SIMULATION AND SAFETY ANALYSIS OF THE LEAKAGE OF LIQUEFIED HYDROGEN FROM HIGH-PRESSURE CONTAINER

by

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In this paper, the leakage and diffusion of liquefied hydrogen (LH2) which is stored in high-pressure container were investigated and the safety arrangement in cosmodrome focused on the effects of external flow on the above process was proposed. The phase transition process of leakage of LH2 at the initial stage was first analyzed by considering the motion of single particle and particle group. Furthermore, the rule of leakage and diffusion of LH2 under different conditions was thoroughly examined by CFD modeling. Through this work, the leakage pressure, leakage location, external airflow direction and external airflow velocity are found to have great effects on the diffusion of leaking hydrogen. By increasing the leakage pressure and putting leakage port closer to ground, the diffusion and dilution of leaking hydrogen would be strongly expedited to spread much further away. By adopting upper air blow and raising the external air speed, the concentration can be fairly reduced.

Key words: *liquefied hydrogen (LH2), leakage, CFD, phase transition*

Introduction

As a clean propellant, LH2 possesses high energy density and has the good cooling and combustion performance [1]. In 1903, hydrogen and oxygen were first proposed to be used as a propellant by Konstantin and Byrne; American company “Pratt and Whitney” carried out the attempt to use LH2 as rocket fuel in 1955; by 1960, LH2 became one of the qualified fuels for rocket engine [2].

The leakage accident of LH2 will generate large amounts of hydrogen gas due to phase change resulting from the evaporation. Due to the low molecular weight and viscosity, the leakage rate of LH2 is 50 times that of water, and 10 times that of liquefied nitrogen [3]. In addition, the gasification rate of LH2 is 6.1 times than that of the liquefied nitrogen, and 7.5 times that of liquid hydrogen [4]. Considering the large density of LH2, downwind area in leakage case easily become combustible area, where the volume fraction of hydrogen in the mixture of gasified hydrogen and air is 4%-75% [5]. Due to the high energy density, hydrogen combustion is characterized by high flame

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temperature and fast flame spread, which often appears as deflagration especially the detonation and result in serious human injury and equipment damage [6-7]. In 1988, Raymond [8] analyzed the fracture pressure of storage tank, and the heat flux in the process of LH2 explosion. Since the evaporation of LH2 is the premise of combustion, Nakamichi [9] used high-speed CCD camera to measure the evaporation rate after LH2 ejection. It was found that the diameter of LH2 droplet, which is affected by the temperature and the leakage hole size of LH2 jet. Raj [10] analyzed the diffusion feature of the liquefied natural gas (LNG) in the water and especially studied the gasification process of the LNG. The complete gasification time and distance of the LNG was obtained by theoretical calculation in this study. Ichard [2] predicted the evaporation and diffusion of LH2 based on two-phase simulation in FLACS. The study found that the cooling effect of LH2 on the ambient air will induce the rise of LH2 and the behavior of hydrogen cloud in the air will present more obvious buoyancy effect. The studies of Najjar [11] and Lowesmith et al. [12] were focused on the security of the liquefaction, transportation and use of LH2 and emphasized that safety assessment. Giannaissi [13] simulated both horizontal and vertical diffusion of LH2 leakage based on the CFD software "ADREA-HF" and investigated the influence of the humidity in the air on LH2 diffusion. Hallgarth et al. [14] compared the simulation results of LH2 leakage with the experimental data from of NASA in 1980, and found atmosphere stability plays an important role in the formation of hydrogen cloud.

In addition to the leaking process, a serious research was to study the safety of LH2. Zhang et al. [15] and Wang et al. [5] investigated the risk of low temperature, deflagration and detonation of LH2 in the leakage and gasification progress and suggested some technical safety control methods. They also found that the appearance of oxygen-solid and air-solid as the low temperature of LH2 would easily cause the explosion. Through experimental analysis, Hu et al. [16] studied the explosion limit of flammable mixture gas and the transition condition between deflagration and detonation, which showed that the detonable range of the hydrogen and oxygen mixture is 25%-84% in volume ratio. Du et al. [17] studied the effects of storage tanks layout on the damage size and range of the explosion based on the analysis of shock wave in the explosion hazard of LH2.

The leakage and diffusion of LH2 in a space filled by air is a quite complex process, which include phase transition, component transport and multiphase flow. Most of past experimental studies were focused on the flow evolution after the full gasification of LH2, and only theoretical analysis and some simple numerical simulation studies on the phase transition process have been done. In this study, the process of LH2's leakage and diffusion was studied based on CFD modeling. In this work, we studied different leaking conditions with different effect factors, including leakage pressure, the position of leakage hole, the flow velocity and direction of ambient air. Especially, the phase transition process of LH2 at the initial stage was analyzed in view of single particle and particle group.

