LES SIMULATION OF BUOYANCY JET FROM UNINTENDED HYDROGEN RELEASE WITH GASFLOW-MPI

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ABSTRACT

Hydrogen leakage is a key safety issue for hydrogen energy application. For hydrogen leakage, hydrogen releases with low momentum, hence the development of the leakage jet is dominated by both initial momentum and buoyancy. It is important for a computational code to capture the flow characteristics transiting from momentum-dominated jet to buoyancy dominated plume during leakage. GASFLOW-MPI is a parallel computational fluid dynamics (CFD) code, which is well validated and widely used for hydrogen safety analysis. In this paper, its capability for small scale hydrogen leakage is validated with unintended hydrogen release experiment. In the experiment, pure hydrogen is released into surrounding stagnant air through a jet tube on a honeycomb plate with various Froude numbers (Fr). The flow can be fully momentum-dominated at the beginning, while the influence of buoyancy increases with the Fr decreases along the streamline. Several quantities of interest including velocity along the centerline, radial profiles of the time-averaged H_2 mass fraction are obtained to compare with experimental data. The good agreement between the numerical results and the experimental data indicates that GASFLOW-MPI can successfully simulate hydrogen turbulent dispersion driven by both momentum and buoyant force. Different turbulent models i.e. k-ε, LES, and DES model are analyzed for code performance, the result shows that all these three models are adequate for hydrogen leakage simulation, k-ε simulation is sufficient for industrial applications, while, LES model can be adopted for detail analysis for a jet/plume study like entrainment. The DES model possesses both characters of the former two model, only the performance of its result depends on the grid refinement.

1.0 INTRODUCTION

A small unintended hydrogen release has been identified as an important phenomenon for codes and standards development in hydrogen energy industry [1] because it may lead to combustion hazard and also it is often too small to detect for hydrogen measurement. Many studies have been focused on this issue, both experiment and simulation [2][3].

Leaks of hydrogen from break sources form turbulent jets that are dominated by both monument and buoyancy, which can be described with Froude number.

$$Fr = u_{inlet}/(gd(\rho_\infty - \rho_{inlet})/\rho_\infty)^{1/2} \quad (1)$$

where u_{inlet} – velocity of jet exit, m/s; g – gravity accelerator, m/s^2; ρ_∞ - density of the surrounding air, kg/m^3; ρ_{inlet} – density of injected gas.

If Fr < 10, the injected flow is more plume like, dominated by buoyancy generated from density difference between hydrogen and surrounding air; if Fr>1000, the injected flow is more jet like, dominated by initial monument; and if 10<Fr<1000, the injected flow is dominated by both buoyancy and initial monument in this intermediate range [1]. How the jet is developed and how to predict the turbulent mixing are interesting issues that have drawn lots of intension. Researchers have conducted experiments with gases with different densities like hydrogens, helium, methane injecting into air or nitrogen, to discuss behaviour of turbulent jets [4][5]. Previous research tended to solve this problem with integral model [6] taking account of assumptions for entrainment velocity, density or velocity distributions or so. A classic plume theory of MTT has been widely adopted and validated by many

researchers, also been extended deal with a range of different physical phenomena through years of development [4]. Furthermore, a new theory is developed and validated by van den Bremer & Hunt to provide universal solution for both Boussinesq and non-Boussinesq plumes, through solving for the variation with height of solving Γ, a local Richardson number [7].

Another approach is numerical modelling, which became increasingly important for better understanding plume behaviour, as the development of computational prowess. CFD method can provide more detail information of turbulent plume, in terms of entrainment, distributions of various properties, also to resolve fields that are extremely difficult to measure directly, e.g. pressure fields [8], [9]. GASFLOW-MPI is a parallel computational fluid dynamics (CFD) code developed in Karlsruhe Institute of Technology, which is a best-estimate tool for predicting transport, mixing, and combustion of hydrogen [10].

In this paper, GASFLOW-MPI is validated with small-scale hydrogen release experiment, three different turbulent models are discussed i.e. k-ε, LES, and DES model, in order to discuss the code performance of GASFLOW-MPI for both buoyancy jet and turbulence mixing of different species.

