Research on Influence Factors of Leakage and Diffusion of 5 m³ High Pressure Hydrogen Cylinder

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Abstract. According to the characteristics of 5m³ hydrogen cylinder in a hydrogenation station, the influence factors of high-pressure hydrogen leakage and diffusion under different leakage aperture, cylinder pressure and wind speed were studied by using the safety analysis software PHAST. The results show that the area of downstream dangerous cloud cluster and diffusion isolation area increases with the increase of leakage diameter, cylinder pressure and wind speed. The aperture has a great influence on the mass leakage rate and the distribution range of cloud clusters, while the cylinder pressure mainly affects the distribution of cloud clusters. The influence of pressure on mass leakage rate is not as obvious as the influence of aperture. The wind speed has no effect on the mass leakage rate, and has only a slight impact on the downstream cloud cluster distribution.

1 Introduction

Compared with traditional fossil energy, hydrogen energy has the advantages of clean and environmental protection, wide sources, convenient transportation, and efficient combustion [1]. It is considered to be the most promising alternative energy source in the 21st century. In recent years, many countries have made great progress in hydrogen catalysis, hydrogen fuel cell and hydrogen engine technology, and began to build corresponding hydrogenation stations to meet the fuel filling requirements of hydrogen fuel vehicles. By the end of 2019, 66 hydrogenation stations have been built in China. The hydrogen in these stations is stored in high-pressure gas state, and the storage pressure is not less than 35MPa.

The main safety risks of hydrogen refueling station include hydrogen leakage and diffusion, fire (including jet fire, pool fire, flash fire) and explosion (limited and unrestricted) caused by hydrogen diffusion [2, 3]. Among them, leakage and diffusion is the inducement of other disasters in hydrogen refueling station, so it is necessary to carry out research on the diffusion of high-pressure hydrogen leakage. In this paper, the influence factors of leakage and diffusion of a single 5m³ hydrogen cylinder are studied, and then the overall safety research of hydrogen refueling station can be carried out on this basis.

Due to the high risk of hydrogen and the high cost of experimental research, there are few experimental studies on hydrogen leakage and diffusion [4]. At present, numerical calculation method can be used to study the leakage and diffusion of hydrogen [5-10]. According to literature research, scholars have carried out research on leakage, diffusion and hazard of hazardous fluids as early as 1960s, and proposed many calculation models, such as BM model, Gaussian model, shallow model, FEM3 model, UDM (Unified dispersion model) model, etc. [11]. The advantages and disadvantages of
the above models will not be discussed in this paper, and the corresponding literature can be queried for the specific model research. Since the content of this article is biased towards engineering applications, corresponding models or mature safety analysis software can be used directly in the research process.

2 Boundary Conditions and Research Conditions

In this paper, the safety analysis software PHAST (Process Hazard Analysis Software Tool) is used to study the influence factors of high-pressure hydrogen leakage and diffusion. The software is independently developed by the Det Norske Veritas (DNV) and is mainly used in hazard analysis and safety calculations in the petrochemical industry. The PHAST software leakage diffusion module adopts the UDM model. By calculating the concentration distribution of hazardous chemicals at various locations at different times, the safe area, quasi-hazardous area, and flammable and explosive area are obtained. Based on calculation results, the technicians can take corresponding emergency measures in different areas to reduce and eliminate the adverse effects of the accident.

2.1 Boundary Conditions

This paper selects a 5 m³ high-pressure hydrogen cylinder at a hydrogen refueling station as the research object, which is currently the largest high-pressure hydrogen storage container in China. The hydrogen temperature is 20°C, and the explosion limit is 4.0%~75.0%. In order to study the influence of the pressure of the storage cylinder, 4 pressures are selected, namely 10MPa, 20MPa, 35MPa and 45MPa (the pressures used in this article are all gauge pressures), of which 35MPa is the highest working pressure, 45MPa is the cylinder design pressure.

In order to study the influence of the leakage aperture on the diffusion of hydrogen, three apertures of 10mm, 30mm and 50mm were selected. The leak hole is located at a height of 1m. The direction of the hydrogen jet is horizontal.

The ambient wind speed and direction also have a great influence on the size of the cloud formed after hydrogen diffusion. The annual average wind speed at the location of the gas cylinder is 3m/s. On this basis, two wind speeds of 1m/s and 5m/s are used for research. The direction of the wind speed is the same as the direction of the hydrogen jet.

