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CFD Simulation and ANN Prediction of Hydrogen Leakage and Diffusion Behavior in a Hydrogen Refueling Station

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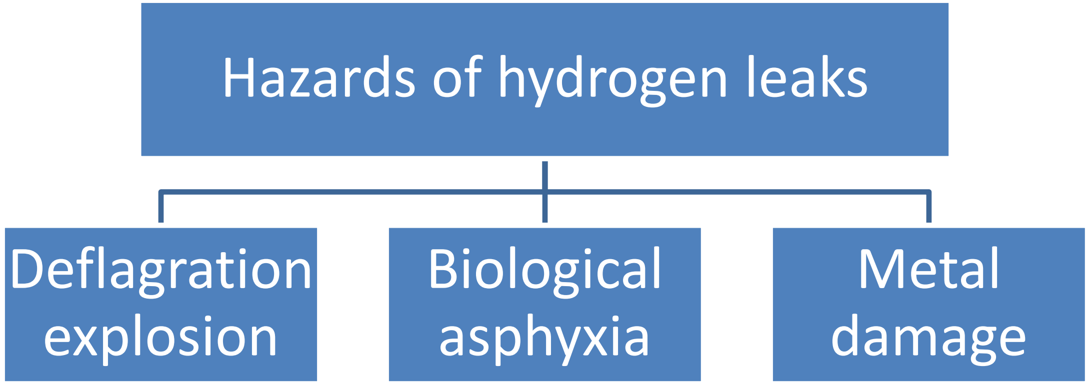
Introduction

Hazardous Properties of Hydrogen

● Hydrogen has a **wide flammable range** (4% -74%) **, low ignition energy, small molecular weight**, **high diffusion coefficient, fast leakage rate, high combustion heat** and **fast flame propagation speed**.

● CFD simulation helps to **explore the diffusion laws of gas hydrogen leakage**.

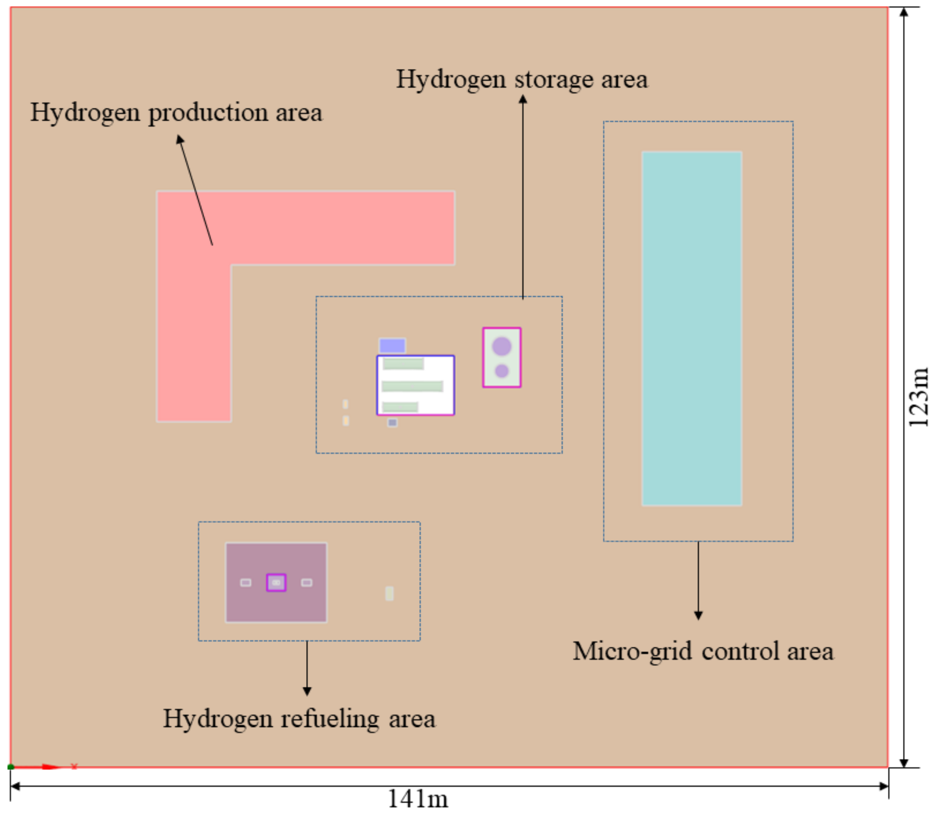
●Establishing a combustible hydrogen cloud prediction model helps to **quickly determine the danger range and promote the safe application of hydrogen energy**.

