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Simulation Study on the Effects of Methane Blending on the Auto-Ignition Mechanism of High-Pressure Hydrogen Leakage

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Abstract: As a clean energy source, hydrogen plays a crucial role in driving energy transitions. However, its highly flammable and explosive characteristics limit its safety in applications. This paper employs numerical simulation to investigate the influence of methane blending at varying concentrations on the auto-ignition and flame propagation characteristics of high-pressure hydrogen. The study focuses on analyzing the mechanisms by which methane blending affects shock wave intensity, ignition delay, and flame propagation behavior. The results indicate that methane blending significantly reduces shock wave intensity, prolongs ignition delay, and suppresses the integrity and intensity of flame propagation both inside and outside the pipeline. Furthermore, these effects are enhanced with increasing methane concentration. These findings provide theoretical support for safe design under conditions of high-pressure hydrogen blended with methane, contributing to the safer application of hydrogen energy in industrial and transportation fields.

Keywords: hydrogen, methane blending, shock wave intensity, flame propagation characteristics

1. Introduction

Hydrogen energy, as a clean energy source, holds broad application prospects and market potential [1]. At present, many developed countries are vigorously developing hydrogen energy and hydrogen fuel cells [2]. However, a series of unsafe characteristics of hydrogen, such as its extremely low ignition energy (only 0.017 mJ [3]), a wide flammability range (volume ratio of 4%–75%), and strong leakage properties, make hydrogen highly prone to fires and explosions. These risks constrain the widespread use and development of hydrogen, and ensuring hydrogen safety remains a significant challenge in its promotion and application [4].

Currently, hydrogen is primarily used as an intermediate chemical product, such as in the synthesis of ammonia, methanol, and petroleum refining. In industrial applications, high-precision purification is often unnecessary, resulting in the presence of trace impurity gases like CH_4, CO, and N_2 during hydrogen utilization. Previous studies have partially examined the impact of impurity gas blending on the auto-ignition characteristics of high-pressure hydrogen leakage [5-9]. However, the influence of varying concentrations of CH_4 blending on hydrogen auto-ignition, especially on the flame

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propagation behavior of mixed gases, remains unexplored. Therefore, this study investigates the auto-ignition characteristics of high-pressure hydrogen accidentally released with different concentrations of CH_4 under varying discharge conditions.

2. Numerical Model for Auto-Ignition of Methane-Blended Hydrogen Leakage

2.1. Physical Model Development

A symmetric modeling approach was adopted to develop the physical model of the auto-ignition process for high-pressure hydrogen blended with different concentrations of methane during leakage. The model includes three regions: the hydrogen storage area, the discharge pipeline, and the atmosphere. The dimensions of each region are shown in Figure 1.

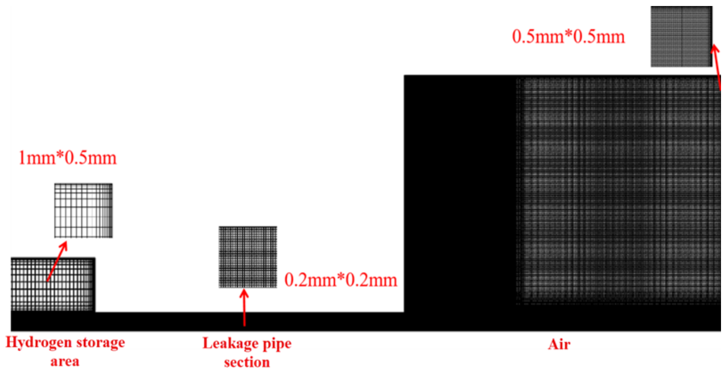

Figure 1: Mesh distribution for a pipe length of 120 mm and a diameter of 10 mm.

The Fluent software was used for simulations, with the initial conditions set as follows: an initial temperature of 300 K and a velocity of 0 m/s. The air composition was set to 21% O_2 and 79% N_2. The gas composition in the hydrogen storage area was configured for different scenarios: 97.5% H_2 and 2.5% CH_4, 95% H_2 and 5% CH_4, and 92.5% H_2 and 7.5% CH_4. The chemical reaction mechanism employed the CKL 1.1 methane-hydrogen combustion mechanism developed by Sichuan University. The rupture process of the burst disc was simulated using an instantaneous rupture mode.

2.2. Grid Independence Verification

Figure 2 compares the computational results for different grid sizes in the downstream pipeline. The results show that when the minimum grid size in the pipeline was set to 0.4 mm or 0.3 mm, significant deviations occurred compared to grid sizes of 0.2 mm or 0.1 mm. However, the results for grid sizes of 0.2 mm and 0.1 mm were similar, and the temperature trends within the pipeline were consistent. Considering the balance between solution accuracy and computational resource consumption, the grid size was set to 0.2 mm in this study.

