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3D CFD analysis of the hydrogen releases and dispersion around storage facilities

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Abstract−Unexpected hazards often arise from hydrogen storage and distribution facilities, and latent dangers induced by handling of hydrogen. This paper represents the results of CFD (computational fluid dynamics) modeling of hydrogen releases and dispersion at model storage facilities with simple geometries. Numerical results for model storage facility were compared with the reported data on the hydrogen dispersion. In addition, the hydrogen concentration in a real industrial environment, such as in the hydrogen energy station (HES), was estimated with 3D CFD modeling. The risk assessment was achieved under hypothetical hydrogen leakage scenarios.

Key words: Hydrogen Release, 3D CFD, Risk Assessment, Hydrogen Energy Station

INTRODUCTION

Uncertainties in the availability of fossil fuels have spurred research in alternative energy carriers for transportation applications and other industrial facilities. The use of hydrogen has specific advantages over petroleum-based fuels, including diversification of potential primary energy sources and reduced tail pipe emissions.

Hydrogen is therefore an ideal energy resource in which mobile applications are stored in units of hydrogen and other industrials. The usefulness of hydrogen can be seen by issues such as energy sourcing, including fossil fuel use, greenhouse warming, and sustainable energy generation, because hydrogen is an environmentally friendly energy, particularly in transportation applications, without release of pollutants. Advantages of using hydrogen are as follows:

1. Hydrogen can be easy to transport as a gas or liquid, as well as various storage conditions like a high-pressure gas, cryogenic hydrogen and metal hydride.

2. Water as a hydrogen resource is virtually unlimited and it is possible to recycle the used water.

3. Hydrogen as a fuel is not published as any polluted material except a small quantity of NO_x. Applications of hydrogen energy are unlimited.

Even though hydrogen energy has a variety of advantages, one of the major issues affecting the acceptance of hydrogen for public use is the safety of hydrogen installations as well as its applications. The actual effect of a leakage in a confined space, such as hydrogen stored tanks, would generate a hazardous situation, which may cause severe damage to the environment and human health. Therefore, many researchers are attempting to develop simulations on hydrogen dispersion as 1D or 2D computational analyses [1,2]. In fact, the properties of hydrogen gas dispersed from a storage facility are changed with 3D geometry, whereas the risk estimation for a storage tank imposes the presence of obstacles within the flow field. In this study, several chemical hazards associated with hydrogen storage facilities and distribution systems are described.

Powerful computational tools based on fluid dynamics have been developed, allowing for an integrated approach on complex geometries and/or physicochemical transport phenomena [3]. In this study, computations on dispersion of a hydrogen facility were carried out for a hypothetical hydrogen release scenario, using the validated CFD (computational fluid dynamics) code named by Fluent.

PRELIMINARY SCENARIO FOR HYDROGEN RELEASE

Hydrogen is stored either in gaseous state under high pressure and normal temperature, or in liquid state under low temperature and moderate pressure. Recently, an interesting system for hydrogen production was reported, such as a hybrid adsorbent-membrane reactor compared with a conventional packed-bed reactor for hydrogen production [4]. In any case, there is a significant risk, such as mechanical explosion of hydrogen vessels when exposed at high temperature or thermal radiation. In addition, there are various elemental for the hydrogen hazards.

At hydrogen refilling stations and vehicles, hydrogen has to be compressed at high pressures (typical 400 bar), due to the low-energy content per unit volume. Nevertheless, in some applications, hydrogen as well as other gases (i.e., carbon dioxide, nitrogen, helium, and methane) needs to be stored in liquid state at very low temperature for a volumetric restriction. Hydrogen is kept liquefied at extremely low temperatures below −240 °C and moderate pressures (20-30 bar). Hydrogen release and dispersion at cryogenic conditions have a unique behavior according to its physical properties. The scenario is shown in Fig. 1.