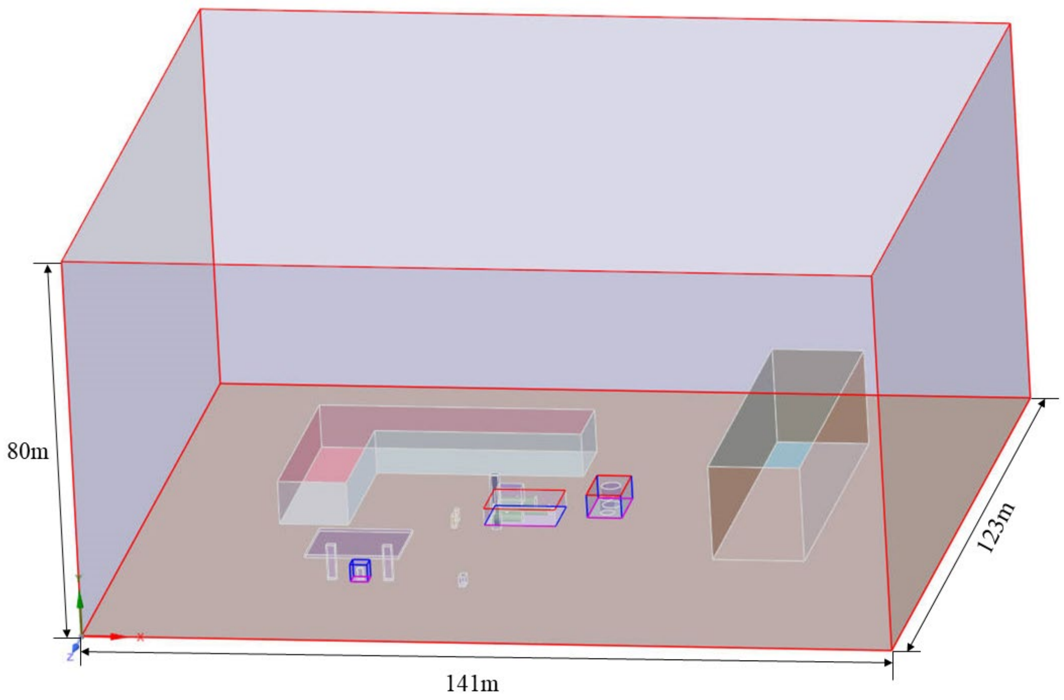


CFD Model Description

Hydrogen Refueling Station Model

The external area of the hydrogen refueling station mainly includes **hydrogen production area**, **micro-grid control area**, **hydrogen storage area**, and **hydrogen refueling area**. Assuming that both the hydrogen production area and the micro-grid control area are enclosed, leaked hydrogen will not enter both areas.





