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Investigations of the influence of leakage and diffusion of hydrogen-doped natural gas pipelines by numerical simulation

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Abstract

The leakage of natural gas pipelines will waste energy and damage the environment. Research on the leakage and diffusion features of hydrogen-doped natural gas is beneficial to the safe management of natural gas pipelines. This paper established a numerical model used for simulating and computing the diffusion of hydrogen-doped natural gas. Then, simulation experiments were conducted. First, the model accuracy was verified through experiments, and the appropriate mesh number of the model was determined. Then, the influence of different hydrogen blending ratios and various leakage hole diameters on the leakage and diffusion of gas was calculated. Under the same diffusion time, the higher the hydrogen content in the gas, the higher the diffusion rate of methane and hydrogen, and the diffusion rate of hydrogen had the most obvious change. Under the same diffusion time, the closer to the leakage hole, the higher the concentration of natural gas, and the concentration at the monitoring points at the same level differed little.

Keywords: Hydrogen mixing; Natural gas; Leakage; Numerical simulation

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1. Introduction

With the continuous adjustment of the global energy structure and rapid development of clean energy, natural gas, as an environmentally friendly and efficient form of energy occupies an important position in the energy supply system [1]. Methane is the primary constituent of natural gas, and the products after combustion are carbon dioxide and water, which will not pollute the environment. Hydrogen, as a flammable gas, will not pollute the environment because its combustion product is water [2]. For the two combustible gases mentioned above, pipelines are usually used to transport them, and the addition of hydrogen to natural gas has the potential to enhance the efficiency of combustion, cut down carbon emissions, and make hydrogen and natural gas share a set of transportation pipelines, saving construction costs. However, natural gas pipelines will be damaged during use due to ageing or other unexpected factors. The damage may lead to natural gas leakage, which will not only cause energy waste but also may cause fire once the concentration of leakage is too high [3]. Meanwhile, high-concentration natural gas will also pose a threat to human health. Thus, investigating the characteristics of leakage and diffusion of hydrogen-doped natural gas pipelines has great practical significance and can offer a theoretical background for engineering practice and safety

Nomenclature

A – diagonal matrix of M
B – resultant external force, N/m^3
$C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$ – turbulence constants
D – non-diagonal matrix of M
G_b – production of turbulent kinetic energy by buoyancy, J/(m^{3}s)
G_k – production of turbulent kinetic energy by flow, J/(m^{3}s)
J_i – diffusion flux of the i-th component, kg/(m^{2}s)
k – turbulent kinetic energy, J/kg
M – molar mass of gas, kg/mol
M – coefficient matrix,
p, P– pressure, Pa
p' – corrected pressure, Pa
R – gas constant, J/(mol K)
S_i – source of mass, kg/(m^{3}s)
S_m – source of momentum, N/m^3
S_k – source term, J/(m^{3}s)
S_ε – source term, J/(m^{3}s^2)
t – time, s
T – pipe temperature, K
U – velocity field, m/s
v – gas velocity, m/s
x – gas displacement, m
Y_i – mass fraction of the i-th gas component
Y_M – contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, J/(m^{3}s)

Greek symbols

γ – specific heat ratio
ε – dissipation rate of turbulent kinetic energy, J/(kg s)
μ_{eff}, μ_l, μ_t – effective, laminar, turbulent viscosity, Pa s
ρ – gas density, kg/ m^3
σ_k – turbulence constant

administration in related fields. Moortgat et al. [4] described the scenario of shallow groundwater pollution caused by natural gas leakage due to horizontal drilling and hydraulic fracturing in the process of exploitation. They used the numerical model of gas phase migration related to leaking natural gas wells to simulate working conditions, which provides an effective contribution to evaluating the leakage frequency of faulty natural gas wells and reducing leakage events. Shan et al. [5] designed a practical approach combining a Bayesian network with a bow-tie model for assessing the risk of natural gas pipeline leakage. The analysis of the case revealed that negligence in signage, implicit signage, excessive load, and design flaws in auxiliary equipment were identified as the primary factors inducing natural gas pipeline leakage. Wu et al. [6] established a Bayesian inference-iterative ensemble Kalman filter model for estimating source terms (leak location and leakage rate) and forecasting gas concentration distribution. Lee et al. [7] utilized a restricted quantity of sensors for the early detection of chemical leaks, thereby facilitating prompt and suitable initial response. Zandi et al. [8] conducted research on natural gas leaks resulting from pipeline failures in both atmospheric and porous conditions using a three-dimensional simulation methodology. Li et al. [9] compared the disparities in the distribution of hydrogen-blended natural gas flow fields released from three pipeline leakage sources: gas flowing downwards in a vertical pipe with a leak hole on the pipe wall, gas flowing upwards in a vertical pipe with a leak hole on the pipe wall, and a leak hole at the end of a horizontal pipe. In this article, a numerical model was designed to simulate the diffusion of hydrogen-doped natural gas, and simulation experiments were also conducted.