2.0 GASFLOW-MPI

Three turbulent models are employed in this paper. First two models, the Large Eddy Simulation Large (LES) model and Detached Eddy Simulation (DES) model are recently developed and validated to capture more details of turbulence and flow features in applications of scientific research and engineering problems. Another model is the k-ε model which is well-accepted in industrial applications.

2.1 Large Eddy Simulation Model

LES model has been adopted to simulate buoyancy plume in many research since most of the turbulent fluctuation could be resolved directly and only the turbulence eddy at sub-grid scale should be modelled by sub-grid scale model. The Smagorinsky model is employed in GASFLOW-MPI to calculate the SGS turbulent viscosity due to its simplicity and practicality [11]. And the turbulent viscosity could be expressed by Eq.(2).

$$\mu_t = \rho L_s^2 |S| \tag{2}$$

Where L_s- mixing length for subgrid scales; $|S|$ - an inner product of strain rate tensor;

$$L_s = C_s \Delta \tag{3}$$

$$\Delta = V^{1/3} = \left(\Delta x \Delta y \Delta z\right)^{1/3} \tag{4}$$

$$|S| = \sqrt{2 S_{ij} S_{ij}} \tag{5}$$

Where C_s - the Smagorinsky constan; Δ- the filter width.

In LES model, the turbulent viscosity is related to the mesh size. Theoretically, the Smagorinsky constant C_s is computed either from turbulence statistical theories or from DNS data base. However, in applications, C_s is set to 0.1 which has been found to yield the best results for a wide range of flows [11]. The filter width Δ is computed according to the volume of the computational cell using Eq. (5).

2.2 *k-ε* Model

k-ε turbulence model is one of the most common models to simulate the mean characteristics of the turbulent flow. It is a kind of two equation models which gives a general description of turbulence by turbulence energy transport equation and turbulence dissipation rate equation, as shown in Eq. (6) and (7). The turbulent viscosity coefficient μ_t is calculated by Eq. (8) [12].

$$\frac{\partial}{\partial t}(\rho k)+\nabla\cdot(\rho k\mathbf{U})=\nabla\cdot\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\nabla k\right]+G_k+G_b-\rho\varepsilon \tag{6}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\cdot(\rho\varepsilon\mathbf{U})=\nabla\cdot\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right]+C_{\varepsilon 1}\frac{\varepsilon}{k}(G_k+G_b)-C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \tag{7}$$

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \tag{8}$$

Where k - the turbulent kinetic energy, ε - the rate of dissipation; G_k – turbulence generation due to viscous forces; G_b- turbulence generation due to buoyancy.$C_{\varepsilon 1}, C_{\varepsilon 2}, C_\mu, \sigma_k, \sigma_\varepsilon$ are constant coefficients in *k-ε* Model.

2.3 Detached Eddy Simulation Model

Detached Eddy Simulation (DES) model is a kind of hybrid turbulence model. The main feature of DES model is that it could switch between RANS and LES adaptively according to the local turbulent information. When the mesh size is fine enough to resolve the turbulent information, the DES model approaches to the LES model. In the opposite condition, DES model approaches to the k-ε model. In this paper, the k-ε based DES model is employed to model the turbulence behaviour, as shown in Eq. (9) and (10).

$$\frac{\partial}{\partial t}(\rho k)+\nabla\cdot(\rho k\mathbf{U})=\nabla\cdot\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\nabla k\right]+G_k+G_b-\frac{\rho k^{3/2}}{l_{des}} \tag{9}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon)+\nabla\cdot(\rho\varepsilon\mathbf{U})=\nabla\cdot\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right]+C_{\varepsilon 1}\frac{\varepsilon}{k}(G_k+G_b)-C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k} \tag{10}$$

$$l_{des}=\min(l_{rke},l_{les}),\quad l_{rke}=\frac{k^{3/2}}{\varepsilon},\quad l_{les}=C_{des}\Delta_{\max},\quad \Delta_{\max}=\max(\Delta x,\Delta y,\Delta z) \tag{11}$$

$$\mu_t=\rho C_\mu\frac{k^2}{\varepsilon} \tag{12}$$

Where l_{des} - DES length scale; C_{des} - DES coefficient.

