulation, and they were the average temperature of the outer wall of experimental data. Each face has a time-dependent temperature during the transient simulation, as shown in Fig. 8b for case 1 and 8c for case 2. Furthermore, the experimental data showed that the temperature on the flanges differs from the main vessel wall since a cooling jacket did not cover the flanges. Thus, temperature boundary conditions at the surface of the flanges must also be prescribed explicitly during the transient simulation. The actual number of primary flanges in the CIGMA facility is 36 flanges. However, in the present model domain, the total number of flanges was only 32. The rest of the flanges, which are located at elevation 0.9 m, were not discretized due to technical difficulty during the meshing process.

Fig. 8b–c indicate that the outer wall temperature at the cooled region decreases rapidly after the water-cooling injection, i.e., $t = 0$ s. The temperature at the noncooled region also decreases due to heat loss. However, the temperature gradient at the noncooled region is not steep compared to the cooled region. The slight decrease in temperature proves that the heat loss at the noncooled region is relatively small.

At the interface between solid and fluid regions, an appropriate boundary condition is required to couple the energy equations in both regions. In order to couple heat transfer simulations on their interface, Dirichlet–Neumann coupling was used in the simulation. To derive the equations for this boundary condition, consider the two cells at either side of the interface, such as in Fig. 9. $T_{cf}$ and $T_{cs}$ are the temperatures at the cell center of fluid and solid. $T_f$ and $T_s$ are the temperatures on the patch for the fluid and solid, and $T_{int}$ is the temperature at the interface. $q_f$ is the heat flux out of the fluid region, and $q_s$ is the heat flux that enters the solid region. In the Dirichlet–Neumann coupling, the continuity of the temperature and the heat flux on the fluid-solid interface is assumed, therefore by simplifying with $T_f - T_s = T_{int}$, the value of $T_{int}$ and heat flux $q$ at the interface can be calculated as follow

\[
q = \lambda_f \Delta_x (T_{cf} - T_{cs}) = \lambda_s \Delta_x (T_f - T_s)
\]

(39)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Base mesh</th>
<th>Fine mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of fluid cells</td>
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<td>1,676,300</td>
</tr>
<tr>
<td>Number of solid cells</td>
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<td>828,868</td>
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<tr>
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<tr>
<td>Wall-adjacent cell $y^+$</td>
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</tr>
</tbody>
</table>

---

**Table 5**

**Computational meshes.**

---

**Fig. 6.** The initial condition of the temperature.

---

**Fig. 5.** The detail of near-wall mesh resolution.
where $\Delta_f = 1/\delta_f$ and $\Delta_s = 1/\delta_s$. $\delta_f$ and $\delta_s$ are the distance between the cell centers and wall interfaces of the solid and fluid domain, $\lambda_f$ and $\lambda_s$ are the thermal conductivity of the fluid and solid, respectively.

### 3.7 Numerical methods

The numerical discretization of the governing equations on "chtMultiRegionFoam" and "containmentFoam" is second-order accurate in time and space. The gradient terms were discretized by the central differencing scheme, and the divergence terms were discretized by the linear scheme with the total variation diminishing (TVD) scheme. The implicit backward Euler scheme was used for temporal discretization. The coupling between velocity and pressure fields was solved using the PIMPLE algorithm, which combines the PISO (pressure implicit with splitting of operator) and SIMPLE (semi-implicit method for pressure linked equations) algorithms. The stabilized preconditioned bi-conjugate gradient (PBiCGStab) method is used for solving all the discretized equations except the pressure correction equation, which is solved using preconditioned conjugate gradient (PCG) method. The convergence criteria are set to be $10^{-6}$. The time step was adjusted during the transient simulations. The maximum Courant number in the fluid region was less than 0.5, and the maximum diffusion number in the solid region was less than 1.

