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Investigation of the Combustion Characteristics of Hydrogen-blended Natural Gas

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ABSTRACT

During the initial phases of the energy transition, blending hydrogen into operational natural gas pipelines proves to be an efficient method for hydrogen delivery. Nevertheless, the blending of hydrogen raises the reactivity of the gas and escalates the fire hazard. A jet fire occurs when a leakage and accidental ignition of a hydrogen/natural gas mixture within a pipeline. Flame length, as one of the key parameters to measure fire safety, is of great significance for evaluating the impact range of fire. A numerical model of horizontal jet fire of hydrogen-blended natural gas, including hydrogen content of 0%、10%、20%、50% and 100%, is established to analyze the effect of hydrogen on flame length from the perspective of combustion intermediate. The research results may provide reference for the risk assessment of hydrogen-blended natural gas pipelines.

Keywords: natural gas, hydrogen, jet fire, flame length, safety

NONMENCLATURE

Abbreviations	
HBNG	Hydrogen-blended Natural Gas
Symbols	
V	The fuel velocity at the nozzle
γ	The gas adiabatic index
M	The molar mass
R	Gas constant
P_0	The gas pressure in the pipeline
P_∞	The ambient pressure

1. INTRODUCTION

To reduce greenhouse gas emissions, great attention has been paid to new energy technologies and the search for alternatives to fossil energy sources [1]. Hydrogen, because of its unique advantages of being pollution-free and renewable, has become the most promising energy carrier in the 21st century [2]. Hydrogen can be blended into natural gas and transported via these existing long-distance natural gas pipelines at low cost [3]. However, the addition of hydrogen increases the failure probability of the pipeline [4] by promoting fuel reactions and raising the risk of fire [5]. It is necessary and urgent to study the combustion characteristics of HBNG and the impact of hydrogen addition on the flame for better prediction and assessment of potential fire risks.

The effect of H2 on combustion characteristics has often been discussed in previous studies. Francis et al. [6] and Dong et al. [7] studied the concentration of H2/CH4 flame intermediate radical in a burner. They found that the concentration of OH, O, and H increased significantly with the volume fraction of H2. The amount of added hydrogen has a direct effect on the combustion characteristics. Zhao et al. [8] conducted experimental studies on premixed H2/CH4 gas combustion. Results showed that the gas combustion characteristics were slightly affected when the hydrogen content was less than 15%. Lowesmith et al. [9] concluded that the flame profile of natural gas blended with 22% hydrogen content was generally similar to pure natural gas.

The flame length, as one of the key parameters to measure fire safety, is the main factor affecting the impact range of jet fire and the distribution of thermal radiation, which is of great significance for evaluating the impact range of fire. Choudhuri et al. [10] performed H2/CH4 turbulent combustion experiments in a combustion chamber and found that the flame height decreased with hydrogen content. Wu et al. [11] found an 8.9% decrease in flame length when the volume fraction of H2 was raised from 0% to 50%, suggesting that this could be related to the reduction in carbon soot production. Ouyang et al. [12] numerically simulated the hydrogen/methane mixture flames and found that the

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maximum reduction in flame length was 11% when the H2 volume fraction ranges from 0% to 20%. However, no analysis on the distribution of combustion intermediates along the flame length of HBNG are conducted. Thus, a numerical model of horizontal jet fire of HBNG with hydrogen content of 0%、10%、20%、50% and 100%, is established to analyze the effect of hydrogen on flame length from the perspective of combustion intermediate. The research results may provide reference for the risk assessment of HBNG pipelines.

2. PHYSICAL AND MATHEMATICAL MODELS

2.1 Physical model

The simulation domain size of the non-premixed jet diffusion flame is 4m×2m×2m, the jet nozzle is 0.5m above the ground, and the flow direction of fuel is along the X-axis. A monitoring surface is set on the jet center line in order to obtain the various of intermediate products. The operating pressure of HBNG is 600 Pa, the nozzle diameter is 8 mm, and 5 groups of hydrogen content, including 0%, 10%, 20%, 50% and 100% are set to analyze the effect of hydrogen content on the combustion intermediate.

