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Unsteady Reynolds-Averaged Navier-Stokes Simulation of Turbulent Buoyant Jets Issued into a Model HTGR Cavity with Bottom Venting

Bo Liu,^{a*} Shuisheng He,^b Jundi He,^b Charles Moulinec,^a and Juan Uribe^c

^a Daresbury Laboratory, Scientific Computing, Science and Technology Facilities Council, United Kingdom

^b Department of Mechanical Engineering, The University of Sheffield, Sheffield, United Kingdom

^c Rolls Royce SMR, Warrington, United Kingdom

Correspondence:

Daresbury Laboratory, Keckwick Lane, Daresbury WA4 4AD, United Kingdom

*E-mail: bo.liu@stfc.ac.uk

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As one of the six proposed designs for Generation IV nuclear reactors, the High-Temperature Gas Reactor (HTGR) is being designed to have various passive safety features. Its system safety performance has been investigated both experimentally and numerically, particularly under depressurisation scenarios that may occur during postulated accident conditions. In this study, we consider a pipe break accident in the main loop, in which high-temperature and high-pressure helium is discharged into the reactor cavity, resulting in complex flow phenomena involving helium filling, gas mixing and natural circulation within the cavity.

To investigate the jet discharging behaviour near the break and the resulting gas mixing in the reactor cavity, a scaled HTGR reactor cavity test facility was constructed at the City College of New York, and relevant experimental investigations are being carried out. In parallel, Unsteady Reynolds-averaged Navier-Stokes (URANS) models are developed based on geometry and operating conditions of the experimental setup. Numerical simulations are conducted to reproduce representative test cases, include a mild-buoyant case and a strong-buoyant case with injection of 75°C nitrogen and 300°C helium, respectively, into the cavity initially filled with room-temperature air. Due to the nature of the flow which becomes quasisteady during the long transient, a relatively large Courant–Friedrichs–Lewy number of up to 30 is used to accelerate the simulations, ensuring the long transient process to be captured at a reasonable computational cost. Overall, the URANS predictions show good agreement with the experimental data in terms of time evolution of local gas temperature and oxygen concentration at various sensor locations within the cavity.

Keywords: URANS; HTGR; reactor cavity; buoyant jet; gas mixing

I. INTRODUCTION

Jets and the related physical phenomena widely exist in many natural and industrial processes. Early studies of the behaviours of jets can date back to the 1920s and 1930s. In 1926, Tollmien ¹ obtained the analytical solution of a plane jet issuing into a quiescent environment with

the aid of the Plandtl mixing length theory, starting the era of intensive studies of jets. Jets are free shear flows that are usually originated from localised momentum sources which drive the fluid to discharge into the ambient with part of the surrounding fluid continuously entrained into the flow path. This causes the interface between the jet-affected region and the quiescent environment to expand with the downstream distance, forming a tapered shear layer. Most real-world jets are turbulent due to the inherent instability of the shear layer, where the radial velocity gradient leads to the formation, evolution and pairing of vortices. Ball et al. ² claims that these vortices are interlinked with the longitudinal vorticity to create braids-shaped turbulent structures. As the momentum spreads and decays, the jet terminates until the point where the viscous motions dominate the flow and dissipate energy.

When there is a density difference between the discharged fluid and the ambient fluid, buoyancy may play an important role in shaping the flow pattern of a jet. One example is the discharge of hot effluent into a cold water reservoir in an power plant, resulting in a rising jet. According to the classification of Turner ³, a jet is called a pure jet when the flow at the discharging location is dominated by momentum, while it is called a plume when the flow is dominated by buoyancy. For intermediate situations when flows are driven by both momentum and buoyancy, the jet is referred to as a buoyant jet. The flow regime of a buoyant jet can be further characterised by a non-dimensional number, that is, the Richardson number, which quantitatively measures the ratio of buoyant-to-inertial strengths at the discharge location. For very small Richardson numbers (far less than 1), the jet is close to a pure jet. For very large Richardson numbers (much greater than 1), the jet becomes a plume. Over the past few decades, researchers have put great efforts to study the effects of buoyancy on the behaviours of jet both theoretically and experimentally.

One of the earliest theoretical models to describe jet and plume flows in an unbounded ambient fluid was proposed by Morton et al. ⁴ in 1956. Their model is based on solving a set of integral conservation equations with assumptions of self-similar velocity profile and buoyancy effect, small density variation and constant entrainment coefficient. The method was later extended by Fox ⁵, Hirst ⁶, So and Aksoy ⁷, and more recently Jirka ⁸. In addition to theoretical analyses, experimental investigations were carried out on vertical ^{9,10}, inclined ^{11,12} and horizontal ^{13–15} buoyant jets to quantitatively study into the buoyancy effects. Carazzo et al ¹⁶ carried out an comprehensive review on the published experimental data of the jet flow dynamics and argued that the global evolution of both jet and plume tends to follow a universal route towards complete self-similarity in the far field. Such a regime was believed to be driven by the large-scale turbulent coherent structures and the appearance of buoyancy excited the large-scale turbulence modes.