### 4. Results and discussion

#### 4.1 Mesh convergence study

Two model domains were tested on case 2 to study the mesh convergence, i.e., base and fine mesh. The effect of mesh resolution on the helium molar fraction and temperature along the vertical axis are depicted in Figs. 10 and 11. The simulation on the fine mesh was only performed for 1500 s to save computational time. Then each result on each mesh was compared with the experimental data.

Figs. 10 and 11 show that both base and fine mesh predict the general trend in helium molar fraction and temperature. However, the comparison results between the base and fine mesh show a slight discrepancy. The relative error between the base and fine mesh is less than 0.5%. Therefore, the results obtained with the base mesh will be discussed in the following chapters to reduce numerical costs.

#### 4.2 The effect of outer cooling on pressure

Figs. 12 and 13 depict the time history of pressure in both case 1 and case 2. The numerical simulation was carried out using...
Fig. 10. Helium molar fraction distribution along the center vertical axis in case 2 at t = 100 s and t = 1500 s.

Fig. 11. Temperature distribution along the center vertical axis in case 2 at t = 100 s and t = 1500 s.

“chtMultiRegionFoam” and “containmentFoam” solver. The Sc number is dynamically changed in the “chtMultiRegionFoam,” and constant Sc = 1 is set in the “containmentFoam”.

The experimental results are indicated by a black dashed line. The numerical result using “chtMultiRegionFoam” is indicated by a solid red line, and “containmentFoam” is indicated by a solid blue line. The pressure history using “chtMultiRegionFoam” and “containmentFoam” agrees well on cases 1 and 2. All results show a gradual decrease in pressure due to outer cooling. The temporal pressure profile in case 2 is faster than in case 1 since the cooling area is wider. Although the simulation results show the same trend as the experimental data, we can observe that the depressurization rate is faster than the experimental data. The discrepancy might be due to the effect of solid internal structure, i.e., injection nozzle, on the overall heat transfer inside the vessel was not considered in the present simulation.

4.3. Helium molar gas and fluid temperature distributions

The temporal profile of helium molar fraction and temperature along the centerline axis in case 1 and case 2 are depicted in Figs. 14, 15, 17 and 18, respectively. The molar fraction data are provided by concentration sensors located at the center axis. The temperature data are provided by the thermocouples located at 0.9 m away from the center axis. They are plotted every 1000 s to see the evolution of helium molar fraction and gas temperature inside the vessel.

Fig. 14 shows the vertical helium molar fraction of case 1 from t = 0 s–5000 s. Numerical results show fair agreement with the experimental data. The helium-rich layer is expanding to the lower part while decreasing the concentration. At t = 1000 s to t = 4000 s, we can see that the numerical results show a faster erosion rate than the experimental data. One possible reason to explain the discrepancy between numerical and experimental data is that numerical simulations do not match experiment conditions in terms of initial and boundary conditions. The initial condition was assumed to be quiescent, which means that the initial velocity was set to zero in the present analysis. Nevertheless, it was probable that a weak natural convection flow occurred at the initiation of the cooling, and the initial velocity was expected to include uncertainty. Also, the present model did not consider the internal structure inside the actual CIGMA vessel, i.e., the nozzle. Therefore, the residual heat of the CIGMA structure during the preheating may affect the flow pattern. Afterward, at t = 5000 s, the numerical results agree well with the experimental data. A visible discrepancy between “chtMultiRegionFoam” and “containmentFoam” is observed at t = 3000 s. The different turbulent Schmidt numbers at the density gradient layer cause the distinction between them.

Fig. 15 shows the vertical temperature profile of case 1 from t = 0 s–5000 s. The general trend of predicted temperature is in fair agreement with the experimental data. At t = 1000 s, the predicted temperature at the top vessel is underestimated. It might be due to the initial solid temperature at the top vessel being lower than the actual temperature. The initial temperature of the solid region at the top vessel was probable that a weak natural convection flow occurred at the initiation of the cooling, and the initial velocity was expected to include uncertainty. Also, the present model did not consider the internal structure inside the actual CIGMA vessel, i.e., the nozzle. Therefore, the residual heat of the CIGMA structure during the preheating may affect the flow pattern. Afterward, at t = 5000 s, the numerical results agree well with the experimental data. A visible discrepancy between “chtMultiRegionFoam” and “containmentFoam” is observed at t = 3000 s. The different turbulent Schmidt numbers at the density gradient layer cause the distinction between them.

