Research on Leakage and Diffusion characteristics of Liquid Hydrogen Based on Gaussian Diffusion Model

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Abstract: In order to analyze the diffusion characteristics of the hydrogen cloud during a liquid hydrogen leakage accident, the Matlab calculation program of liquid hydrogen leakage and diffusion was compiled based on the Gaussian diffusion theory, and analyzed the influence of wind speed, pressure, leakage area and other factors on the size of the dangerous area after liquid hydrogen leakage. The calculation results show that: the wind speed accelerates the diffusion, and the higher the wind speed, the stronger the dilution effect on the hydrogen cloud, and the smaller the dangerous area formed; the increase of pressure and leakage port area will increase the leakage of liquid hydrogen, and as a result, the scope of the dangerous area is increased.

1. Introduction
As an important clean energy, hydrogen has been widely used in many fields such as chemical industry, clean energy and aerospace propulsion. As a cryogenic propellant, liquid hydrogen has important application value in space launch sites. Once the stored liquid hydrogen leaks, it will quickly evaporate into hydrogen and mix with the surrounding air to form flammable and explosive gas, which poses a huge potential threat to surrounding personnel and equipment. Studying the characteristics of the diffusion law after liquid hydrogen leakage has very important practical significance for formulating emergency plans after an accident, delimiting emergency evacuation areas, and assessing the consequences of accidents.

Liquid hydrogen has the characteristics of ultra-low temperature (-253°C), easy to vaporize, inflammable and explosive. After a leakage accident, the ambient air and solid walls around the liquid hydrogen exchange heat and quickly vaporize, low-temperature hydrogen and air are quickly mixed, and the concentration gradually drops below the safe concentration (<4%). The continuously leaking liquid hydrogen will form a quasi-steady hydrogen cloud in the wind direction area below the leak through evaporation and heat absorption. The cloud with the volume fraction in the range of 4%-75% [1] is a dangerous area where combustion may occur. Clouds with a volume fraction in the range of 18.3%-59% [1] are dangerous areas that may explode.

In order to explore the characteristics of the law of leakage and diffusion of liquid hydrogen, researchers conducted research through methods such as liquid hydrogen leakage and diffusion experiments and numerical simulation of leakage and diffusion. In 1981, the National Aeronautics and Space Administration (NASA) [2] conducted a series of large-scale liquid hydrogen leakage experiments, and recorded the dynamic diffusion process of visible hydrogen clouds after the liquid hydrogen leakage; British HSL [3] adopted diameter A leakage diffusion test was conducted for a 26.3mm pipeline connected to a liquid hydrogen storage tank, and the influence of the leakage height
on the diffusion characteristics of the hydrogen cloud was compared and analyzed by adjusting the height of the outlet of the pipeline. Sklavounos [4] used CFX software to simulate NASA’s large-scale liquid hydrogen experiment, and obtained that the hydrogen at the initial stage of diffusion behaves as heavy gas diffusion; Wu Mengxi [5] analyzed the influence of the nitrogen-oxygen phase transition on the liquid hydrogen overflow process and was considered The simulation results of the nitrogen-oxygen phase transition are more consistent with the experimental data; Shao Xiangyu [6] studied the diffusion law of the hydrogen cloud formed after the leakage of liquid hydrogen in the air, and obtained the spatial distribution of the hydrogen cloud at different times. Fan Shuangyu [7] used ALOHA software based on Gaussian plume model to study the influence of wind speed, temperature, and leakage on the leakage and diffusion of liquid hydrogen, and verified the effectiveness of the model through experiments.

Based on the Gaussian smoke model, this paper divides the continuous leakage into multiple instantaneous leakage sources at a certain time interval. The hydrogen concentration in the space at a certain time is the superposition of the concentration field formed by these instantaneous leakage sources. Based on this, the continuous leakage and diffusion mathematics of liquid hydrogen is established. The model and the Matlab numerical calculation program were compiled. By changing the initial conditions, the characteristics of the leakage and diffusion of liquid hydrogen affected by different factors were studied, and the dangerous area formed after the leakage of liquid hydrogen under the conditions of different wind speeds, leakage pressures and leakage opening diameters were analyzed.