In the last couple of decades, various researchers started to use advanced numerical simulation tools, particularly the Computational Fluid Dynamics (CFD), to study the behaviour of buoyant jets and plumes. (Unsteady) Reynolds-Averaged Navier-Stokes ((U)RANS) approaches were first used and gained success in many engineering flow scenarios. For example, Nam et al. ¹⁷ and Hara and Kato ¹⁸ simulated thermal plumes using the standard k-ε turbulence model and their results were in good agreement with experiments. Large Eddy Simulation (LES) was then used to capture more detailed physics and provide a clearer picture of the transition and evolution of the turbulence structures. Most of the LES studies are focused on vertical buoyant jets, while those on horizontal ones are relatively scarce. For example, Zhou et al. ¹⁹ simulated vertical turbulent buoyant jets with two different ambient-to-jet density ratios and found that an increased density ratio resulted in increased self-similar turbulence intensities and hence higher plume spreading and entrainment rate. Soleimani et al. ²⁰ looked at the asymmetry effects of vertical

buoyant jets formed through a realistic pipe geometry. Both air and helium jets were found to have higher spreading rates and enhanced mixing compared to the axisymmetric cases. Ghaisas et al.²¹ studied the effects of Richardson number and Reynolds number on horizontal buoyant jets. They found that stable stratification appears on one side of the jet centre line and unstable stratification appear on the other side, leading to an asymmetric development of horizontal buoyant jets. The coherent ring-like vortices tend to persist on the stable stratification side and breakdown on the unstable stratification side.

Another case of considerable interest to researchers is where buoyant jets happen in confined or semi-confined spaces. This is of particular relevance in some of the lighter-than-air flammable gas leakage accidents, such as hydrogen leakage in large fuel cell cabinets ²². A quantitative description of the light gas dispersion and its mixing with air in confined enclosures is crucial for the assessment of potential hazardous combustion and explosion. Due to safety concerns, inert gases are usually used as simulants in many experimental studies of such phenomena. For example, helium was intensively used to replace hydrogen owing to their similar density and diffusion properties. The distribution of a buoyant gas in an enclosure is in general more complex than that in an large stationary ambient fluid, as it depends not only on the momentum and buoyancy fluxes of the jet, but also the volume of the enclosure, the location of the source, and the ventilation conditions ²³.

Baines and Turner ²⁴ first carried out a theoretical analysis of turbulent buoyant plume in a sealed enclosure. The method proposed was later referred to as the filling-box model. For pure plumes that are completely driven by buoyancy, a filling front can form between a stratified layer at the upper part and a dense layer at the lower part of the enclosure and move downward with the injection of gas during the filling process. However, when the jet is energetic, i.e. with a strong

momentum flux, a homogeneous layer can form over the entire height of the enclosure due to strong mixing created. For intermediate situations, the homogeneous layer is only produced at the top of the enclosure. The thickness of the homogeneous layer depends on the size of the enclosure, the orientation of the jet and the volume Richardson number introduced by Cleaver et al. ²⁵. Cleaver and co-authors also proposed a correlation to estimate the thickness of the homogeneous layer and classified the filling regimes into three groups, that is, stratified, stratified with a homogeneous layer and homogeneous. Cariteau et al. ²⁶ verified Cleaver's theory experimentally for a helium jet injected in a 1 m³ enclosure. They found that the correlation is in good agreement with experiment for volume Richardson numbers lower than 0.01 but under-estimated the homogeneous layer thickness when the volume Richardson number ranges from 0.01 to 1.

Similar to Baines and Turner's filling box theory for fully confined spaces, Linden et al. ²⁷ studied the buoyant jet issued in semi-confined enclosures with one or two openings connected to a large bulk of ambient fluid. Their model considered not only the filling mechanism but also the emptying process due to natural ventilation. Cariteau et al. ²⁸ carried out experiments using a 1 m³ enclosure with helium inject at the centre of the floor and venting near the ceiling. They investigated the effects of venting shape and size on the stratification transient in the enclosure. It was found that a top vent had some effect on the homogeneous layer formed at the upper part of the enclosure for large Richardson number buoyant jets, but the effects become small with the decrease of the jet Richardson number. Liu et al. ²⁹ focused on the dispersion of low-density gases, particularly hydrogen and helium, in large-aspect ratio semi-confined spaces like tunnels. A 4m × $0.3m \times 0.3m$ dispersion chamber was used in their experiments, with helium injected at the floor centre and monitored using sensors at different locations. They found that helium dispersion forms a homogeneous upper layer, influenced significantly by buoyancy and vent locations. Liang et al.

³⁰ investigated the dispersion of helium in a much larger vented domain. They found that the shortterm transient of helium distribution is in good agreement with Baines and Turner's prediction. The helium distribution always reached a steady state with a homogeneous layer overlaying a stratified layer under the flow conditions they considered.