2.2 Research Conditions

According to the selected boundary conditions, the leakage aperture, cylinder pressure and wind speed are orthogonal combined, and eight working conditions are designed as shown in the table below.

| Working Condition No. | Leakage Aperture(mm) | Cylinder Pressure(MPa) | Wind Speed(m/s) |
|-----------------------|-----------------------|------------------------|-----------------|
| 1                     | 10                    | 10                     | 3               |
| 2                     | 10                    | 20                     | 3               |
| 3                     | 10                    | 35                     | 3               |
| 4                     | 10                    | 45                     | 3               |
| 5                     | 10                    | 35                     | 1               |
| 6                     | 10                    | 35                     | 5               |
| 7                     | 30                    | 35                     | 3               |
| 8                     | 50                    | 35                     | 3               |

3 Result Analysis

After inputting the corresponding parameters into the software, the leakage and diffusion simulation
results can be obtained. Since the shape of the downstream cloud cluster is roughly the same for each working condition, the difference is only the size of the affected area, so a certain working condition can be used as an example to illustrate the analysis idea. Figure 1 shows the calculation results of Working Condition 3, that is, when the wind speed is 3m/s, the cylinder pressure is 35MPa, and the leak hole diameter is 10mm, the downstream side and top view of the cloud cluster distribution and the horizontal concentration distribution along the center line of the leak hole.

Because the density of hydrogen is less than air, hydrogen will not only move in the horizontal direction but also in the vertical direction after it leaks from the high-pressure gas cylinder to the atmosphere. The area between the dotted line and the solid line in Figure 1 is A, and its concentration is 20000~40000ppm, of which 20000ppm is the 1/2 lower explosive limit. Although this area is a safe area, it is an area that needs to be isolated, that is, the diffusion isolation area. The area within the dotted line is B, and its hydrogen concentration is greater than the lower explosion limit of 40000 ppm. This area can be divided into dangerous and quasi-hazardous areas according to the upper and lower explosion limits. The area where the hydrogen concentration is greater than 750,000ppm is the quasi-dangerous area, but this area cannot be displayed because of its small size. The hydrogen concentration of 40,000 to 750,000 is a dangerous area. Once an open flame source appears in this area, the gas will ignite and explode. It can be seen from Figure 1 that the diffusion range of the dangerous zone is 19.3m downstream, and the maximum cloud cluster height is 6.8m; the maximum width of the cloud cluster in the diffusion isolation zone on the ground is 4.4m. Along the centerline, the concentration of hydrogen gradually decreases from near to far.

![Figure 1](image)

**Figure 1** Downstream cloud cluster distribution and centerline concentration when the wind speed is 3m/s, the cylinder pressure is 35MPa and the leakage aperture is 10mm (a) side view (b) top view of the ground

### 3.1 Influence of leakage aperture

Figures 2 and 3 show the distribution of dangerous cloud clusters and concentration along the centerline of the leak hole under different leakage apertures when the wind speed is 3m/s and the cylinder pressure is 35MPa. It can be seen that under the same wind speed and storage cylinder pressure conditions, the influence range of the hydrogen cloud cluster expands from 19.3m to 34.1m when the hole diameter increases from 10mm to 50mm. The maximum height of the dangerous cloud cluster also increases from 6.8m to 10.6m. The area of the ground diffusion isolation zone and the dangerous zone has increased significantly, because the size of the leakage aperture directly determines the amount of hydrogen leakage. The larger the aperture is, the more leakage mass will be, and the concentration and influence range of the downstream cloud cluster will be.
Figure 2 Downstream cloud cluster distribution and concentration along the centerline of the leak hole under different leakage apertures when the wind speed is 3m/s and the cylinder pressure is 35MPa (a) side view (b) top view of the ground

Figure 3 Concentration along the centerline of the leak hole under different leakage apertures when the wind speed is 3m/s and the cylinder pressure is 35MPa

Figure 4 shows the comparison of mass release rate and release time under different leakage apertures when the wind speed is 3m/s and the cylinder pressure is 35MPa. The hydrogen mass release rate of the gas cylinder is mainly related to the pressure of the gas cylinder. As the pressure continues to decrease, the hydrogen mass release rate also continues to decrease. However, when the leakage aperture is 10mm, the hydrogen at the leakage port will flow at supersonic speed and form a blockage. At this time, the leakage rate is small and there will be no major changes in the whole process, so the leakage maintenance time is longer than the other two conditions. When the leakage aperture is 50mm, the hydrogen mass release rate during the leakage process will change drastically. The initial mass release rate of the leakage is 35.2kg/s, which is much greater than 1.4kg/s when the diameter is 10mm. In addition, the entire leakage process under 50mm aperture is relatively short, only 21.6s.
Figure 4 Mass release rate and release time under different leakage apertures when the wind speed is 3m/s and the cylinder pressure is 35MPa (a) Mass release rate (b) Release time