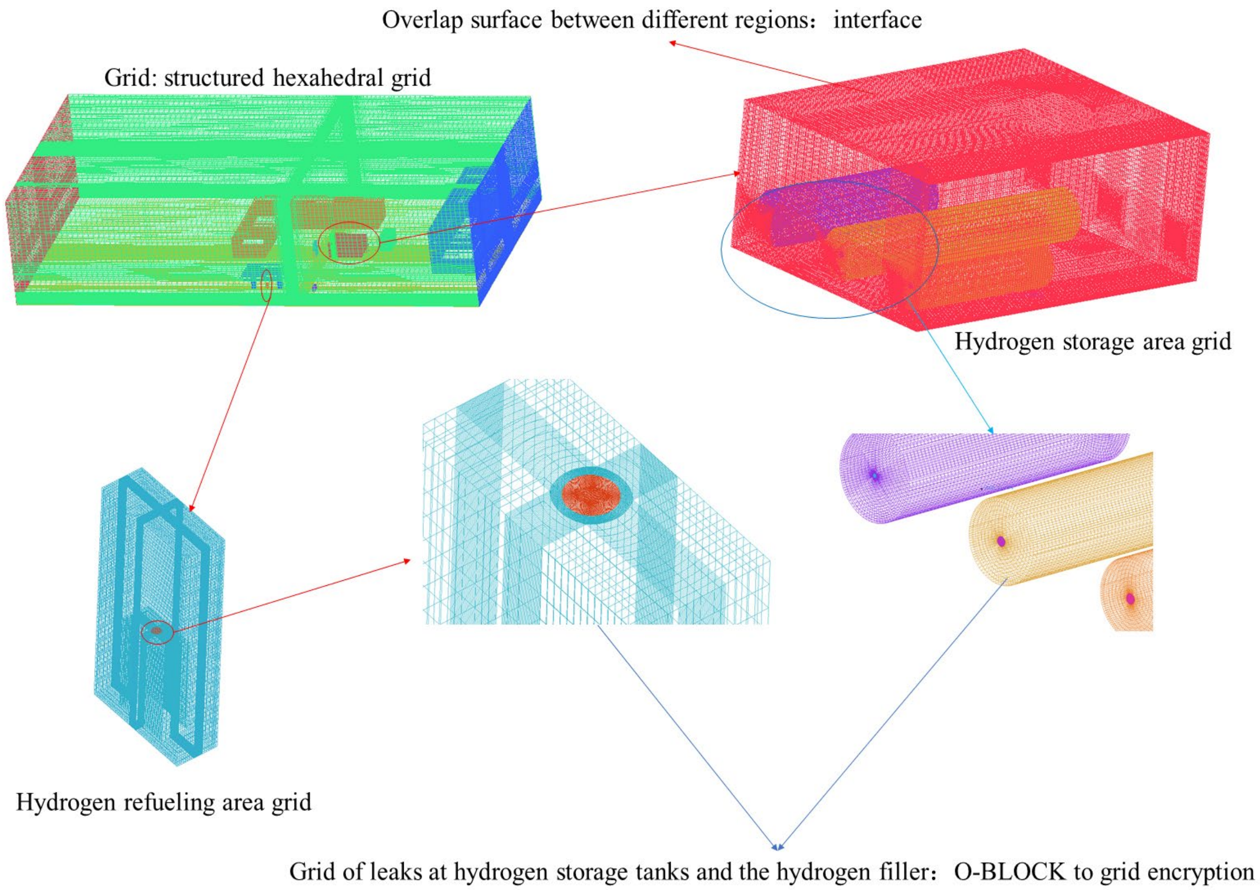
CFD Model Description

Meshing and Independence Verification

- **ICEM software** was used to construct the external model for meshing.

- Considering the difficulty of meshing and the number of meshes, **the model was divided into different parts:** hydrogen refuelling area, hydrogen storage area and air domain.

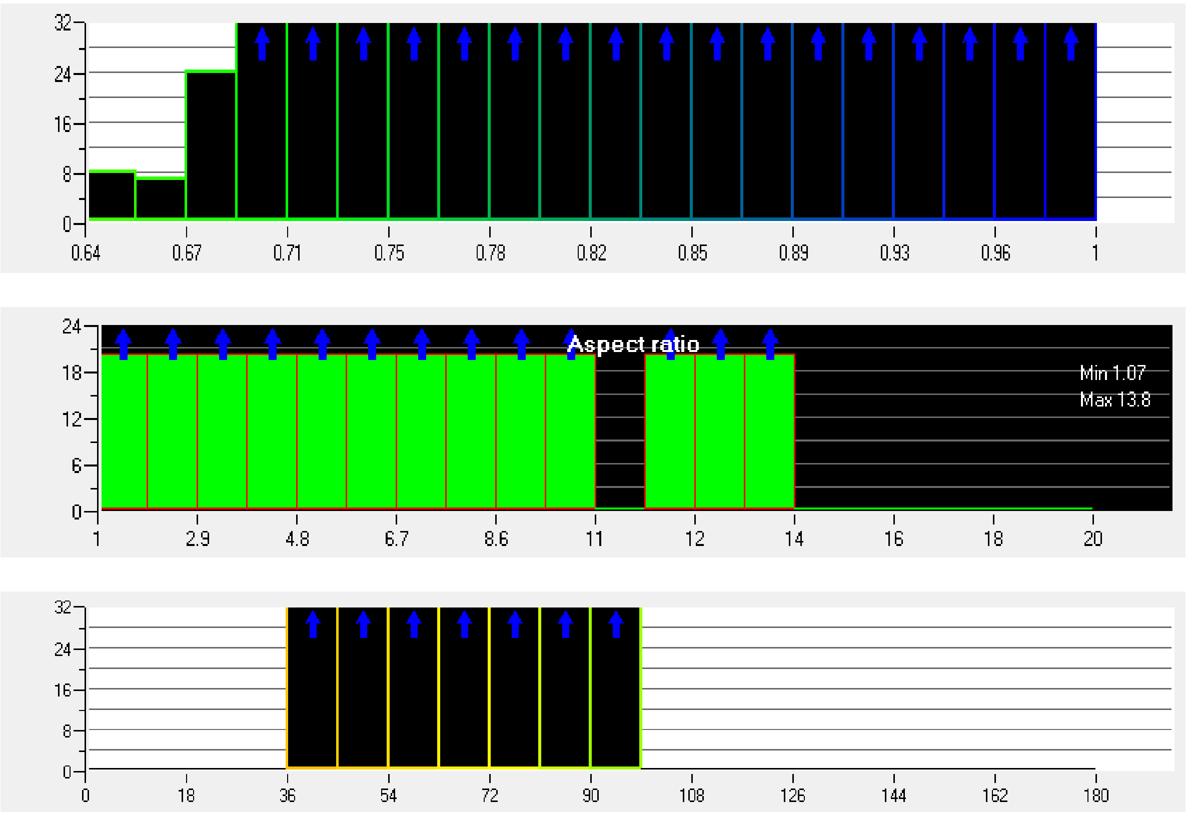
- According to the principle of hybrid meshing technology, the meshes of these parts were divided independently.