3.0 MODELING

The experiment of small-scale unintended releases of hydrogen was conducted by Sandia National Laboratories for the validation of CFD models to predict unintended hydrogen release scenarios [1], [5], [13], as shown in Figure.1. In the experiment, pure hydrogen is injected into surrounding still air through an inlet with a diameter of 1.91 mm. The temperature of hydrogen and surrounding air was maintained constant at 21 ℃ and the pressure of the ambient room was 100 kPa. For the selected case analysed in this paper, the injection velocity is 133.9m/s with a mass flow rate 3.82e-4 m^3/s. The value of initial Fr is 268, which falls into the intermediate range, as mentioned above. And the Reynolds number of the jet is with the value of 2384, indicating fully turbulent. The measurement system provides flow velocity field, the mole fraction of gas, and fluctuating quantities for code validation. We use the Cartesian coordinate system to model this problem with the computational domain size of 30*30*115mm. This domain is divided into 90*90*150 grids, with a total cell number 1,215,000, as shown in Fig.2.

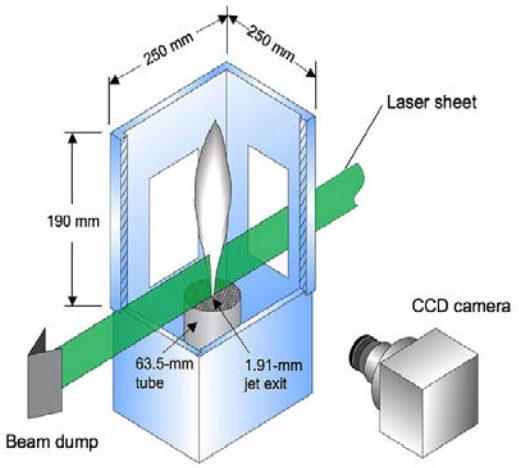

Figure 1. Experiment of small-scale unintended releases of hydrogen

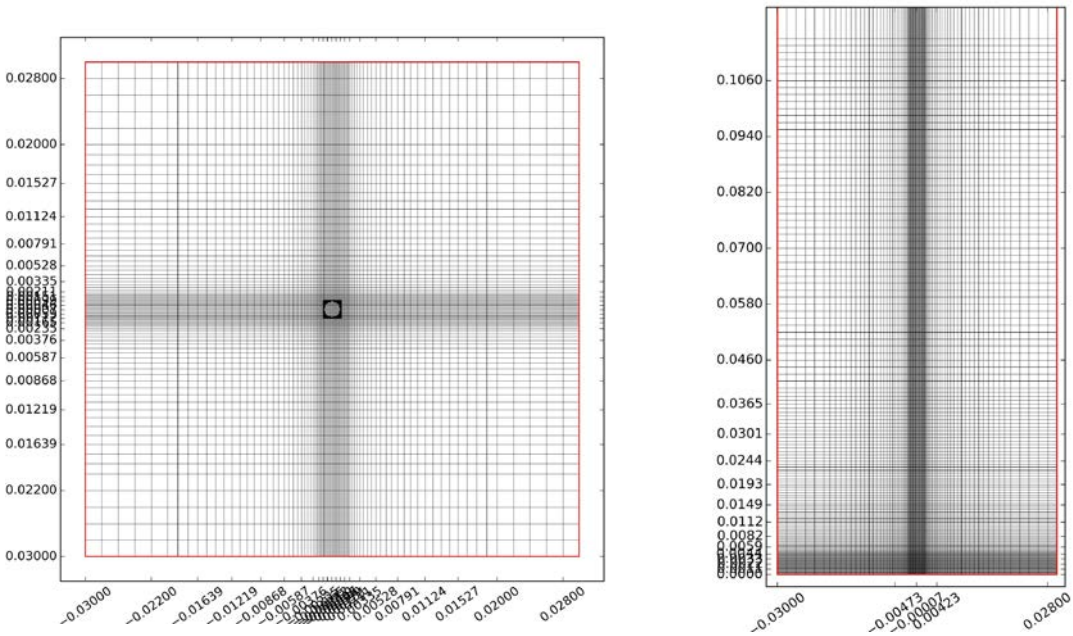

Figure 2. diagram of mesh (a) X-Y view; (b)X-Z view

4.0 NUMERICAL RESULTS

4.1 LES simulation

As described in section 3, pure hydrogen is injected into air through a cylindric inlet at constant velocity with a diameter of 1.91mm. with Fr number of 268 in this case, hydrogen is mainly dominated by monument at the beginning. In this paper, we focus on the height of 0-40*D*, that ensures there is a region in which the jet becomes fully developed sufficiently far above the source that a meaningful comparison with experimental data, where *D* is the inlet diameter.