2. Numerical calculation method

When the liquid hydrogen storage tank is damaged, a liquid hydrogen leakage accident will occur. If the liquid pressure in the storage tank is $P_1$, the ambient pressure is $P_0=101325pa$, the density of liquid hydrogen is $\rho = 70.85kg/m^3$, the leakage area is $A$, the height of the upper liquid level from the leakage opening is $h$, the acceleration of gravity is $g$, and the liquid leakage coefficient is $C_0$, the flow rate at the leakage port is:

$$u = C_0 \left( \frac{2(P_1 - P_0)}{\rho} + 2gh \right)$$

(1)

The mass flow rate of the leakage source:

$$Q_m = C_0 \rho A \left( \frac{2(P_1 - P_0)}{\rho} + 2gh \right)$$

(2)

The Gaussian smoke model uses statistical methods to study the concentration distribution of the diffusion medium. It can calculate the diffusion results of light gases or gases that are not much different from air density. Due to the earlier proposal time, there are many experimental data, simple and easy to calculate, and the calculation results, compared with the experimental value and other advantages, it is widely used. The Gaussian smoke cluster model can describe the leakage and diffusion of the instantaneous leakage source. The leakage process is completed in a short time, forming a gas cloud, which moves and diffuses continuously along the wind direction. At time $t$, the calculation formula of the gas concentration in space is:

$$C(x,y,z,t) = \frac{Q_m}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp\left[ -\frac{(x - ut)^2}{2\sigma_x^2} \right] \exp\left[ -\frac{(y - u)^2}{2\sigma_y^2} \right] \times \exp\left[ -\frac{(z - H)^2}{2\sigma_z^2} \right] + \exp\left[ -\frac{(z + H)^2}{2\sigma_z^2} \right]$$

(3)

Where: $C(x,y,z,t)$ is the stable concentration of toxic and hazardous substances at any point $(x,y,z)$ in space at time $t$, $Q_m$ is the total amount of instantaneous release of liquid hydrogen, $u$ is the ambient wind speed, and $H$ is The effective height of the gas cloud, $\sigma_x$, $\sigma_y$, and $\sigma_z$ respectively are the diffusion coefficients in the x, y and z directions, which can be selected with reference to the literature [8].

The continuous leakage process of liquid hydrogen can be regarded as a combination of multiple instantaneous leakage processes. If the total leakage time is $T$, the total amount of liquid hydrogen leakage per unit time is regarded as an instantaneous leakage source, and the i-th leakage source is at time $t$ The
concentration field is:

$$C_i(x,y,z,t) = \frac{Q}{(2\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left[ -\frac{(x-u(t-i))^2}{2\sigma_x^2} \right] \exp \left[ -\frac{y^2}{2\sigma_y^2} \right] \times \left\{ \exp \left[ -\frac{(z-H)^2}{2\sigma_z^2} \right] + \exp \left[ -\frac{(z+H)^2}{2\sigma_z^2} \right] \right\}$$

(4)

The concentration field of the hydrogen cloud formed at time $t$ is the concentration superimposed field formed by the previous $n$ instantaneous leak sources in space:

$$C(x,y,z,t) = \sum_{i=1}^{n} C_i(x,y,z,t)$$

(5)

Compile the above diffusion model into a Matlab calculation program. By changing the initial conditions, the distribution of hydrogen clouds after different liquid hydrogen leakage accidents can be calculated. This paper mainly considers the wind speed, storage tank pressure, leakage hole diameter and other factors to the liquid hydrogen leakage and diffusion impact.

3. The influence of wind speed on the leakage and diffusion characteristics of liquid hydrogen

Liquid hydrogen has the characteristics of ultra-low temperature (-253°C), easy to vaporize, flammable and explosive. After a leakage accident, the ambient air and solid walls around the liquid hydrogen exchange heat and quickly vaporize, and the vaporized low-temperature hydrogen is with the surrounding. There is a large temperature difference between the air, which makes the two mix quickly, and accelerate the mixing and diffusion under the action of atmospheric turbulence, until it diffuses to a safe concentration (<4%).

In order to study the influence of different factors on the leakage and diffusion characteristics of liquid hydrogen, a Matlab program was compiled based on the above mathematical model. By changing the initial conditions, the range of the dangerous area of hydrogen cloud under different factors was given. The flammable limit range of hydrogen is 4%~75%, and the explosion limit range is 18.3%~59%.