Apart from theoretical analyses and experimental studies, there are a few CFD simulations reported in the open literature, that investigate the predictive capability in reproducing the steadystate and transient mixing of lighter-than-air gases in vented enclosures. One of the most significant challenges of the numerical simulations is the substantially high requirement in computing time especially when they are aimed for predictions of long transient behaviours of large-scale enclosures. Apart from experimental investigations, Liu et al. ²⁹ also conducted CFD simulations of helium dispersion in their $4m \times 0.3m \times 0.3m$ dispersion chamber and Patel et al.³¹ further extended the simulation to hydrogen in the same configuration and compared the dispersion behavious between helium and hydrogen. Molkov and Shentsov ³² investigated no-model, RANS and LES in their work for laminar, transitional and turbulent releases of buoyant gas in an enclosure with one vent. They found that LES produced the best results for a wide range of experimental conditions and reproduced well the measured concentrations even with large Courant-Friedrichs-Lewy (CFL) numbers. Saikali et al. 33 carried out a Direct Numerical Simulation (DNS) of a buoyant helium jet in an enclosure with two vents. They found that Linden et al.'s model predicts the gas density of the homogeneous layer reasonably well compared to the simulation, which was only 10% away from the DNS results.

Jet dynamics and buoyant gas distribution in confined enclosures are relevant to an engineering process that is of interest in the present study. Here, we focus on the discharge of helium coolant and its mixing with air in a High Temperature Gas-cooled Reactor (HTGR) cavity

during a postulated accident of pipe break in its primary loop. Following the beak, a buoyant jet forms at the rupture location due to the pressure difference between the reactor pressure vessel and the reactor cavity. As a result, high-temperature and high-pressure helium gas is continuously discharged into the reactor cavity. To ensure the overall safety of the system, a venting system is usually employed to reduce pressure within the reactor cavity and to facilitate decay heat removal. Since helium as a reactor coolant has a much higher temperature and lower density than air, buoyancy is expected to play a dominant role in both the discharge dynamics and the subsequent gas mixing within the reactor cavity. In addition, the distribution of helium concentration in the cavity is influenced by various parameters, such as size, shape and location of the vent. The entire process is highly complex due to the combined effects of turbulence, buoyancy, shear and entrainment, confinement, and venting path. As the system pressure decreases over time, an equilibrium is eventually established between the reactor cavity, the reactor pressure vessel and the external environment. Under such conditions, air may re-enter the cavity and potentially the reactor pressure vessel through the venting path. This air ingress could lead to oxidation reactions with the graphite structures inside the core, posing a risk of core damage. Therefore, an in-depth understanding of the evolution of the helium jet and the following gas mixing in the reactor cavity is crucial for predicting the helium-oxygen distribution during the accident and thus of utmost importance for optimising the design of the reactor.

In this paper, we create URANS models based on the experiment carried out at the City College of New York (CCNY) and perform numerical simulations to closely look at the behaviours of helium jets in a vented model HTGR cavity. Findings will be useful to enrich the current theory and understanding of buoyant jets in confined spaces. Experimental data obtained can be used effectively to validate the numerical analyses. The rest of the paper is organised as follows, Section II shows some details of the experimental rig and data acquisition, Section III deals with the numerical model development, simulation results are presented and discussed in Section IV, and conclusions are drawn in Section V.

II. THE CCNY EXPERIMENT

At CCNY, a reactor cavity test facility has been designed and built based on a scaled down modular HTGR, to investigate gas mixing phenomena that happen during pipe break accidents. Pre-heated helium (apart from helium, nitrogen is also used in some of the tests) was injected into the cavity through a valve/nozzle located at the lower part of one of the walls of the rectangular cavity that mimicked the break. Gas temperature and oxygen concentration were measured against time at various elevations in the cavity to monitor the evolution of helium discharge and its mixing with air in the cavity. A vent was created close to the cavity bottom at the wall opposite to the injection nozzle to represent a potential design of the venting path.

II.A Apparatus

In the experiment, a gas cylinder was used to supply helium/nitrogen to the cavity which was initially filled with air at room temperature. Before discharging into the system, the gas was heated using an ultra-high temperature mineral insulated heating cable to get a jet inlet temperature of up to 320 °C. This was maintained throughout the experiments (lower than that of a typical HTGR operating temperature for safety reasons). The mass flow rate was also maintained at a chosen level throughout the test. The experimental tests were typically run for 20 to 50 minutes until most of the air in the cavity was displaced by the jet gas. The test facility consists of two cavities that are interconnected to each other through a horizontal tube close to the bottom, as shown in Figure 1 (see Cavity 1 and Cavity 2), to simulate the reactor pressure vessel and the

steam generator cavities in the reactor building of a typical HTGR system. The experiments considered in this work were conducted with the solenoid valve of the connection tube kept open throughout the gas injection. Since the physical phenomena of utmost interest happen in Cavity 1, optional large openings in Cavity 2 were left open to maintain its pressure at the atmospheric pressure, ensuring its impact on Cavity 1 is negligible.



Figure 1. Schematic of the experimental apparatus.