3.2 Influence of cylinder pressure

Figures 5 and 6 show the distribution of dangerous cloud clusters and concentration along the centerline of the leak hole under different cylinder pressures when the wind speed is 3m/s and the leakage aperture is 10mm. It can be seen that under the same wind speed and leakage aperture conditions, when the pressure increases from 10 MPa to 45 MPa, the influence range of the hydrogen cloud cluster expands from 13.8m downstream to 20.1m downstream, and the maximum height of the cloud cluster in the isolation area also increases from 4.7m to 6.9m. m, the width of the cloud cluster in the isolated area on the ground surface has increased from 2.6m to 4.6m, which shows that the pressure of the storage cylinder has a more significant impact on the horizontal diffusion of the cloud cluster. Similar to the effect of the leakage aperture on the area of the diffusion isolation zone, the pressure of the storage cylinder increases, and the area of the diffusion isolation zone and the danger zone will also become larger, because both can directly affect the leakage of hydrogen.

Figure 5 Downstream cloud cluster distribution under different pressures when the wind speed is 3m/s and the aperture is 10mm (a) side view (b) top view of the ground
Figure 6 Concentration along the centerline of the leak hole under different pressures when the wind speed is 3m/s and the aperture is 10mm

Figure 7 shows the mass release rate and release time under different pressures when the wind speed is 3m/s and the aperture is 10mm. It can be seen that when the pressure increases from 10MPa to 45MPa, the mass release rate increases from 0.4kg/s to 1.8kg/s, and the release leakage time also increases from 479.8s to 542.0s. It should be noted that the hydrogen density of 45MPa is 28.8kg/m$^3$, which is much greater than the density of 10MPa hydrogen of 7.8kg/m$^3$. Under the same volume condition, the mass of the former is 3.7 times that of the latter.

Figure 7 Mass release rate and release time under different pressures when the wind speed is 3m/s and the aperture is 10mm (a) Mass release rate (b) Release time

3.3 Influence of wind speed

Figures 8 and 9 show the distribution of dangerous cloud clusters and concentration along the centerline of the leak hole under different wind speeds when the leakage aperture is 10mm and the cylinder pressure is 35MPa. It can be seen that under the same leakage aperture and storage cylinder pressure, when the wind speed increases from 1m/s to 5m/s, the influence range of the hydrogen cloud cluster decreases from 17.0m downstream to 20.2m downstream, and the maximum height of the cloud cluster also increased from 5.6m to 6.9m, the cloud cluster width in the isolated area on the ground increased from 3.8m to 4.6m. The same as the impact of leakage aperture and cylinder pressure, when the wind speed increases, the area of the diffusion isolation zone and the danger zone increases. Finally, wind speed has little effect on the centerline concentration distribution of the leak hole. Since the mass release rate is only determined by the pressure difference between the inside and outside of
the cylinder, the wind speed has no effect on the mass release rate.

![Figure 8](image1.png)  ![Figure 8](image2.png)

**Figure 8** Downstream cloud cluster distribution under different wind speed when the leakage aperture is 10mm and the cylinder pressure is 35MPa (a) side view (b) top view of the ground

![Figure 9](image3.png)

**Figure 9** Concentration along the centerline of the leak hole under different wind speeds when the leakage aperture is 10mm and the cylinder pressure is 35MPa

4 Conclusion

A study on the leakage and diffusion of a 5m³ high-pressure hydrogen gas cylinder in a hydrogen refueling station was carried out. Using PHAST software, the side view cloud cluster distribution, the mass leakage rate change and the concentration distribution of the leakage hole in the horizontal direction under 8 different working conditions were calculated. The effects of different leakage apertures, cylinder pressure and ambient wind speed on these parameters are compared in detail. The study found that the area of the downstream danger zone and diffusion isolation zone increases with the increase of the leakage aperture, storage cylinder pressure and wind speed. The aperture has a great influence on the mass leakage rate and the distribution range of cloud clusters, while the change in pressure mainly affects the distribution of the cloud clusters. The influence of pressure on mass leakage rate is not as obvious as the influence of aperture, while wind speed has no effect on the mass leakage rate. The wind speed has only a slight impact on the downstream cloud cluster distribution.

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