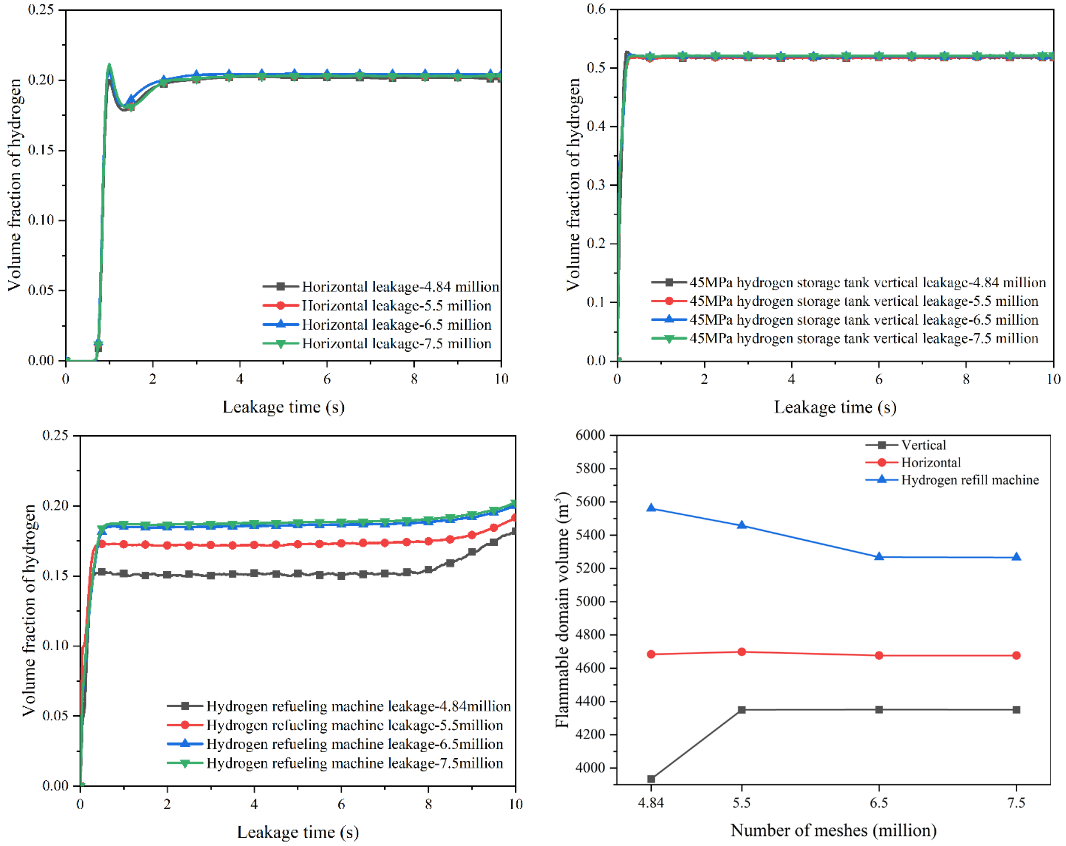


CFD Model Description

Meshing and Independence Verification

- The overall orthogonal quality of the mesh is between **0.64 and 1**.
- The maximum aspect ratio of the overall grid is **13.8**.
- The minimum angle of the overall grid element is **36°** .
- Through irrelevance verification, **6.5 million grids** were ultimately selected for subsequent calculations.





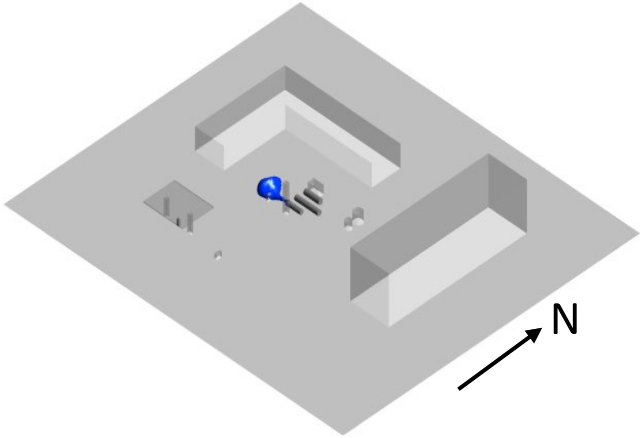
Parametrical Study of Hydrogen Leakage and Diffusion Behavior

Leakage Direction—Horizontal leakage of 45MPa hydrogen storage tank

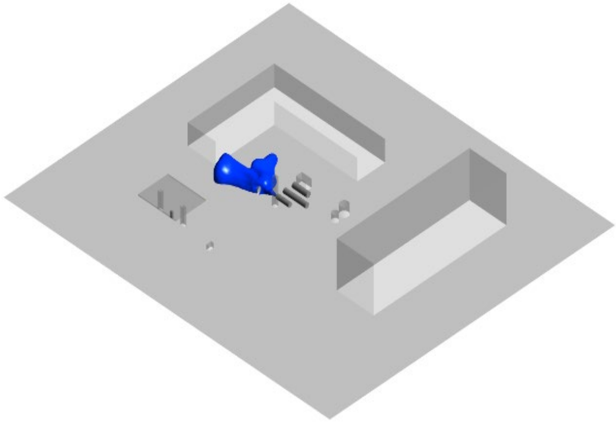
● At **0.2 s,** the hydrogen has diffused into the pressure reducing valve and **wrapped around it**.

● At **1 s,** the hydrogen diffuses **forward** along the **side of the device** and **upward** along the **front of the device**, respectively.