II.B. Instrumentation and Data Acquisition

Data acquired in the experiment include time histories of gas temperature and oxygen volume concentration at various locations in the cavity. They are measured using thermal couples and oxygen sensors, respectively. The oxygen sensors used have a maximum temperature rating of 400 $^{\circ}$ C and a response time of ~3 s. They measure the oxygen concentration distribution continuously in the cavity. Figure 2 shows the exact spatial coordinates of these sensors with respect to a coordinate system where the origin coincides with the centroid of the exit plane of the injection nozzle. It can be seen that four sets of thermal couples and oxygen sensors are scattered

from bottom to top at the side wall parallel to the injection tube, whereas two sets are installed at the higher part of the cavity and are on the same side of the injection nozzle. An additional oxygen sensor is inserted into the cavity through the opposite wall of the injection nozzle and directly facing the exit of the nozzle.



| Sensor | | Y (m) | Z (m) |
|--------------------|--------|--------------|--------|
| Inlet Gas TC | -0.254 | 0.000 | 0.000 |
| $O_2 - 1$ | 0.302 | -0.272 | -0.112 |
| TC – 1 | 0.302 | -0.363 | -0.112 |
| O ₂ - 2 | 0.302 | 0.094 | -0.112 |
| TC – 2 | 0.302 | 0.185 | -0.112 |
| $O_2 - 3$ | 0.302 | 0.826 | -0.112 |
| TC – 3 | 0.302 | 0.734 | -0.112 |
| $O_2 - 4$ | 0.302 | 1.191 | -0.112 |
| TC – 4 | 0.302 | 1.100 | -0.112 |
| $O_2 - 5$ | 0.191 | 0.643 | 0.000 |
| TC – 5 | 0.196 | 0.551 | 0.000 |
| O_2-6 | 0.191 | 1.008 | 0.000 |
| TC – 6 | 0.196 | 0.917 | 0.000 |
| $O_2 - 7$ | 0.236 | 0.000 | 0.000 |
| | | | |

Figure 2. Location of the thermal couples and oxygen concentration sensors.

III. CFD MODELLING

In the present work, the CFD modelling is closely aligned with the experimental setup in terms of both geometry and flow conditions, with the objective of achieving sufficient validation of the numerical approach. Once validated, the CFD simulations could be used in the future as a powerful complement to experimental investigations, to acquire new knowledge, physical insights, and providing guidance for future improvements of the experimental design. The numerical simulations are conducted using Code_Saturne, ³⁴ an open-source finite-volume CFD software developed by EDF. Code_Saturne provides a wide range of turbulence models, numerical schemes

and gradient reconstruction methods, and has demonstrated excellent scalability on highperformance computing platforms, making it well-suited for the simulations required in this work.

III.A. Model Geometry and Mesh

Considering the fact that the axes of the injection tube and the vent are located in the same vertical plane (which is also a symmetry plane of the cavity), the simulation domain is created based on half of the full geometry, as highlighted on the left side of Figure 3. Key geometrical dimensions are also indicated and consistent with those of the experimental rig. The computational domain is then mapped using a hexahedral mesh consisting of about 1.7 million cells, as shown on the right side of Figure 3. Mesh refinement is applied near the nozzle exit and the high shear zones that are expected to appear in the far field, to accurately capture the jet flow (see the zoom-in cross-sectional meshes normal to the jet path).



Figure 3. Geometry and mesh. Left: computational domain with key dimensions indicated, right: hexahedral mesh with refinement near the jet path and solid walls.

III.B. Fluid Physical Properties

Variable thermal-physical properties of the gas mixture are used in the present CFD simulations. Density, molecular viscosity, specific heat capacity and thermal conductivity of the individual gas components are first calculated using temperature-based look-up tables generated from the NIST database REFPROP v9 ³⁵ where air is treated as a pseudo-pure gas. Then, mixing laws are used to compute the corresponding properties for the gas mixture based on local mass or mole fractions of the gas components. Table I shows the specific mixing laws used for each of the physical properties. For the binary diffusion coefficient, representing the diffusion of the injection (i.e. helium or nitrogen), the following expression is used ³⁶,

$$D = \frac{D_0}{(298/T)^m}$$
(1)

where D_0 is the binary diffusion coefficient at 25 °C, *m* is a constant, taking a value of 1.75 for nitrogen-air diffusion and 1.73 for helium-air diffusion.

| Property | ρ (density) | μ (viscosity) ³⁷ | <i>C_p</i> (specific heat capacity) | λ (thermal conductivity) ³⁷ |
|---------------|--|---|---|---|
| Mixing law | $\rho_m = \frac{1}{\sum_{i=1}^2 y_i / \rho_i}$ | $\mu_m = \frac{\sum_{i=1}^{2} x_i \mu_i M_i^{1/2}}{\sum_{i=1}^{2} x_i M_i^{1/2}}$ | $C_{p,m} = \sum_{i=1}^{2} y_i C_{p,i}$ | $\lambda_{m} = \sum_{i=1}^{2} \frac{x_{i} \lambda_{i}}{\sum_{j=1}^{2} x_{j} A_{ij}}, \text{ where}$ $A_{ij} = \frac{\left[1 + (\lambda_{i} / \lambda_{j})^{1/2} (M_{i} / M_{j})^{1/4}\right]^{2}}{\left[8(1 + M_{i} / M_{j})\right]^{1/2}}$ |

Table I. Mixing laws of thermal-physical properties for the gas mixture

Note: y denotes the mass fraction of the individual gas component, x the mole fraction of the individual gas component, M the molecular weight of the individual gas component.