Initial Phase Transition

Single Particle of LH2

When LH2 leaks from the storage tank to environment, it is a transition process from a cryogenic environment to a normal temperature environment. Due to the high ambient temperature, evaporation of LH2 drops will be achieved in a very short time. Although the phase transition process is rapid, it is not a simple step, which consists of the initial appearance of LH2 particles with different diameters, the following shrinking and eventually complete evaporation.

In this part, the evaporation process of a single drop of LH2 was studied in order to get the time of full evaporation. The evaporation and gasification follow the occurrence of leakage, thus, the calibration of the leakage process is essential for the following gasification. The leakage velocity was calculated by

$$\vec{u}_J = C_0 \sqrt{\frac{2gPg}{\rho_J}} \tag{1}$$

where Pg is pressure change between inside and outside of storage tank, MPa; ρ_J is the density of leakage LH2, [$\mathrm{kg/m^3}$]; C_0 is the leakage factor, which is decided by the Re number and the diameter of leakage hole, in the case of some sharp mouth or leakage with $Re > 30000$, $C_0 = 0.61$, which is the value used in our study.

Table 1. Phase transition parameters of LH2 particle

	Case 1	Case 2	Case 3
Leakage temperature (K)	21	22	24
Leakage pressure (MPa)	0.15	0.2	0.3
LH_2 density in leakage case (kg/m^3)	70	68.5	66
Leakage velocity (m/s)	118.38	169	243
Surface tension coefficient (N/m)	0.002	0.0019	0.0015
Dynamic viscosity (Pa/s)	0.000013	0.0000122	0.0000116
Evaporation heat (J/kg)	440000	426000	412000
Saturation temperature (K)	21.672	22.805	24.571
Largest liquid drop diameter (m)	2.26e-6	2.04e-6	1.55e-6
Complete gasification time (s)	0.00052	0.00046	0.00027
Complete gasification distance (m)	1.41e-5	1.19e-6	5.5e-7

In order to describe the evaporation process of a single drop, the diameter, the full evaporation time and distance, and evaporation frequency are required, which were calculated based on the processing procedure of Raj and Bowdoin [10]. The evaporation process of LH2 particle was calculated with different leakage temperature and pressure. These temperature and pressure were selected following the experiments conducted by HSL in Buxton, UK in 2010 [18], in which the leakage temperature is 20K and the leakage pressure is 0.2MPa. The parameters for the phase transition of LH2 particle are shown in table 1.

Particle Group

The phase transition process of liquid hydrogen is the emission of liquid hydrogen from a low temperature environment to a high temperature environment to produce hydrogen and spread in the air entrainment, which is a process with multi-phase and multi-component. In the simulation, we defined the function to calculate this process focused on the heat needed for the evaporation of LH2.

Based on saturation temperature shown in table 1 in three cases, the phase transition happens when the temperature, detected in some calculation element, is larger than the saturation temperature. The volume fractions of LH2 and hydrogen gas in every calculation element were calculated based on the defined functions in CFD.

Simulation Details

The simulation domain is a 8000×2000×2000mm rectangular flow region (Fig. 1). In this figure, the leakage hole described by the inlet is a circular hole with diameter of 2 mm, the X direction shows the centerline of hydrogen jet evolution. The face, where the inlet locates, and the ground face are set to be wall boundary; other faces are set to be pressure outlet. The governing equations of leakage and diffusion of LH2 includes the conservation equation of mass, momentum and energy for the multi-phase mixture.

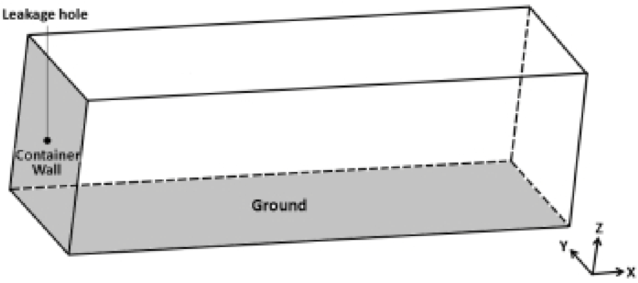


Fig. 1 Schematic of simulation calculation region

Table 2. Initial condition of experiment and simulation

	LH_2 temperature(K)	Air temperature(K)	Diameter of leakage hole (mm)	Leakage velocity (m/s)
HSL[18]	20	280	26.3	163

Results and Analysis

Grid Independence Study and Simulation Results Verification

The simulation was carried out with four different grid densities and Fig 2 shows the volume fraction along the centerline at the symmetry face. It shows that good grid convergence is achieved in the simulation. In the following analysis, result data is from simulation with grid number N=845600. The simulation result shows similarity with HSL’s experiment data. Due to the uncertainly in the leakage experiment, the simulation data demonstrated in Fig. 3 is considered to be accurate.