SIMULATION AND RESULTS

CFD computational tools have been successfully used for providing hydrogen gas dispersion estimations [5,6]. A CFD method in Fluent code, particularly, follows a general deterministic procedure to approximate the problem; it considers the fundamental governing equations for mass, momentum, and heat transfer processes, in conjunction with other partial differential equations for describing

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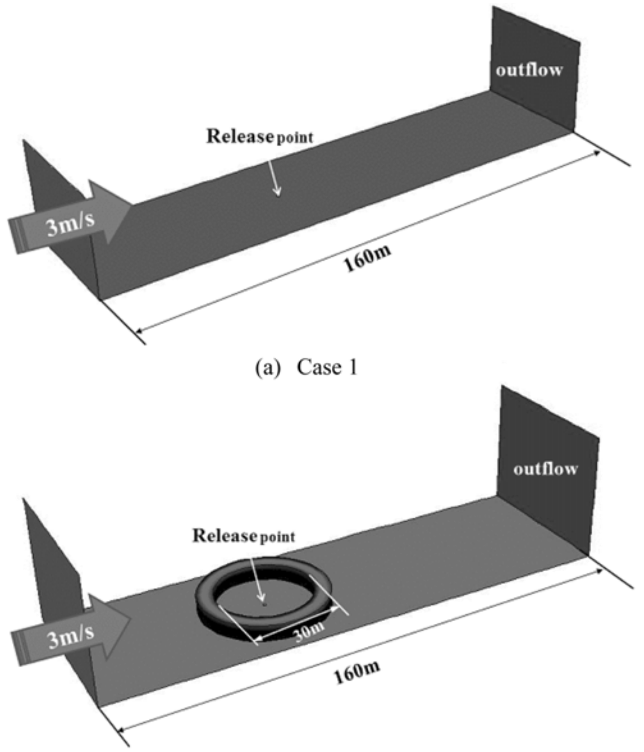

Fig. 1. Schematic drawings for present scenarios of hydrogen release.

further processes such as turbulence. Fluent code incorporates the κ-ε model for turbulence modeling. The first step in a CFD simulation project includes the definition of the 3D geometry (computational domain), in addition to the sub-division of the entire domain into a number of smaller control volumes (cells) that form a mesh. The geometry consists of a unified set of parametric surfaces built in GAMBIT CAD software suitable for Fluent.

The code runs for a typical accidental release scenario, which includes hydrogen discharge under pressurization and liquefaction conditions in a 160×50×40 m^3 computational domain, which was subdivided as shown in Table 1. Hydrogen release was modeled as a ground-level area source with inflow rate equal to 2 kg/s for 5 s, whereas typical atmospheric conditions (1atm, 20 °C), ground temperature equal to 15 °C and wind speed equal to 3 m/s were considered. The time step used for the transient problem solution was 0.2 s and total simulation time was 60 s. Two scenarios were considered in the CFD simulations: a hydrogen release at cryogenic conditions without any obstacle (case 1) and with a obstacle (case 2) (see Fig. 1).

1. Turbulence Modeling (κ-ε)

Turbulence flow can be defined as the viscous flow in which fluid particles move in a random and chaotic way within the flow field.

Table 1. Computational domain for present geometries

Case	Volume cell	Face cells	Node
1	32840	102464	36861
2	36015	150342	45369

The designation of viscous flow refers to the flow of a real fluid regardless of its viscosity value. Velocity and all other fluid properties vary continuously, with strong concurrent molecular mixing between adjacent fluid layers. In atmospheric flows, turbulence is the dominant mechanism in the mixing and dilution of gaseous releases [7], associated with the presence of natural obstacles, human structures and ground surface roughness.

The κ-ε model is one of the most prominent turbulence prediction tools implemented in many general purpose CFD codes. It has proven to be stable and numerically robust, having a well established predictive capability. The κ-ε model uses the scalable wall-function approach instead of standard wall functions, improving robustness and accuracy when the near-wall meshes in very fine. The κ-ε model introduces two new variables into the system of conservation equations, which take the form [8,9]:

$$\frac{\partial p}{\partial t} + \nabla(\rho U) = 0, \quad (1)$$

$$\frac{\partial \rho U}{\partial t} + \nabla(\rho U \otimes U) - \nabla(\mu_{eff}\nabla U) = \nabla p' + \nabla(\mu_{eff}\nabla U)^T + B, \quad (2)$$

where B is the sum of body forces and p' the modified pressure given by

$$p' = p + \frac{2}{3}\rho k, \quad (3)$$

and

$$\mu_{eff} = \mu + \mu_t, \quad (4)$$

The κ-ε model assumes that the turbulence viscosity is linked to the turbulence kinetic energy and dissipation via the relation

$$\mu_t = \frac{C_\mu \rho k^2}{\varepsilon} \quad (5)$$

The values of κ and ε are directly calculated from the differential transport equations for the turbulence kinetic energy and turbulence dissipation rate

$$\frac{\partial(\rho k)}{\partial t} + \nabla(\rho U k) = \nabla\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + P_k - \rho\varepsilon, \quad (6)$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla(\rho U\varepsilon) = \nabla\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right] + \frac{\varepsilon}{k}(C_{\varepsilon 1}P_k - C_{\varepsilon 2}\rho\varepsilon), \quad (7)$$

where P_k is the turbulence production due to viscous and buoyancy forces, which is modeled by using

$$P_k = \mu_t \nabla U(\nabla U + \nabla U^T) - \frac{2}{3}(\nabla U)(3\mu_t\nabla U + \rho k) + P_{kb}. \quad (8)$$