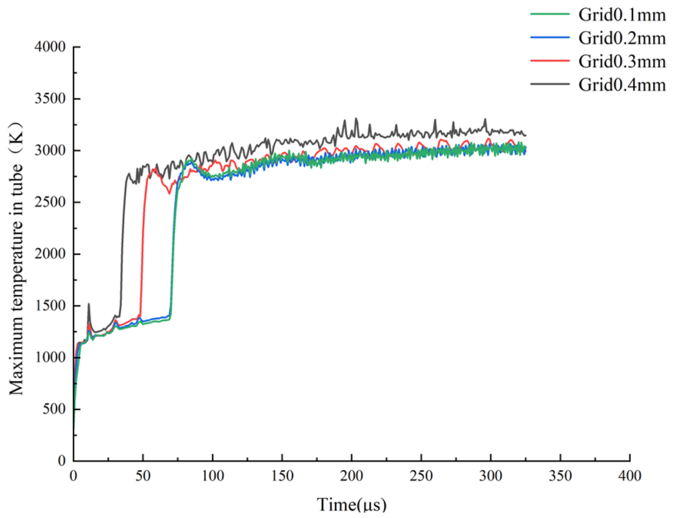

Figure 2: Maximum temperature distribution in the pipeline for different grid sizes.

2.3. Model Accuracy Validation

Figure 3 compares the shock wave Mach numbers obtained in this study with experimental and simulation results from previous studies, as well as theoretical values under different pressures [10]. The results show that the shock wave Mach numbers in this study were slightly higher than the theoretical values, with an error of less than 10%. The higher Mach numbers may be attributed to the numerical simulation treating high-pressure hydrogen and air as ideal gases, neglecting dissipative effects such as fluid viscosity and pipe wall friction. Additionally, experimental uncertainties may have influenced the results. The sufficiently small error demonstrates the accuracy of the model.

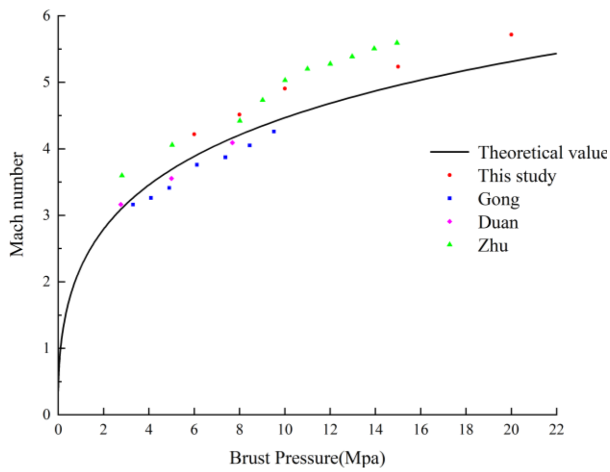

Figure 3: Comparison of the relationship between shock wave Mach numbers and discharge pressures in this study and previous studies.

3. Numerical Simulation Results Analysis

3.1. Impact of Methane Blending on Shock Waves

This study investigates the effect of different methane concentrations (0%, 2.5%, 5%, and 7.5%) on hydrogen autoignition characteristics by simulating hydrogen mixed with methane. The analysis was conducted under a release pressure of 6 MPa, pipeline length of 120 mm, and diameter of 10 mm for four different conditions. Four monitoring points were set along the pipeline (located 30 mm, 60 mm,

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90 mm, and 120 mm from the release pipe) to record pressure variations during the shock wave propagation downstream. The results indicate that the maximum pressure at the monitoring points after the shock wave passed reached the highest value of 3.07 MPa under pure hydrogen conditions. As the methane blending concentration increased, the pressure peak gradually decreased. Under the conditions of 2.5%, 5%, and 7.5% methane blending, the peak pressures were 2.63 MPa, 2.56 MPa, and 2.51 MPa, respectively. Shock wave intensity is a key factor in determining hydrogen autoignition. In this study, the shock wave overpressure Ps, which represents the average dynamic pressure on the pipe wall in the shock wave region, was used. As shown in Table 1, for the same release pressure, the shock wave overpressure Ps decreases as the methane blending ratio increases. Moreover, with the increase in release pressure, the reduction in shock wave overpressure Ps becomes more significant.