2.2 Mathematical model

The FLUENT is used for numerical simulation. The governing equations for the jet flame simulation are Navier-Stokes for turbulent flows related to the reaction. The governing equations are as follow:

Mass conservation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0 \qquad (1)$$

Momentum balance:

$$\frac{\partial(\rho u)}{\partial t}+\operatorname{div}(\rho u u)=-\frac{\partial p}{\partial x}+\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{yx}}{\partial y}+\frac{\partial \tau_{zx}}{\partial z}+F_x \qquad (2)$$

$$\frac{\partial(\rho v)}{\partial t}+\operatorname{div}(\rho v u)=-\frac{\partial p}{\partial y}+\frac{\partial \tau_{xy}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{zy}}{\partial z}+F_y \qquad (3)$$

$$\frac{\partial(\rho w)}{\partial t}+\operatorname{div}(\rho w u)=-\frac{\partial p}{\partial z}+\frac{\partial \tau_{xz}}{\partial x}+\frac{\partial \tau_{yz}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}+F_z \qquad (4)$$

Energy balance：

$$\frac{\partial \rho E}{\partial t}+\frac{\partial\left(\rho u_j E+u_j p\right)}{\partial x_j}=\frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_j}+u_i \tau_{ij}\right)+S_h \qquad (5)$$

2.3 Numerical methods

(1) Mesh generation

The ICEM is used to generate structural grids in the computing domain. The computational efficiency and mesh quality of structured grids are generally more favorable than those of unstructured grids. In addition, the O-grid division method is applied near the leak hole to better deal with the circular area, and the grid is locally encrypted at the leak port. In order to improve the calculation efficiency, a gradually sparse grid division method is carried out for the places far away from the nozzle while ensuring the calculation accuracy. The final grid generation for the computation domain is shown in Fig.1.

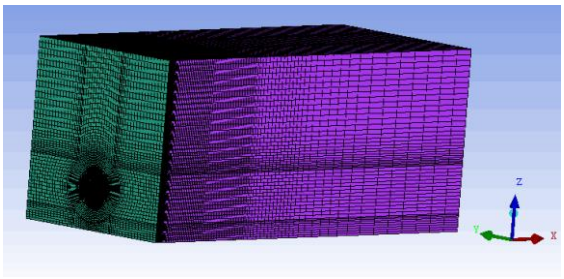

Fig.1 Grid division

(2) Boundary conditions

Considering that the velocity inlet boundary condition is more convergent than that of the pressure inlet, the pressure inlet is converted to the velocity inlet boundary condition for calculation. For small leakage, when the gas flow rate at the nozzle is large, the heat transfer process with the outside world during the leakage process can be ignored, and the gas flow process is assumed to be isentropic. The gas flow rate at the nozzle can be calculated by the following formula:

$$V=\sqrt{2\frac{\gamma R T_0}{M(\gamma-1)}\left[1-\left(\frac{P_\infty}{P_0}\right)^{\frac{\gamma-1}{\gamma}}\right]} \qquad (6)$$

Where, V is the fuel velocity at the nozzle，$m\cdot s^{-1}$; γ is the gas adiabatic index; M is the molar mass，$kg\cdot mol^{-1}$; R is gas constant, R=8.3145 $J\cdot(mol\cdot K)^{-1}$; T_0 is the temperature in the pipe，K; P_0 and P_∞ respectively refer to the gas pressure in the pipeline and ambient pressure, Pa.

(3) Numerical method and combustion reaction model

In this paper, the three-dimensional transient solver is used for calculation. Considering the stability and accuracy of the calculation, the κ-ε turbulence model is selected to simulate the gas flow state due to the large gas flow velocity and the relatively small influence of the viscous action of gas molecules. This model has been

widely used in the simulation of un-premixed turbulent jet fire [13]. The EDM model is used for the preliminary calculation of the jet fire of HBNG in chemical reaction, and the initial distribution of the flame temperature field is obtained. The EDC model is used for the further calculation to get accurate distribution of the intermediate products of the combustion reaction.

3. MODEL VALIDATIONS

3.1 Grid independence verification

In this paper, hexahedral mesh is used to divide the geometric model, and four kinds of mesh numbers, 65 thousand, 910 thousand, 1.22 million and 1.61 million, are selected to verify the grid independence. The temperature distribution at the centerline of the flame is obtained by using different mesh numbers to calculate the working condition with 50% hydrogen content, as shown in Fig. 2. When the number of grids is greater than 910,000, the calculation results are very close, and it can be considered that further mesh encryption has no significant impact on the calculation results. In this paper, a grid with 1.22 million units is used for simulation calculation.