III.C. Turbulence model

The near-wall turbulent flow is expected to vary significantly in different regions of the cavity. For example, wall-bounded shear flows develop within the injection and venting tubes, while a weakly impinging jet may form on the wall opposite the injection nozzle. In other regions near the remaining cavity walls, natural convection boundary layer flows are expected to dominate. To ensure accurate simulation of the turbulence in all regions of the cavity, the k- ω SST model is used, which was found to be one of the best-suited RANS models for turbulent jet or impinging jet flows ^{38,39}. In addition, an two-layer all-y⁺ wall function, based on a continuous formulation covering from the viscous sublayer to the logarithmic region is employed to reduce the sensitivity of the turbulence model to the near-wall mesh resolution, specifically the first layer y⁺ values. This approach allows the turbulence model to perform well across the entire cavity, despite the varied behaviours of the near-wall turbulent flow.

III.D. Boundary Conditions

III.D.1. The inlet

The flow at the nozzle exit is assumed to be fully developed. To achieve that within a short injection tube, a recycling method is used, where the flow field at a downstream location in the tube is continuously mapped back to the inlet plane, to generate fully developed flow profiles.

III.D.2 The walls

The cavity walls are made of thin steel and have no thermal insulation measures applied to the outer surfaces. So, heat losses through the cavity walls to the environment could be significant and need to be considered in the numerical simulation. The Heat Transfer Coefficient (HTC) between the wall and the environment is estimated based on empirical Nusselt number correlations for natural convective heat transfer between air and large flat surfaces. For the vertical walls, the following Nusselt number correlation is used,

Nu =
$$\left\{ 0.825 + \frac{0.387 \text{Ra}^{1/6}}{\left[1 + (0.492 / \text{Pr})^{9/16} \right]^{8/27}} \right\}^2$$
(2)

For the horizontal walls, the Nusselt number is calculated differently for the top and bottom walls as follows,

$$\begin{cases} Nu = 0.54 Ra^{1/4} & \text{top wall} \\ Nu = 0.27 Ra^{1/4} & \text{bottom wall} \end{cases}$$
(3)

In these correlations, Pr is the Prandtl number, Ra is the Rayleigh number defined as $\text{Ra}=\rho\beta(T_w-T_\infty)L^3g/\mu\alpha$, where ρ is the density of air, β is the volume expansion, T_w-T_∞ is an estimated average temperature difference between the outer surface of the wall and the environment, obtained based on the observations during the experiment, L is a characteristic length of the wall, g is the gravitational acceleration, μ is the dynamic viscosity, and α is the thermal diffusivity.

III.E. Numerical simulations

III.E.1 Cases investigated

Two representative experimental conditions are investigated, including: Case 1, with mild buoyancy influences, in which nitrogen is injected into the cavity at a mean velocity of 9.98 m/s and a mean temperature of 75 °C at the nozzle exit. The corresponding jet inlet Reynolds number and Richardson number are 6,325 and 0.000146, respectively; Case 2, with a stronger buoyancy influence, in which helium is injected into the cavity at a mean velocity of 12.5 m/s and a mean temperature of 300 °C at the nozzle exit. Due to the low density of helium, the jet inlet Reynolds number is only 441 in Case 2, which is much lower than that of Case 1, while the jet inlet

Richardson number is 0.00527, which is much higher than that of Case 1. As a result, a stronger buoyant jet is expected to form in Case 2. The jet inlet Richardson number Ri_0 and volume Richardson number Ri_v are calculated based on Cleaver et al. ²⁵ as follows,

$$\operatorname{Ri}_{0} = \frac{r_{0}g_{0}'}{U_{0}^{2}} \qquad \operatorname{Ri}_{v} = \frac{V^{1/3}g_{0}'}{U_{0}^{2}}$$
(4)

where r_0 is the radius of the injection tube, $V^{1/3}$ a characteristic length based on the cavity volume V, U_0 the gas injection velocity, g_0 ' the reduced gravity given by

$$g_0' = \frac{g \left| \rho_a - \rho_g \right|}{\rho_g} \tag{5}$$

with g the gravitational acceleration, ρ_a the density of ambient air filled initially in the cavity and ρ_g the density of the injection gas. The reduced gravity compares the ratio of the gravitational potential energy to the kinetic energy of the injection.

An additional case (Case 3) with helium injected at a significantly higher injection velocity (107 m/s) and a slightly higher temperature (400 °C) is added to the simulations, in order to get better understanding of the role of Richardson number in gas mixing within the cavity. Experimental data are not available for this case because of safety reasons. Table II lists the key parameters of the cases simulated.

Table II. Flow and thermal conditions of the cases simulated.

| Case | <i>U</i> ₀ (m/s) | <i>T</i> ₀ (°C) | <i>T_a</i> (° <i>C</i>) | Re ₀ | Rio | Riv |
|-------------------|-----------------------------|----------------------------|------------------------------------|-----------------|-----------|--------|
| Case 1 (nitrogen) | 9.98 | 75 | 20 | 6325 | 0.000146 | 0.0193 |
| Case 2 (helium) | 12.5 | 300 | 25 | 441 | 0.00527 | 0.695 |
| Case 3 (helium) | 107 | 400 | 25 | 2876 | 0.0000839 | 0.0111 |

In this study, a second-order upwind linear scheme is used to ensure spatial accuracy in the numerical simulations. A backward Euler time marching scheme is used to capture the flow transient. To accelerate the simulations, a maximum CFL number of approximately 30 is used, which produces satisfactory accuracy based on a time step sensitivity test. Similar observations regarding the use of large CFL numbers have been reported in the LES study by Molkov et al.³² on gas release and dispersion in a vented enclosure.