At the beginning, the flow near the inlet is a steady axisymmetric laminar flow, then the development of the instability generated at the shear layer, leads to interaction between injected hydrogen and the surrounding air. Thus, with entrainment of surrounding air, the mole fraction of hydrogen begins to decay, as well as centerline velocity, as shown in Fig.3 and Fig.4. Meanwhile, the radius of hydrogen

flow begins to grow, generating an inversely conical shape as shown in Fig 3. In Fig.4, as the z-velocity *u* decays with height, there is also a small negative velocity near the boundary of the main up going flow. This indicates the turbulence vortexes that are captured near the interface between hydrogen and air. The time averaged centerline velocity u_{cl} and mole fraction of hydrogen vf_{h2} are compared with experimental data as given in Fig.5 and Fig.6. In Fig.5, the velocity remains constant near the inlet where the turbulence is not fully developed after that u_{cl} decays linearly along 1/*z*. The similar tendency is also found in mole fraction as shown in Fig.6. This consists of the experimental data, that in monument dominated region, for both velocity and fraction, the decay rate follows a 1/*z* dependence.

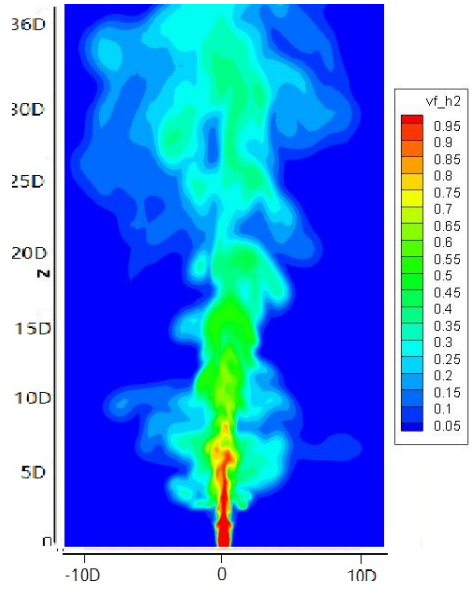

Figure 3 Instantaneous mole fraction of hydrogen in Z/D 0-40.

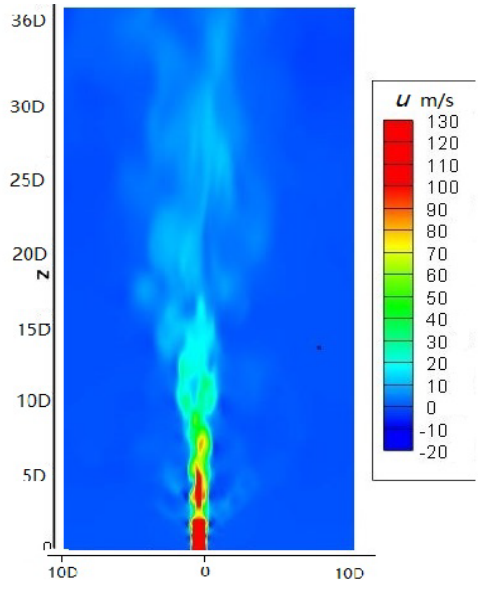

Figure 4 Instantaneous z-velocity contour in Z/D 0-40.

