Study on the influence of barriers in the diffusion process of liquid hydrogen leakage

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Abstract: Based on the computational fluid dynamics method, a numerical model of large-scale liquid hydrogen leakage and diffusion is established. By simulating the diffusion process of hydrogen cloud when the obstacle is located at different positions, we get the motion law of cloud and the important time parameters of Cloud Diffusion reaching the dangerous range (combustible concentration). Compared with the process of liquid hydrogen leakage and diffusion under barrier-free conditions, it was found that setting an obstacle in the wind direction of the leakage port can accelerate the diffusion speed of the hydrogen cloud. The time to reduce the cloud concentration below the flammable range is reduced by 15%, therefore, can decrease the risk of fire; however, setting barrier in the downwind direction will lead to the accumulation of hydrogen cloud near the ground, and the time when the cloud concentration drops below the flammable range is 64% longer than the barrier-free working conditions, the possibility of serious secondary accidents was increased.

1. Introduction
Hydrogen energy has the advantages of large reserves, high calorific value, zero pollution, etc., and can well solve the problems of energy shortage and environmental pollution. At present, hydrogen energy has been increasingly used in power sources of cryogenic liquid rockets, ships, aircraft, and fuel cells [1]. Due to the physical and chemical properties of hydrogen itself, once the stored liquid hydrogen leaks, the leaked liquid hydrogen will form a low-temperature liquid pool on the ground, and at the same time, the hydrogen formed by the rapid evaporation of liquid hydrogen will accumulate under certain conditions, which is easy to form explosive gas mixture and poses a huge potential threat to the surrounding people and environment. By setting barriers near the location of the liquid hydrogen leakage, observing the diffusion law after the liquid hydrogen leaks, and predicting the explosion time range of the flammable hydrogen cloud, it can provide a certain theoretical basis for reducing the occurrence of fire and other secondary accidents and for the space layout of the liquid hydrogen storage tank.

At present, researchers at home and abroad have carried out some experimental research on liquid hydrogen leakage. The National Aeronautics and Space Administration (NASA) [2] conducted experiments that on the open space large-scale liquid hydrogen leakage diffusion process affected by different environmental factors, and statistically obtained the law of liquid pool evaporation and hydrogen cloud diffusion after liquid hydrogen leakage. The German Material Monitoring Association (BAM) [3] has measured the data of the hydrogen content near some buildings and the change of ambient temperature with time by studying the leakage of liquid hydrogen among numerous buildings. The British Health and Safety Laboratory [4] [5] (HSL) experimented in the valley to simulate the...
leakage of the connecting hose during the transfer of the liquid hydrogen storage tank, and found the desublimation of the air components (oxygen and nitrogen) near the leak phenomenon. Flame speed, heat radiation flux and other data were also obtained in the ignition experiment.

Numerical simulation research is also mainly carried out based on the experimental results of the above three organizations. Giannissi et al. [6] established the leak source as a two-phase state in which liquid hydrogen and hydrogen are mixed. Considering the ground heat conduction, the simulation reproduced the NASA liquid hydrogen leak test, and the results were compared with the experimental data to verify the feasibility of the numerical simulation method. Ichard et [7] conducted a numerical simulation on the liquid hydrogen leakage experiment of HSL, and set the mass fraction of hydrogen in the two-phase flow of the leakage outlet to be 5.6%, 14%, 31%, 65%, and 100% respectively. The simulation result is closest to the test when the mass fraction is 31%, and it is found that the energy released by the condensation of oxygen and nitrogen makes the hydrogen cloud more buoyant. Statharas et al. [8] numerically simulated the BAM hydrogen diffusion experiment and found that the hydrogen diffusion between buildings is affected by natural wind and the backflow near the building, and the heat exchange between the ground and hydrogen will significantly affect the hydrogen cloud diffusion process. To sum up, it can be seen that there is currently no research on whether the installation of barriers reduces or increases the risk of liquid hydrogen leakage and the characteristics of hydrogen cloud diffusion behavior. The presence of barriers will affect the shape of the liquid pool on the ground after the liquid hydrogen leaks, as well as the subsequent evaporation and diffusion process and the shape of the hydrogen cloud. Therefore, this paper is focused on studying the influence of barriers on the diffusion process and characteristic parameters of hydrogen cloud by establishing a three-dimensional CFD mathematical model describing the large-scale liquid hydrogen diffusion process.