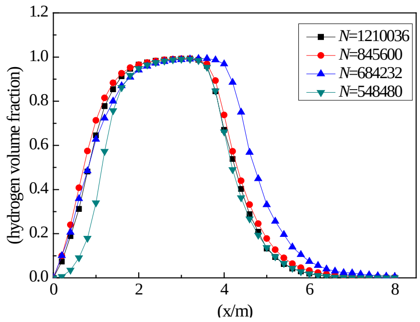


Fig. 2 Volume fraction of hydrogen with different grid number

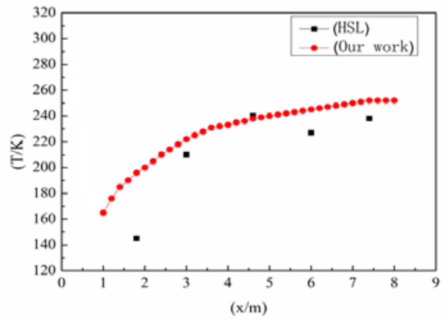


Fig. 3 Temperature along the centerline at the symmetry face

Cases with Different Leakage Pressure

In the section, the effect of leakage pressure is investigated by analyzing a set of different storage pressure conditions, which are given in Tab. 2. When the leakage pressure is varying in the simulation cases, the diameter of leakage hole is 2 mm and the leakage position off the ground is 1m for different cases.

Table 3. Cases with different leakage pressure

	Leakage pressure(MPa)	Leakage velocity (m/s)	Atmosphere Pressure (MPa)	Velocity of ambient air (m/s)
1	0.15	118.38	0.1	0
2	0.2	169	0.1	0
3	0.3	243	0.1	0

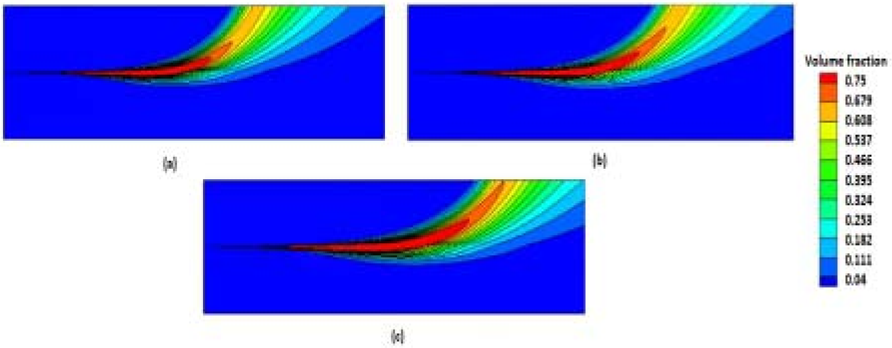


Fig. 4 Volume fraction of hydrogen at the symmetry face: (a)0.15MPa; (b) 0.2MPa; (c) 0.3MPa

Based on the results of Fig. 4, because of the increase of the leakage pressure of LH2, the corresponding saturation temperature will increase. As shown in Tab. 3, the difference between ambient temperature and saturation temperature is small, which is easy for LH2 to reach its evaporation temperature. With the increase of leakage pressure, hydrogen leakage distance is extended, and the hydrogen flammable area (4%-75%) with the increase of pressure is bigger.

Fig. 5 shows the temperature distribution for the leakage of LH2 under three different leakage pressure conditions. In the contour, the deep red color represents the ambient air zone with higher temperature, and the dark blue represents the LH2 zone with lower temperature. With leakage pressure increases from 0.15MP to 0.3MP, the relatively low temperature zone gets extended and larger LH2 leakage area is formed. Therefore, the increase of leakage pressure can increase the hazard area by enforcing the leaking of LH2 in larger extent.