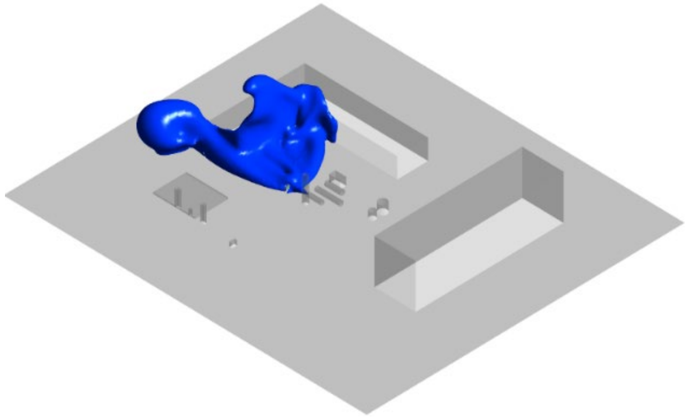
● At **30 s,** the **maximum distance** for horizontal diffusion is **67.2 m**, and the **highest position** for vertical diffusion is at the corner of the factory building, reaching **34 m**.



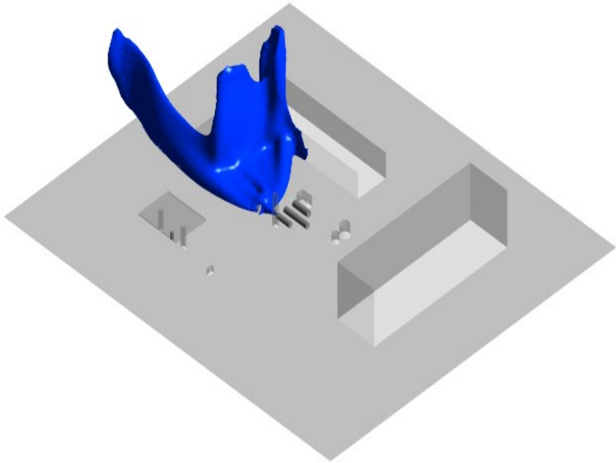
0.2s



1s



10s

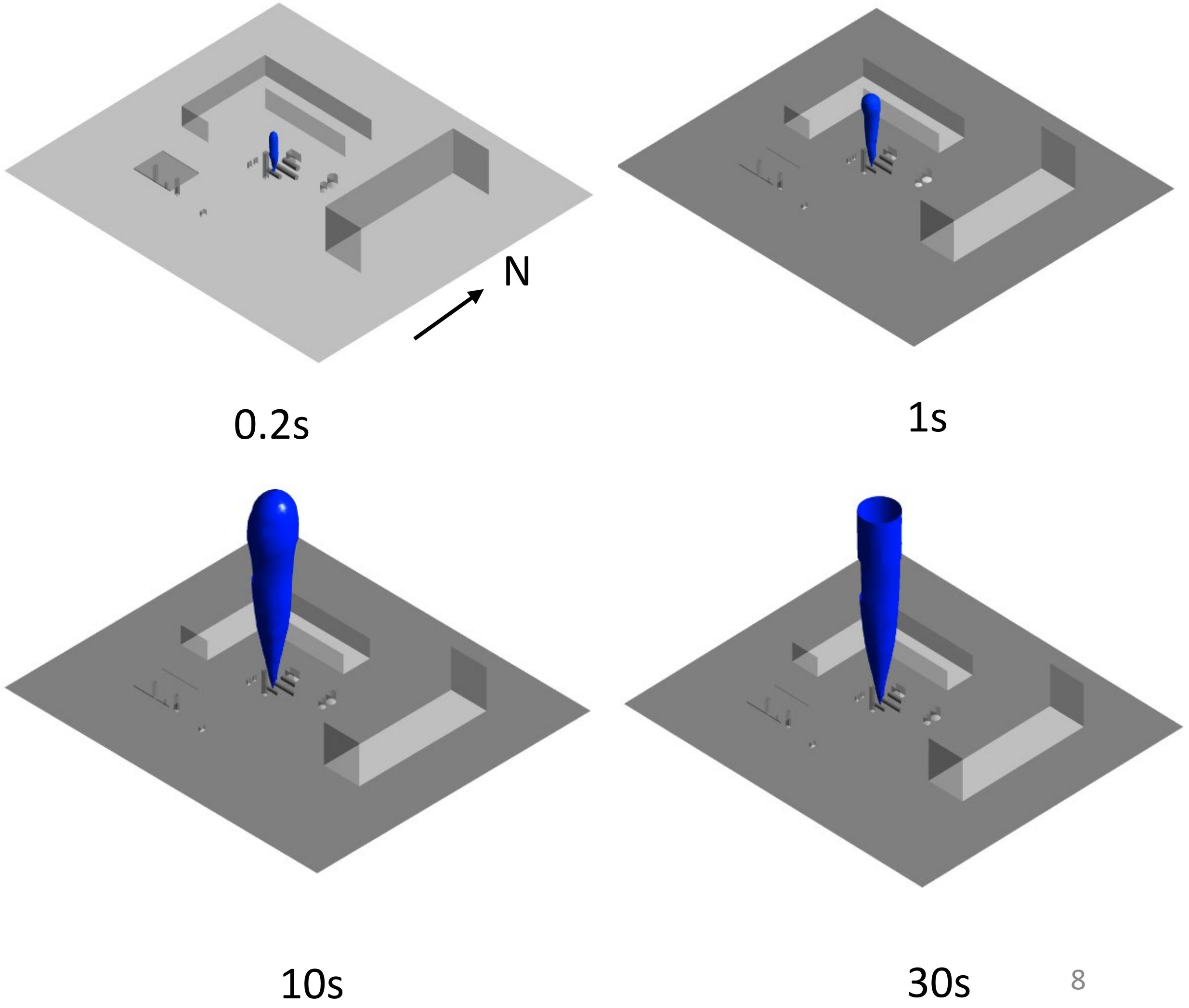


30s

Parametrical Study of Hydrogen Leakage and Diffusion Behavior

Leakage Direction—Vertical leakage of 45MPa hydrogen storage tank

- From **0.2s to 1s**, a spherical area appears at the top of the flammable domain and continuously moves up over time.
- When the leak occurred for **10 s**, the combustible hydrogen cloud had already spread to the boundary of the computational domain, reaching up to **76 m**.
- At a **height of 60 m**, the hydrogen cloud reaches a maximum width of approximately **17 m**.



Parametrical Study of Hydrogen Leakage and Diffusion Behavior

Leakage Mass Flow Rate

● When the leakage **mass flow rate** increases from 1.5589 kg/s to 4.5589 kg/s, the horizontal diffusion distance increases **from 30.417 m to 67.2 m**, and the combustible cloud volume increases **from 2277.48 m^3 to 6140.46 m^3** .

● When the mass flow rate is 1.5589 kg/s, the vertical diffusion distance is the highest, reach **42.41 m**.

● When the mass flow rate is 2.5589 kg/s, 3.5589 kg/s, and 4.5589 kg/s, the vertical diffusion distance has no significant difference, ranging from **33 to 34 m**.

Table 1. Hydrogen diffusion results under different leakage mass flow rates