2. Hydrogen Releases

Figs. 2 and 3 show the concentration distributions of hydrogen and flow configurations at cryogenic conditions. The results demonstrate substantial dissimilarity between open and closed hydrogen release conditions as far as cloud dispersion is concerned. Hydrogen cloud spreading is similar to that of liquefied natural gas that has been experimentally observed in field-scale trials [8], namely, horizontal cloud shift at low height. The great inertia of the heavy cryogenic gas reduces the rate of turbulent mixing leading to delayed

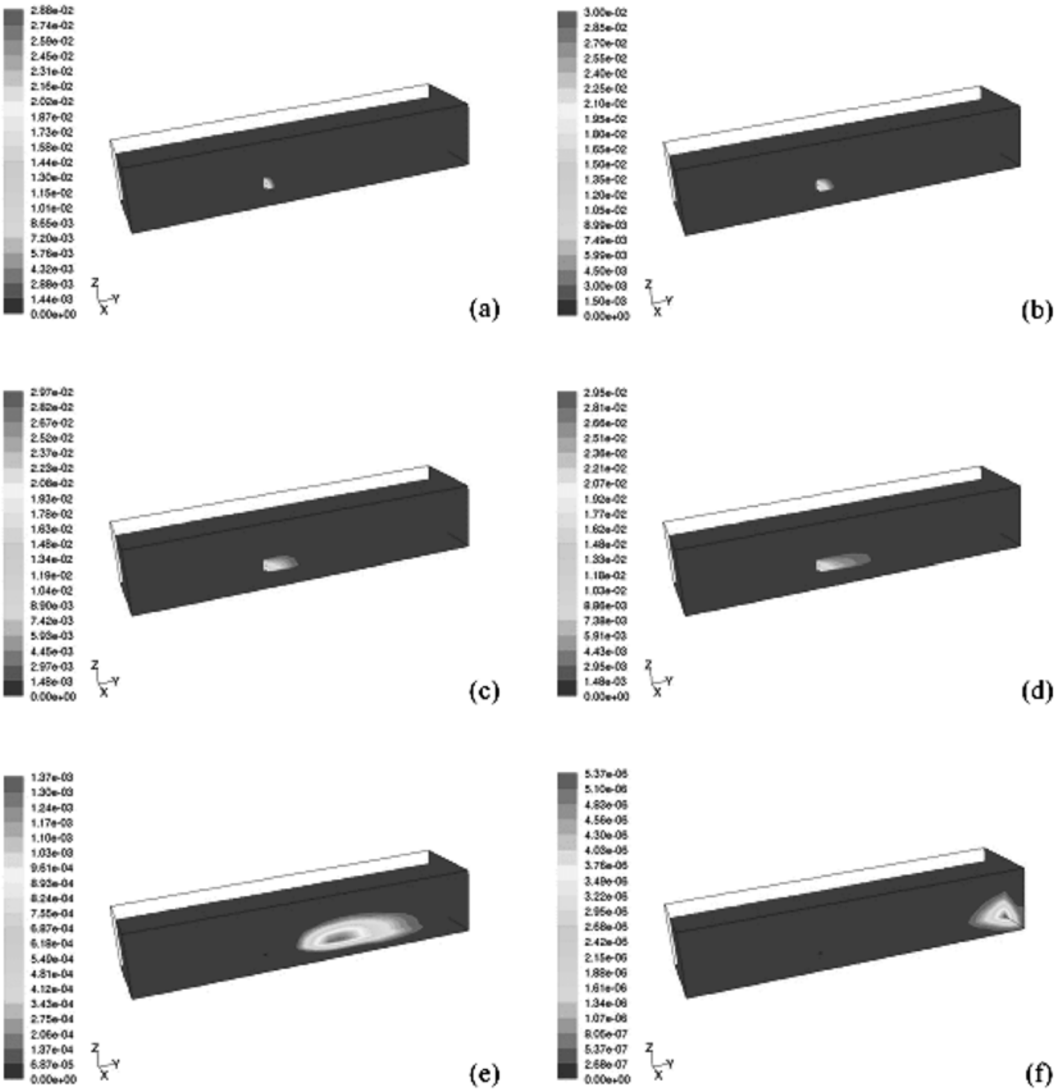

Fig. 2. Simulated dispersion snapshots following cryogenic hydrogen release at time (a) 1 s, (b) 2 s, (c) 5 s, (d) 10 s, (e) 20 s and (f) 60 s after release.