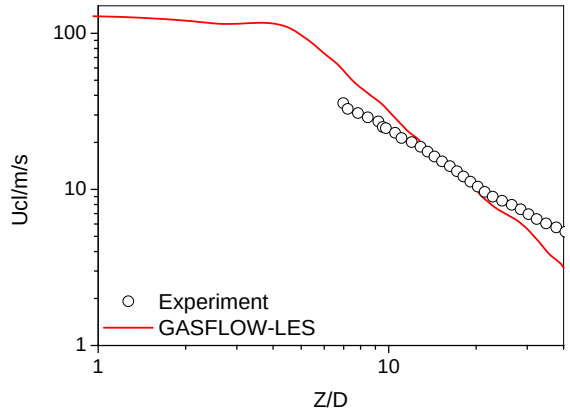

Figure 5 z-direction velocity along centerline -time averaged

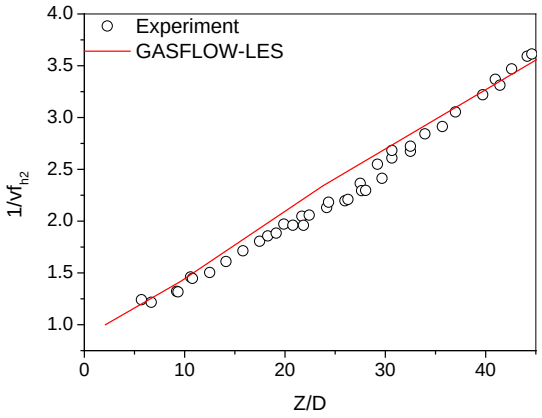

Figure 6 $1/vf_{h2}$ along centerline- time averaged

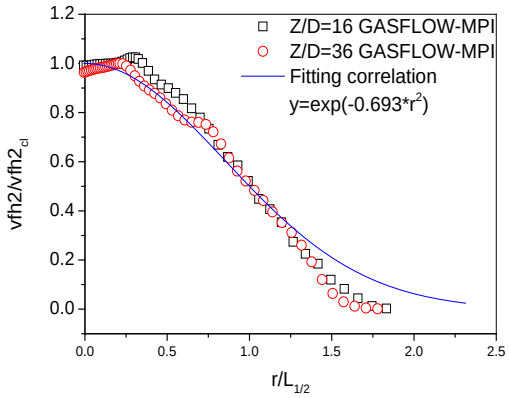

Figure 7 radius profile of hydrogen -time averaged

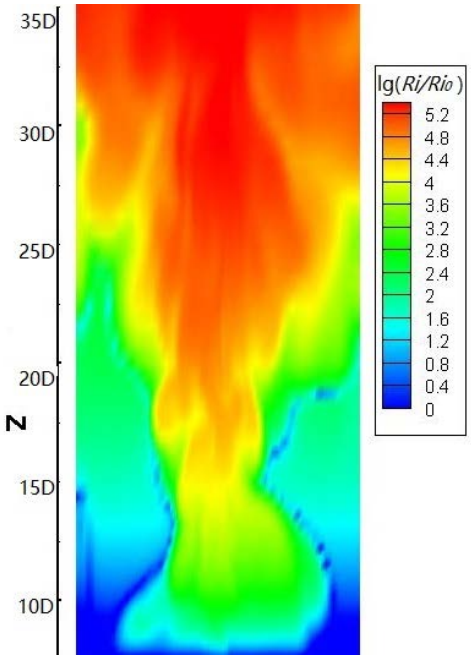

Figure 8 Contour of local Richardson number

The time-averaged radius profile of vf_{h2} is given in Fig.7, where $vf_{h2}(r)$ is normalized with centerline vf_{h2}, and the radius r is normalized with mole fraction half radius $L_{1/2}$. Previous research shows that radial profiles of the fraction collapse on to the same curve when plotted against the appropriate similarity variables. The equation fitting from experimental data is given in Eq. (13), and compared with simulation result. The results show that the simulated vf_{h2} profiles at different downstream locations reach the self-similar state and agree quite well with Eq. (13).

$$vf_{h2}(r)/vf_{h2cl} = \exp[-0.693(r/L_{1/2})^2] \quad (13)$$

Where vf_{h2}- mole fraction of hydrogen; $L_{1/2}$ - half radius; r – radius.