2. Large-scale numerical calculation method of liquid hydrogen diffusion

2.1. Liquid hydrogen leakage diffusion process

The schematic diagram of the liquid hydrogen leakage and diffusion process in an open space is shown in Figure 1, which is mainly divided into four stages [9] [10]: liquid hydrogen flash evaporation stage, part of the liquid hydrogen is quickly converted into hydrogen vapor; heavy gas diffusion stage, low-temperature liquid hydrogen exchanges vigorously with air and ground to evaporate to form extremely low-temperature gas. At this stage, the tail of the hydrogen cloud is close to the surface, and the head is floating, and it is at an angle with the surface in the downwind direction. Within a short period of time after the leak, the hydrogen concentration dropped rapidly, the tail of the cloud detached from the surface, and then quickly floated to a certain height, which was the main phase in the diffusion process of the hydrogen cloud; the passive diffusion phase, which lasted a long time and maintained at a certain height and drifting downstream driven by wind, the hydrogen concentration drops slowly.

![Figure 1. Schematic diagram of macroscopic diffusion of hydrogen cloud.](image-url)
2.2. Mathematical model of liquid hydrogen leakage and diffusion

The liquid hydrogen leakage and diffusion process is simulated using the multiphase flow Mixture model and the Realizable $k$-$\varepsilon$ turbulence model [11] [12], and the interphase mass transfer process uses the evaporation-condensation model. The control equation of the Mixture model is

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \bar{v}_m) = 0$$  \hspace{1cm} (1)

$$\frac{\partial}{\partial t} \left( \rho_m \bar{v}_m \right) + \nabla \cdot \left( \rho_m \bar{v}_m \bar{v}_m \right) = -\nabla p + \nabla \cdot \left[ \mu_m \left( \nabla \bar{v}_m + \nabla \bar{v}_m^T \right) \right] + \rho_m g + F + \nabla \cdot \left( \sum_{k=1}^{n} \alpha_k \rho_k \bar{v}_{k,m} \bar{v}_k \right)$$  \hspace{1cm} (2)

$$\frac{\partial}{\partial t} \left( \sum_{k=1}^{n} \alpha_k \bar{v}_k \right) + \nabla \cdot \left[ \sum_{k=1}^{n} \alpha_k \bar{v}_k \left( \rho_k E_k + p \right) \right] = \nabla \cdot (k_{eff} \cdot \nabla T) + S_g$$  \hspace{1cm} (3)

The volume fraction equation of the liquid phase is

$$\frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) + \nabla \cdot \left( \alpha_k \rho_k \bar{v}_k \right) = -\nabla \cdot \left( \alpha_k \rho_k \bar{v}_{k,p} \right) + \sum_{i=1}^{n} \left( \dot{m}_{l-s} - \dot{m}_{l-s} \right)$$  \hspace{1cm} (4)

Where $\rho_m$ is the mass average density, $\bar{v}_m$ is average speed, $\alpha_k$ is the volume fraction of phase $k$, $\bar{v}_{k,m}$ 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; $\dot{m}_{l-s}$ and $\dot{m}_{l-s}$ are mass flow rate from liquid to gas and gas to liquid.

