

NUMERICAL SIMULATION ON HYDROGEN LEAKAGE AND DISPERSION BEHAVIOR IN HYDROGEN ENERGY INFRASTRUCTURES

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ABSTRACT

Unexpected hydrogen leakage may occur in the production, storage, transportation and utilization of hydrogen. The lower flammability limit (LFL) for the hydrogen is 4% in air. The combustion and explosion of hydrogen-air mixture poses potential hazards to personnel and property. In this study, unintended release of hydrogen from a hydrogen fuel cell forklift vehicle inside a enclosed warehouse is simulated by fireFoam, which is an LES Navier-Stokes CFD solver. The simulation results are verified by experimental data. The variation of hydrogen concentration with time and the isosurface of hydrogen concentration of 4% vol. are given. Furthermore, the leakage of hydrogen from a storage tanks in a hydrogen refueling station is simulated, and the evolution of the isosurface of hydrogen concentration of 4% vol. is given, which provides a quantitative guidance for determination the hazardous area after the leakage of hydrogen.

1.0 INTRODUCTION

The non-renewable fossil fuels, including coal, oil, natural gas, become gradually depleted as its excessive exploitation and use, which bring a series of severe ecological and environmental problems. In order to solve these problems, the development of new energy sources has become extremely urgent. Hydrogen is a clean and renewable energy with high energy conversion rate. It has been preliminarily applied in some important fields such as automobile, forklift, backup power and distributed generation, and has shown great potential applications [1]. However, hydrogen is prone to leakage and dispersion, and has a wide flammable range . When the concentration of hydrogen in air exceeds 4%, the combustion generally occurs. Meanwhile, hydrogen features a high thermal radiation value and a large explosion energy, which can cause heavy casualties and damage. There have been many reports on hydrogen leakage accidents. On June 10, 2019, a hydrogen leakage accident occurred at a hydrogen refueling station in the outskirts of Oslo, Norway, which caused an explosion and left two injuries.

Therefore, safety issues on the production, storage, transportation, and utilization of hydrogen cannot be ignored. Analyzing hydrogen leakage and dispersion behaviors, obtaining an accurate concentration distribution and estimating whether the lower flammability limit is reached or not are vital to determination the hazardous area and protective measures. Therefore it is necessary to conduct deep research into these behaviors.

Hydrogen leakage and dispersion behaviors initiate many severe accidents, and have attracted great attention of many researchers at home and abroad. Prankul et al. [2] performed simulation of slow leakage, subsonic jet, and high-pressure sonic jet of hydrogen in a garage with FLACS-HYDROGEEN. Researchers at Sandia National Laboratory used FUEGO [3], fireFoam [4], and experimental methods [5] to study the unintended release of hydrogen from a hydrogen fuel cell forklift vehicle inside a enclosed warehouse. Xuefang Li et al. [6] studied the leakage and dispersion of high-pressure hydrogen of a two-dimensional axisymmetric geometric model with Fluent. Zhang et al. [7] carried out a research on the transmission and mixing process of hydrogen in a containment under severe accidents in nuclear power plants based on Gasflow-MPI.

The CFD tool, fireFoam, is an open source Large Eddy Simulation (LES) transient flow solver based on OpenFOAM [8]. In the article, the leakage and dispersion behaviors of hydrogen from a hydrogen fuel cell forklift vehicle inside a enclosed space are simulated using fireFoam. The results are compared with experimental data. Then, the leakage of hydrogen from a storage tanks in a hydrogen refueling station is simulated. The evolution of flammable hydrogen cloud is given.

2.0 SIMULATION ON HYDROGEN LEAKAGE AND DISPERSION BEHAVIOR IN ENCLOSED SPACE

2.1 Geometric Modeling

Simulations on hydrogen release from the fuel-cell poared forklift inside an enclosed warehouse are performed in the present section. The research object is a scaled test facility located at the SRI Corral Hollow Experiment Site in Livermore California [5], which measures 3.64 m wide, 4.59 m long, 2.72 m high, and has a total internal volume of 45.4 m³. A photograph of the test facility is provided in Fig. 1a, while a schematic of the warehouse geometry is given in Fig. 1b.

