Numerical simulation study on shock wave induced spontaneous combustion of high pressure hydrogen-doped natural gas leakage

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Abstract. Incorporating a specific percentage of hydrogen to natural gas and utilizing current natural gas pipelines to transport hydrogen-natural gas mixtures can achieve an effective way of transporting hydrogen on a large scale, long distances, and with high efficiency, which is one of the most significant ways to promote the efficiency of hydrogen energy utilization. However, high-pressure storage and transportation and suitable hydrogen doping ratios have become one of the safety issues that threaten the stable implementation of this technological option. Therefore, based on numerical simulation, the spontaneous combustion of high-pressure hydrogen-doped natural gas was investigated at different hydrogen doping ratios and discharge pressures. The effects indicate that the higher the hydrogen doping ratio and the higher the discharge pressure, the greater the shock wave pressure and the greater the average propagation velocity of the shock wave. The higher the hydrogen blending ratio and the higher the discharge pressure, the more conducive to the occurrence of spontaneous combustion, and the initial spontaneous combustion ignition is more likely to occur near the position of the bursting disc. When the discharge pressure is 25 MPa, the pure methane gas with a hydrogen blending ratio of 0% does not undergo spontaneous combustion in the tube. When the hydrogen blending ratio is from 5% to 30%, the temperature of spontaneous combustion is reduced from 1130 K to 1087 K, the time of spontaneous combustion is shortened from 157 μs to 110 μs, and the distance of spontaneous combustion is reduced from 134 mm to 100 mm (from the bursting disc). When the discharge pressure is 13 MPa, the hydrogen-doped natural gas with a hydrogen blending ratio of 20% does not spontaneous combustion in the tube. When the discharge pressure is from 19 MPa to 40 MPa, the time of spontaneous combustion is shortened from 194 μs to 61 μs, and the distance of spontaneous combustion is reduced from 166 mm to 60 mm (from the burst disc).

Keywords: High pressure hydrogen-doped natural gas; leakage; shock wave propagation; spontaneous combustion characteristics; hydrogen blending ratio; relief pressure.

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1 Introduction

As a clean and pollution-free secondary energy, hydrogen energy is one of the main strategies to solve energy problems. Due to the high construction cost, high safety risk and insufficient operation experience of hydrogen transportation and storage facilities, the large-scale application of hydrogen energy is hindered to a certain extent[1]. Therefore, it is proposed to mix a certain proportion of hydrogen into natural gas and use the existing natural gas tube to transport hydrogen-natural gas mixture, which can achieve an effective way of large-scale, long-distance and efficient transportation of hydrogen, and is one of the important ways to promote the utilization efficiency of hydrogen energy. The potential for spontaneous combustion is high when hydrogen embrittlement or pressure relief device failure results in accidental leakage from a high-pressure hydrogen storage device, and the addition of hydrogen will inevitably increase the risk of spontaneous combustion of hydrogen-doped natural gas.

China has not yet defined the upper limit of hydrogen blending ratio. Elaoud et al.[2] numerically simulated the steady-state and transient flow of hydrogen-natural gas mixture in the annular tube network. The study found that 30% hydrogen does not put the API X52 tube at risk of failure. Leicher et al.[3] suggested that the addition of hydrogen to natural gas would affect the safety performance of gas appliances and that there was a need to establish acceptable hydrogen concentration limits. Molnarne et al.[4] found that adding 1% hydrogen had little effect on the safety of natural gas. Gondal et al.[5] believed that automobile engines, boilers and other equipment can accept 20% hydrogen addition.