Fig. 16 shows the 2D contour density gradient snapshot and Sc number at t = 3000 s in case 1. Figs. 16a–b are a result obtained by “chtMultiRegionFoam” and “containmentFoam”. The minimum turbulent Schmidt number, i.e., Sc = 0.85, of “chtMultiRegionFoam” is located at the zero gradient density region. The maximum turbulent Schmidt number, i.e., Sc = 20, is located at the non-zero density
gradient region. Meanwhile, the turbulent Schmidt number of “containmentFoam” is uniformly unity over the whole vessel. The more considerable turbulent Schmidt number in the non-zero gradient density region makes the turbulent mass diffusivity smaller. It means that the erosion rate of density stratification is suppressed. Therefore, the erosion rate of the “chtMultiRegionFoam” is slightly faster than “containmentFoam”. However, the difference is relatively small and hardly observed after \( t = 3000 \) s since the density gradient at the interface decreases over time and becomes steeper at \( t = 5000 \) s.

Fig. 17 shows the vertical helium molar fraction of case 2 from \( t = 0 \) s–5000 s. Numerical predictions on the helium molar fraction show fair agreement with the experimental data. The temporal profile of the helium molar fraction indicates that the helium-rich layer shrinks to the upper part. Meanwhile, the helium concentration at the upper part decreases slowly, and the helium concentration at the lower part gradually increases. Similar results are obtained in both “chtMultiRegionFoam” and “containmentFoam” simulations, and a discrepancy between them is not significant. We can see in Fig. 17 that the numerical results agree well with the experimental data at \( t = 1000 \) s to \( t = 2000 \) s. However, the numerical results show a faster erosion rate at \( t = 3000 \) s to \( t = 4000 \) s. Moreover, at \( t = 5000 \) s, the simulation result over-predicts the upper vessel’s helium molar fraction. The discrepancy might be because of a different volume at the top vessel. The top vessel of the numerical domain was simplified for the sake of convenience during the meshing process. Therefore, the computational domain has a smaller volume at

**Fig. 14.** Spatial and temporal profile of helium molar fraction distribution along the centerline axis in case 1.

**Fig. 15.** Spatial and temporal profile of gas temperature distribution along the vertical axis in case 1.

**Fig. 16.** The 2D contour of density gradient and Sct number at \( t = 3000 \) s in case 1.
the top vessel than the actual design. Consequently, the predicted molar fraction at the top vessel is higher than the experimental data.

Fig. 18 shows the vertical temperature profile of case 2 from \( t = 0 \) s–5000 s. The predicted gas temperature is in reasonably good agreement with experimental data. The cooling area in case 2 is wider than in case 1. Therefore, both temperatures at both helium-rich and poor decrease over time. The gas temperature in the helium-rich layer decreases faster than in the helium-poor layer because the heat transfer rate at the upper part is more dominant than the lower part. However, at \( t = 1000 \) s, the predicted temperature deviates from the experiment. It might be due to the initial internal solid temperature being assumed to be the same as gas temperature. Still, there is a high possibility that the solid internal temperature at the top vessel is higher than the gas temperature. The slight discrepancy between “chtMultiRegionFoam” and “containmentFoam” is mainly due to the different turbulent Prandtl numbers in the bulk fluid. The turbulent Prandtl number in “chtMultiRegionFoam” is smaller than “containmentFoam”. Hence, the thermal diffusivity in the “containmentFoam” is slightly suppressed.