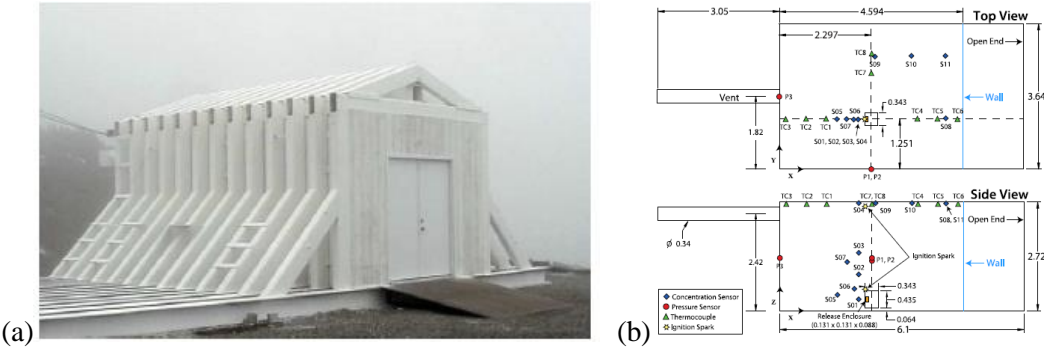


Fig. 1 (a) Photograph of the SRI subscale warehouse test facility. (b) Scaled warehouse schematic that illustrates the forklift model placement along with the locations of the concentration sensors.

In order to simplify the simulation, the release process is treated as hydrogen being exhausted from the side of the forklift through a 131 mm by 131mm opening with a uniform velocity that is directed toward the back wall of the warehouse. The geometric modeling of the scaled warehouse test facility is shown in Fig. 2a. The structured grids are generated by ICEM, and the number of the grids is 780,000. The area near the release point is refined. The surface mesh of the scaled warehouse is shown in Fig. 2b.

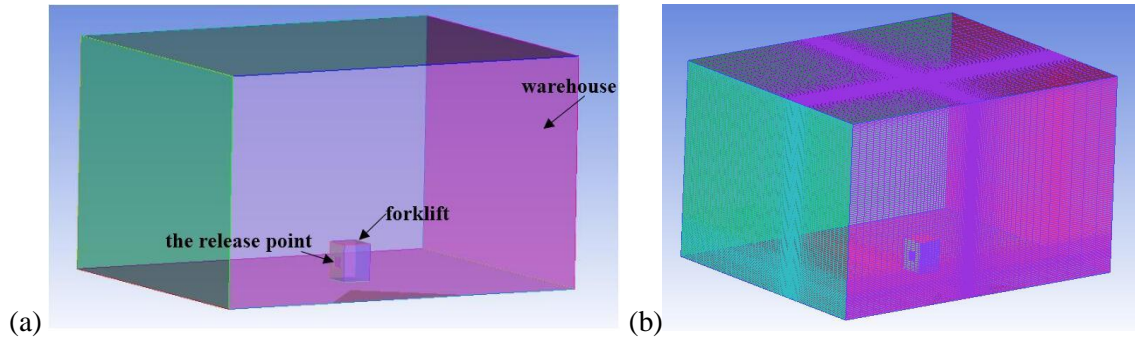


Fig. 2 (a) The geometric modeling of the scaled warehouse. (b) The surface mesh of the scaled warehouse.

2.2 Results and Analysis

At the beginning, the scaled warehouse is filled with air. The pressure is 1atm and the temperature is 297K. Release velocity is obtained by measured mass release rates. During the calculation, the mass fractions of hydrogen, oxygen and nitrogen at s01- s11 sensor locations are monitored. Hydrogen mole fraction from select sensors near the point of release is shown in Fig. 3a, and hydrogen mole fraction from select sensors along the ceiling is shown in Fig. 3b. In Fig. 3, the simulation results are compared with experimental data [5]. The solid line represents the simulation results and the dashed line represents the experimental data. It can be seen from Fig. 3 that the peak values of the hydrogen mole fraction from the numerical calculations are close to that of the experimental data, and the variation trend of the numerical results is consistent with that of the experimental data. The accuracy of the numerical simulation method is thus verified.