Mass flow rate	Horizontal diffusion distance	Vertical diffusion distance	Volume of flammable hydrogen cloud
1.5589 kg/s	30.417 m	42.41 m	2277.48 m^3
2.5589 kg/s	43.092 m	33.13 m	3664.88 m^3
3.5589 kg/s	54.283 m	33.08 m	4876.71 m^3
4.5589 kg/s	67.2 m	34 m	6140.46 m^3

Parametrical Study of Hydrogen Leakage and Diffusion Behavior

Ambient Wind Direction

It can be seen from the Table 2 that when the wind direction is **opposite** to the leakage direction, hydrogen gas cannot diffuse smoothly, thus gathering between the **hydrogen storage tank** and **hydrogen production area**, greatly **increasing the danger**.

Table 2. Diffusion distance results of flammable hydrogen clouds in different wind directions

Wind direction	Horizontal diffusion distance	Vertical diffusion distance	Volume of flammable hydrogen clouds
East wind	47.19 m	32.91 m	9160.21 m^3
West wind	25.02 m	28.76 m	9419.06 m^3
South wind	30.61 m	40.12 m	8124.44 m^3
North wind	41.93 m	39.22 m	9251.27 m^3

Parametrical Study of Hydrogen Leakage and Diffusion Behavior

Ambient Wind Speed

- Table 3 shows that as the wind speed increases, the **vertical diffusion distance** gradually **decreases** and the **horizontal diffusion distance increases**.

- The main reason is that when the wind speed reaches a certain value, **a backflow will form on the side wall of the hydrogen production area**, accumulating hydrogen on the side wall to form a flammable zone, thereby increasing the horizontal diffusion distance along the leakage direction.