2. Materials and methods

2.1. Experimental environment

The numerical simulation of hydrogen-doped natural gas pipeline leakage and diffusion was conducted on a laboratory server with the Windows 10 operating system, 32 G memory, and Core I7 processor.

2.2. The numerical model of gas diffusion

The relevant mathematical models involved in the simulation of leakage and diffusion of hydrogen-doped natural gas pipelines include the governing equations and the turbulent motion equations, where the governing equations are:

$$\begin{gathered}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0,\\ \frac{\partial(\rho v)}{\partial t} + \nabla \cdot (\rho v^2) = -\nabla p' + \nabla \cdot (\mu_{eff} \nabla v) + B + S_m,\\ \frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho v Y_i) = -\nabla J_i + S_i.\end{gathered} \quad (1)$$

The first governing equation is a continuity equation, the second is a momentum conservation equation, and the third is a component conservation equation. ρ represents the gas density, v – gas velocity, t represents time, μ_{eff} represents the effective viscosity, p' is the corrected pressure, B is the resultant of all the external forces, S_m is the source of momentum, Y_i is the mass fraction of the i-th component in the gas, J_i is the diffusion flux of the i-th component, and S_i is the source of mass [10].

The governing equations ensure the basic rules to be followed by the gas in the numerical simulation process [11], and the simulation of the gas flow needs the application of the turbulent motion equations. In this paper, a common k-ε turbulence model [12] is adopted. The reason for choosing this turbulence model is that it is a semi-empirical formula summarized from experimental phenomena, so it has extensive applications, low computational cost, and reasonable accuracy. Its formula is:

$$\begin{gathered}\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x}(\rho k v) = \frac{\partial}{\partial x}\left(\left(\mu_l + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x}\right) + \\ + G_k + G_b - \rho\varepsilon - Y_M + S_k,\\ \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x}(\rho \varepsilon v) = \frac{\partial}{\partial x}\left(\left(\mu_l + \mu_t + \frac{\mu_t}{\sigma_k}\right)\frac{\partial \varepsilon}{\partial x}\right) + \\ + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k + C_{3\varepsilon}G_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon,\end{gathered} \quad (2)$$

where k denotes the turbulent kinetic energy, ε denotes the dissipation rate of turbulent kinetic energy, μ_l is the laminar viscosity coefficient, μ_t is the turbulent viscosity [13], G_k is the turbulent kinetic energy produced by mean velocity gradients, G_b is the turbulent kinetic energy produced by buoyancy, Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, S_k, S_ε are source terms, $C_{1\varepsilon}$, $C_{2\varepsilon}$, $C_{3\varepsilon}$ and σ_k are turbulence constants.

The governing equations and turbulent motion equations are used to simulate the leakage and diffusion of the blended gas. This paper adopts the SIMPLE algorithm to solve the equation iteratively. The basic flow is as follows:

① The subject of numerical simulation is modelled. In order to facilitate the calculation, the model is simplified, and the side of the damaged pipe opening facing the atmosphere forms a closed two-dimensional rectangular space with the atmospheric space (The closure here is used to limit the spatial range of calculations rather than to enclose atmospheric space) [14].

② After the two-dimensional rectangular space is divided into grids and given boundary conditions, the initial working conditions are set, including the initial velocity distribution and pressure distribution.

③ The velocity field is predicted according to the initial pressure, and the prediction equation [15] is:

$$MU = -\nabla p, \tag{3}$$

where U is the velocity field, p is the pressure field, and M is the coefficient matrix.

④ The new pressure field is obtained using the pressure correction equation:

$$\nabla(A^{-1}\nabla p) = \nabla(A^{-1}D), \tag{4}$$

where A is the diagonal matrix of M and D is the non-diagonal matrix.