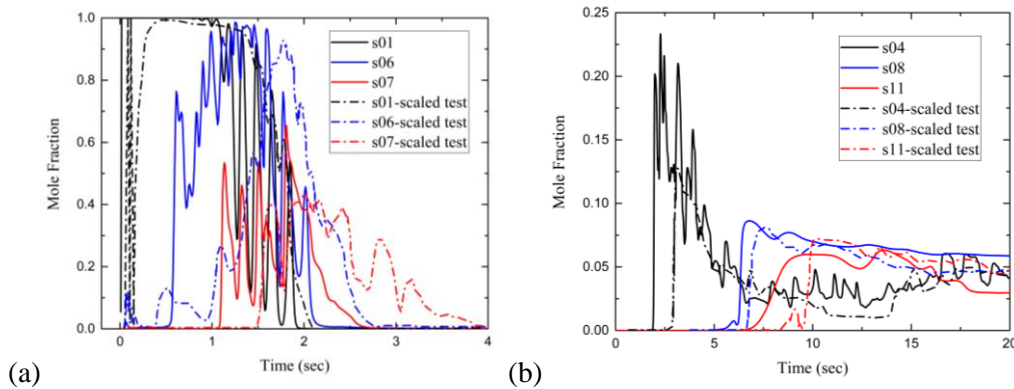


Fig. 3 (a) Hydrogen mole fractions from select sensors near the point of release. (b) Hydrogen mole fractions from select sensors along the ceiling.

A comparison between numerical calculated values (cal) and experimental data (exp) of the peak hydrogen mole fractions at each sensor location is shown in Table 1. As shown in Table 1, there is a bigger difference between numerical calculated values and experimental data of the peak hydrogen mole fractions at the locations of S02 and S03, while a smaller difference at other sensor locations [5].

Table 1 Comparison between numerical calculated values (cal) and experimental data (exp) of the peak hydrogen mole fractions at each sensor location.

	S01	S02	S03	S04	S05	S06	S07	S08	S09	S10	S11
exp	1	0.336	0.187	0.128	0.917	0.923	0.441	0.082	0.09	0.067	0.072
cal	1	0.853	0.535	0.23	0.991	0.99	0.65	0.048	0.08	0.085	0.063

Since the flammable range of hydrogen in air is from 4% to 75%, the isosurface of hydrogen concentration of 4% vol. can be considered as the quantitative index for the prediction of combustion or explosion risk. The evolution of the isosurface of hydrogen concentration of 4% vol. in the scaled warehouse for the first 4 seconds after the hydrogen releasing are shown in Fig. 4. As we can see from Fig. 4, the flammable cloud rises from the side vent on the forklift and collects along the ceiling in the corner of the warehouse.

