Influence of flash evaporation on safety Characteristics of Liquid Hydrogen Leakage and Diffusion

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Abstract: During the storage and transportation of liquid hydrogen, damage of pipeline or sealing failure of valve may cause liquid hydrogen leakage. The cryogenic and combustible hydrogen produced by the leakage are dangerous. Because the storage pressure is higher than atmospheric pressure, flash will occur in leakage accident, resulting in LH2 / H2 two-phase flow at the leakage port. In order to study the effect of flash evaporation on the hydrogen diffusion characteristics, the CFD method is used to simulate the liquid hydrogen leaking and diffusing process at different mass fractions of flash evaporation. The results show that the horizontal distance of combustible cloud diffusion is 15.6m when the liquid hydrogen leaking amount is 60L / min. When 14% liquid hydrogen flashes, the horizontal distance of hydrogen diffusion reaches 24.1m, and with the increase of flash evaporation, the horizontal distance increases significantly. With the increase of flash evaporation, the horizontal distance of cryogenic hazardous zone increased from 6.3m to over 9m. It can be concluded that flash evaporation has adverse influence on the safety after a liquid hydrogen leakage accident, which greatly increases the distance of combustible cloud dispersion and cryogenic hazardous areas.

1. Introduction
As a cryogenic propellant, liquid hydrogen has the advantages of large specific impulse and environmental protection, and has important application value in the aerospace launch site. During the production, storage, transportation and filling of liquid hydrogen, leakage may occur at the transportation pipelines and valves. Hydrogen is colorless and odorless, and it is difficult to find when a small amount of liquid hydrogen leaks. When the leak is slightly larger, the leaked liquid hydrogen cools the water vapor in the surrounding air. There is obvious water mist near the leak and condensation on the wall water droplets. The continuous leakage of liquid hydrogen will form a quasi-steady-state hydrogen cloud in the downwind direction. Clouds with a volume fraction in the range of 4% -75% [1] are dangerous areas where explosions may occur. The temperature below 233.16K [2] may cause frostbite of workers and brittle fracture of pipeline equipment.

At present, researchers mainly study the leakage and diffusion of liquid hydrogen through experiments and numerical simulations. Due to the difficulties in production and storage of liquid hydrogen, high cost and high risk, a few tests of LH2 spills have been carried out. Typical experiments include the experimental of large-scale liquid hydrogen spills by NASA [3] in 1981 and the experimental releases of liquid hydrogen by HSL [4 ] in 2010. The NASA test recorded the dynamic process of visible hydrogen clouds generated by the liquid hydrogen evaporation, and obtained the data of the size of the liquid pool and the hydrogen concentration at measure tower. A pipe with a
diameter of 26.3mm used to releases the liquid hydrogen from storage tank by HSL. The effect of the leak height on the diffusion characteristics of the hydrogen cloud was analyzed by adjusting the height of the pipe.

In order to investigate the influence of various factors on the dispread of flammable clouds when liquid hydrogen spills, the researchers simulated the process of liquid hydrogen leakage and diffusion through CFD method. Sklavounos [5] used CFX software to simulate the large-scale LH2 spills and concluded that the initial stage of diffusion hydrogen is manifested as heavy gas. Ichard et al. [6] simulated the liquid hydrogen leakage experiment of HSL through FLACS software, and verified the feasibility of numerical simulation. Wu Mengxi [7] analyzed the influence of nitrogen and oxygen phase transition on liquid hydrogen spills, and conclusion that the simulation results considering the phase transition of nitrogen and oxygen are more consistent with the experimental data. Shao Xiangyu [8] studied regular of hydrogen cloud diffusion after the leakage of liquid hydrogen, and obtained the distribution of hydrogen cloud at time history.