The Lee model is used to calculate the phase change of the liquid hydrogen leakage and diffusion process. It is judged that if the fluid in the flow field is higher than the set phase change temperature, it is considered to evaporate, and if it is lower than the phase change temperature, condensation will occur. The gas-liquid mass transfer equation is

$$\frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) + \nabla \cdot \left( \alpha_k \rho_k \bar{v}_k \right) = \dot{m}_{l-s} - \dot{m}_{l-s}$$  \hspace{1cm} (5)

$$\dot{m}_{l-s} = \text{coeff} \cdot \alpha_k \rho_k \left( T_c - T_{sat} \right) / T_{sat}, \text{if} T_c > T_{sat}$$

$$\dot{m}_{l-s} = \text{coeff} \cdot \alpha_k \rho_k \left( T_c - T_{sat} \right) / T_{sat}, \text{if} T_c < T_{sat}$$  \hspace{1cm} (6)

In the formula, $T_{sat}$ is the saturation temperature, and coeff is the phase change mass transfer coefficient. In this paper, the method of numerical calculation is compared with the experimental results, and the evaporation coefficient is 0.5.

3. Analysis of Influence of Barriers on Hydrogen Cloud Diffusion Process

Establish a calculation area of $250 \times 60 \times 100$ m. The liquid hydrogen storage area is $0.3 \times 0.6 \times 0.07$ m. According to the size of the explosion-proof wall of the liquid hydrogen storage tank placement area of the Hainan launch site, the wind direction is 7 m above and below the storage tank respectively. Barriers were set up with a width of 1 m, a height of 7 m and a length of 30 m. The diffusion process of the hydrogen cloud after the liquid hydrogen leaked was studied. The schematic diagram of the model is shown in Figure 2.

Using the stabable wind field as the initial field to calculate the liquid hydrogen leakage diffusion process, the liquid hydrogen leakage conditions are

$$\begin{cases} m = 4.76 \text{ kg/s}, & 0 < t \leq 38 \text{s} \\ m = 0, & t > 38 \text{s} \end{cases}$$  \hspace{1cm} (7)
The temperature of the liquid hydrogen is 19.5 K, the transient calculation adopts the pressure and velocity coupled PISO algorithm. The time step is 0.001 s, and the convergence residual is $10^{-6}$. The ambient temperature is 288 K, the pressure is 101325 Pa, the ground temperature is 283 K and the wind speed is 2.2 m/s. The phase change of other components in the air occurs near the outlet of liquid hydrogen has little effect on the entire process of liquid hydrogen leakage and diffusion. The time for the hydrogen cloud to diffuse out of the explosion range is mainly affected by the wind speed and surface temperature in the space environment, so phase change of other components of air could be ignored. And because the large-scale liquid hydrogen leakage belongs to low Mach number flow, it is calculated by incompressible flow.

![Figure 2. Schematic diagram of large-scale liquid hydrogen leakage after adding barriers](image)

Based on the results of the stable wind field, the simulation of the liquid hydrogen leakage and diffusion process in the presence of unobstructed objects was carried out. The comparison of the hydrogen cloud concentration changes is shown in Figure 3. For barrier-free, the right column is the barrier in the downwind direction. The duration of liquid hydrogen leakage is 38 s. We selected the hydrogen concentration cloud diagrams of 10 s, 25 s, 43 s and 53 s after the start of the leak to compare the influence of the position of barriers on the diffusion process of the hydrogen cloud.

![Figure 3. The diffusion concentration of the hydrogen cloud changes with different position of barrier](image)
When liquid hydrogen begins to leak for 10 s, the liquid hydrogen pool formed after the leak exchanges heat with the ground, air and evaporates violently. These extremely low temperature (near boiling point) hydrogen gas is mixed with a small amount of air to form a "cold air cloud" with a large temperature and low density. When the obstacle is located in the upwind direction, it is not affected by the wind force. As the hydrogen cloud clusters are attracted by the vortex on the leeward side of the obstacle, the cloud entrained air diffuses toward the height direction. When the height of the gas cloud exceeds the obstacle, it is affected by the natural wind. When there is no barrier or barrier are located in the downwind direction, the gas cloud formed by the leakage of liquid hydrogen hovering near the ground, the diffusion degree is low, and the accumulation of hydrogen cloud clusters on the windward side of the downwind obstacle which is very bad for the gas cloud diffusion.

