Numerical Analysis of Hydrogen Leakage from Hydrogen Storage Container under Various Circumstances

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Abstract. A numerical simulation method by using the realizable k-ε model of computational fluid dynamics (CFD) proposed by establishing the model of hydrogen leakage of a high-pressure hydrogen storage container is presented in this paper. By setting different environmental wind speeds, leakage apertures, and leakage locations, multiple simulation calculations are performed to compare test results. As the wind speed increases, the degree of turbulence of hydrogen increases. Large aperture and bottom side leakage cause more serious hazardous area of personnel than small aperture and top leakage do. Base on the results, it can provide reference for dealing with the leakage of high-pressure hydrogen storage containers.

Keywords: Hydrogen leakage, CFD, Hazard analysis.

1. Introduction

Hydrogen energy is regarded as the clean energy with the most development potential in the 21st century. Hydrogen energy has many characteristics such as a wide range of sources, a high calorific value, convenient to storage and transportation. In the context of coping with global warming and the transformation of the energy system, it has important strategic significance for a country's technological development and economic benefits. With the continuous emergence of fuel cell vehicles that use hydrogen as energy, hydrogen refueling stations and hydrogen storage containers are booming to meet the demand for hydrogen supplies [1-4].

Due to the low density, the large volumetric content of combustion and explosion range (4%-74%), hydrogen is regarded flammable and explosive, meanwhile the hydrogen refueling station systems currently in use often have huge amounts of hydrogen storage and high filling pressure. Therefore, the consequences of an accident caused by a hydrogen leak will be incalculable. In 2019, there was an explosion accident at a hydrogen refueling station in Norway. It was found that a large amount of hydrogen was leaked and diffused and exploded due to the sealing failure of the high-pressure hydrogen storage unit, which shows that the damage is extremely enormous. In traditional chemical industry, the description and calculation of the leakage process are mostly based on empirical formulas, with varying degrees of deviation. Nevertheless, it is difficult to guarantee the safety factor of hydrogen leakage test, and there are high requirements for space and facilities. This paper is based on computational fluid dynamics to numerically simulate the leakage of hydrogen storage container in multiple scenarios, and to compare the leakage results under different environmental wind speeds, different sizes of leakage.
holes, with a view to detecting hydrogen leakage points, estimating leakage and risk assessment provides reference [5-12].

2. Modeling strategy

2.1. Numerical methodology

The process of hydrogen leakage from the hole of hydrogen storage container obeys the mass conservation equation (1), momentum conservation equation (2) and energy conservation equation (3).

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} + \frac{\partial (\rho u_j)}{\partial y_j} + \frac{\partial (\rho u_z)}{\partial z} = 0
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = - \frac{\partial p}{\partial x_i} + s_i
\]

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\bar{u}(\rho E + p)] = \nabla \cdot \left[ k_{eff} \nabla T - \sum_j h_j \mathbf{j}_j + (\tau_{eff} \cdot \bar{u}) \right] + S_h
\]

Due to the high pressure in the container, a jet is formed at the leak, so the Realizable k-ε turbulent flow model in Fluent is applicably used. The transport equations for turbulent kinetic energy (4) and the turbulence dissipation rate (5) are as follows:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho k u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + \rho C_1 \varepsilon S - \rho C_2 \frac{\varepsilon^2}{k + \sqrt{\varepsilon}} + C_1 \frac{\varepsilon}{k} C_3 \varepsilon G_b + S_\varepsilon
\]

This paper only analyzes the process of hydrogen leakage, ignores the influence of chemical reactions and combustion, and activates the use of component transport model (6) for simulation with equations for mass diffusion in laminar flow (7) and in turbulent flow (8) are as follows:

\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \bar{v} Y_i) = -\nabla \cdot \bar{J}_i + R_i + S_i
\]

where \( Y_i \) is the mass fraction of the component \( i \). \( R_i \) represents the net production rate of the product \( i \). \( S_i \) is the additional generation rate caused by discrete phases and user-defined source terms and \( J_i \) means the diffusion flux of substance \( i \).

\[
\bar{J}_i = -\rho D_{i,m} \nabla Y_i
\]

Where \( D_{i,m} \) is the diffusion correlation coefficient of component \( i \) in the mixture.

\[
\bar{J}_i = -\left( \rho D_{i,m} + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla Y_i
\]

2.2. Model settings

Referring to the simulation parameters of a hydrogen storage container, the simulation flow field area of this paper is 100 meters in length and 50 meters in height. The center line of the hydrogen storage
container is 50m from the left side of the simulation area, and the diameter of storage container is 1.2m, the height is 3m, the diameter of leakage hole is 0.008mm, and the leakage hole is located on the top of the container. The pressure in the container is 25MPa, and the temperature is 300K. The ambient pressure is 0.1MPa, and the ambient wind speed is 2m/s.

2.3. Mesh refinement test
The calculation domain after gas leakage is the large rectangular surface to remove the space occupied by the hydrogen storage container in the middle. Fig. 1 shows the triangles mesh view of xy plane.

![Figure 1. Triangles mesh view of xy plane.](image)

High-quality meshing can accelerate the process and save the resources of calculation. The mesh quality is checked, and Fig. 2 element quality by mesh metric shows the average is above 0.945, which is qualified and a certain calculation accuracy can be achieved.