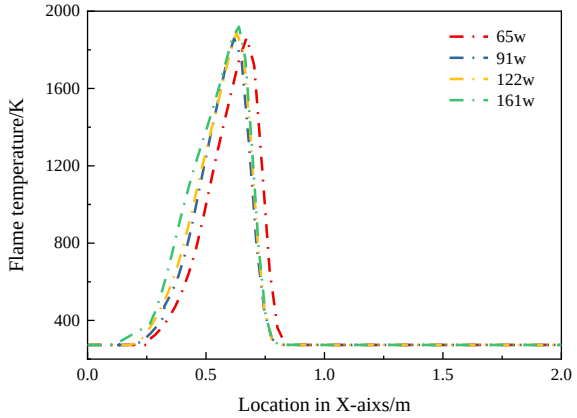

Fig. 2 Flame temperature profiles with different mesh numbers

3.2 Verification of combustion reaction mechanism

To solve the combustion problem numerically, it is necessary to select a suitable chemical reaction mechanism. GRI-Mech 3.0 is a mechanism document widely accepted by scholars, which includes 53 components and 325 primitive reactions [14]. The GRI-Mech 3.0 mechanism includes detailed reaction mechanisms, but at the same time leads to a lot of unnecessary calculations, which affects the efficiency of numerical simulation. Researchers have proposed a series of simplification mechanisms based on GRI-Mech 3.0, such as the 84-step reaction simplification mechanism and the 104-step reaction mechanism [15].

In order to select a suitable simplification mechanism, the temperature distribution at the center of the flame after the jet flame stabilization is obtained by taking the condition of hydrogen content of 50% as an example, as shown in Fig.3. The temperature distribution of the flame center obtained by the two simplified mechanisms is basically consistent with the results of GRI-Mech 3.0. In order to improve the efficiency of numerical calculation without affecting the accuracy of simulation results, the 84-step reaction simplified mechanism is selected as the combustion mechanism file for simulation calculation.

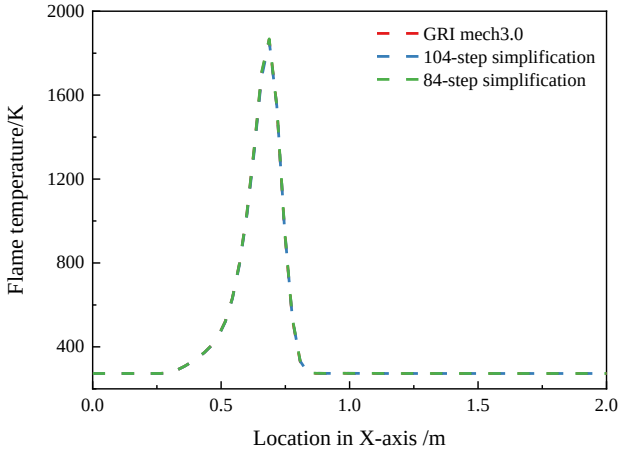

Fig.3 Flame temperature profiles with different combustion mechanisms

4. RESULTS AND DISCUSSION

4.1 Simulation result analysis

In order to verify the accuracy of the calculation model, the calculation results of the jet flame formed by the immediate ignition of HBNG after leakage were compared with the experimental data of Kong et al. [16]. In the experiment, HBNG is sprayed horizontally through a nozzle 1.5 m above the ground, and an igniter is used to ignite the gas at the outlet of nozzle. The operating pressure of the experimental study ranges from 200 Pa to 600 Pa, and the nozzle diameter is 8 mm.

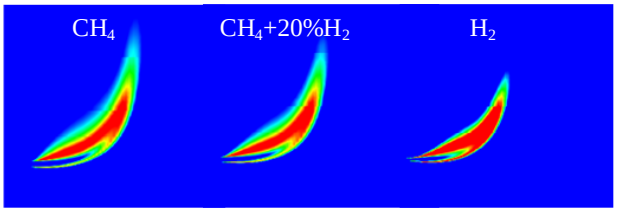

Fig. 4 The morphology of flame

Fig.4 shows the flame morphology of 0%, 20% and 100% hydrogen content calculated under the condition of pipeline pressure of 600 Pa and nozzle diameter of 8 mm. For flame boundaries, researchers usually use specific temperature profiles as flame shape boundaries.