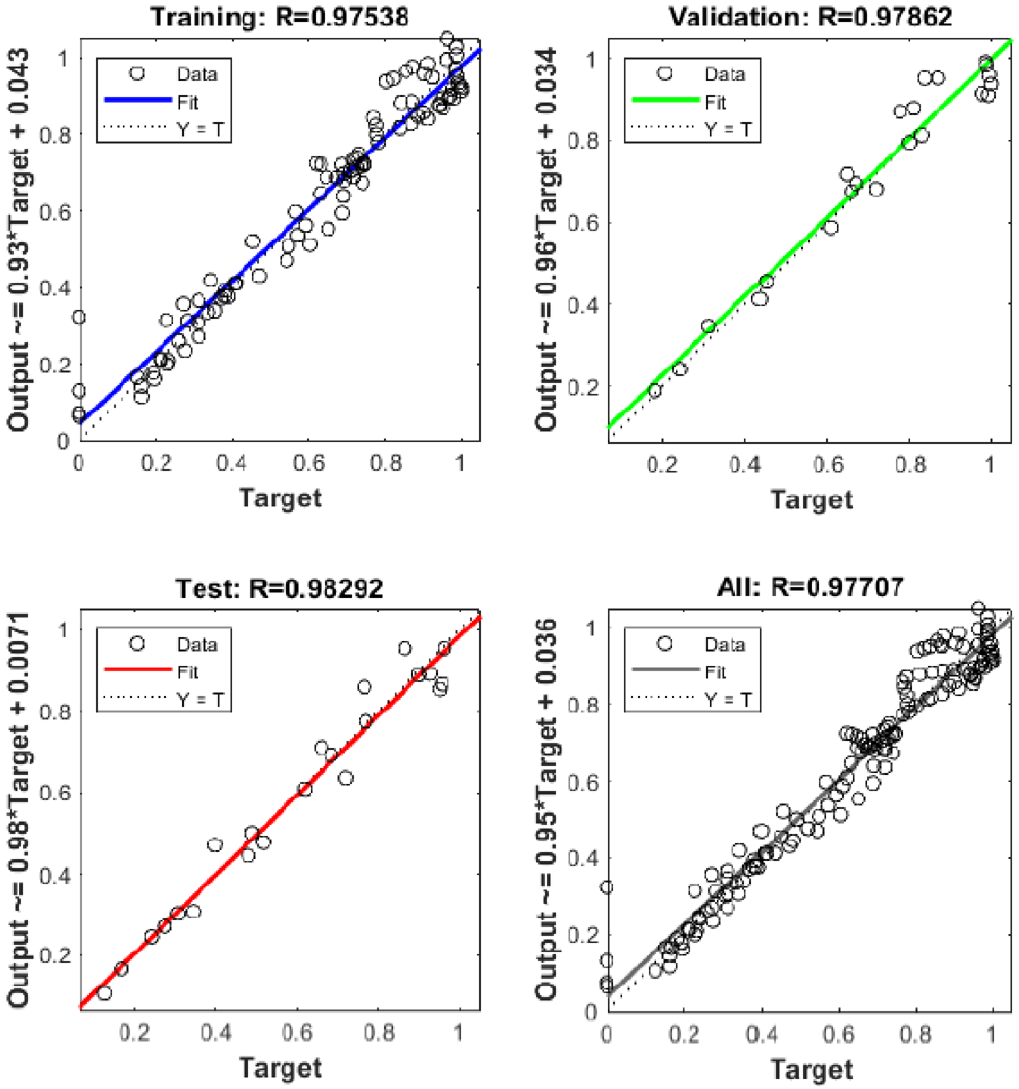
Table 3. Diffusion distance results of flammable hydrogen clouds in different wind speed

Wind speed	Horizontal diffusion distance	Vertical diffusion distance	Volume of flammable hydrogen clouds
2 m/s	25.02 m	28.76 m	9419.06 m^3
5 m/s	29.59 m	18.799 m	8259.45 m^3
8 m/s	35.843 m	15.58 m	6568.19 m^3
10 m/s	36.423 m	15.14 m	5738.24 m^3

Prediction of Flammable area Based on Artificial Neural Network Model

Establishment and Training of BP Artificial Neural Network(BP-ANN)

- The number of hidden layers is selected to 1.
- The number of neurons in the input, hidden and output layers is 3, 8 and 2.
- The hidden and the output layers adopt different activation functions, namely ***tansig* and *purelin***.
- The correlation coefficient **R** during **training, validation and testing** are 0.97538, 0.97862, and 0.98292. The correlation coefficient **R** for the entire process is 0.97707.