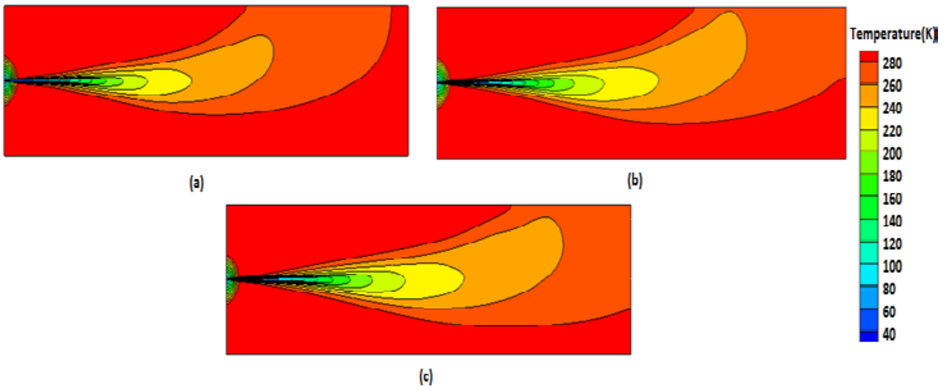


Fig. 5 Diffusion temperature at the symmetry face: (a) 0.15MPa; (b) 0.2MPa; (c) 0.3MPa

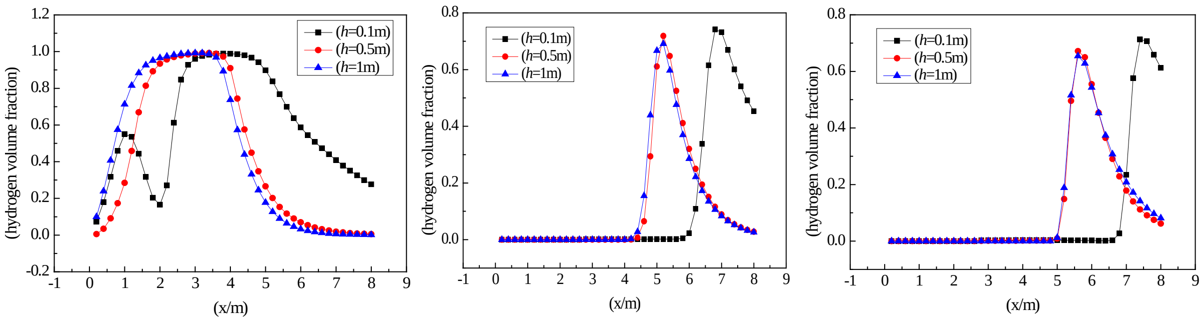
With the increase of leakage pressure, the upper part of low temperature zone extends backwards, the leakage rate increases and more liquid hydrogen leaked from the container. The entrainment of ambient air increases as the leakage rate of hydrogen increases; moreover, the heat transfer is strengthened which produce larger low temperature zone. Therefore, the hazard of the low temperature of LH2 will increase with the increase of leakage pressure.

Cases with Different Leakage Hole Position

Table 4. Cases with different height of leakage hole

	Leakage pressure (MPa)	Atmosphere Pressure (MPa)	Velocity of ambient air (m/s)	Height of leakage hole (m)
1	0.2	0.1	0	0.1
2	0.2	0.1	0	0.5
3	0.2	0.1	0	1

The change of the location of leakage hole "*h*" will significantly affect the characteristics of the diffusion of LH2. When the leakage hole is close to the ground, the concentration distribution changes dramatically. Therefore, the concentration accumulation behavior near the ground should be focused in this study. In this section, LH2 leakage and diffusion under different leakage locations will be given. The initial condition of cases considered is given in Tab. 4.



(a) (b) (c)

Fig. 6 Volume fraction of hydrogen along the horizontal line off leakage hole at the symmetry face: (a) axis line along leakage hole；(b) 0.5m from leakage hole；(c) 1m from leakage hole

The Fig. 6 shows the volume fraction distribution along the horizontal line at three different vertical locations. One obvious observation is that in case “c” the peak value of volume fraction along the horizontal line gets significantly pushed downstream by about 2 meters. From the finding in Fig. 7, it is confirmed that the closer the leakage hole is against ground, the further the leaking can pass down.