The storage pressure of liquid hydrogen is higher than atmospheric pressure. After the liquid hydrogen leaks, due to the sudden decrease in pressure, the liquid hydrogen vaporizes rapidly, and the current status of flash evaporation occurs. At the same time, the large temperature difference near the leakage port will exacerbate the vaporization phenomenon. Therefore, the fluid at the leakage port can be regarded as a gas-liquid two-phase flow of liquid hydrogen and cryogenic hydrogen. In this paper, the numerical model of liquid hydrogen leakage and diffusion is established, and the diffusion characteristics of hydrogen cloud under different mass fractions of flash vaporization are analyzed.

2. Numerical calculation method

The liquid hydrogen spills is a gas-liquid flow process. The Mixture model is used to simulate the multiphase flow, and the phase slip and surface tension balance are considered. The liquid hydrogen evaporation phase transition model uses the Lee model and the evaporation coefficient is set to 0.25. Hydrogen diffusion in air adopts the component transportation model, and the turbulence model adopts the Realizable $\kappa - \varepsilon$ model. The specific control equations are as follows:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \left( \rho_m \bar{v}_m \right) = 0$$

$$\frac{\partial}{\partial t} \left( \rho_m \bar{v}_m \right) + \nabla \cdot \left( \rho_m \bar{v}_m \bar{v}_m \right) = -\nabla p + \nabla \cdot \left[ \mu_m \left( \nabla \bar{v}_m + \nabla \bar{v}_m^T \right) \right] + \rho_m g + F + \nabla \cdot \left( \sum_k \alpha_k \rho_k \bar{v}_k \cdot \bar{v}_k \right)$$

$$\frac{\partial}{\partial t} \sum_k \left( \alpha_k \rho_k E_k \right) + \nabla \cdot \left( \sum_k \alpha_k \bar{v}_k \left( \rho_k E_k + p \right) \right) = \nabla \cdot \left( k_{eff} \cdot \nabla T \right) + S_g$$

The volume fraction equation of the liquid phase is

$$\frac{\partial}{\partial t} \left( \alpha_l \rho_l \right) + \nabla \cdot \left( \alpha_l \rho_l \bar{v}_l \right) = -\nabla \cdot \left( \alpha_l \rho_l \bar{v}_g \right) + \sum_{\nu=1}^{n} \left( \bar{m}_{l-v} - \bar{m}_{v-l} \right)$$

Where $\rho_m$ is the mass average density, $\bar{v}_m$ is average speed, $\alpha_k$ is the volume fraction of phase $k$, $\bar{v}_{k,\bar{v}}$ is the slip velocity of the $k$-th phase relative to the centroid of the mixture, $T$ is temperature, $E_k$, $f_{drag}$, $F$ and $g$ are the energy, drag coefficient, volume force and gravitational acceleration of the $k$-th phase in the mixture, $\mu_m$ is mixture viscosity, $k_{eff}$, $p$ and $S_g$ are effective thermal conductivity, pressure and heat source items. $\bar{m}_{l-v}$ and $\bar{m}_{v-l}$ are mass flow rate from liquid to gas and gas to liquid.

Liquid hydrogen will undergo phase change and mass transfer through heat exchange with the ground and air. Here Lee model is adopted in the present study and the equations is

$$\frac{\partial}{\partial t} \left( \alpha_l \rho_l \right) + \nabla \cdot \left( \alpha_l \rho_l \bar{v}_l \right) = \bar{m}_{l-v} - \bar{m}_{v-l}$$

$$\begin{cases} \bar{m}_{l-v} = \text{coeff} \cdot \alpha_l \rho_l \left( T_l - T_{sat} \right) / T_{sat}, & \text{if } T_l > T_{sat} \\ \bar{m}_{v-l} = \text{coeff} \cdot \alpha_l \rho_l \left( T_v - T_{sat} \right) / T_{sat}, & \text{if } T_l < T_{sat} \end{cases}$$
Where $T_{sat}$ is the saturation temperature, and $coeff$ is the mass transfer coefficient.