Figs. 19 and 20 show the time transients of helium molar fraction at EL = 6.3, 7.1, 7.5, and 9.3 m in case 1 and case 2, respectively. The experiment data is shown in a solid line, and CFD data is shown in a solid line with a circle marker. The time transient in case 1 (Fig. 19) indicates that the helium molar fraction in the upper part of the vessel, i.e., EL = 9.3 m, decreases monotonically. Meanwhile, the helium molar fraction in the lower vessel (EL = 6.3 m, 7.1 m, and 7.5 m) increases exponentially. Then, they decrease monotonically after the fraction is equivalent.
to the helium molar fraction in the upper vessel (EL = 9.3 m). The exponential increase in helium molar fraction at the lower vessel suggests that the helium layer expands downward. The CFD results show similar trends compared to the experimental data. However, an exponential increase in the helium molar fraction at EL = 6.3 m, 7.1 m, and 7.5 m starts earlier than the experimental data. It indicates that the erosion rate in the present CFD simulation is overestimated. The relative errors time required for the complete dissolution of the helium gas were within 15%.

In case 2 (Fig. 20), the time transient of the helium molar fraction shows a different trend than case 1. Before discussing the detailed trend, it is worth mentioning that the initial helium stratification layer is above EL = 7 m (see Fig. 7c). Hence, sensors at EL = 7.1, 7.5 m, and 9.3 m are located in the helium stratification layer. The sensor at EL = 6.3 is located below the helium stratification layer. In case 2, the exponential increase of helium molar fraction is not observed at the lower vessel. It suggests that the helium stratification layer does not expand but shrinks. Fig. 20 shows that the helium molar fraction in the helium stratification layer (EL = 7.1, 7.5, and 9.3 m) decreases, and the helium molar fraction at EL = 6.3 m increases linearly. The helium molar fraction at EL = 9.3 m decreases slowly. The helium molar fraction at EL = 7.1 m and 7.5 m decreases rapidly and then increases monotonically after the fraction is equivalent to the helium molar fraction in the lower vessel (EL = 6.3 m).

The helium molar fraction at EL = 7.1 m and 7.5 m decrease rapidly right after cooling is initiated because they are located in the transition region (see Fig. 7c). In the transition region, the density gradient is large. Thus, the helium molar fraction in the transition region becomes relatively easier to change when the perturbation is introduced, e.g., shear flow. The CFD results show a similar trend compared to the experimental data. A good agreement between CFD simulation and experimental results is found at EL = 6.3 m and EL = 7.1 m. However, a distinct discrepancy is observed at EL 7.5 m and EL = 9.3 m. As mentioned in the previous section, the discrepancy might be due to the volume domain in CFD, i.e., at the top vessel, being smaller than the actual volume. This effect can be clearly seen in the helium molar fraction at EL = 9.3 m. The experimental data shows that, at EL = 9.3 m, the helium molar fraction decreases significantly after $t = 4000$ s. This behavior is similar to the helium molar fraction at EL = 7.1 m and 7.5 m. The experimental data suggest that the transition region moves upward and reaches at EL = 9.3 m after $t = 4000$ s. However, CFD simulation shows that the helium molar fraction at EL = 9.3 m decreases linearly with time.

### 4.4. Inner wall temperature and wall heat flux

The numerical results on the inner wall and wall heat flux are only obtained from the “chtMultiRegionFoam”. The inner wall temperature and wall heat flux in case 1 and case 2 are plotted in Figs. 21 and 22. Four different elevations are selected, as shown in Figs. 21a and 22a. In case 1, two profiles are located at the cooled region, i.e., EL = 9.3 m, 8.4 m, and two more are located at the noncooled region, i.e., EL = 6.7 m, 3.9 m. In case 2, three profiles are located at the cooled region, i.e., EL = 9.3 m, 8.4 m, and 6.7 m. Only one profile is located at the noncooled region, i.e., EL = 3.9 m. In this regard, it is crucial to evaluate whether the CFD with the conjugate heat transfer model is able to predict the heat transfer.