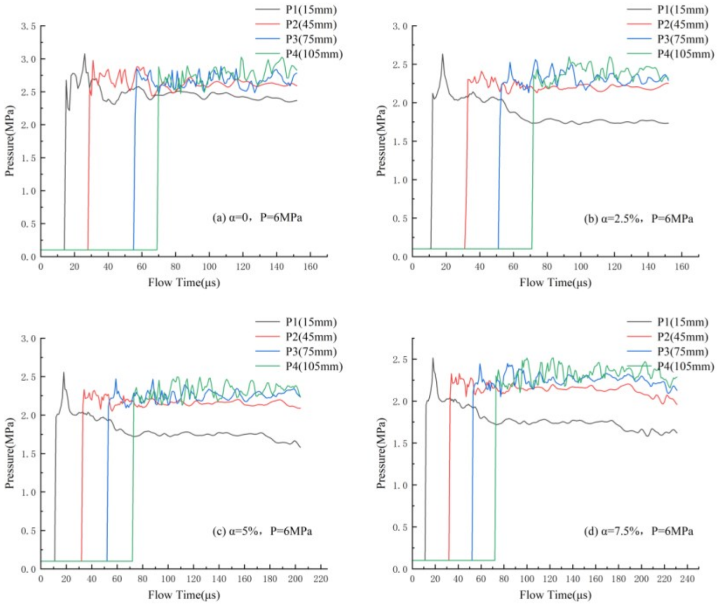

Figure 4: Pressure distribution at monitoring points within the pipe under different methane concentrations and a release pressure of 6 MPa.

Table 1: Shock wave overpressure at different methane concentrations and release pressures.

Release Pressure (MPa)	Ps (H2) (MPa)	Ps (2.5% CH4) (MPa)	Ps (5% CH4) (MPa)	Ps (7.5% CH4) (MPa)
6	2.76	2.29	2.16	2.13
10	3.46	3.07	2.98	2.96
20	5.23	4.57	4.49	4.37

3.2. Flame Propagation Characteristics in the Pipe

Bragin et al. [11] pointed out that visible flames are produced when the OH mole concentration exceeds 0.001. Based on this standard, this study observed the hydrogen flame under different CH_4 concentrations (release pressure 6 MPa, pipeline lengths 60 mm and 120 mm, pipeline diameter 10 mm). Figure 8 presents the distribution of OH mole fractions at different times. The results show that CH_4 blending significantly reduces shock wave intensity and suppresses hydrogen combustion kinetics.

At different blending concentrations, the ignition time of the flame gradually delayed as the CH_4 concentration increased. Under pure hydrogen conditions, ignition occurred at 24 μs at the pipe wall boundary layer, which is consistent with the ignition time in the study by Golovastov S V [8]. When 2.5% CH_4 was added, ignition was delayed to 42 μs, to 43 μs with 5% CH_4, and to 48 μs under the high concentration of 7.5% CH_4. In terms of flame propagation, at T = 49 μs, under pure hydrogen conditions, the flame propagated radially from the boundary layer of the pipe wall to the mixed gas front. When 2.5% and 5% CH_4 were added, the flame intensity significantly weakened, and the flame appeared in a faint form. Especially under 7.5% CH_4 conditions, the flame only formed a weak flame kernel attached to the pipe wall boundary layer.

Under a release pressure of 6 MPa, pipeline length of 120 mm, and pipeline diameter of 10 mm, when comparing pure hydrogen with 2.5% methane mixing, the effect of methane blending on flame propagation pattern was clearly observed. The increased pipeline length extended the compression wave return time, further delaying the ignition time under the CH_4 mixing condition. Under pure hydrogen conditions, the shock wave reflection formed a stable vortex structure at the center of the pipeline, effectively promoting the mixing of cold hydrogen and heated air, generating a high-temperature flammable region. At 74 μs, the ignition kernel appeared at the center of the pipeline, and the flame expanded radially from the boundary layer, gradually covering the entire cross-section of the pipeline. In contrast, under 2.5% CH_4 blending, due to the interaction between the hydrogen/air mixture and the pipe wall boundary layer, the flame developed along the boundary layer. Although the blending of CH_4 slightly inhibited combustion, the effect was minimal. However, during the period from 74 to 96 μs, the flame still showed noticeable suppression. The weakened shock wave intensity led to a decrease in the temperature and flammable gas concentration at the center of the pipeline, making it difficult to maintain the vortex structure, and the flame remained primarily attached to the boundary layer area, with almost no radial expansion.