Domestic and foreign scholars have carried out corresponding research on the high-pressure leakage process of combustible gas and the spontaneous combustion characteristics of combustible gas induced by shock wave. Jiang et al.[6] analyzed the shock wave propagation chaCompared with the straight pipe, the propagation of the leading shock wave in the L-shaped pipe becomes more complicated due to the presence of the reflected shock wave, and the intensity of the reflected shock wave is much higher than that of the leading shock wave. Wen et al.[7] investigated the effect of bursting disc rupture time, release pressure, tube length and tube diameter on the spontaneous combustion of hydrogen leakage at high pressure. It was found that the occurrence of spontaneous combustion can be inhibited by using a bursting disc with a slower rupture speed and reducing the aspect ratio of the tube. Gong et al.[8][9] utilized numerical simulation and experimental research methods to analyze the shock wave propagation characteristics and spontaneous combustion phenomena of high-pressure hydrogen leakage in U-tubes and L-tubes of the same length and diameter. Zeng et al.[10] studied the effect of the addition of methane, carbon monoxide and nitrogen on the spontaneous combustion of high-pressure hydrogen leakage under the condition of the same size of the discharge tube. The results show that the addition of three same volume gases leads to the decrease of shock wave intensity in the tube, which will inhibit the occurrence of spontaneous combustion.

At present, the research on hydrogen-doped natural gas at domestic and international is limited to the feasibility of hydrogen-doped natural gas, the safety of transportation, and the reasonable hydrogen blending ratio. There are few experimental studies and numerical simulation studies on the spontaneous combustion of hydrogen-doped natural gas leakage. A few researches on the spontaneous combustion of methane/hydrogen mixture leakage only focus on the impact of methane addition on the spontaneous combustion characteristics of high-pressure hydrogen. Due to the high storage pressure in the current high-pressure hydrogen storage technology, on the other hand, the critical pressure of spontaneous combustion of hydrogen-doped natural gas leakage with natural gas as the main body is also relatively high, which puts forward higher requirements for the related experimental equipment of hydrogen-doped natural gas high-pressure leakage. Therefore, the study of spontaneous combustion of high-pressure hydrogen-doped natural gas leakage through the numerical simulation system can contribute to the experimental research of hydrogen-doped natural gas and provide a scientific basis for the safe application of hydrogen-doped natural gas.

2 Control equations and numerical methods

2.1 Turbulence model

Aiming at the flow problem of high-pressure gas leakage shock wave, in order to accurately reflect the gas flow and flow field changes in the tube, the RNG k-ε model is used for numerical simulation. The RNG k-ε model is as follows:

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_i}(\rho k u_i)=\frac{\partial}{\partial x_j}\left(\alpha_k \mu_{eff}\frac{\partial k}{\partial x_j}\right)+G_k+G_b-\rho\varepsilon-Y_M+S_k \tag{1}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon)+\frac{\partial}{\partial x_i}(\rho \varepsilon u_i)=\frac{\partial}{\partial x_j}\left(\alpha_\varepsilon \mu_{eff}\frac{\partial \varepsilon}{\partial x_j}\right)+C_{1\varepsilon}\frac{\varepsilon}{k}(G_k+C_{3\varepsilon}G_b)-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}-R_\varepsilon+S_\varepsilon \tag{2}$$

where G_k is the turbulent kinetic energy generated under the laminar velocity gradient, J; G_b is the turbulent kinetic energy generated by buoyancy, J; Y_M is the turbulent pulse constant of compressible fluid; $C_{1\varepsilon}$, $C_{2\varepsilon}$ and $C_{3\varepsilon}$ are empirical constants. α_k and α_ε are the Prandtl numbers of k equation and ε equation; S_k and S_ε are user-defined.

Compared with the standard k-ε model, the RNG k-ε model adds a correction term:

$$R_\varepsilon=\frac{C_\mu \rho \eta^3(1-\eta/\eta_0)\varepsilon^2}{1+\beta\eta^3}\frac{\varepsilon^2}{k} \tag{3}$$

Where: $\eta=S_k/\varepsilon$, $\eta_0=4.38$, $\beta=0.012$.