It is noted that 800 K and 1300 K are usually selected as flame boundaries for natural gas and hydrogen jet fires respectively. In this paper, the flame boundaries under different hydrogen contents are determined by interpolation method. It can be seen that due to the effect of buoyancy, the end of the flame will be bending. The horizontal flame length and vertical flame length decrease gradually with the increase of hydrogen content, which is consistent with the experimental results.

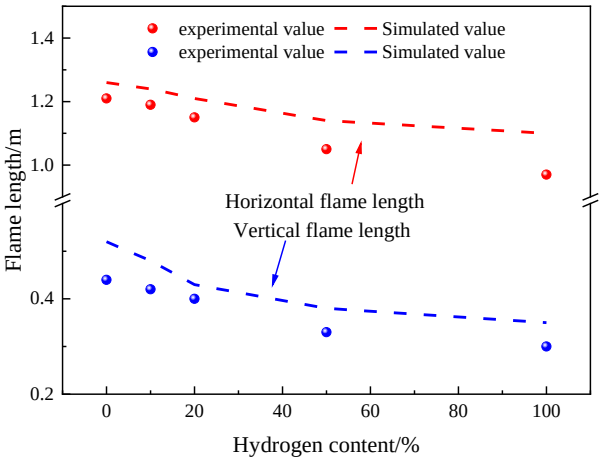

Fig. 5 Comparison of simulated and experimental value

Fig.5 shows the comparison between experimental and simulated results. The maximum errors of horizontal flame length and vertical flame height are 11.8% and 15.38% respectively, which are within the acceptable range. The error may be due to the unclear tail contour of the flame image in the experiment, resulting in a short flame length. In addition, uncontrollable factors such as ambient wind speed in the experiment may also lead to certain differences between the experimental and calculated results.

4.2 Analysis of combustion intermediates

The combustion intermediates play an important role in the combustion reaction. Fig.6 shows the distribution of OH, H, CO and O2 molar fractions and flame temperature on the centerline of HBNG jet flame. It can be seen that with the increase of hydrogen content, OH, H and CO are formed closer to the leakage nozzle, and the peak value of OH, H and CO molar fractions increases with the increase of hydrogen content. The addition of hydrogen provides more OH and H, promotes the combustion reaction, and makes the combustion reaction occur closer to the nozzle. From the view of the combustion intermediates, it is verified that the flame lifted-off distance decreases with the increase of the hydrogen content. In addition, the mole fraction of CO increased slightly with the addition of hydrogen, indicating that hydrogen mixing did not reduce CO production, which was consistent with the conclusions of El-Ghafour et al. [17].

With the increase of hydrogen content, the gas flow rate increases, the O_2 on the jet axis near the nozzle is replaced by fuel gas, and the mole fraction of O_2 near the nozzle is basically 0. Then the molar fraction of O_2 increases gradually, and its peak value decreases with the increase of hydrogen content. According to the