⑤ The velocity field is corrected using the corrected pressure field:

$$U = A^{-1}D - A^{-1}\nabla p. \tag{5}$$

⑥ It is determined whether the corrected velocity field satisfies Eq. (1). If not, it returns to step ③; if it does, then the iteration stops.

2.3. Numerical simulation

The schematic plot of the numerical simulation model of the simulation experiment is displayed in Fig. 1.

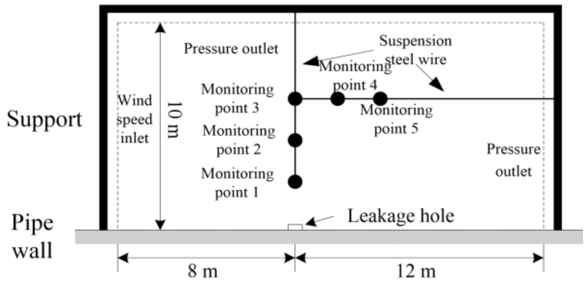

Fig. 1. Schematic plot of the numerical simulation model.

The model was simplified into a closed two-dimensional rectangular space, i.e. the two-dimensional rectangular space composed of the pipe wall and dashed line frame in Fig. 1, to simplify the calculation. The space is 10 m high and 20 m long, and the leakage hole is 8 m away from the left side. In the rectangular space, the left boundary is the wind speed inlet, the upper and right boundaries are pressure outlets, and the leakage hole is the natural gas velocity inlet. In addition, the thick black lines in Fig. 1, as well as the black dots and thin connecting lines, are part of the actual scaled model that will be validated for effectiveness later. Here, the numerical model was overlapped with the actual scaled model. The numerical model is represented by the region formed by pipe walls and dashed lines in the figure.

2.4. Experimental items

(1) Validation of numerical model

To facilitate operation during the numerical simulation, the model was simplified to some extent, which led to some errors between the calculated results and the actual results. Therefore, to guarantee the precision of the simulation under various working conditions, the validity of the numerical model was verified first. To assess the effectiveness of the numerical model, an equal scale model was built, and then a support was set up outside the two-dimensional rectangular space as shown in Fig. 1. A gas sensor was set on the monitoring points 1–5 using the support. The monitoring point 1 was 2 m above the leakage hole, and the interval between adjacent monitoring points was 2 m. The sensors on the monitoring point were fixed by suspending steel wires according to Fig. 1. The steel wires were as thin as possible to guarantee the sensors' stability.

Because the wind speed in the natural environment is difficult to control, the test environment was wind-free, the pressure in the pipeline was 3.0 MPa, the diameter of the leakage hole was 10 mm, the hydrogen mixing ratio of natural gas was 5%, and the leakage rate was 2.3 m^3/h. The same conditions were substituted into the numerical model. In the numerical model, the number of grid cells in the two-dimensional rectangular space was set to 4 875, 5 425 and 6 387, respectively. The deviation between the calculation results of the numerical model at the monitoring point and the actual results was compared under different grid numbers when the diffusion was carried out for 5, 10, and 15 seconds.

(2) Influence of hydrogen mixing ratio on leakage and diffusion

During the numerical simulation, the hydrogen blending ratio was set to 0%, 5%, 10%, 15% and 20%, the pressure in the pipeline was set to 3.0 MPa, the diameter of the leakage hole was 10 mm, and the number of grid cells was set to 5 427. The computation formula for the gas leakage velocity [16] at the leakage hole is:

$$v = \frac{P}{\rho}\sqrt{\frac{M}{RT}\cdot\gamma\cdot\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}}, \tag{6}$$

where P is the pipeline pressure, ρ is the gas density, M is the molar mass of the gas, γ is the specific heat ratio, R is the gas constant, and T is the pipe temperature.

(3) The change of diffusion concentration when gas leaks

When conducting the numerical simulation, the hydrogen mixing ratio was set to 20%, the diameter of the leakage hole was set to 10 mm, the pipeline pressure was set to 3.0 MPa, and the number of grid cells was set to 5 427. The mass fraction change of natural gas and hydrogen at each monitoring point within 20 s after the diffusion began was simulated.