III.E.2 Mesh sensitivity test

The mesh used in this study, as shown in Figure 3, is optimised based a mesh sensitivity test to ensure a balance between simulation efficiency and accuracy. Three meshes with different number of cells are created for the test: Mesh 1 (0.9 million cells), Mesh 2 (1.7 million cells) and Mesh 3 (3.5 million cells). To assess mesh independency, simulations with the three meshes are conducted for Case 1 (as detailed in Table II) until a physical time of 20 seconds is reached.

The x-direction velocity and gas temperature are plotted along two vertical lines perpendicular to the main jet trajectory, located at x/d = 20 and x/d = 40 downstream of the nozzle outlet. The results, are shown in Figure 4, indicating that the x-direction velocity profiles at x/d = 20 are in good agreement across all three meshes. However, at x/d = 40, a slight deviation is observed between the Mesh 1 result compared to those of Mesh 2 and Mesh 3. A similar trend is observed for the temperature predictions, where Mesh 2 and Mesh 3 results follow well with each other, while Mesh 1 result deviate noticeably from the other two. Based on these observations, Mesh 2 (1.7 million cells) is considered to be sufficient to ensure accuracy of the simulation, and therefore, it is selected for all subsequent simulations in this study.



Figure 4. Mesh sensitivity test

IV. RESULTS AND DISCUSSION

IV.A. Overview of the Flow Features

The transient flow in the cavity can be characterised using two distinct time scales. The first determines the jet time scale, $t_j = L/U_0$, where *L* is a characteristic length scale over which the flow behaves with jet-like features in an unconfined environment, and U_0 is the gas injection velocity. *L* is estimated as $3r_0 / \sqrt{\text{Ri}_0}^{25}$, and the resulting jet time scale, t_j , at an order of lower than 1 second in all three cases: $t_j = 0.160$ s for Case 1, $t_j = 0.021$ s for Case 2 and $t_j = 0.020$ s for

Case 3. The second is the filling time scale, $t_f = V/Q_0$, where V is the cavity volume and Q_0 is the injection flow rate. This scale characterises the time required to fill the cavity with injected gas. In the present cases, t_f is of O(100 s), much larger than t_j : specifically, $t_f = 475 \text{ s}$ for Case 1, $t_f = 380 \text{ s}$ for Case 2 and $t_f = 44 \text{ s}$ for Case 3. The flow in the cavity can be considered "well established" after a period at an order of t_f , allowing typical features to be identified through snapshots of the CFD results. Accordingly, Figures 5, 6 and 7 show snapshots of the CFD results taken at 600 s for Case 1 and 2, and at 90 s for Case 3.

In Case 1, nitrogen is used as the injection gas, and buoyancy effects mainly arise from the temperature difference between the jet gas and the environment. Since the temperature difference is relatively small (only 55 °C), the flow behaves predominantly as a forced jet. The calculated characteristic length scale, L = 1.6 m, is significantly larger than the cavity width of 0.61 m. Therefore, the momentum force dominates over the buoyancy force throughout most of the jet trajectory until the point where it impinges on the wall opposite the nozzle, resulting in the jet gas being diverted to the area around. This creates large-scale circulations in both the lower and upper regions of the cavity (see the left side picture of Figure 5). The circulations significantly enhance the dispersion of the injection gas and hence its mixing with the surrounding air. The observed behaviour is further evidenced in the temperature and oxygen concentration distributions within the cavity, both of which are appear relatively uniform in regions away from the jet, as shown in middle and right pictures of Figure 5, respectively.



Figure 5. Snapshots of velocity magnitude, temperature and oxygen volume concentration at t = 600 s in Case 1.

In Case 2, the situation is substantially different due to the increased influence of buoyancy. The buoyancy force becomes dominant after a short distance away from the nozzle exit, causing the jet to turn upwards. The corresponding length scale, L = 0.27 m, is less than half of the cavity width, indicating a rapid transition from momentum-driven to buoyancy-driven flow. As shown in Figure 6, the jet starts to turn upward near the midpoint of its trajectory across the cavity and ascends along the wall, rather than impinging directly on it, creating a large circulation throughout the entire upper part of the cavity above the nozzle. Similar to Case 1, the circulation enhances gas dispersion and mixing, resulting in uniform distributions of both temperature and oxygen concentration in the upper part of the cavity. In contrast, in the lower part of the cavity where the

jet influence is minimal, the flow shows some stratification features. This is evident from the vertical gradients of temperature and oxygen concentration between the nozzle height and the floor of the cavity.



Figure 6. Snapshots of velocity magnitude, temperature and oxygen volume concentration at t = 600 s in Case 2.

In Case 3, the jet behaviour more closely resembles that of Case 1 than Case 2, although stronger buoyancy is expected to occur due to the higher jet gas temperature. This is because the significant increase in gas injection velocity (about 9 times higher than that of Case 2) leads to a substantial reduction in the jet inlet Richardson number. Consequently, the jet length scale, L = 2.1 m, becomes much larger than the cavity width. As a result, the flow maintains jet-like until it

impinges on the wall. Accordingly, the flow pattern and gas mixing within the cavity are also similar to those of Case 1 and not repeated here for brevity.



Figure 7. Snapshots of velocity magnitude, temperature and oxygen volume concentration at t = 90 s in Case 3.