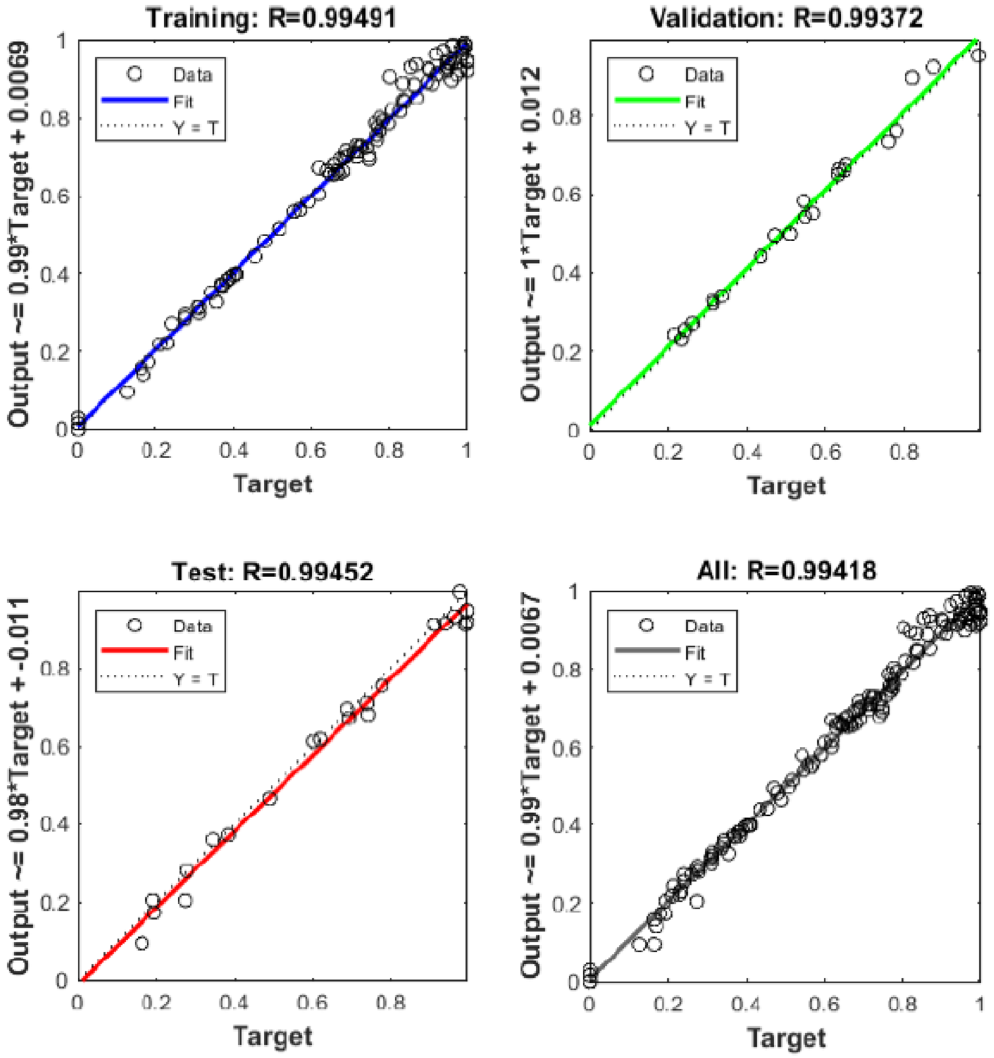


Prediction of Flammable area Based on Artificial Neural Network Model

Neural Network Optimization Based on Sparrow Search Algorithm (SAA)

● The correlation coefficient R of the neural network optimized using **SAA** during training, testing and validation are 0.99491, 0.99372 and 0.99452, respectively, and the overall correlation coefficient R is 0.99418.

● All the correlation coefficient **R** are **higher** than that of the BP-ANN before optimization, indicating that the BP-ANN optimized using the SAA has **a better correlation**.



Prediction of Flammable area Based on Artificial Neural Network Model

Neural Network Optimization Based on Sparrow Search Algorithm (SAA)

● Table 4 shows, for the prediction of **horizontal diffusion** distance, the Mean absolute error (MAE) between the prediction result of BP-ANN and the actual value is 1.6367 m. Mean squared error (MSE) is 6.4573%, and Mean absolute percentage error (MAPE) is 9.7864%.

● However, the MAE between the prediction result of the optimized BP-ANN (**SAA-BP-ANN**) and the actual value is 0.4991 m, MSE is 2.7818%, and MAPE is 2.4801%.

Table 4. Comparison of model evaluation indicators before and after optimization (horizontal diffusion distance prediction)

Model	MAE	MAPE	MSE
BP-ANN	1.6367	9.7864%	6.4573%
SAA-BP-ANN	0.4991	2.4801%	2.7818%

Prediction of Flammable area Based on Artificial Neural Network Model

Neural Network Optimization Based on Sparrow Search Algorithm (SAA)

● Table 5 shows that for the prediction of **vertical diffusion** distance, the MAE between the prediction result of the BP-ANN and the actual value is 1.2924 m, MSE is 5.3698%, and MAPE is 6.6092%.

● However, the MAE between the prediction result of the optimized BP-ANN (**SAA-BP-ANN**) and the actual value is 0.1698 m, MSE is 1.0871%, and MAPE is 1.9337%.

Table 5. Comparison of model evaluation indicators before and after optimization (vertical diffusion distance prediction)

Model	MAE	MAPE	MSE
BP-ANN	1.2924	6.6092%	5.3698%
SAA-BP-ANN	0.1698	1.9337%	1.0871%

Conclusions

● For **leaking vertically**, the maximum diffusion distance in the **horizontal direction** is **17 m**, but the diffusion distance in the **vertical direction** is much **larger than 80 m**. For **leaking horizontally**, the diffusion range of combustible hydrogen was **wider**, with the maximum distance of 67.2 m horizontal and 34 m vertical.

● The higher the **mass flow rate**, the farther the hydrogen spreads horizontally. The **wind direction** will result in a wider spread of the flammable hydrogen cloud in the wind direction. The **wind speed** affects the horizontal and vertical spreading distance of the leaking hydrogen.

●The mean absolute error (MAE), mean squared error (MSE) and mean absolute percentage error (MAPE) between predicted and the actual values for the horizontal and vertical diffusion are less after using the **SAA to optimize BP-ANN**.

Thanks for your attentions!