2.5. Experimental results

Before using the model to simulate the leakage, the validity of the model was verified first, and the calculation error and time consumption of the numerical model under different grid cell numbers were compared. The final results are presented in Table 1. Under the same number of grid cells, with the increase of simulated diffusion time, the average error between the mass fraction of methane and hydrogen at the monitoring point calculated by the model and the actual value did not change significantly, nor did the standard deviation of the error change significantly. In other words, the model's simulated calculation of gas diffusion was relatively stable. Under the same simulated diffusion time, although the calculation time of the model under the 4 875 grid count was the least, the calculation error and the standard deviation of the error were large, while the model under the 5 425 grid count and the 6 387 grid count had relatively smaller calculation errors and standard deviations, with little difference between them. However, the model under the 6 387 grid count consumed more simulated calculation time. Therefore, this paper used a model with a grid size of 5 425 cells for the subsequent simulated calculation.

Table 1. Validity verification of the numerical model with different grid cell numbers.

Diffusion time, s	Number of grid cells	Average error of methane mass fraction, %	Standard deviation of methane mass fraction error, %	Average error of hydrogen mass fraction, %	Standard deviation of hydrogen mass fraction error, %	Simulation time, s
5	4 875	2.34	1.11	2.33	1.12	1.22
	5 425	1.53	0.53	1.52	0.52	1.23
	6 387	1.52	0.53	1.51	0.53	1.48
10	4 875	2.53	1.22	2.52	1.23	1.89
	5 425	1.61	0.52	1.60	0.51	1.90
	6 387	1.51	1.23	1.51	0.52	2.05
15	4 875	2.52	1.25	2.50	1.24	2.03
	5 425	1.62	0.53	1.61	0.52	2.06
	6 387	1.53	0.56	1.51	0.53	2.41

The numerical model was employed to simulate the leakage and diffusion of gas under various hydrogen mixing ratios. The diffusion rates of methane and hydrogen are shown in Fig. 2. With the passage of leakage diffusion time, the diffusion rates of methane and hydrogen in natural gas eventually tended to be stable, and the rates of methane and hydrogen diffusion tended to be consistent in the end. Under the same diffusion time, the higher the hydrogen proportion in the gas, the higher the diffusion rate of methane and hydrogen, and the diffusion rate of hydrogen had the most apparent change.

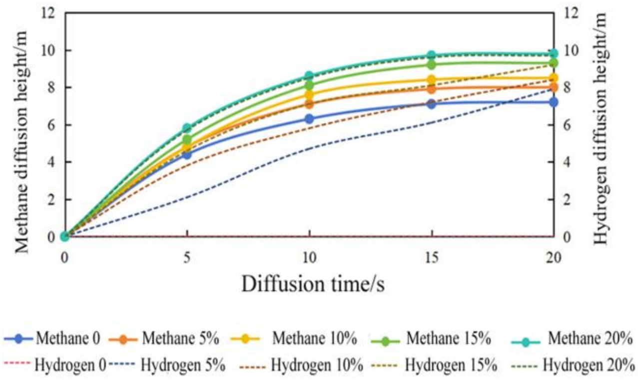

Fig. 2. Diffusion rates of methane and hydrogen under various hydrogen mixing ratios.

The numerical model was employed to simulate the natural gas leakage and diffusion with 20% hydrogen and 10 mm leakage hole diameter. The concentration variation at the monitoring points during diffusion is shown in Table 2. With the passage of diffusion time at each monitoring point, the gas concentration presented a trend of rapid rise at first, then a slow decline, and finally stability. At the same time after the beginning of diffusion, the gas concentration at the monitoring points closer to the leakage hole was higher, while the gas concentration at the monitoring points at the same height level was not significantly different.

Table 2. Changes in concentration at the monitoring points.