IV.B. Validation of the CFD Model against Experiment

To further assess the reliability of the CFD model, simulation results are compared with experimental data in terms of the time evolution of the gas temperature and oxygen concentration at the sensor locations shown in Figure 2. The comparisons for Case 1 are shown in Figure 8. As shown in the left side pictures of Figure 8, the CFD predicted time histories of gas temperature at different sensor locations are closely aligned with each other, suggesting that the hot jet gas and

cold air mix well throughout the cavity, with no clear thermal stratification observed, during the entire injection process. This is consistent with the experimental observations, where the temperature evolution at locations, such as TC-1, TC-3 and TC-4, follows a similar pattern. However, at TC-2, the experimental result exhibited some distinct features, specifically larger fluctuations compared to other locations. The exact cause of this is not clear, but one possible explanation is that thermocouple TC-2 is located near the outer shear layer of the jet, where large temperature gradients are expected and Kelvin-Helmholtz instabilities could amplify the temperature fluctuations. Such a localised behaviour is not captured by the CFD simulations. Overall, both the experimental and numerical results show an initial gas temperature rises followed by a gradual approach to a plateau, indicating a thermal equilibrium between the cavity and the external environment. The CFD model reproduces the general trend, but it over-predicts the temperature rise, leading to an overestimation of the plateau temperature.

Good gas mixing is more clearly illustrated through plots of the oxygen concentrations, as shown in the right side pictures in Figure 8, where the curves representing oxygen concentrations at different sensor locations exhibit very similar features. The CFD predictions and the experimental observations are in good agreement in both the timing and magnitude of the oxygen concentrations. It can also be seen from these plots that the oxygen concentration is reduced to approximately half of its initial value when the injection time reaches the cavity-filling time scale.

Figure 9 shows CFD predictions compared against the experimental data for Case 2. In contrast to Case 1, the time histories of the gas temperature at various sensor locations exhibit significantly different behaviours. At TC-1, located below the jet in the stratified layer of the cavity (as shown in Figure 6), the gas temperature remains significantly lower than that of the other locations. One of the most notable features is a distinct temperature peak occurring about 6 minutes

after the start of the injection. The CFD model successfully captures not the overall trend but also the timing and magnitude of the peak temperature. At TC-2, located close to the edge of the jet core and is directly affected by the jet, the gas temperature is higher than that at TC-1 and exhibits noticeable oscillations due to the instability of the jet. These are also reasonably well predicted by the CFD model. At TC-3 to TC-6, located in the upper part of the cavity, where the jet gas and air are well mixed, gas temperatures are very close to each other, higher than those at TC-1 and TC-2. They rise rapidly in the first 2 to 3 minutes and then level off into a plateau. However, about 15 minutes after the start of the injection, the CFD predictions for TC-3 to TC-6 begins to deviate from the experimental data and exhibits increased oscillations thereafter. Further investigation is required to understand the underlying causes of this discrepancy.





Figure 8. Experimental measurements versus CFD predictions of time evolutions of temperature (left) and oxygen concentration (right) at some probe locations in Case 1.

Figure 9. Experimental measurements versus CFD predictions of time evolutions of temperature (left) and oxygen concentration (right) at some probe locations in Case 2.

Overall, good agreement is also observed between the CFD predictions and experimental data for oxygen concentration. At sensors O_2 -1 and O_2 -2, located below the jet, the oxygen concentration is significantly higher than that in the region above the jet. It is worth noting that the CFD predicted boundary of the vertical stratification layer is slightly different from that observed in the experiment. Specifically, both O_2 -1 and O_2 -2 are located within the stratified layer as indicated from the experimental data, while the CFD model predicts that O_2 -2 is located in the well mixing region above the jet. For the other sensors, namely, O_2 -3 to O_2 -6, the CFD predictions align well with the experimental measurements, capturing the expected trends in oxygen distribution throughout the upper cavity region. In the case of sensor O_2 -7, located opposite the nozzle, the experimental data appear to be unreliable, showing an unexpected increase in oxygen concentration during the later phase of the injection (after approximately 15 minutes), so the results for O_2 -7 are not presented here.

To further evaluate the accuracy of the CFD simulations, the deviation between simulation results and the experimental data is quantified using a normalised time-accumulated error for Case 1 and Case 2. Given the fact that data collection in the experiments is conducted at a larger time interval compared to the time step sizes used in CFD simulations, the simulation results are first interpolated onto the experimental time series, and then error is calculated as follows,

$$Err = \frac{\sum_{i} \left| \phi_{s,i} - \phi_{e,i} \right| \Delta t_{i}}{\left| \phi_{0} - \phi_{a} \right| t}$$
(6)

where ϕ represents the parameters of interest, namely temperature and oxygen concentration, Δt is the time step, *t* is the total gas injection time, subscriptions *s* and *e* denote the simulation and experimental results, respectively, *0* refers to the value of a parameter at the jet inlet (nozzle outlet), *a* represents the initial value of the parameter in the ambient within the cavity, and *i* corresponds to the *ith* time step in the time series.