In the case of source term flashing evaporation, the mass fraction of gas phase and the density of the mixture are:

$$q_v = \frac{H_{1u} - H_{2l}}{H_{2v} - H_{2l}}$$  \hspace{1cm} (7)

$$\frac{1}{\rho_{mix}} = \frac{q_v}{\rho_v} + \frac{q_l}{\rho_l}$$  \hspace{1cm} (8)

Where $H_{1u}, H_{2l}, H_{2v}$ are the liquid phase enthalpy before leakage, liquid phase and gas phase enthalpy after leakage, $q_v$, $q_l$, $\rho_v$, and $\rho_l$ are the gas phase mass fraction, liquid phase mass fraction, gas phase density and liquid phase density.

3. Physical model and boundary conditions

As shown in Figure 1, the computational domain $33m \times 6m \times 10m$ used for the calculation. In order to simulate the liquid hydrogen leakage caused by the looseness of valve or the broken of transportation pipeline on the ground. The leakage port is placed on the ground at a height of 0.5m, and set it as a mass inlet of LH2 / H2 multiphase flow. The ground is made of concrete, and set its density to 2371kg / m$^3$, specific heat capacity to 880J / (kg • K), thermal conductivity to 1.13W / (m • K). The plane $Z = 0$, $Z = -6$ and $Y = 10$ set as symmetry. The air inlet is set to a logarithmically distributed wind speed, the wind speed is 2.5 m / s at a height of 3 m, and the air outlet is set to a pressure outlet. The physical model adopts structured grid division. As shown in Figure 2, the grid near the leak is thinner, and the grid away from the leak gradually becomes widen. The grid growth rate is less than 1.2. After the grid independence test, the total number of grids is 151063.

The environmental parameters are set the atmospheric pressure is $P_0 = 100960pa$ and the temperature is $T_0 = 296.9K$. When the leakage port is pure liquid hydrogen, the leakage volume is 60L / min, and its temperature and liquid hydrogen saturation vaporization temperature are both set to 20.324K. The H2 / Air mixed gas uses incompressible ideal fluid, the pressure-velocity coupling solution uses the PISO algorithm, and the transient time step is set to 0.005s.
4. Analysis of numerical simulation results

The area with a hydrogen volume fraction greater than 4% is defined as a combustible hazard area, and the area with a temperature below 233.16K is defined as a cryogenic danger area. To simulate the leakage of liquid hydrogen at a height of 0.5m above the ground, different leak source items are set. The leakage source is a two-phase flow of LH2 / H2 with different proportions. Specific parameters of leakage source term are shown in Table 1.

| Source term | Mass flow rate (kg/s) | Temperature (K) | Gas volume fraction (%) | Gas mass fraction (%) |
|-------------|-----------------------|-----------------|-------------------------|----------------------|
| ST1         | 0.071                 | 20.324          | 0                       | 0                    |
| ST2         | 0.071                 | 20.324          | 0.9                     | 0.14                 |
| ST3         | 0.071                 | 20.324          | 0.96                    | 0.31                 |
| ST4         | 0.071                 | 20.324          | 1                       | 1                    |

4.1. Diffusion characteristics and concentration distribution of hydrogen cloud

When the pipeline full of liquid hydrogen is damaged, the continuous leakage and diffusion will form a quasi-steady state hydrogen cloud in the space area. The size of the cloud and the range of the cryogenic area are basically stable. As shown in Fig. 3, they are the quasi-steady-state hydrogen volume fraction distribution formed on the symmetry plane under the four simulated working conditions. It can be seen that flash vaporization increases the risk of leakage and diffusion of liquid hydrogen. When the leakage source is completely liquid hydrogen (ST1), the horizontal diffusion distance of combustible clouds is 15.6m; when 14% liquid hydrogen flashes (ST2), the horizontal diffusion distance of combustible clouds increases to 24.1m; when 31% liquid hydrogen flashes (ST3), the horizontal diffusion distance of combustible clouds exceeds the calculation domain, but it can be predicted that its horizontal diffusion distance is slightly greater than 30m; and when the leaks are all cryogenic hydrogen (ST4), its horizontal diffusion distance will be much greater than 30m; the diffusion distance in the vertical direction also increases with the increase of flash evaporation of liquid hydrogen. As shown in Table 2, it can be seen that the flashing of liquid hydrogen will increase the diffusion range of combustible clouds, especially the diffusion distance in the horizontal direction, greatly increasing the risk of hydrogen explosion after liquid hydrogen spills.
4.2. Temperature distribution characteristics