dissolution times, whereas the greater density of the cloud produces a gravity-driven flow which tends to reduce the cloud height and increase width. In contrast with lighter-than-air gas, the residence of a heavy cloud at low height increases significantly the risk of ignition.

The releases of cryogenic hydrogen gases differ from conventional hydrogen releases. The releases consist of different component mixtures of gases and liquids. There may be heat and/or mass transfer with the ground surface and the ambient air. Phase changes of the released material during the cloud formation typically take place. The density difference between the released cryogenic hydrogen and the atmospheric air results in specific physical processes influencing the heavy hydrogen gas dispersion in the atmosphere. Major physical processes specific for negatively buoyant clouds include the gravitational velocity field, wind shear at the cloud interfaces, turbulence dumping and inertia of the released material.

The gravitational velocity field is produced due to horizontal density gradients. It is an additional transport mechanism to the ambient wind field. It results in heavy hydrogen gas clouds with an increase in the horizontal and a reduction in the vertical dimensions in comparison to gravitational flow which causes the shear at the ground cloud interface and at the air cloud interface. It may result in intermingling of a heavy gas cloud with the surrounding air and eventually in turbulence generation. This mechanism becomes important when the wind velocity is small and the self generated velocity large. The stable clouds have negative vertical density gradients. This phenomenon results in dumping the turbulence and turbulent mixing in the clouds and in the wind flow over them. One more obvious point is the density difference between the released hydrogen and the atmospheric air passive dispersion. In addition to the volume, or the volume plays an important role not only in delineating the cloud behavior but also in releasing the heavy hydrogen gas or flux of the released substance, parameters characterizing the ambient flow such as the wind velocity and the source dimensions are needed.

In Figs. 2 and 3, in the first case the hydrogen cloud was raised immediately with horizontal direction (Fig. 2), while in the second case, it remained within the bank for a long time period (Fig. 3).