Figs. 21b–22b depict the temporal profile of averaged inner wall surface temperature in case 1 and case 2, respectively. The predicted inner wall temperature by “chtMultiRegionFoam” is presented in solid lines, and the experimental data is presented in dashed lines. The simulations results show reasonable agreement with the experimental data. The inner wall temperature at the cooled region drops exponentially for 1000 s, and it is monotonically constant until 5000 s. In addition, we can observe that the inner wall temperature at the noncooled region slightly decreases due to the heat loss. It proves that the heat loss at the noncooled region is not significant because the vessel wall is well insulated. Figs. 21c–22c depict the temporal profile of the wall heat fluxes in case 1 and case 2, respectively. The wall heat flux is calculated from the temperature difference between the inner and outer wall, and the wall thickness is as follows

$$q = -\lambda_\delta \frac{T_{in} - T_{out}}{\delta} \quad (40)$$

where $\lambda_\delta$ is the thermal conductivity of the solid wall and $\delta$ is the wall thickness.
4.5. Flow field analysis

One of the objectives of the CCPL30 (case 1) and CCPL34 (case 2) experiment is to understand the effect of different cooling regions on helium mixing. However, the lack of experimental data on the flow field leads to assessing the helium mixing solely from the spatial and temporal profile of helium molar fraction and temperature. Therefore, a prediction on flow field by CFD simulation is beneficial to understand the mechanism of helium mixing driven by natural convection. In this regard, the normalized velocity vectors from 0 s to 5000 s in case 1 and case 2 are presented in Figs. 23–26.

Fig. 23 depicts the 2D contour velocity and normalized velocity vectors in case 1 for every 1000 s. Fig. 23 shows that velocity magnitude in the upper vessel becomes higher while the lower vessel shows the opposite behavior. It indicates that the turbulent mixing in the upper vessel is enhanced with time. On the contrary, the convection flow in the helium-poor zone becomes weaker with time.

Fig. 24 depicts the 2D contour helium molar fraction and normalized velocity vectors in case 1 for every 1000 s. Fig. 24 reveals that the counter-rotating pair vortex is observed at the beginning of time in the upper vessel (helium-rich zone). A stagnant fluid is kept between helium-rich and helium-poor zones at the interface region. It is mainly due to a large density gradient in the interface region suppressing the heat and mass exchange between the upper and lower regions. A single counter-rotating pair vortex in the helium-rich region is maintained over 1000 s. After 1000 s, the helium molar fraction in the helium-rich zone becomes homogenous, and the gradient between the upper helium-rich and the lower helium-poor zone becomes steeper (see Fig. 14). Then, after 1000 s, the stratification layer starts to expand downward. Later, the gas between the upper and lower regions starts to mix, and the helium molar fraction at the helium-rich layer decreases with time.

The counter-rotating pair vortex is characterized by a downward flow along the cooled wall and an upward flow in the center region. In Fig. 24, in the beginning, one counter-rotating pair vortex is created in the upper vessel (depicted in the blue color). After that, at t = 2000 s, as cooling progresses and the density stratification spreads downward, another counter-rotating pair vortex is newly generated beneath the first counter-rotating pair vortex (depicted in the yellow color). The flow direction of the lower counter-rotating pair vortex is opposite to the upper counter-rotating pair vortex. The upper counter-rotating pair vortex is relatively quickly established because the radial temperature distribution can easily be created by cooling the outer wall. At the same time, in the lower counter-rotating pair located below the cooling region, the radial temperature difference is only established when the center fluid is cooled. It can be achieved either by the ingress in the downward flow of the upper counter-rotating pair vortex or the fluid mixing between the upper and lower counter-rotating pair vortexes in the horizontal flow toward the center axis. The ingress of the downward flow in the upper counter-rotating pair vortex into the center region of the lower counter-rotating pair vortex creates instability. Thus, counter-balanced by the ingress of the lower counter-rotating vortex upward flow into the center region of the upper counter-rotating pair vortex (see Fig. 24 at t = 5000 s).