2.2 Combustion model

The combustion model used is the Eddy Dissipation Concept (EDC). In the spontaneous combustion phenomenon of high-pressure leakage of hydrogen-doped natural gas, the thermal effect of methane+hydrogen spontaneous combustion process is studied, so the methane-air reaction mechanism and the total package reaction of hydrogen are adopted. The reaction mechanism used in the combustion reaction model is shown in the formula:

$$CH_4 + 20_2 = CO_2 + 2H_2O \tag{4}$$

$$2H_2 + O_2 = 2H_20 \tag{5}$$

2.3 Numerical methods

The flow of gas in the tube is a high-speed compressible flow, and the solution method is based on the implicit solution of the density method. The gas component model selects the species transport model, the volume reaction, the module selects the methane-air type, and adds the H_2 component to the material module, and the gas density option is set to the ideal gas. Roe-FDS is selected for Flux-Type, and the second-order upwind scheme is used for flow field discretization.

3 Modeling

In this paper, the leakage process of high-pressure hydrogen-doped natural gas is taken as the research object. The calculation area is separated into two zones: high-pressure zone (driving) and the low-pressure zone (driven), which have the following initial conditions: high-pressure zone (P4, T4) and low-pressure zone (P1, T1). The high-pressure zone has a length of 200 mm and a width of 40 mm. The low-pressure zone has a length of 300 mm and a length of 10 mm. Figure 1 shows the structure. In the simulation, the gases in the high-pressure zone are set to be methane and hydrogen, and the gas in the low-pressure zone is set to be air. The initial temperature in the high-pressure zone is set to 300 K, and different discharge pressures and mass fractions of methane and hydrogen are set according to the operating conditions. The mass fraction of oxygen in the low-pressure zone is 0.23 and the mass fraction of nitrogen is 0.77.

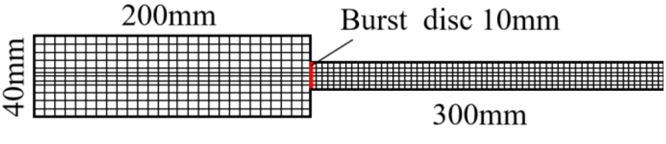
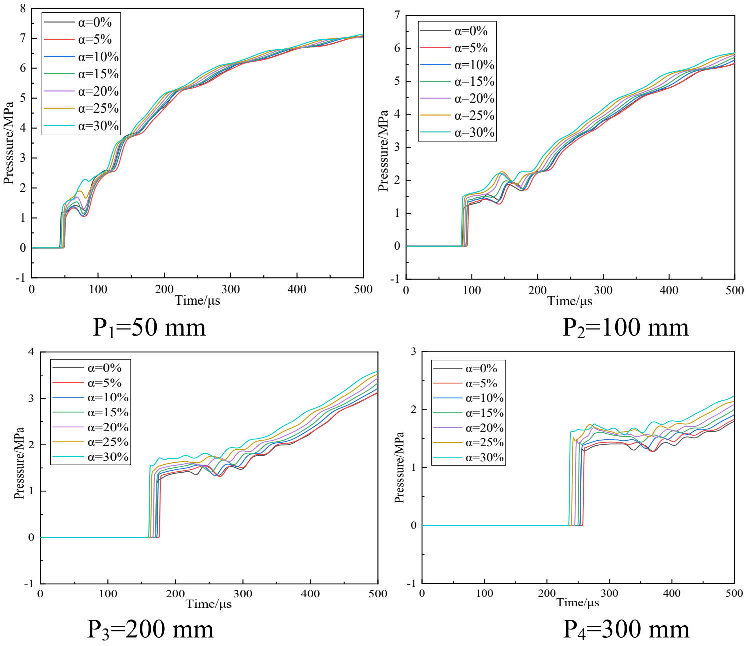


Fig. 1. Physical model

4 Results and analysis

4.1 Effect of hydrogen doping ratio on shock wave propagation characteristics

In order to investigate the shock wave transmission characteristics and spontaneous combustion characteristics of high-pressure hydrogen-doped natural gas leakage at different hydrogen-doping rates, with four hydrogen mixing ratios (*α*=0%, 5%, 10%, 15%, 20%, 25%, 30%) and the discharge pressure fixed at 25 MPa to study the effect of hydrogen mixing ratio on the propagation characteristics of shock waves.