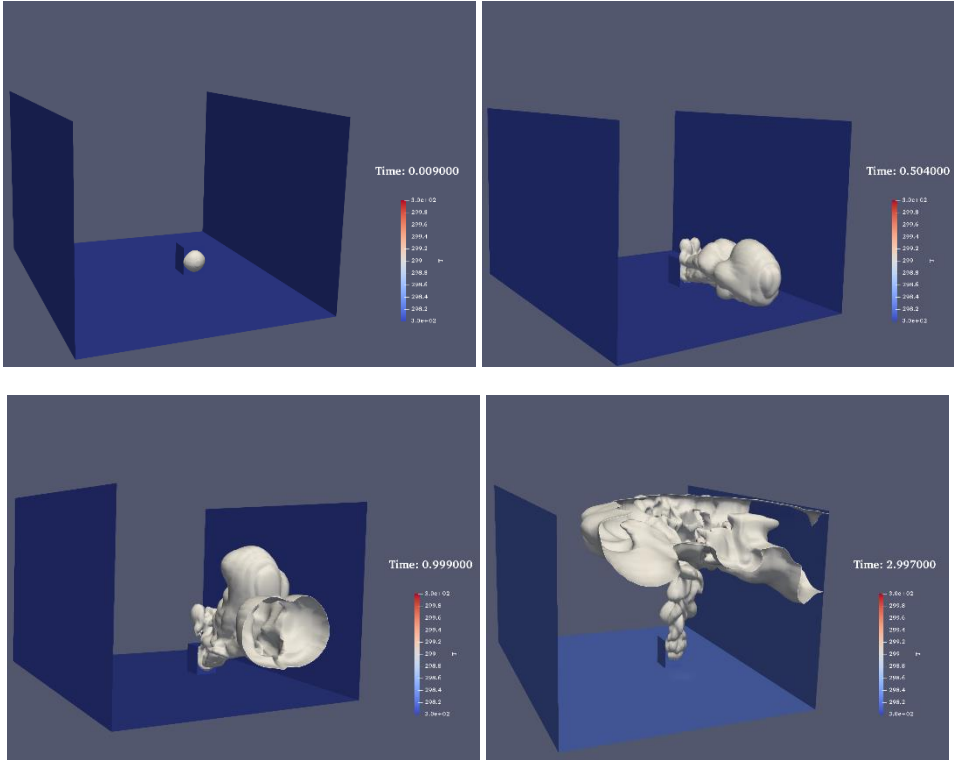


Fig. 4 The evolution of the isosurface of hydrogen concentration of 4% vol. in the scaled warehouse for the first 4 seconds after the hydrogen releasing.

3.0 SIMULATION ON HYDROGEN LEAKAGE AND DISPERSION BEHAVIOR IN OPENED SPACE

3.1 Geometric Modeling

Hydrogen refueling station (HRS) is an important hydrogen energy infrastructure. Accurate simulation of dispersion behavior and concentration distribution after hydrogen leakage is of great significance to the prediction of dangerous area and design optimization of HRS. This section simulates the dispersion behavior after hydrogen leakage of a hydrogen refueling station simplified model. The HRS covers an area of about 2352 m² and provides dispensing pressure of 35 MPa and 70 MPa. The high-pressure hydrogen storage vessels consist of two 98.5 MPa cylinders, two 45 MPa 3*3 bundles and two 20 MPa long tube trailers. To simplify the geometry, the bundles and trailers are treated as cuboids, and 98.5 MPa hydrogen storage vessels are modeled as cylinders. Keep the canopy and the firewall. The simplified model of the hydrogen refueling station is shown in Fig. 5, with dimensions of 20 m*25 m*6 m.

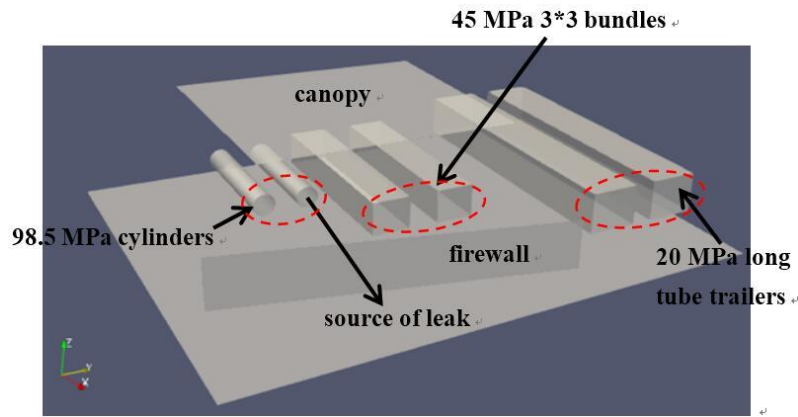


Fig. 5 The geometric modeling of the hydrogen refueling station simplified model.

3.2 Results and Analysis

Hydrogen leakage and dispersion behavior from a 98.5 MPa hydrogen storage tank are simulated. Fig. 5 shows the location of the source of the leak. The diameter of the leakage source is 15 cm. The rate of hydrogen leakage is 132m/s. The evolution of hydrogen cloud with concentration of 4% vol. is shown in Fig. 6. It can be seen that a high-speed jet driven by momentum appears firstly after the release of hydrogen. Then it turns into a buoyance-driven plume gradually. At about 2.5s, the hydrogen cloud with concentration of 4% vol. will cross the firewall and enter the dispensing area, which brings a potential threat to the dispensing area. Due to the frequent activities of personnel and vehicles, the conditions of the dispensing area are relatively complicated and the flammable cloud is more likely to be ignited. Therefore, it is necessary to take measures to restrict the dispersion of flammable cloud to the dispensing area, such as heightening the firewall or installing fans.

