Research on hydrogen leakage and dispersion characteristics in indoor thermal stratification environment

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Abstract. The leakage of hydrogen in a room is a key issue of hydrogen safety, and ventilation plays an important role in hydrogen dispersion. The hydrogen leakage usually builds a thermal stratification environment due to the low temperature of liquid hydrogen or throttling effect. This study attempts to develop a fast-computational theoretical model of hydrogen dispersion motion in an indoor thermal stratification environment based on the classical buoyant jet model and to carry out an experimental to verify model. The research results show that the developed theoretical model can well predict the trajectory of slowly releasing hydrogen leakage. The motion trajectory of the hydrogen leak oscillates in the thermally stratified environment at a certain height, called as the "lock height". The smaller the leak port in the uniform environment the larger the horizontal diffusion distance, and the smaller the leak port in the thermally stratified environment the higher the locking height. The research results are expected to predict the hydrogen leakage safety prediction problem and the formulation of related standards and help make ventilation strategies to ensure the hydrogen safety.

1 Introduction

As a renewable and sustainable energy source, hydrogen energy has been widely used in aerospace, energy, chemical and machinery industries. Hydrogen energy is also used in indoor household energy, fuel cell vehicles, and the mixing of natural gas with hydrogen has also become a social hotspot. The best way to reduce the safety risk of hydrogen in indoor applications is ventilation [1].

The relationship between hydrogen and indoor ventilation has been attracting much attention, and some experimental results have reiterated the occurrence of hydrogen leakage concentration stratification [2-6], but the mechanism of hydrogen leakage and stratification in a thermally stratified environment is still unclear. Numerical simulation of hydrogen leakage is also an important means to study hydrogen safety, and many studies use the most commonly used k-ε model [7-9], LES model [10]. However, the temperature of the air conditioning vents and leaking hydrogen is usually lower than the ambient air temperature, resulting in thermal stratification, i.e. cooler air at the bottom and warmer air at the top, with an air temperature gradient. The phenomenon of jet dispersion in a thermally homogeneous environment is quite different from that in a thermally stratified environment. Qian et al. [11-14] theoretically predicted and observed that in a thermally stratified indoor environment, the respiratory airflow and virus appeared to be highly oscillated indoors. The same phenomenon is observed in the outdoor atmospheric inversion layer, which restricts vertical airflow and traps aerosols, air pollutants [15,16]. The studies of the above scholars have found that temperature stratification is a very common phenomenon in both indoor and outdoor environments.

This paper focuses on the dispersion trajectory of hydrogen in indoor homogeneous and thermally stratified environments, and determines the locking height of hydrogen dispersion through theoretical models, thereby providing technical reference for indoor ventilation interventions.

2 Methodologies and Verification

In indoor environments such as hydrogen fuel cell car garages, home hydrogen-infused gas kitchens, and hydrogen storage tanks in factories, the potential for thermal stratification is high. In this work, a hydrogen leak in a thermally stratified environment in a garage is taken as an example, as shown in Fig. 1. The research expects to determine the locking height of hydrogen in the thermally stratified environment through the predictive analysis of the theoretical model, so as to set up indoor mechanical ventilation intervention at the...
locking height to reduce the accumulation of hydrogen and reduce the risk of explosion. Due to different application environments, the temperature gradient of thermal stratification is also quite different. The relationship between thermal stratification and locking height is determined by prediction model.

Fig. 1. Caption of the Figure 1. Below the figure.

### 2.1 Modelling

A buoyant jet mathematical model is used to describe the movement of hydrogen leaking from a small hole. The dispersion of hydrogen leakage can be simplified as the dispersion process of buoyant jets. To reveal the essential characteristics of the buoyant jet, the dimensionless form of the above-mentioned governing equation is derived to facilitate the subsequent solution. The following parameters are dimensionless:

\[
\begin{align*}
  u_\text{m} &= \frac{U_\text{m}}{B}, b^* = \frac{b}{B}, s^* = \frac{s}{B}, \rho_\text{a}^* &= \frac{\rho_\text{a}}{\rho_0}, x^* = \frac{x}{B}, y^* = \frac{y}{B}, \Delta \rho_\text{m} = \frac{\Delta \rho_\text{m}}{\rho_0}.
\end{align*}
\]

where, \(U\) is the initial velocity, m/s; \(B\) is the radius of the leakage source, m; \(\rho_\text{a}\) is the density of hydrogen, kg/m\(^3\); \(\Delta \rho_\text{m}\) is the density difference between the expiratory jet at the outlet and the surrounding air, kg/m\(^3\).

Bring the above-mentioned dimensionless parameters into the governing equation to obtain the governing equation in dimensionless form.

- Dimensionless continuity equation:
  \[
  \frac{d}{ds^*}(u_\text{m} b^* \Delta \rho_\text{m}) = 0
  \quad (13)
  \]

- Dimensionless buoyancy flux equation in thermally stratified environment:
  \[
  \frac{d}{ds^*}(u_\text{m} b^* \Delta \rho_\text{m}) = 1 + \frac{\Delta \rho_\text{m}}{\rho_\text{a}^*} - \frac{\rho_\text{a}^* \beta}{\rho_0} \left(\frac{dT}{dy}\right) \sin \theta
  \quad (14)
  \]

where, the density gradient is calculated approximately by Boussinesq: \(\frac{dT}{dy} = -\rho_0 \beta \frac{dT}{dy}\). \(\beta\) is the thermal expansion coefficient of air, and \(dT/\text{dy}\) is the temperature gradient, °C/m.