When liquid hydrogen leaked to 25 s, the hydrogen cloud settled to the ground under the control of gravity effect. As the stratification of the concentration inside the cloud is obvious, the concentration drop and the temperature rise are very slow, in this process the gravity effect plays a leading role, and the atmospheric turbulence effect plays an auxiliary role. With the hydrogen cloud located on the leeward side of the upwind obstacle further diffuses, the area near the leak boasts a higher concentration while the hydrogen cloud volume is smaller. Under the condition of unobstructed objects, the hydrogen gas cloud diffuses downstream due to the influence of natural wind. The gas cloud becomes flat and wide, and its volume grows rapidly. Due to the barrier effect, there are still hydrogen cloud clusters on the windward side of the downwind barrier, resulting in a high concentration of hydrogen cloud clusters, which is restricted between the leak and the barrier. The object will bounce upstream, the gas near the ground has a large width, and the diffusion speed is very slow.

At 43s, liquid hydrogen has stopped leaking. At this time, due to the combined effect of atmospheric turbulence and gravity settling, the hydrogen cloud shifts from heavy gas diffusion to non-heavy gas diffusion. As more and more air is sucked into the cloud and mixed, and the heat exchange among the cloud, the ground and air, the cloud is gradually diluted, the concentration drops rapidly as well as the temperature increase accompanied by the density also decreases. Then, strengthen the buoyancy effect of the hydrogen gas for the effect of gravity gradually weakened. Therefore, the cloud cluster diffuses significantly in the vertical direction, the lateral diffusion rate slows down, the volume of the cloud cluster expands further, and the ability to entrain air is enhanced. When the barrier is set upwind, the volume of hydrogen cloud increases less, and the areas with higher concentration gradually break away from the ground. Under the condition of no barrier, the volume of hydrogen cloud continues to grow, and it fully diffuses downstream and vertically. The areas with high gas cloud concentration formed when the barrier is set downwind are still concentrated near the ground. After a part of the gas clouds spread over the barrier, they begin to spread downstream.

At 53 s, the hydrogen cloud belongs to the passive diffusion stage. This stage occupies most of the time during the diffusion process of the hydrogen cloud. The cloud diffuses significantly downstream under the action of wind drive and buoyancy. In this stage, the conditions of setting up barrier in the upwind direction are similar to the cloud conditions of unobstructed conditions. The volume of gas clouds continues to increase and spread rapidly downstream. With the mixing of hydrogen clouds and air, the cloud concentration further decreases and gradually off the ground. However, under the conditions of downwind barrier, the liquid hydrogen evaporates at a slower rate and has a low degree of diffusion. Only the clouds that bypass the barrier are diffused downstream by the wind field.

In general, the presence of barriers reduces the volume growth of hydrogen cloud clusters and plays a guiding role in the diffusion direction of gas clouds relative to the working conditions of barrier-free objects. Barriers are installed in the upwind direction of the leakage location, and the gas cloud grows faster when it is relatively unobstructed in the vertical direction. When the height of the gas cloud exceeds the barrier, the hydrogen cloud quickly diffuses downstream and the concentration drops rapidly under the influence of the wind field. Under the conditions of downwind barriers, due to the obstruction of the barriers, the hydrogen cloud is blocked on the side of the barrier in the windward direction, and gathers between the leak and the barrier, which is not conducive to the dissipation of the
hydrogen cloud, but if there is a building in the wind direction, which can play a certain role in protecting the building.

4. Analysis of the Influence of Barriers on the Diffusion Characteristics of Combustible Clouds

The flammable concentration range of hydrogen cloud is 4% ~ 75%. We focus on the rapid diffusion phase of hydrogen cloud after liquid hydrogen leakage stops (the risk in this stage is higher for the wider diffusion and changing concentration). Given the stoppage of liquid hydrogen leakage as the starting moment, that is, from 38s, the time parameters of the diffusion characteristics of combustible hydrogen clouds when the barriers are located at different positions as shown in Table 1, and the cloud concentration and minimum temperature changes, shown in Figure 4.