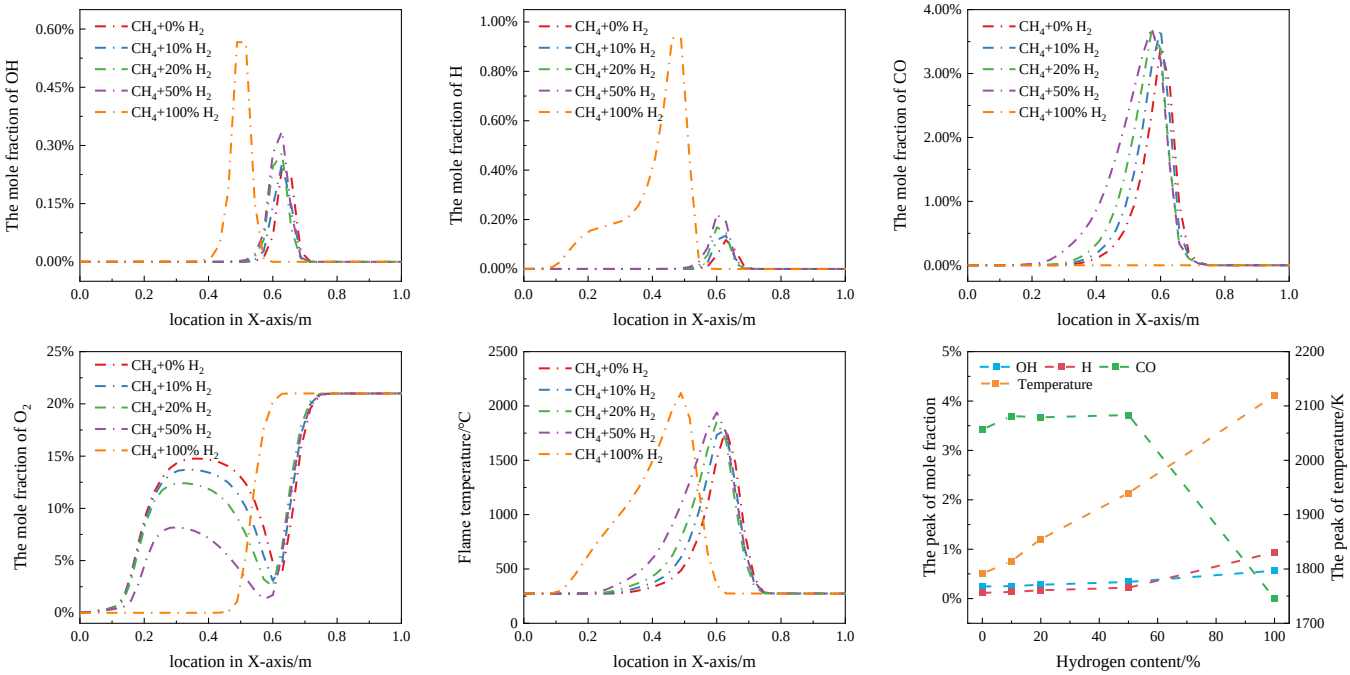

Fig.6 Combustion intermediates and flame temperature distribution and their peaks

corresponding temperature distribution, there is no combustion reaction near the nozzle. The entrainment of the fuel gas near the nozzle forms premixed combustible gas, which leads to premixed combustion near the bottom of the flame, that is consistent with the research results of Wang et al. [18]. In addition, with the increase of hydrogen content, the position of flame peak temperature moves forward to nozzle, which further verifies that the increase of hydrogen content will reduce flame length.

The last figure shows the changes of OH, H and CO molar fractions on the centerline of HBNG jet fire and the flame temperature peak with the hydrogen content. The peak molar fractions of OH and H increased exponentially with the addition of hydrogen. The peak molar fraction of OH increased from 2.45×10^{-3} to 2.82×10^{-3}, 3.37×10^{-3} and 5.66×10^{-3}, respectively, with increases of 15.01%, 37.55% and 131.02% when the hydrogen increased from 0% to 30%, 50% and 100%, respectively. The peak molar fraction of H increased from 1.17×10^{-3} to 1.56×10^{-3}, 2.20×10^{-3} and 9.37×10^{-3}, respectively, with increases of 33.33%, 88.03% and 700.85%, respectively. The peak H molar fraction increased from 1.17×10^{-3} to 1.56×10^{-3}, 2.20×10^{-3} and 9.37×10^{-3}, respectively, with increases of 33.33%, 88.03% and 700.85%, respectively. The molar fraction of CO changed slightly when the hydrogen content is less than 50%, and hydrogen had little effect on CO production. The peak flame temperature increases linearly with the increase of hydrogen content. Because the flame temperature of hydrogen is higher than that of methane, the addition of hydrogen will cause the flame temperature to rise.

5. CONCLUSIONS

A numerical model of horizontal jet fire of HBNG, including hydrogen content of 0%、10%、20%、50% and 100%, is established to analyze the effect of hydrogen on flame length from the perspective of combustion intermediate. The results show that the length of the jet flame is shorter and the flame temperature is higher after hydrogen mixing, and the bottom of flame is closer to the nozzle than that of pure methane flame. After hydrogen addition, OH and H are formed closer to the nozzle, and the peaks of OH and H molar fractions increase with the increase of hydrogen, which promotes the combustion reaction and makes the combustion reaction occur closer to the nozzle.

It was found that the molar fraction of CO shows a slightly increase with the increase of the hydrogen when the hydrogen content is less than 50%, which verified that the hydrogen couldn't uninhibited the generation of CO. With the increase of hydrogen content, the combustion reaction is advanced, which consumes part of the oxygen and leads to the decrease of O_2 molar fraction near the nozzle. In addition, hydrogen addition leads to the flame temperature rise, and the position of flame peak temperature moves forward as the increase of hydrogen content.

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