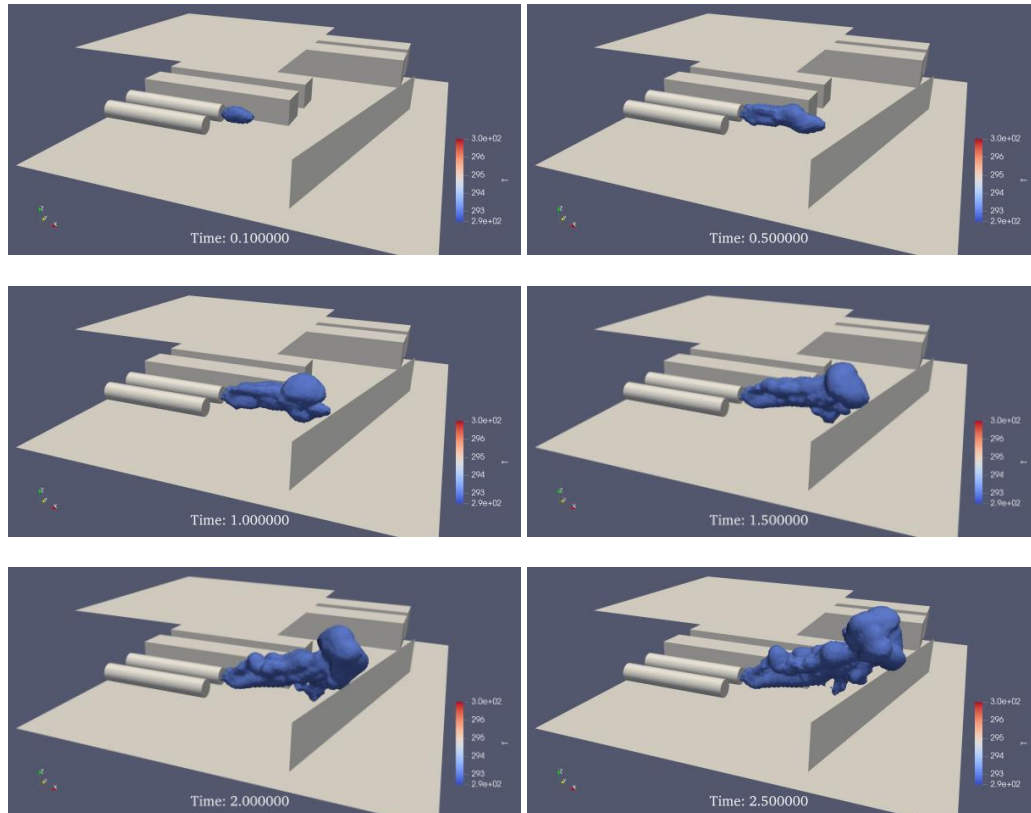


Fig. 6 The evolution of hydrogen cloud with concentration of 4% vol..

4.0 SUMMARY

As the rapid development of hydrogen energy, the frequency of hydrogen accidents is increasing. It is imperative to accelerate the research of hydrogen safety. In this paper, the fireFoam solver is used to analyze the hydrogen leakage and dispersion behavior. An enclosed warehouse model and an open hydrogen refueling station model are simulated respectively. In the warehouse model, the variation of the molar fraction of hydrogen at different locations over time are obtained. By comparing simulation results with experimental data, it can be seen that the numerical method can accurately predict the leakage and dispersion process of hydrogen. In the hydrogen refueling station model, the evolution of the isosurface of hydrogen concentration of 4% vol. is given, which provides a quantitative guidance for determination the hazardous area. Those results can provide technical support for the design optimization of hydrogen energy facilities.

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