We use local Richardson number to analyse the influence of buoyancy. The normalized Ri/Ri_o defined as Eq. (14) [14]. If Ri is smaller than unity, the buoyance is not important in the flow, while the buoyancy is dominant when Ri is much greater than unity.

$$Ri/Ri_o = \frac{g(\rho_\infty - \rho_i)/\rho_\infty d(z)}{{u_{cl}}^2(z)} / \frac{(gd(\rho_\infty - \rho_{inlet})/\rho_\infty)}{{u_{inlet}}^2} \quad (14)$$

Where $d(z)$ - local width of hydrogen jet, which is proportional to height above the injection; ρ_i – local gas density; $u_{cl}(z)$ – centerline velocity at z height, time-averaged velocity is used in the calculation.

The contour of $\lg(Ri/Ri_o)$ is given in Fig.8. At the beginning, this flow is dominated by initial momentum, while local Richardson number Ri increases along with height, which indicates the increase of effects of buoyancy. Meanwhile, the decay rate of centerline velocity and hydrogen fraction obeys 1/z dependence, as shown in Fig.5 and Fig.6, indicating that the momentum is still in a dominant position.

In this section, the LES model is validated with small unintended hydrogen release experiment. Several key parameters compared with experimental data, both axially and radially. The result shows that numerical simulation has a good agreement with experiment. Therefore, LES model of GASFLOW-MPI can provide a reasonable prediction for a plume driven by monument and

buoyancy, also turbulence mixing of different species.

4.2 Turbulence model discussion

The results of DES and *k-ε* Model are discussed below. As a RANS-based turbulent model, all turbulence information is modelled in *k-ε* Model. Therefore, in *k-ε* simulation, the turbulent vortexes are averaged, and the mole fraction of hydrogen is symmetrical in theta-direction for an instantaneous result, as shown in Fig.8 (a), where the hydrogen jet shows a perfectly reverse-cone. As for DES simulation, as described in section 1.3, the results show the characters of both LES model and *k-ε* Model. As given in Fig.8 (b), near the inlet, the hydrogen distribution is similar to the LES simulation, while at the far field, the instantaneous result reveals the symmetric distribution similar to *k-ε* simulation. The numerical results are compared with experimental data as shown in Fig 9 and 10. The *k-ε* result is instantaneous while the DES result is time averaged. the decay rate of centerline velocity and mole fraction shows the same *1/z* discipline as mentioned above, and agree quite well with the experimental data.

Based on the analysis above, all these models are adequate for small unintended hydrogen release simulation. The *k-ε* model can achieve a reasonable prediction for industrial application, only detail flow information like turbulent fluctuation that is lost. However, this information can be captured by LES model. Therefore, LES model can be adopted for detail analysis for a jet/plume study like entrainment. The DES model possesses both characters of the former two model, only the performance of its result depends on the grid refinement.