The upward flow along the noncooled wall in the lower counter-rotating pair vortex is mainly due to the inner gas being heated by the
residual heat of the CIGMA structure. Hence, the lower counter-rotating pair vortex size is constrained between the bottom edge of the upper counter-rotating pair vortex and the boundary of the stratified layer. At the same time, the size of the upper vortex is constrained between the upper wall’s vessel and the bottom edge of the cooling region, i.e., EL = 8.2 m. In this case, the vortex sizes are mainly constrained by the size of the cooling region, the initial helium layer elevation, and the vessel size.

The cooling region in case 2 is wider than in case 1. Consequently, the dynamic flow evolution and the mixing mechanism differ in case 1. Fig. 25 shows 2D contour velocity and normalized vector in case 2 every 1000 s. The predicted flow field reveals that the convective flow in the lower vessel (helium-poor) region is more dominant than the upper vessel (helium-rich) region. Normalized velocity shows that the convective flow in the helium-rich zone is maintained all the time even though the velocity magnitude is relatively small.

Fig. 26 depicts the 2D contour helium molar fraction and normalized vector in case 2. At t = 1000 s, in the helium-poor zone, we can observe the downward flow along the cooled region and upward flow along the noncooled region. The lower counter-rotating pair vortex’s radial temperature distribution is established by the ingress in the downward flow of the upper vortex flow. Later, at t = 2000 s, the convective flow in the helium-rich zone becomes more complicated, and a newly single counter-rotating pair vortex is generated (depicted in the yellow color). Later, at t = 3000, the ingress of the downward flow in the upper counter-rotating pair vortex into the center region of the lower counter-rotating pair vortex creates instability. Hence, the upper counter-rotating pair vortex collapses and creates a more complicated convective flow.

Fig. 27 shows the temporal profile of gas density near the inner wall surface at a different elevation for every 1000 s in case 2. As shown in Fig. 27a, the first elevation is located in the helium-rich zone, i.e., EL = 9.2 m, and the second is located in the helium-poor zone, i.e., EL = 5 m. Fig. 27b shows an almost flat density gradient in the helium-poor zone. Fig. 27c shows a steeper density gradient in the helium-rich region. These suggest that the convective flow is more enhanced and prominent in the helium-poor zone. The overall density at EL = 9.2 m increases with time since the fluid is cooled by outer surface cooling. On the other hand, the overall density at EL = 5 m decreases with time since the helium stratification layer is eroded from the bottom, and then the helium is mixed uniformly with the gas at the lower stratification layer.

Fig. 28 shows a qualitative behavior of the counter-rotating vortex velocity vectors in case 2 for every 1000 s. In the beginning, the vortex flow is generated in the helium-poor zone, and a single counter-rotating pair vortex flows in the helium-rich region (depicted in the blue color). At t = 1000 s, in the helium-poor zone, we can observe the downward flow along the cooled region and upward flow along the noncooled region. The lower counter-rotating pair vortex’s radial temperature distribution is established by the ingress in the downward flow of the upper vortex flow. Later, at t = 2000 s, the convective flow in the helium-rich zone becomes more complicated, and a newly single counter-rotating pair vortex is generated (depicted in the yellow color). Later, at t = 3000, the ingress of the downward flow in the upper counter-rotating pair vortex into the center region of the lower counter-rotating pair vortex creates instability. Hence, the upper counter-rotating pair vortex collapses and creates a more complicated convective flow.
pair in case 1 at \( t = 4000 \) s and case 2 at \( t = 2000 \) s. Fig. 28 illustrates a similar behavior between case 1 and case 2. In case 1, the two counter-rotating pair vortexes are located in the helium-rich region. In case 2, the two counter-rotating pair vortexes are located in the helium-poor region. Two counter-rotating pair vortexes consist of an upper vortex and a lower vortex. The edge of the cooled region maintains the vortex center, which separates the upper vortex and lower vortex. Therefore, the downward flow occurred near the cooled region, and an upward flow occurred in the central region. Otherwise, the upward flow occurred near the noncooled region, and a downward flow occurred in the central region. The lower counter-rotating pair vortex’s radial temperature distribution is only established when the center fluid is cooled. Therefore, it appears that case 1 requires more time to establish the lower counter-rotating vortex. A time difference in the vortex establishment between case 1 and case 2 depends on the initial stratification and cooling locations. In case 2, because the cooling area is wider than in case 1, the cooled fluid is more significant than in case 1. As a result, the colder fluid momentum ingress into the lower region is more prominent than in case 1. It is the main reason the lower counter-rotating vortex in case 2 is established faster than in case 1.