For continuous leakage sources, after a certain period of time, the hydrogen concentration field gradually stabilizes, and the dangerous area is the largest at this time. Assuming that the liquid pressure in the tank is $P_1=0.3$Mpa, the leakage port is on the ground, and the diameter is 10cm, regardless of the influence of the liquid hydrogen level. As shown in Figure 1, it is the range of the dangerous area of liquid hydrogen leakage and diffusion under different wind speed conditions. It can be seen from the figure that the wind speed has a relatively obvious impact on the leakage and diffusion of liquid hydrogen, as follows:

1. After the liquid hydrogen leaks, with the increase of time, the dangerous area formed by the downwind direction gradually increases, and finally stabilizes;

2. The greater the wind speed, the faster the diffusion rate. When $t=20$s, the wind speed $u=1$m/s hydrogen combustible concentration area will diffuse to 25m in the farthest downwind direction, while $u=3$m/s, 5m/s, the downwind direction is dangerous. The ranges are 72m and 108m respectively;

3. The greater the wind speed, the smaller the scope of the dangerous area. The wind speed is $u=1$m/s and the distance to the dangerous area reaches 503m, while $u=3$m/s, 5m/s, and the dangerous range of the downwind is 276m, respectively: 202m;

The influence of wind speed on the process of gas cloud diffusion is mainly manifested in the transportation of cloud clusters, concentration dilution and air entrainment. When the gas concentration distribution is not stable, the concentration value in the space still has the potential to increase. The high wind speed has a stronger effect on the transport of the leaked material, so in the same time, the leaked material will be transported to a farther location. So that the concentration value in the area down the wind direction of the leak continues to increase, thereby forming a larger dangerous area. After the gas cloud concentration distribution is stable, the greater the wind speed, the smaller the range of stable hazard areas.

For example, when the time is 1000s (concentration has stabilized), the corresponding hazard area, the minimum wind speed is 5m/s, and the wind speed is 1m/s is the largest. This is because the greater the wind speed, the stronger the dilution effect on the gas cloud, the faster the gas diffusion speed, and the smaller the dangerous area that is formed.
4. The influence of tank pressure on the leakage and diffusion characteristics of liquid hydrogen

The liquid hydrogen storage pressure will directly affect the leakage rate, and thus the size of the leakage. The larger the leakage, the larger the scope of the downwind danger zone. When the diameter of the leak is 10cm and the ambient wind speed is 2m/s, Figure 2 shows the leakage and diffusion process of liquid hydrogen under different leakage pressure conditions can be seen:

1) Leakage pressure has no effect on the diffusion speed. The diffusion distance of hydrogen in the downwind direction at different leakage pressures is 50m at 20s, and the diffusion distance in the downwind direction at 100s is about 203m;

2) The greater the leakage pressure, the greater the range of the dangerous area when the gas concentration distribution does not reach stability. When the leakage pressure is 0.2Mpa, the farthest distance to the dangerous area downwind is 302m, and when the leakage pressure increases to 0.6Mpa, the wind direction is dangerous. The longest distance in the area reaches 410m.
The influence of leakage opening diameter on the leakage and diffusion characteristics of liquid hydrogen

The size of the leakage port directly affects the leakage rate and leakage rate. When the pressure of the storage tank is 0.3Mpa and the wind speed is 2m/s, the hydrogen cloud diffusion process after the liquid hydrogen leakage accident occurs in the leakage ports with diameters of 5cm, 10cm, and 15cm, as shown in Figure 3. As shown in the figure, it can be seen that the diameter of the leak has a greater impact on the largest dangerous area formed by diffusion. When the diameter of the leak is 5cm, the hydrogen cloud diffusion distance in the downwind direction is 143m; the diameter of the leak is 10cm When the maximum diffusion distance of the hydrogen cloud in the downwind direction is 307m, when the diameter of the leakage opening increases to 15cm, the maximum diffusion distance of the hydrogen cloud in the downwind direction is 475m. This is because when the diameter of the leakage opening is doubled, the area of the leakage opening is increased by 3 times, which in turn increases the leakage volume by 3 times, so the range of the dangerous area of the hydrogen cloud is greatly increased.
6. Conclusion
Based on the Gaussian diffusion theory, this paper establishes a continuous leakage and diffusion model of liquid hydrogen, and analyzes the influence of factors such as ambient wind speed, leakage pressure and leakage port size on the distribution of dangerous areas in the downwind direction. The following conclusions are specifically obtained:

1. The greater the wind speed, the faster the gas diffusion speed, the stronger the dilution effect on the hydrogen cloud, and the smaller the dangerous area formed;
2. The greater the leakage pressure, the faster the liquid hydrogen leakage rate, and the larger the scope of the dangerous area formed;
3. The larger the area of the leakage opening, the greater the leakage of liquid hydrogen, and the larger the scope of the dangerous area formed.

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