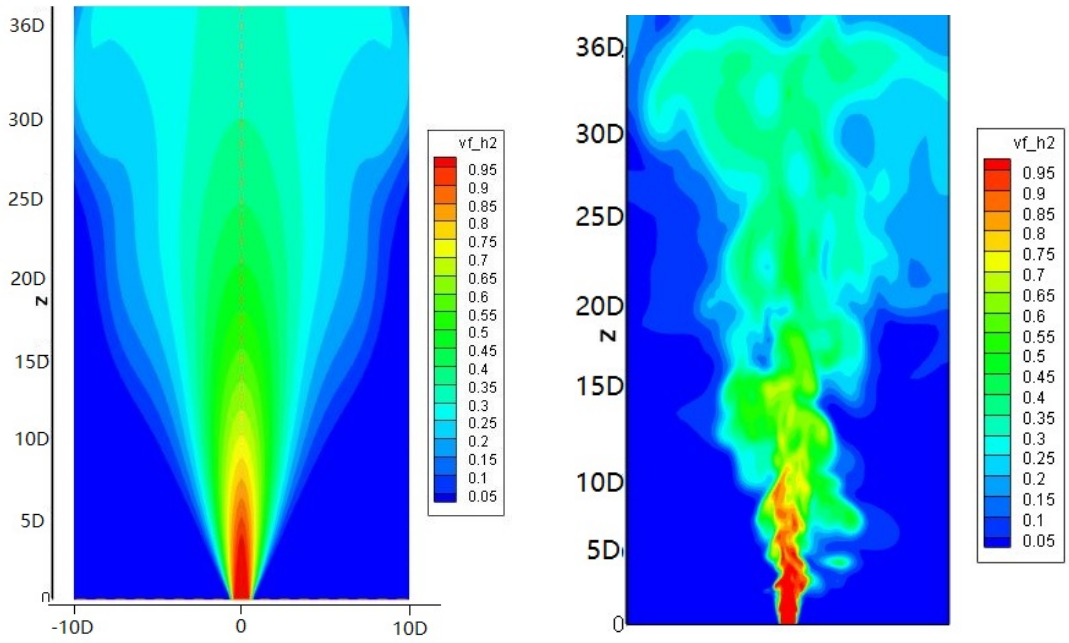

Figure 8 instantaneous mole fraction of hydrogen: (a) *k-ε* Model (b) DES Model

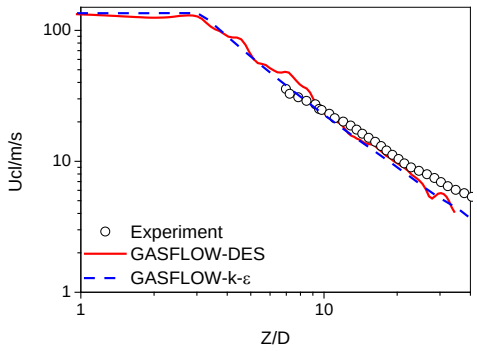

Figure 9 z-direction velocity along centerline -time averaged

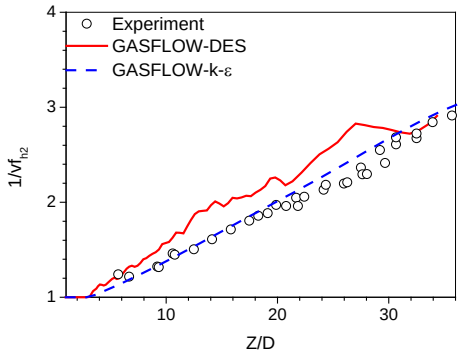

Figure10 $1/vf_{h2}$ along centerline- time averaged

5.0 CONCLUSION

The small unintended release is an important safety phenomenon for codes and standards development in hydrogen energy industry. To simulate this issue, we validate the CFD code GASFLOW-MPI with the small-scale hydrogen release experiment to evaluate the code performance for buoyancy jet and turbulence mixing. Three different turbulent models are discussed, i.e. LES model, DES model and k-ε Model. Several quantities of interest including velocity along the centerline, radial profiles of the time-averaged H_2 mass fraction are obtained to compare with experimental data. The good agreement between the numerical results and the experimental data indicates that GASFLOW-MPI can successfully simulate hydrogen turbulent dispersion driven by both momentum and buoyant force. Different turbulent models i.e. k-ε, LES, and DES model are analysed for code performance, the result shows that all these three models are validated, *k-ε* simulation is sufficient for industrial applications, while, LES model can be adopted for detail analysis for a jet/plume study like entrainment. The DES model possesses both characters of the former two model, only the performance of its result depends on the grid refinement.

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