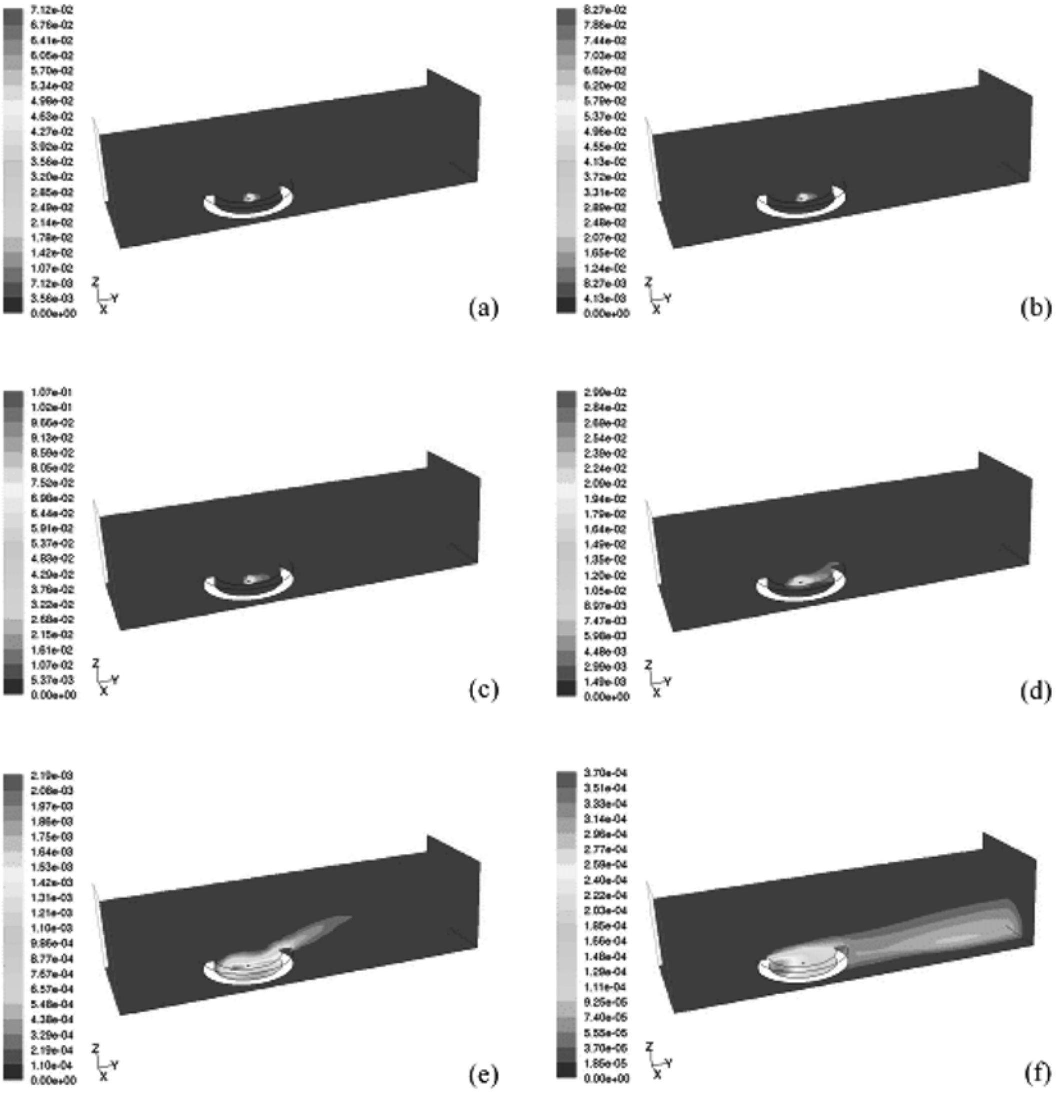

Fig. 3. Simulated dispersion snapshots following cryogenic hydrogen release with a bank at time (a) 1 s, (b) 2 s, (c) 5 s, (d) 10 s, (e) 20 s and (f) 60 s after release.

When the cryogenic hydrogen flowed at the dispersion constraint bank, hydrogen dispersion was restrained due to the obstacle. It should be noted that hydrogen was not transported to the atmosphere and its explosion possibility was also increased at the surroundings of the release point. It is very important to exclude an ignition material when we construct a restraint obstacle at the cryogenic hydrogen surrounding. As shown in Fig. 3, the spreading hydrogen cloud is similar to that of liquefied natural gas that has been simulated by Rigas and Sklavounos [1], where horizontal clouds were transported low height. It is considered that the greater inertia of the heavy cryogenic hydrogen reduced the rate of turbulent mixing, whereas the lighter density of the cloud produces a buoyancy-driven convection which tends to enlarge the cloud height and decease its width [10]. At a short time period of up to 5 s, which is the release time, the dispersion behaviors are similar to each other, as shown in Figs. 2 and 3. After 5s, a drifting flow over the bank was described in (d), (e) and (f) of Fig. 3. And also, a highly concentrated point of hydrogen without a bank moves downwards along the wind after release while the hydrogen remains within a bank in Fig. 3.

Fig. 4 shows the concentration distributions of cryogenic hydrogen release during the flow time. In the first case, the hydrogen concentration distribution is reached a little to the right side, due to the wind flow effect at the start of release, while in the second case, its distribution is located at the center of the dispersion point (at 60 m from lift side). As a result, it is the effect of the constraint obstacle. After that, the hydrogen distributions for the formal case are spread over the whole area and, finally, disappear after 60 s, while latter case's hydrogen concentration remain also after the 60 s. The hydrogen concentration for the latter case remains constant after 60 s. It is obvious that even if a hydrogen release constraint obstacle is used to limit the dispersion of hydrogen, it is more dangerous due to the high concentration of hydrogen around the emission point.

Furthermore, as shown in Fig. 4, case 2 still has high concentrations after a release. It is evident that the experimental variability for the dispersion of liquefied hydrogen releases is very important, whereas computational maxima are obtained from single point meas-