P_1=50 mm

P_2=100 mm

P_3=200 mm

P_4=300 mm

Fig. 2. The pressure of each measuring point in the tube varies with time under different hydrogen blending ratios

At four monitoring points (P_n=50 mm, 100 mm, 200 mm and 300 mm from the bursting disc) in the tube, Monitoring of shockwave pressure variation with time after high-pressure hydrogen-doped natural gas leakage at different hydrogen blending ratios By comparing with the case of pure methane release (*α*=0), as can be seen in Figure. 2, the shock wave pressure values under different hydrogen blending ratios are continuously detected at four monitoring points and rise rapidly, which indicates that a leading shock wave is produced and transmitted downstream of the tube. With the continued propagation of the shockwave, the multiple reflects of the shockwave from the surface of the tube wall become lower and lower as the gas flows downstream until it disappears. The pressure value of shock wave is evenly distributed under different hydrogen blending ratios, showing that the leading shock wave takes a dominant role in the pressure distribution in the tube. The higher the hydrogen blending ratio, the greater the pressure released into the tube, indicating the more powerful the compression effect of the shock wave and the greater the shock wave pressure. Therefore, the higher the hydrogen blending ratio, the stronger the shockwave intensity.

The average propagation velocity of the shock wave can be calculated from the location of the monitoring points and the time it takes for the shock wave to reach each monitoring point. As illustrated in Figure 3, the higher the hydrogen ratio, the greater the propagation velocity of the shock wave. When the bursting disc ruptures, the propagation velocity of the shock wave increases. With the continuous rupture of the bursting disc until completely open, the propagation velocity of the shock wave is generally in a constant state, but in the case of hydrogen mixing ratio is very small there will be a small decrease. This is because with the increase in the propagation distance of the shock wave, the wall of the pipe blocking and shock wave attenuation will weaken the intensity of the shock wave, reducing the propagation speed of the shock wave. When the hydrogen mixing ratio is high, the propagation velocity of the shock wave will continue to increase. This is because during the propagation of the shock wave, the phenomenon of shock wave reflection in the discharge tube and the interaction between the shock waves increase the intensity of the shock wave. Therefore, the propagation velocity of the shock wave tends to stabilize under the dual effect of shock wave attenuation and enhancement.

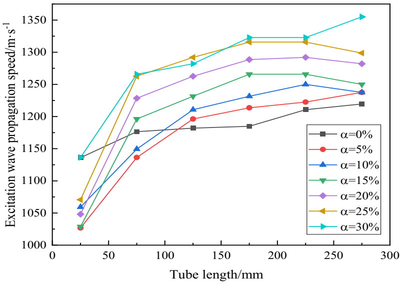


Fig. 3. Relationship between shock wave propagation velocity and propagation distance