Due to the extremely low temperature of liquid hydrogen, a cryogenic zone will be formed near the leakage port after a liquid hydrogen leak accident. Figure 4 shows the temperature fields of 4 simulation conditions. It can be seen that the cryogenic hydrogen exchange heat with ground and air. The shape of the cryogenic zone is close to the shape of the hydrogen cloud, and the hydrogen concentration is high, the temperature is low.

The horizontal and vertical range of the cryogenic hazardous area with the temperature below 233.16K is shown in Table 3. A certain amount of liquid hydrogen flash vaporization increases the horizontal distance of the cryogenic hazardous area. When the leakage source is completely liquid hydrogen (ST1), the horizontal distance of the cryogenic hazardous area is 6.3m. When has 31% liquid hydrogen flashed (ST3), the horizontal distance of cryogenic hazardous area increased to 10m. When the leaks are all cryogenic hydrogen (ST4), the horizontal dangerous distance is only 9.1m. The reason is that when the spills without hydrogen, the formed hydrogen cloud is small, and its horizontal cryogenic dangerous area is small. When a amount of liquid hydrogen flashes, the horizontal diffusion distance of hydrogen increases, and large area of low-temperature hydrogen increases the risk of frostbite. However, when the leakage port is only hydrogen(), due to no liquid hydrogen evaporate, the hydrogen temperature away from the leakage source quickly rises to exceed 233.16K, so the cryogenic danger zone of this condition is smaller than when 31% liquid hydrogen flash occurs. The horizontal and vertical ranges of the cryogenic hazardous area are shown in Table 3.
Figure 4. Temperature field on symmetry plane: Z=0

![Temperature field on symmetry plane: Z=0](image)

(a) ST1  
(b) ST2  
(c) ST3  
(d) ST4

Table 3. Cryogenic zone

| Max distance | ST1  | ST2  | ST3  | ST4  |
|--------------|------|------|------|------|
| Horizontal distance (m) | 6.3  | 9.0  | 10.0 | 0.91 |
| Vertical distance (m) | 0.8  | 0.52 | 0.7  | 0.75 |

Figure 5 shows the temperature distribution at a height of 0.25 m above the ground. Under the horizontal distribution distance below 233.16 K is close with different conditions. When less liquid hydrogen flashing, the dangerous temperature zone is close to the leakage source. When leakage is only liquid (ST1), there is a liquid hydrogen pool on the ground, which undergoes a phase change mainly through heat exchange with the ground, and its cryogenic area is mainly concentrated near the ground. It can be seen that the minimum temperature value of ST1 at Y = 0.25 m is higher than condition of ST2 in Figure 5. With considering the liquid hydrogen flash evaporation, the greater flashing amount, the more uniform of temperature distribution at Y = 0.25, but the horizontal distance with temperature lower than 233.16 K is close.
5. Conclusion

It is of great significance to study the safety characteristics of liquid hydrogen leakage for accident prevention and post disaster disposal of liquid hydrogen storage and transportation sites. Through the simulation with different source term of liquid hydrogen flash evaporation, the following conclusions are obtained:

1. When liquid hydrogen is continuously released, the flash evaporation of liquid hydrogen increases the range of flammable explosive areas and cryogenic hazardous areas, which has a very adverse impact on safety.

2. With more flash evaporation of liquid hydrogen, the horizontal distance of flammable cloud diffusion greatly increased, and the horizontal distance of flammable cloud diffusion increased slightly.

3. With more flash evaporation of liquid hydrogen, the horizontal distance of cryogenic hazardous area increased from 6.3m to more than 9m, and it has small impact on vertical distance.

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