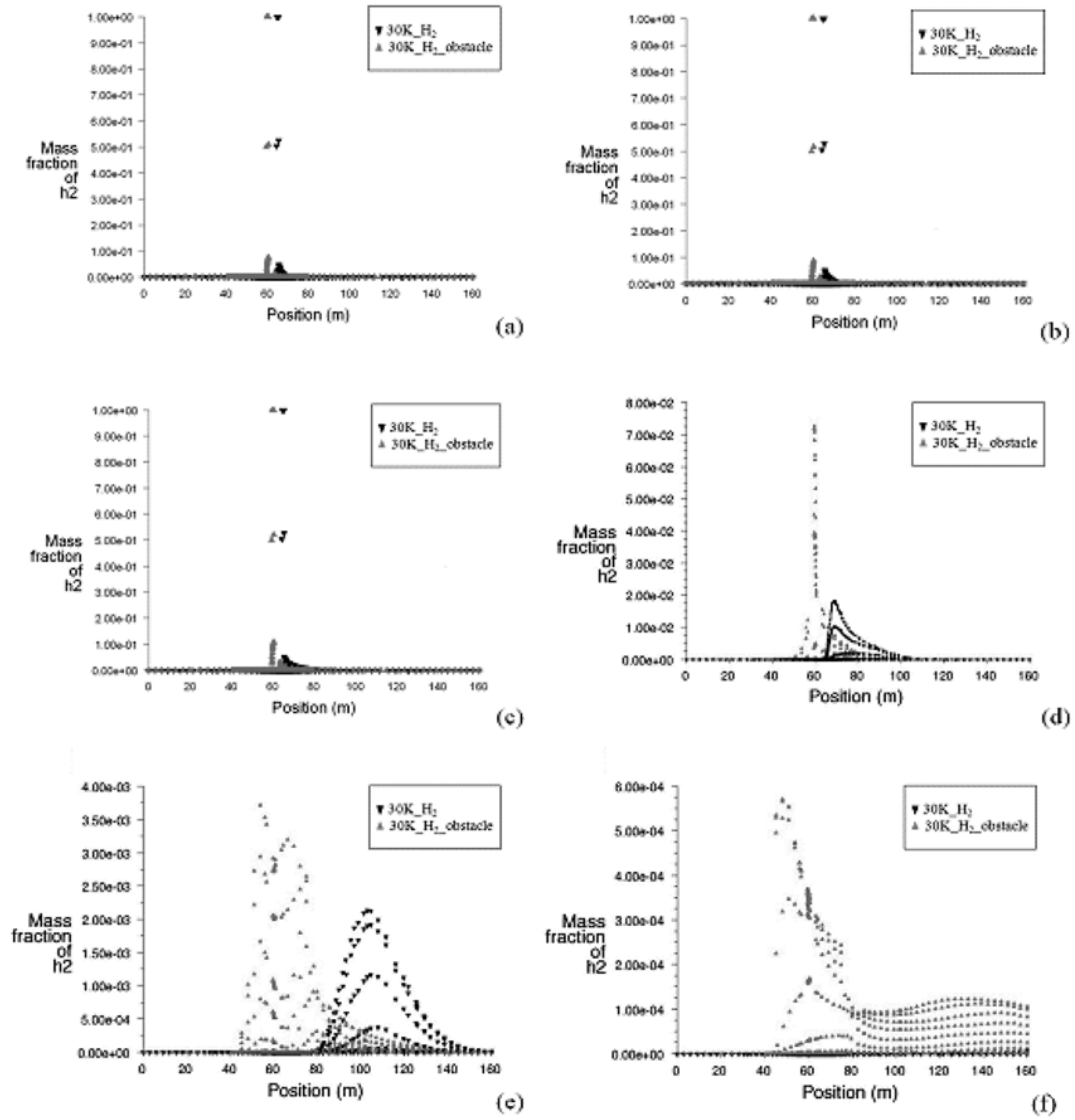

Fig. 4. Simulated concentration distributions of cryogenic hydrogen release during the flow at time (a) 1 s, (b) 2 s, (c) 5 s, (d) 10 s, (e) 20 s and (f) 60 s after release.

urements. Therefore, the deviations between the reported data by Rigas and Sklavounos [1] and the present results may not be as great as they appear.

CONCLUSION

In this study, the main flow configuration and hydrogen distributions associated with hydrogen storage procedures were analyzed. The atmospheric dispersion of cryogenic hydrogen released was simulated also by using the computational fluid dynamics code Fluent. The results showed that hydrogen disperses as a heavier-than-air gas when discharged in cryogenic conditions and dispersion with constraint obstacles. In case 1, hydrogen is spread relatively quickly, as compared with case 2. Visualization of computer-simulated cryogenic hydrogen dispersion demonstrated that hydrogen cloud behavior in this case is similar to that of liquefied natural gas experimental releases. And accidental liquefied hydrogen release scenarios were addressed as heavier-than-air releases by using the appropriate dispersion models.

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