4.2 Comparative analysis of spontaneous combustion characteristics

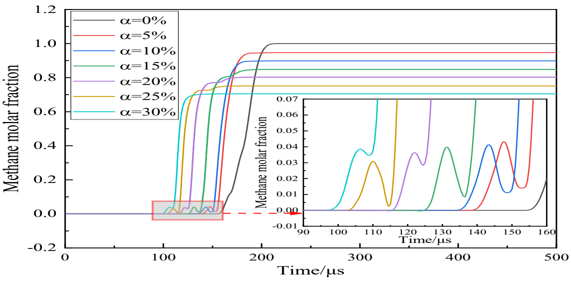
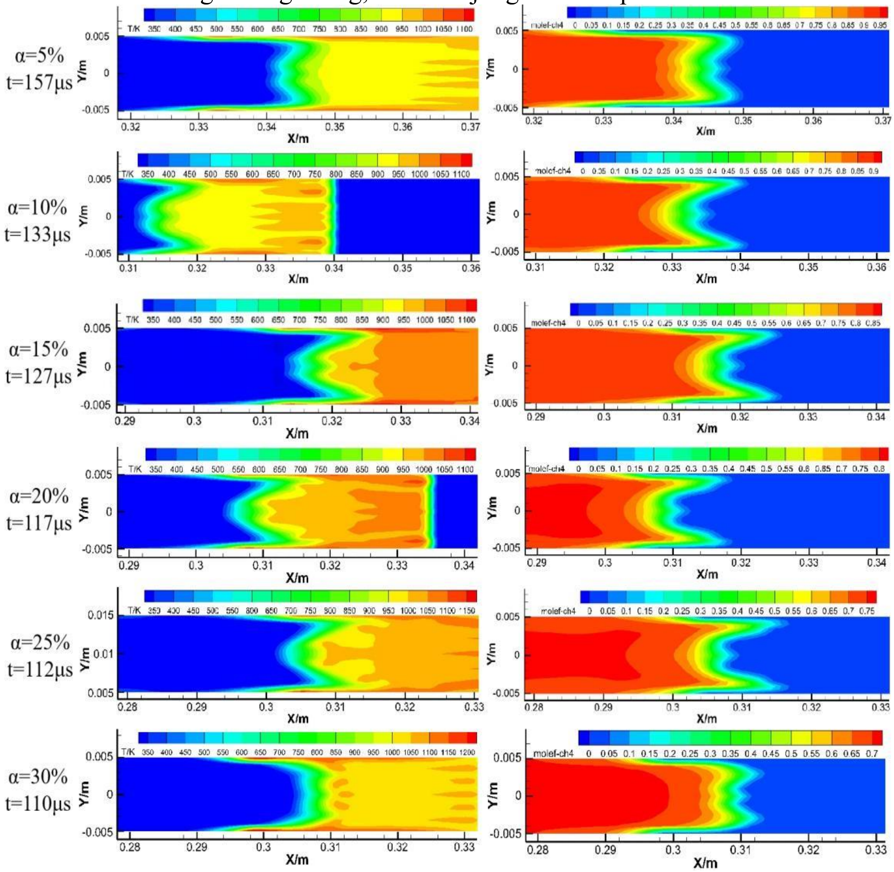


Fig. 4. Methane mole fraction changes with time under different hydrogen doping ratios

In the study of premixed combustible gas explosion, it is generally defined that when the molar fraction of fuel is less than 5% of the initial molar fraction, the corresponding temperature is the ignition temperature. This paper draws on the idea of this definition, combined with the characteristics of high-pressure combustible gas leakage, and defines the characteristic of sudden decline in the process of methane molar fraction rise. It is considered that spontaneous combustion occurs. The time when the methane molar fraction decreases to the lowest value is the time when spontaneous combustion occurs, and the temperature at this time is the ignition temperature. As shown in Figure 4, the variation of methane mole fraction and temperature in the tube with time under different hydrogen blending ratios. When the hydrogen blending ratio is 0% (pure methane), according to the curve change of *α*=0%, the molar fraction of methane shows a gradual upward trend and is stable, so it is determined that no spontaneous combustion occurs. When *α*=5% to α=30%, the change trend of methane mole fraction is rising-falling-rising, which is judged to be spontaneous combustion.