- Dimensionless x-direction centreline trajectory equation:
  \[
  \frac{dx^*}{ds^*} = \cos \theta
  \quad (15)
  \]

- Dimensionless y-direction centreline trajectory equation:
  \[
  \frac{dy^*}{ds^*} = \sin \theta
  \quad (16)
  \]

### 2.2 Verification

Figures 2 and 3 show the comparison of the dimensionless jet width and velocity of centreline calculated by the current prediction model with the experimental result (\(Fr=99\)). The predicted results are in good agreement with the experimental results. Due to the entrainment effect and turbulent instability at the jet boundary, it is difficult to accurately measure the steady seepage width experimentally.

Fig. 2. Comparison of the jet width between the theoretical predictions and experimental results.

Fig. 3. Comparison of the velocity of centreline between the theoretical predictions and experimental results.


3 Results and discussion

3.1 Leakage angle

Due to factors such as pipeline wear and vibration, the hydrogen leakage angle is random, and the leakage angle has a greater influence on the hydrogen diffusion trajectory. Figures 4 and 5 show the centreline trajectories of leaky hydrogen dispersion for different leak angles in thermally homogeneous and layered environments, respectively. It can be seen from Figure 3 that when the leak angle is 0° or 45°, the trajectory of the leaked hydrogen flow continues to move upward in a homogeneous environment. Under the same vertical movement distance, a jet with a leak angle of 0° travels a longer distance in the horizontal direction than a jet with a leakage angle of 45°. Although the Froude number Fr and the initial jet velocity remain unchanged in both cases, the jet with a leak angle of 45° has momentum components in both the horizontal and vertical directions. The vertically upward momentum component helps the leaking hydrogen move up faster. When the leak angle is -45°, the predicted centreline trajectory will move downward at the initial stage due to having a vertically downward initial momentum component, and then start to move upward due to the influence of buoyancy. The model calculation results in Fig. 4 show that the hydrogen leaks and then oscillates at a certain height. In contrast to the experimental results [2][3][5], a clear stratification of more or less hydrogen-rich mixtures can be observed in the room. The upper isothermal restricted area. However, the difference from the simulated respiration of Zhou et al. [11] is that hydrogen is more likely to float in a homogeneous environment due to its lower density and greater buoyancy. Moreover, the "lock height" of hydrogen in a thermally stratified environment is higher than that of respiration.

Fig. 4. Trajectories of hydrogen leakage flow with different angles.

Fig. 5. Trajectories of hydrogen leakage flow with different angles in thermally-stratified.

3.2 Leak port size

Figures 6 and 7 illustrate the hydrogen dispersion trajectory for different leak port sizes. In the uniform and thermally stratified environments, the hydrogen dispersion trajectories are significantly different when the leak openings are 0.2 m, 0.02 m and 0.002 m, respectively. The smaller the leak port in the uniform environment the larger the horizontal diffusion distance, and the smaller the leak opening in the thermally stratified environment the higher the locking height.

Fig. 6. Trajectories of hydrogen leakage flow with different leak port sizes.

Fig. 7. Trajectories of hydrogen leakage flow with different leak port sizes in thermally-stratified.
4 Conclusion

In this work, a hydrogen leakage prediction model is carried out in an indoor homogeneous and thermally stratified environment. Predicting hydrogen leakage trajectories is expected to provide technical strategies for preventing and dealing with hydrogen leakage problems.

It can be used as a reference for leakage and diffusion safety technologies such as household hydrogen energy storage tanks, hydrogen fuel cells, and hydrogen energy vehicles. The trajectories and 'lock heights' of leaking hydrogen were calculated by a hydrogen leak prediction model in a thermally stratified environment, and the accumulation of hydrogen was reduced by ventilation interventions at the 'lock height'.

References

1. S. Gupta, J. Brinster, E. Studer, I. Tkatschenko, Int J Hydrogen Energy 34, 14(2009)
2. J. M. Lacome, D. Jamois, L. Perrette, C. H. Proust, Int J Hydrogen Energy 36, 3(2011)
3. A. Prabhakar, N. Agrawal, V. Raghavan, S. K. Das, Int J Hydrogen Energy 48, 41(2016)
4. C. D. Barley, K. Gawlik, Int J Hydrogen Energy 34, 13(2009)
5. K. Takeno, K. Okabayashi, A. Kouchi, N. Misaka, K. Hashiguchi, Int J Hydrogen Energy 42, 22 (2017)
6. K. Okabayashi, K. Tagashira, K. Kawazoe, K. Takeno, M. Asahara, A. K. Hayashi, M. Komori, Int J Hydrogen Energy 44, 17 (2019)
7. D. Makarov, V. Molkov, Int J Hydrogen Energy 38, 19 (2013)
8. J.J. Keenan, D.V. Makarov, V.V. Molkov, Int J Hydrogen Energy 42, 11 (2017)
9. T Mogi, S Horiguchi, J Loss Prevent Proc 22, 1 (2009)
10. X.P. Li, K. Wu, W. Yao, X.J. Fan, Int J Hydrogen Energy 41, 9 (2016)
11. Q. Zhou, H. Qian, H.G. Ren, Y.G. Li, P.V. Nielsen, Build Environ 116, 1 (2017)
12. F. Liu, H. Qian, Z. Luo, X. Zheng, Indoor Air, 31, 2 (2021)
13. F. Liu, H. Qian, Z. Luo, S. Wang, X. Zheng, Build Environ 180, (2020)
14. Z. Shu, G. Lei, Z. Liu, W. Liang, X. Zheng, J. Ma, F. Lu, H. Qian, Int J Hydrogen Energy 47, 3 (2022)
15. T Jin, YL Liu, JJ Wei, DY Zhang, XX Wang, G Lei, TX Wang, YQ Lan, H Chen, Int J Hydrogen Energy 44, 41 (2019)
16. J. Wallace, D. Corr, P. Kanaroglou, Sci Total Environ 408, 21 (2010)