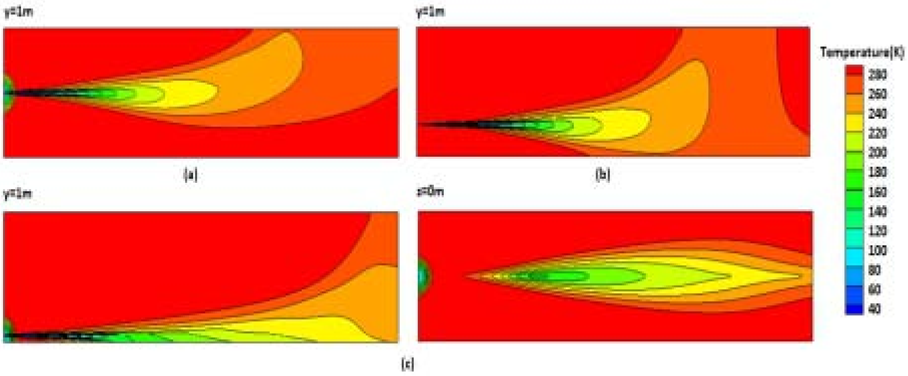


Fig. 7 Diffusion temperature at the symmetry face: (a) *h*=1m; (b) *h*=0.5m; (c) *h*=0.1m and floor

Fig. 7 shows that the leakage position has shorter distance from the ground. The low temperature area spreads further. The low temperature zone represents the leaking LH2 from cold tank. When the leakage position is close to ground, the leaking motion and hydrogen transports in spanwise direction and positive direction of Z will be confined by the ground, shown by Fig. 8(c).

Safety Analysis and Evaluation

In above sections, the leakage of LH2 was simulated in the windless environment. Actually in the real environment one breeze environment generally exists, and the existence of the wind flow is crucial for the spread of LH2 leakage flow. The influence of the wind will make hydrogen concentration distribution greatly change. In this part, we will simulate the liquid hydrogen leakage under different wind directions. “Upper wind” represents the negative direction of z and “Upwind” represents the negative direction of x axis.

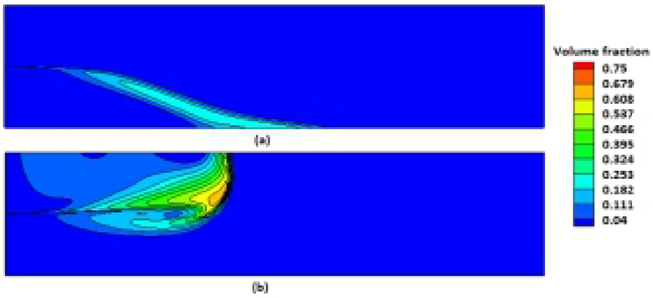


Fig. 8 Volume fraction of hydrogen at the symmetry face: (a) upper wind; (b) upwind

Fig. 8 shows the wind has a great influence on the hydrogen distribution. The wind can induce hydrogen accumulation, and make the diffusion distance shorter. The upper wind can accelerate the diffusion of hydrogen, and make hydrogen concentration lower. The wind is good for the hydrogen diffusion, and the upper wind is better than the upwind case.

Based on above results and analysis, the control strategy of hydrogen diffusion can be proposed as follows：

(1) The leakage height of LH2 storage tanks is proved to affect the hydrogen concentration distribution. Therefore, the storage tank should be designed to have bottom hanging over the ground or adopt enforced material for bottom part. By doing this, the chance of leakage is reduced and even leakage occurs, the hazard effect would be reduced to a low level;

(2) The existence of wind flow will promote the diffusion of hydrogen, and especially the wind is coming from the upper wind direction has the greatest effect on promoting the diffusion. When LH2 leaks, the wind from the upper wind direction can notably dilute the hydrogen. Therefore, the storage tank should be placed on some place which has good venting condition. If possible, fans can be installed to bring in venting flow.

Conclusion

This study is focusing on the leakage and diffusion of LH2 using CFD modeling. The simulation of liquid hydrogen with different leakage pressures and different leakage hole position was performed to characterize the leakage process. From analytical and simulation results, it is shown that the large area range of low-temperature hazard zone of LH2 and hydrogen combustible are induced by large leakage pressure and the location of leakage hole to the ground. It also demonstrates that the external airflow can slow down the accumulation of the hydrogen gas and the upper blow wind is the most favorable way to dilute the concentration of hydrogen. Furthermore, the control strategy of the leakage and diffusion of liquid hydrogen is proposed to reduce the dangers of the leakage and diffusion of liquid hydrogen in cosmodrome. The prominent findings in this work can be used as the fundamental guidance for designing liquid safety forecasting system of hydrogen leakage.

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Nomenclature

$\vec{u}_J$ —leak velocity,[m/s]
ρ_J —the density of leakage LH2,[$\mathrm{kg/m^3}$]
Re—Reynolds number
h —the location of leakage hole, [m]
Pg —pressure change, [MPa]
C_0— leakage factor
N—number of grid

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