The quantitative comparison of the density profile in the axial direction is depicted in Fig. 29. Figs. 29 a and b illustrate the radial density profile at different elevations for case 1 and case 2, respectively. As shown in Fig. 26, EL = 8.5 m in case 1 and EL = 5 m in case 2 are located in the cooled region, and EL = 7 m in case 1 and EL = 3 m in case 2 are located in the noncooled region. A similar trend on the gas density profile is found in both case 1 and case 2. The negative density gradient is observed in the cooled region, and the positive density gradient is observed in the noncooled region. The density is homogenized both in the upper counter-rotating pair vortex and the lower counter-rotating pair vortex regions since the density distribution is observed only near the wall in the radial direction. Also, the overall density differences between the upper and lower counter-rotating pair vortexes are relatively small, suggesting the fluid mixing occurs between the two vortexes.

5. Conclusion

In the present paper, the CFD simulation on the natural convection inside the cylindrical containment vessel CIGMA was performed to understand the helium-air mixing process driven by natural convection. The experimental test series in the CIGMA facility, i.e., CCPL 30 (case 1) and CCPL34 (case 2), were simulated by “chtMultiRegionFoam” and “containmentFoam” solvers in OpenFOAM®. Validation work on helium molar fraction and temperature was performed by using both “chtMultiRegionFoam” and “containmentFoam” to evaluate the dynamic turbulent Schmidt number (Sc_t) model. The simulation results indicated that the dynamic Sc_t model was only affected in the non-zero density gradient. Overall, similar results were obtained by “chtMultiRegionFoam” and “containmentFoam” solvers. The numerical results on spatial-temporal helium molar fraction and temperature showed a good agreement with the experimental data. However, differences in the pressure history were found in both cases. The discrepancy might be related to the initial condition of solid temperature at the top vessel. Hence, the initial condition, including the internal solid part inside the vessel, should be further investigated.

Moreover, the detailed effect of the cooling region on the stratification behavior was numerically investigated. When the cooling region was narrower than the stratification layer thickness, the stratified helium gas layer expanded to the lower part while decreasing the concentration. When the cooling region was broader than the stratification layer thickness, the stratified helium gas layer eroded from the bottom while decreasing the layer thickness. The flow field obtained from the CFD simulation revealed that a similar flow pattern was found in both cases. The upper head cooling caused two counter-rotating vortexes at the helium-rich region. Meanwhile, the upper half body cooling caused two counter-rotating vortexes at the helium-poor region.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Acknowledgments

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Abbreviations

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<tr>
<th>Abbreviation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CIGMA</td>
<td>Containment InteGral effects Measurement Apparatus</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>EL</td>
<td>Elevation</td>
</tr>
<tr>
<td>JAEA</td>
<td>Japan Atomic Energy Agency</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>NEA</td>
<td>Nuclear Energy Agency</td>
</tr>
<tr>
<td>NRA</td>
<td>Nuclear Regulation Authority</td>
</tr>
<tr>
<td>OECD</td>
<td>Organisation for Economic Co-operation and Development</td>
</tr>
<tr>
<td>PISO</td>
<td>Pressure Implicit with Splitting of Operator</td>
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</tbody>
</table>
References