Figure 10 shows the errors computed using Equation (6) between CFD predictions and experimental measurements at the corresponding sensor locations. In Case 1, relatively large errors are observed for temperature, which are around 10% for all four sensor locations, whereas errors for oxygen concentration remain much lower, below 5%. In contrast, errors in Case 2 for temperature predictions are negligibly small, approximately 1%. For oxygen concentration, the errors are slightly larger than those in Case 1, but remain the same level of 5%. The uncertainty in CFD predictions for temperature is likely related to the thermal boundary conditions used for the cavity outer surface, which governs the rate of heat loss from the cavity to the environment, impacting significantly on the temperature evolution within the cavity. This suggests that accurate estimation of the temperature difference between the cavity outer surface and the environment is substantial to ensure the accuracy of the CFD simulations. For species transport, as zero gradient boundary conditions are used in both cases, their impact on oxygen concentration predictions is minimal.





Figure 10. Error analysis of the CFD simulations

IV.C. Effects of Ri₀ on Gas Dispersion and Mixing

The dispersion and mixing of an injected gas in a vented enclosure are affected by many factors, such as the species of the injection source and the surrounding environment, injection flow and thermal conditions, location and orientation of the injection source, venting path, and cavity size. Here, we compare the CFD results of Case 2 and Case 3, in which the same jet source (helium) is used at similar thermal conditions (jet temperature and wall heat loss), but very different inlet Richardson numbers. It is found that the jet inlet Richardson number has a significant impact on the gas flow and mixing behaviour in the cavity, which is in good agreement with the theories of Baines and Turner ²⁴ and Cleaver and co-authors ²⁵ on turbulent buoyant jets in confined enclosures. Their studies suggest that, for an energetic jet with strong momentum flux, a homogeneous layer forms throughout the cavity due to jet-induced mixing, while for a less energetic jet, the homogeneous layer only exists near the top of the cavity with a stratified layer lying underneath.

The characteristic time scales relevant to the investigated cases were described earlier in Section IV.A. Specifically, the filling time scale t_f , defined as the ratio of the cavity volume to the injection flow rate, represents the characteristic time required to fill the cavity with the injected gas. For Case 2 and Case 3, t_f is 380 s and 44 s, respectively. To better account for the thermodynamic effects during the filling process, particularly the temperature difference between the injected gas and the ambient air within the cavity, a modified filling time scale, t_f^* , is introduced and defined as follows,

$$t_f^* = \frac{V}{Q_0} \left(\frac{T_0}{T_a} \right) \tag{7}$$

where T_0 is the gas injection temperature, and T_a is the initial ambient temperature within the cavity. Based on this, t_f^* is estimated to be 730 s for Case 2 and 99 s for Case 3.

Figure 11 shows the vertical distribution of helium volume concentration and gas temperature in the cavity at different time points (normalised by t_f^*) during the injection process for Case 2 and Case 3. In Case 2, a distinct species stratification layer develops below the injection nozzle, while a more uniform, well-mixed region forms above it. In Case 3, however, no such stratification trend appears, and the helium distribution is nearly uniform throughout the entire cavity. Thermal stratification is also observed in Case 2, with a stratified layer forming near the bottom of the cavity, which is thicker than the species stratification layer and extends even above the injection nozzle. This observation suggests that heat and mass transfer respond differently to the jet Richardson number, resulting in distinct stratification patterns. In Case 3, however, no significant thermal stratification is observed. It is also worth noting that, in Case 2, a clear thermal equilibrium between the cavity and the external environment is established when the helium

volume concentration reaches about 30%. In contrast, in Case 3, the thermal equilibrium appears to occur much later.



Figure 11. Vertical distribution of helium volume concentration and temperature in the cavity at a series of time points.

V. CONCLUSIONS

URANS CFD simulations are carried out in the present work to study the gas discharge, dispersion and mixing in a vented cavity fabricated at City College of New York, designed to simulate a pipe break accident in the primary loop of an HTGR. Findings contribute to the existing theoretical framework and enhance our and understanding of buoyant jets in confined environments. Two representative experimental conditions are selected for numerical simulation: a mild buoyant jet, using nitrogen as the injection gas (Case 1) and a strong buoyant jet, using helium as the injection gas (Case 2 and Case 3). The CFD results agree reasonably well with the experimental data in predicting the time evolution of the gas temperature and oxygen concentration at multiple sensor locations within the cavity. Further analysis of the detailed gas distribution allows for deepening the understanding of the underlying physics. On this basis, some key conclusions are drawn and summarised as follows,

- The experimental and numerical simulation results are in good agreement with the theories proposed by Baines and Turner's ²⁴ and Cleaver and co-authors' ²⁵ on turbulent buoyant jets in confined enclosures. In particular, the jet inlet Richardson number is confirmed to be a key parameter to characterise gas mixing and dispersion.
- For highly energetic jets (Case 1 and Case 3), a homogeneous region forms throughout the entire cavity due to strong mixing driven by the jet and its impingement on the wall. In contrast, for a less energetic jet (Case 2), a homogeneous region only exists at the upper part of the cavity and a stratified layer appears at the lower part, as the jet turns upward before reaching the opposite wall.
- The mass transfer and heat transfer within the cavity respond differently to the jet effect at relatively high jet Richardson numbers (e.g. Case 2). Specifically, the region exhibiting thermal stratification tends to be thicker than that exhibiting species (mass) stratification.

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