At 96 μs, the dynamic pressure distribution (see Figure 9) further verified this difference. Dynamic pressure reflects the kinetic energy of a unit volume of gas; the larger the velocity at a given position, the higher the dynamic pressure. Due to the vortex turbulence effect at the center of the pipeline, the hydrogen and air in pure hydrogen conditions were continuously mixed, and the density of the mixture at the jet front increased, resulting in a decrease in speed and dynamic pressure. The reduction in dynamic pressure roughly corresponds to the complete flame form inside the pipe. However, under 2.5% CH_4 mixing, the low-intensity vortex at the center of the pipeline could not sustain the mixing of hydrogen and air, resulting in nearly the same dynamic pressure at the jet front radially. This indicates that methane blending significantly restricted the radial expansion of the flame and suppressed the continued combustion of the flame at the center of the pipeline.

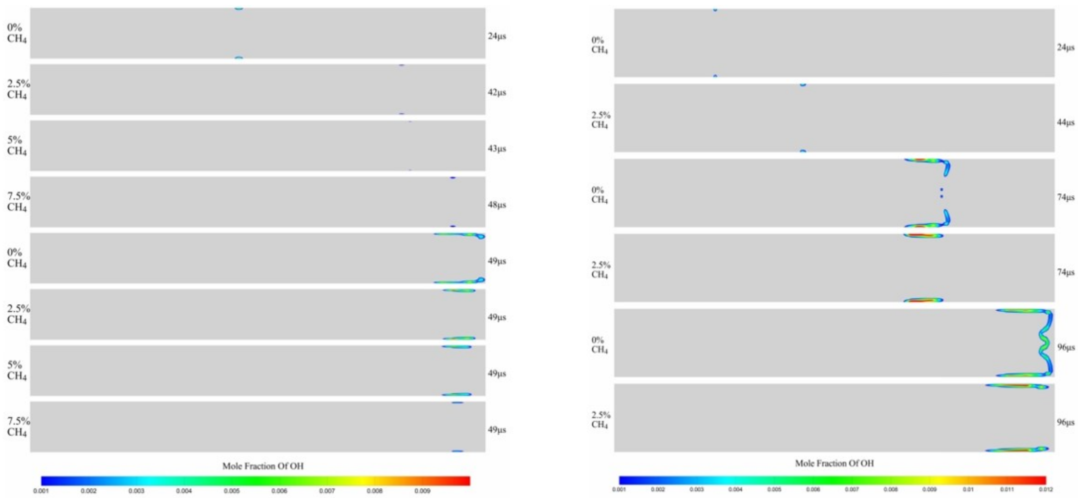

Figure 8: OH mole fraction distribution at different times within the pipe under release pressure 6 MPa, pipeline lengths 60 mm and 120 mm, and pipeline diameter 10 mm.

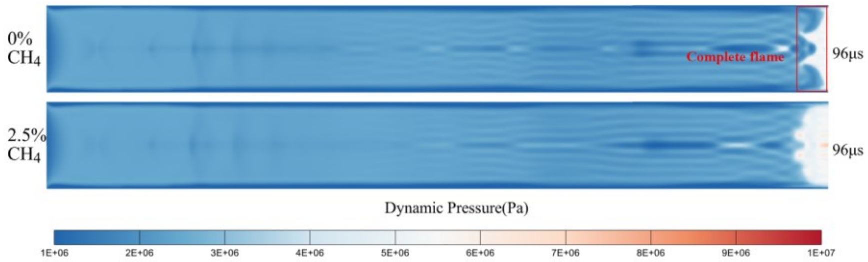

Figure 9: Dynamic pressure distribution at 96 μs within the pipe under release pressure 6 MPa, pipeline length 200 mm, and pipeline diameter 10 mm.

4. Conclusion

This study investigated the autoignition characteristics of high-pressure hydrogen after mixing with different concentrations of CH_4 under various release conditions. The following conclusions were drawn:

(1) As the methane blending concentration increased, the ignition time of hydrogen gradually delayed, and the flame intensity and propagation speed significantly weakened. Under 7.5% methane blending, the shock wave intensity significantly decreased, and the flame existed only as a weak flame kernel, without significant expansion.

(2) Under methane blending conditions, the flame intensity significantly weakened, and the flame primarily propagated along the pipe wall boundary layer, without effectively expanding into the central region of the pipeline. At the end of the flame propagation process, the flame remained confined to the boundary layer, failing to form stable radial flame expansion.

(3) Methane blending resulted in a reduction of shock wave overpressure, thereby weakening the stability of the hydrogen combustion reaction, indicating that shock wave intensity plays a crucial role in high-pressure hydrogen autoignition and flame propagation.

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