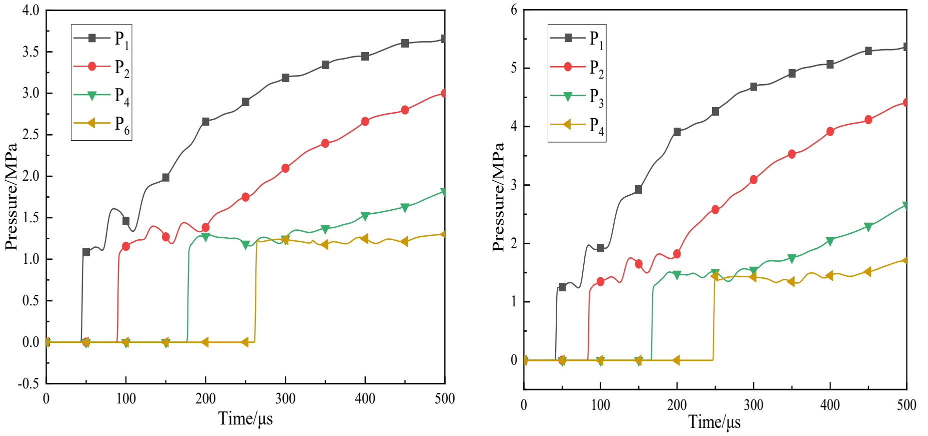
(a) Temperature (b) Methane mole fraction

Fig. 5. Temperature and methane mole fraction contours in the tube

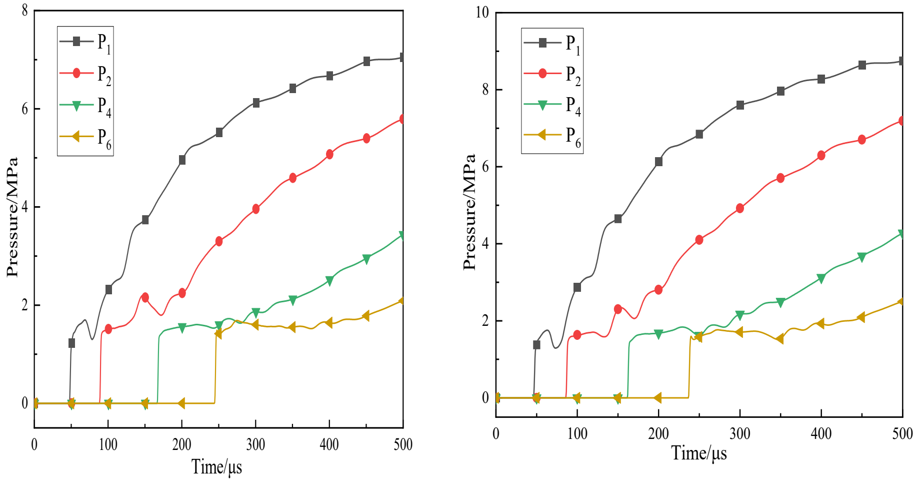
Figure 5 is the ignition temperature cloud diagram and the corresponding methane mole fraction cloud diagram under the condition of each hydrogen blending ratio when spontaneous combustion occurs. The hydrogen blending ratio is reduced from 5% to 30%, the ignition time is reduced from 157 μs to 110 μs, the ignition distance is reduced from 134 mm to 100 mm (from the bursting disc), and the ignition temperature is reduced from 1130 K to 1087 K, which is about 60 K lower. After the rapid rupture of the bursting disc, a boundary layer is formed near the tube wall due to the flow viscosity effect caused by the shock wave. Then, due to the boundary layer interaction on the contact surface of the expanded hydrogenated natural gas and air, a certain volume of hydrogenated natural gas-air mixture is formed. Due to the viscous dissipation of the wall and the effect of the boundary layer, when the hydrogen blending ratio is 20%, two high temperature points appear in the boundary layer of the upper and lower walls at 108 mm from the bursting disc, and the spontaneous combustion first appears on the wall, indicating that the adiabatic wall plays an important role in the process of spontaneous combustion in the high-pressure hydrogen-doped natural gas leakage tube, as shown in Figure 5 (a). It can be seen from this that under the same discharge pressure and tube size, the greater the hydrogen blending ratio, the more prone to spontaneous combustion. In addition, the addition of hydrogen can promote the occurrence of spontaneous combustion in the tube, and the promotion effect increases with the increase of hydrogen blending ratio. As the leading shock wave is formed and propagates downstream, the shock wave heating temperature increases and the shock wave heating range increases.