![Figure 2. Element metrics.](image)

3. Setup and solutions
This simulation experiment using the SIMPLEC discrete solver with considering gravity and the time is selected as transient that the simulation time of hydrogen leakage is 5 seconds. There are 6 simulation tests in total. The variables of the first three tests are wind speed, respectively test 1: 2m/s, test 2: 6m/s and test 3: 10m/s. The variables of the 4th, 5th and 1st test are the diameter of leakage hole, which are test 4: 0.002m, test 5: 0.005m and test 1: 0.008m. The variables of the 6th test and 1st test are the position...
of leakage, which are the top of test 1 and the bottom side of test 6. Iterative calculations are performed according to the equations, with checking that the residuals of each parameter to meet the convergence conditions and the hydrogen leakage calculations have got solutions.

4. Results and discussions

4.1. Influences by wind speed

Set up an observation point 2 meters above the leak, record the transient velocity of the hydrogen cloud passing through this point, and establish a velocity curve with time as the x-axis and velocity as the y-axis. Fig. 6 shows the velocity change of the point from test 1 to test 3.

By comparing the three tests it can be seen that at the beginning of the leak (0~1s), the speed at this point oscillated which is related to the existence of wind. At the same time, the peak velocities are all produced in the interval of 0 to 1 second. When the wind speed was 10m/s, the speed flowing through this point was the largest, reaching 2100m/s, means that the leakage belongs to supersonic flow. When the wind speed was 6m/s, the high airflow velocity was maintained at this point in the middle and late stages of the leakage. When the wind speed was 2m/s, it started to decay monotonously after reaching the maximum speed. The speed at the end of the measurement is 425m/s, which is less than the speed at the end of the measurement when the wind speed is 10m/s(600m/s).

Wind speed has a significant effect on the airflow velocity and the state of hydrogen cloud in the flow field. An increase in wind speed contributes to an increase in air velocity. The airflow velocity reaches its peak at the beginning of the leak and attenuates at the later stage of the leak. The high-speed movement area of the gas in the flow field is different with different wind speeds, so specific analysis

Figure 3. Contour of H2 dispersion.  Figure 4. View of streamline.  Figure 5. View of velocity vector.

The graphic demonstration is used to intuitively analyze the contour of gas flow distribution cloud map, the trace of particle motion and velocity vector in the computing domain. Fig. 3-5 shows the contour of hydrogen leakage, the streamline and the velocity vector at 5s of the leakage.
of specific problems is required. Wind speed is a variable that cannot be ignored in the hydrogen leakage flow field.

4.2. Evaluation of hazardous areas

According to the lower limit of the combustion and explosion limit of hydrogen is 4%. The paper set up three horizontal observation lines at the height of 1m, 10m, 30m which run through the entire flow field to respectively simulate the hazardous areas of personnel (1m), ordinary buildings (10m) and high-rise buildings (30m). Through the first three tests, in test 1(Fig. 7) we could see at the 1s, 3s and 5s that: the hazardous areas of ordinary buildings are larger than or cover the hazardous areas of people, and spread to high-rise buildings in the later stage of the leakage, and the hazardous areas of the ordinary buildings are the largest of the three.

![Figure 7. H₂ mole fraction change during leakage test 1 at 1s, 3s and 5s.](image)

In test 1, it can be seen that the leakage process is in the low-altitude area, which is the hazardous area for personnel, and there is often forms turbulence zone, that is, the actual wind direction upwind area will also have the risk of explosion, so downwind and upwind should not be considered, people should be as far away as possible from the leak point as soon as possible when leakage occurs. The influence of wind can be seen in the mid-to-high altitude area. The higher the downwind area, the farther the hydrogen will spread downwind.

![Figure 8. H₂ mole fraction at 1s during leakage test 1, 2, 3 (variable windspeed).](image)

When leaking for 1 second, the width of the hazardous areas for personnel in test 1 is about 45m and the farthest distance from the leak is about 35m. The width in test 2 is 50m and the farthest is 50m. The width in test 3 is about 65m and the farthest is 50m (Fig. 8). It can be concluded that as the wind speed increases, the danger zone for personnel in the initial stage of the leak gradually expands.
4.3. **Influences by aperture**

The small aperture leakage is distributed in the area where the leakage points are concentrated, and the large aperture has a large spread (Fig. 9). As the leakage aperture increases, the risk area at the initial stage of leakage increases, and the leakage concentration of hydrogen increases.

4.4. **Influences by leakage position**

Comparing the bottom side leakage and the top leakage (Fig. 10), it can be clearly found that the hazardous area of the side leakage is concentrated in the personnel hazardous area within 0–5 seconds, and the gas distribution concentration in this area is the largest. Hazardous areas are more serious (Fig. 11).

![Figure 9](image_url)

**Figure 9.** H₂ mole fraction at 1s during leakage test 1, 4, 5 (variable aperture).

![Figure 10](image_url)

**Figure 10.** H₂ mole fraction at during leakage test 6(bottom side leakage).
5. Conclusions
This paper establishes the leakage and diffusion model of high-pressure hydrogen storage container, and proposes the corresponding numerical solution method. Through the numerical calculation of leakage and diffusion of the high-pressure hydrogen storage container, the change of the diffusion risk area formed after the leakage over time is obtained. Comparing the simulation results with different windspeed, leak apertures and different leak locations, the following conclusions are obtained:

- Through the numerical simulation method, the law of high-pressure hydrogen leakage and diffusion over time can be obtained, and the numerical simulation results can provide references for on-site handling of hydrogen leakage accidents.
- As the ambient wind speed increases, the degree of turbulence of the leaking hydrogen increases, and the low-altitude hazardous area at the initial stage of the leakage increases, and the medium-high-altitude hazardous area gradually shrinks.
- As the leakage aperture increases, the hazardous area at the initial stage of the leakage increases, and the concentration of leakage hydrogen increases.
- For vertical hydrogen storage containers, the hazard of the hazardous area caused by the top leakage is much smaller than the hazardous area caused by the side bottom leakage.

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