Table 1. Comparison of the leakage and diffusion time of the flammable hydrogen cloud under different working conditions

| parameter                          | barrier upwind | no barrier | barrier downwind |
|------------------------------------|----------------|------------|------------------|
| Time to drop to detonation          |                |            |                  |
| concentration 18.3% / s             | 10             | 12         | 25               |
| Time to drop to detonation          |                |            |                  |
| concentration 8% / s                | 14             | 19         | 46               |
| Time to drop to detonation          |                |            |                  |
| concentration 4% / s                | 23             | 27         | 73               |

As can be seen from Table 1 and Figure 4, after the liquid hydrogen stops leaking, the liquid hydrogen gradually evaporates and blends with the air forming a combustible hydrogen cloud. Compared with the barriers, the diffusion speed of the hydrogen cloud is similar. About 5s ~ 12s belongs to the rapid diffusion stage. At this time, the hydrogen cloud and air are rapidly mixed, the concentration drops rapidly, the cloud temperature rises to about 250K, then the hydrogen cloud slowly diffuses out of the combustible concentration range (4%), the temperature also gradually increased to ambient temperature.

It can be found from Table 1 that setting barriers in the wind direction above the leak can make the flammable gas cloud concentration drop to detonation concentration (18.3%), dangerous concentration (8%) and flammable concentration (4%) time [1] Compared to barrier-free condition, they were reduced by 17%, 26%, and 15%, respectively, indicating that installing barriers in the upwind
direction can significantly accelerate the diffusion of combustible hydrogen clouds and reduce the risk of combustible clouds.

Installing barriers in the wind direction under the leak will cause a large amount of combustible gas clouds to accumulate between the storage tank and the barrier. Even if the leak is controlled, it will take a long time for the gas clouds to dissipate. It can be seen from Table 2 that after stopping the leakage, the time for the flammable gas cloud to fall below the flammable concentration (4%) when the obstacle is installed in the downwind direction is 73 s, which is an increase of 46s compared to 27 s when there is no obstacle. The extension is 64%, which increases the risk of fire near the leak and obstacles, and may cause serious secondary accidents such as explosions.

5. Conclusion

Aiming at the follow-up behaviour of large-scale liquid hydrogen leakage, this paper builds a numerical model for large-scale liquid hydrogen leakage and diffusion, and uses numerical simulation software fluent combined with user-defined programs to study the barrier-free objects in the presence of the wind field. The change rule of combustible hydrogen cloud concentration and the influence of barrier at different positions on the leakage and diffusion process of liquid hydrogen were compared. The main conclusions are:

1. Whether an obstacle is set or the position of the obstacle is different, the diffusion behavior after liquid hydrogen leakage is similar. The four stages are flash stage, gravity effect stage, atmospheric turbulence effect and gravity effect stage (buoyancy diffusion) and passive diffusion stage

2. When the barrier is located in the upwind direction, the vortex on the leeward side will cause the hydrogen cloud and air to mix rapidly. When the height of the cloud exceeds the barrier, it will quickly spread downstream due to the influence of natural wind. If the barrier is located downstream of the leak, due to the wind field and the effect of gravity, liquid hydrogen and hydrogen cloud clusters accumulate near the barrier and the ground, which is not conducive to the diffusion of hydrogen cloud clusters.

3. Compared with the process of liquid hydrogen leakage and diffusion under barrier-free conditions, it was found that setting an obstacle in the wind direction of the leakage port can accelerate the diffusion speed of the hydrogen cloud. The time, reducing the cloud to a concentration lower than flammable range, was shorted 15%, therefor, can decrease the risk of fire; and installing barrier in the downwind direction will cause the cloud concentration to fall below the flammable range by 64% longer than the barrier-free conditions.

By studying the influence of barriers on the diffusion process of hydrogen cloud after liquid hydrogen leakage, it can provide a certain theoretical basis for the storage space of liquid hydrogen storage tanks, that is, it can be considered to increase barriers in the wind direction of the storage tank when liquid hydrogen leakage occurs. The hydrogen cloud can accelerate the diffusion according to the predetermined route and reduce the risk and the possibility of serious secondary accidents.

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