4.3 Effect of different relief pressure on spontaneous combustion characteristics of tube leakage

The hydrogen-doped natural gas with α=20% was selected to study the shock wave propagation characteristics of high-pressure hydrogen-doped natural gas leakage and the occurrence of spontaneous combustion. The discharge pressure was selected to be 13 Mpa,19 Mpa,25 Mpa and 31 Mpa. Figure 6 shows the variation curves of shock wave pressure with time at different monitoring points(50 mm, 100 mm, 200 mm and 300 mm from the bursting disc) under different discharge pressures. The time when the first step of the bursting disc is opened is defined as zero. It can be seen that the four monitoring points on the wall of the discharge tube detect the pressure rise in turn, which means that the shock wave is formed in the tube after the leakage of high-pressure hydrogen-doped natural gas and continues to propagate downstream of the tube. At the same time, due to the reflection of shock waves and the interaction of multiple shock waves, the shock waves in the tube continue to develop and maintain a high level.



P=13 MPa *P*=19 MPa



P=25 MPa *P*=31 MPa

Fig. 6. Curves of pressure variation with time at the same monitoring point in the tube under different discharge pressures

Figure 7 shows the change of shock wave propagation velocity in the tube under different discharge pressures. It can be seen that the greater the discharge pressure, the greater the shock wave propagation velocity. In the one-dimensional shock tube flow, the shock wave propagation velocity and shock wave overpressure will gradually become a constant value in the process of shock wave flow, because the strength of the shock wave decreases with time. When the discharge pressure is higher, the time required for the bursting disc to fully open is longer, and the opening size after the bursting disc rupture will also have a significant impact on the shock wave strength and shock wave propagation speed. Therefore, under the condition of high discharge pressure, the possibility of spontaneous combustion is higher, which further promotes the interaction of shock waves and the continuation of combustion.

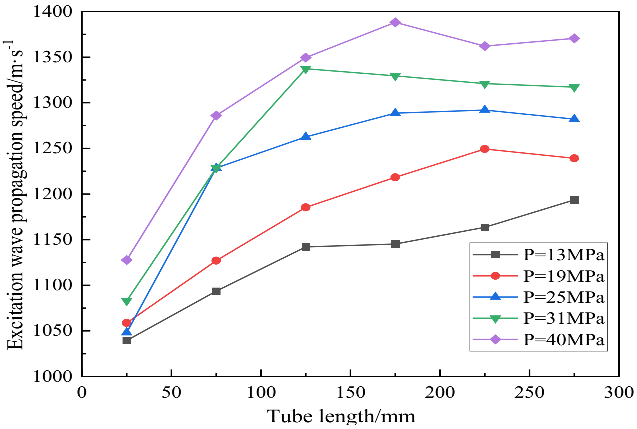


Fig. 7. Propagation velocity of shock wave in tube under different relief pressures.