Monitoring point	Gas concentration, %	0 s	5 s	10 s	15 s	20 s
1	Methane	0	24.5	20.6	18.5	18.3
	Hydrogen	0	6.3	5.2	4.6	4.5
2	Methane	0	22.1	18.9	17.8	17.6
	Hydrogen	0	5.6	4.8	4.4	4.2
3	Methane	0	19.8	17.8	16.9	16.7
	Hydrogen	0	4.9	4.6	4.1	4.1
4	Methane	0	18.9	16.7	13.4	13.2
	Hydrogen	0	4.7	4.2	3.3	3.2
5	Methane	0	18.7	16.6	10.3	10.1
	Hydrogen	0	4.6	4.1	3.2	3.1

3. Discussion

The incorporation of hydrogen into natural gas has the potential to decrease carbon dioxide emissions while maintaining optimal combustion efficiency. At the same time, the two types of gas share a set of transmission pipelines, and there is no need to lay additional pipelines for hydrogen, which greatly saves construction costs [17]. However, unexpected factors during use, such as earthquakes, hail, construction excavation, etc., and ageing due to long-time use may cause cracks or damage to the pipeline. When the pipeline transmits hydrogen-doped natural gas, the high pressure of the gas will produce loads on the inner wall of the pipeline. Once there is a gap in the wall of the pipeline, the gas will escape from the gap under the action of pressure difference, forming a natural gas leakage [18]. The leakage of natural gas will cause energy loss and produce a negative impact on the surrounding environment. In addition, once the leakage concentration reaches a certain level, it may also cause an explosion, further deepening the loss of the pipeline. Therefore, studying the leakage and diffusion characteristics of natural gas pipelines can provide an effective reference for pipeline construction and management.

When analyzing the leakage and diffusion characteristics of natural gas pipelines, the most direct method is to directly observe the leaking natural gas near the pipeline [19]. In this method, on the one hand, natural gas is usually colourless, which is difficult to observe by the naked eye directly, and the detection sensor can only provide the local gas distribution state. On the other hand, the natural gas pipeline is a public facility, and it is impossible to destroy it anytime and anywhere for the purpose of experiment. With the development of technology, the computing power of computers is getting stronger and stronger. By building mathematical models and using computers to perform calculations [20], the characteristics of natural gas leakage and diffusion can be numerically simulated.

The paper used a mathematical model of gas diffusion to simulate the leakage of hydrogen-mixed natural gas. In this process, in order to facilitate calculation, the area where hydrogen-doped natural gas leaks from the pipeline is simplified as a two-dimensional rectangular space. The effectiveness of the numerical model was verified by using an actual scaled model. Subsequently, the numerical model was used to test the influence of hydrogen-doped ratios on leakage diffusion and changes in concentration during the diffusion process. When the number of grid cells increased from 4 875 to 5 425, the error of the numerical model decreased, but the computation time increased. However, when the number of grid cells increased from 5 425 to 6 387, there was no significant change in the error of the numerical model, but the computation time still increased. The reason for this is that an increase in grid quantity means an increase in details in the numerical model, allowing for more accurate calculations. However, this improvement has marginal effects: once a certain number of grid cells is reached, it becomes difficult to further reduce calculation errors while the computational workload continues to rise. In the same diffusion time, the higher the hydrogen content in hydrogen-doped natural gas, the higher the diffusion rate of methane and hydrogen. The variation in diffusion rate was most significant for hydrogen. This is because hydrogen is less dense than natural gas, making it more diffusive. Additionally, the disturbance caused by the rapid diffusion of hydrogen also drives the diffusion of natural gas.

In conclusion, based on the effect of hydrogen content in hydrogen-doped natural gas on the diffusion of leaked natural gas, when preventing the risk of leakage in hydrogen-doped natural gas pipelines, it is advisable to first focus on the concentration of hydrogen in natural gas. While ensuring the combustion performance of hydrogen-doped natural gas, efforts should be made to minimize the concentration of hydrogen as much as possible.

4. Conclusions

This paper established a numerical model used to simulate how the hydrogen-doped natural gas diffuses. Then, simulated experiments were performed. Firstly, the validity of the numerical model was verified through experiments, and the appropriate mesh number of the model was selected. Then, the effect of various hydrogen-doped ratios and different leakage hole diameters on the leakage and diffusion of the hydrogen-doped natural gas was analyzed using simulation. When the number of grid cells was 5 425, there was little difference between the results calculated by the model and the actual results. The errors were relatively stable, and the calculation time was less. Under the same diffusion time, the higher the hydrogen proportion in the gas, the higher the diffusion rate of methane and hydrogen, and the diffusion rate of hydrogen had the most obvious change. The gas concentration in each monitoring point presented a trend of rapid rise at first, then a slow decline, and finally tended to be stable as the diffusion time elapsed. The closer to the leakage hole, the higher the concentration of the natural gas, but there was little difference between the monitoring points at the same level.

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