4.4 Effect of relief pressure on spontaneous combustion characteristics in tube

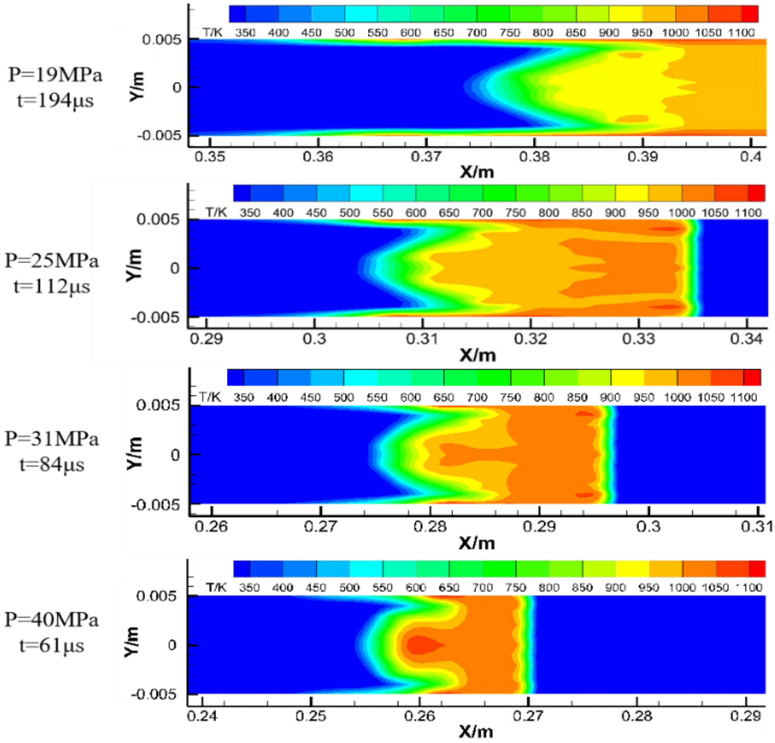


Fig. 8. The temperature distribution in the tube under different discharge pressures

When the discharge pressure is 13 MPa, the temperature in the tube after the shock wave is low, and the possibility of spontaneous combustion is small. Therefore, the temperature distribution cloud map of spontaneous combustion under different discharge pressures is analyzed. It can be seen from Figure 8 that the discharge pressure has a great influence on the location of spontaneous combustion of high-pressure hydrogen-doped natural gas leakage. The higher the pressure is, the closer the location of spontaneous combustion is to the bursting disc. This is because the higher the relief pressure, the higher the intensity of the action of the surge, the higher the speed of the surge propagation, which makes the turbulence intensity of the gas mixture after the surge action higher, increases the mixing rate of high-pressure hydrogen-doped natural gas and high-temperature air in the compression zone, and accelerates the formation of the flammable mixture of hydrogen-doped natural gas-air in the combustible range. On the other hand, the stronger the compression effect of the shock wave generated by the leakage on the air in the tube, the temperature of the shock wave action zone rises step by step, and it is easier to reach the spontaneous combustion ignition temperature of the mixed gas, and the spontaneous combustion ignition phenomenon occurs earlier. Therefore, the higher the discharge pressure, the more prone to self-ignite from high-pressure hydrogen-doped natural gas leakage.

5 Conclusion

In this chapter, the shock wave propagation characteristics and spontaneous combustion characteristics of high-pressure hydrogen-doped natural gas leaking into the discharge tube are studied by two-dimensional numerical simulation method, changing the hydrogen blending ratio and discharge pressure. The conclusions are as follows:

(1)The higher the hydrogen doping ratio, the higher the shock wave strength, the higher the propagation speed of the shock wave, and gradually stabilized during the propagation process. According to the theoretical formula and the simulation results, it is found that the simulation results are slightly higher than the theoretical value.

(2)When the discharge pressure is 25 MPa, pure methane (α=20%) gas does not occur spontaneous combustion during the leakage process. When the hydrogen blending ratio is from 5% to 30%, the ignition temperature is reduced from 1130 K to 1087 K, indicating that the increase of hydrogen content is more prone to spontaneous combustion.

(3)The greater the discharge pressure, the higher the intensity of the shock wave generated in the tube, and the propagation speed of the shock wave shows a trend of increasing first and then stabilizing. The theoretical value of shock wave Mach number in the tube is slightly smaller than the simulated value, and the change trend is consistent.

(4)When the discharge pressure is 13MPa, there is no spontaneous ignition of α=20% hydrogen-doped natural gas. With the increase of discharge pressure, the temperature after shock wave heating is higher, the likelihood of spontaneous combustion is increased, the duration of spontaneous combustion is shortened, and the location of spontaneous combustion is closer to the bursting disc.

6 Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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