Study on Laminar Combustion Characteristics of Ammonia/Hydrogen Premixed Based on Chemical Reaction Kinetics

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Abstract. The combustion characteristics of ammonia/hydrogen premixed laminar flow and the effect of hydrogen on the combustion performance of ammonia fuel were studied. First, the corresponding model of ammonia/hydrogen premixed laminar combustion is established by using GRI3.0 mechanism, Konnov mechanism, Mei mechanism, Okafor mechanism, and Otomo mechanism respectively. Second, the simulation results are compared with the experimental results. It is found that the Mei mechanism and Okafor mechanism are more suitable for ammonia/hydrogen premixed laminar combustion. On this basis, the effects of equivalent ratio, hydrogen ratio, and initial temperature on laminar flame velocity, maximum combustion temperature, and NO mole fraction were studied. The results show that the laminar flame velocity, the maximum combustion temperature, and the mole fraction of NO first increase and then decrease with the increase of the equivalent ratio, and the laminar flame velocity reaches the maximum when the equivalent ratio is 1.1. At the same time, with the increase of hydrogen ratio and initial temperature, the maximum combustion temperature increases first and then decreases. The mole fraction of NO increased with the increase of hydrogen ratio and initial temperature. The results show that mixing hydrogen in ammonia can improve the combustion characteristics of ammonia.

1 Introduction

With the increase of energy consumption in the world, the consumption of fossil fuels has brought great economic benefits, but also accompanied by a series of environmental pollution problems[1]. At the same time, China's external dependence on oil and natural gas is extremely high, and energy security is facing great challenges. Therefore, it is urgent to develop alternative fuels for fossil fuels[2,3]. Many alternative fuels, such as methanol, ether, hydrogen and biodiesel, have been studied by domestic and foreign scholars. Hydrogen is considered to be the ideal clean energy due to its high calorific value, zero carbon emission, wide flammable range and recyclable utilization. However, due to its poor safety performance, high storage and transportation requirements, easy early ignition and tempering problems, the spread of hydrogen fuel is limited[1,4-5].

As a kind of chemical raw material that can be produced on a large scale, ammonia can be used as an ideal substitute for traditional fossil fuel due to its advantages of high energy density, easy compression storage and transportation, zero carbon emission, easy liquefaction storage and low storage and transportation cost. However, because of the low combustion rate, high spontaneous combustion temperature, narrow flammable limit (the volume fraction of air is 15.5%~27%) and other reasons, the wide application of ammonia in internal combustion engine is restricted.

Combustion by mixing ammonia with other accelerants has been an important direction in the development of ammonia combustion flame enhancement technology. Because hydrogen has a fast combustion rate and can be obtained by catalytic reforming of ammonia, it is a good way to improve the combustion characteristics of ammonia fuel by adding hydrogen into ammonia gas[6,7].

At present, ammonia combustion has a wide range of potential applications in combustion equipment such as internal combustion engine, gas turbines and porous medium burners[8,9]. Therefore, the development of the basic theories and technical methods of ammonia combustion has become one of the leading direction in this field. In the past ten years, the research on ammonia combustion and mixed combustion with ammonia has been enriched and developed. In particular, a series of researches have been carried out on the combustion characteristics of ammonia/hydrogen fuel.

Kumar et al.[10] conducted experimental and simulation studies on laminar combustion velocity of ammonia/hydrogen premixed fuel with equivalent ratio in the range 0.5 to 1.1. Sensitivity analysis shows that OH is the key radical leading to the decomposition of ammonia fuel, and the difference in the prediction of OH radical may be the cause of the difference in the prediction results between different models. Joo et al.[11] studied the effect of ammonia replacement of hydrogen/air mixture on the combustion stability limit and NOx emission of premixed flame in stable combustion at normal
temperature and pressure. The results show that although the absolute value of NOx emission increases, the NOx emission remains almost unchanged when the ratio of ammonia to fuel is increased. The NOx emission decreases with the increase of mixing injection velocity under the enriched combustion condition. Sun et al.\[12\] determined the flame extinguishing limit, flame temperature and morphology of non-premixed ammonia/hydrogen/air flame at high temperature and atmospheric pressure through experiments, and calculated the detailed structure and flame extinguishing limit of the flame by using the detailed chemical reaction kinetic mechanism. The results show that in ammonia/air flame, the addition of hydrogen increases the flame blowout limit, the concentration of free radical H, OH, O and the maximum flame temperature. It can be seen that hydrogen as an additive can improve the reactivity and ignition performance of non-premixed ammonia/air flame, thus proving the potential of ammonia/hydrogen mixture as carbon-free fuel.

The laminar combustion velocity of ammonia/hydrogen/air flame under different hydrogen mole fraction was measured by Han et al.\[8\]. The experimental results show that the laminar combustion rate increases non-linearly with the molar fraction of hydrogen, and it is found that the enhanced effect of hydrogen on ammonia flame is not only suitable for the chemical equivalent ratio condition, but also for the wide equivalent ratio range from 0.7 to 1.6. The combustion characteristics and NOx formation law of ammonia/hydrogen mixture fuel under different air-fuel ratios and hydrogen concentration were studied experimentally by Li et al.\[13\]. The results show that hydrogen can be used as fuel to improve the combustion performance of ammonia, and hydrogen and ammonia/hydrogen fuel have good application prospects. The spherical laminar flow premixed ammonia/hydrogen/air flame stability, nitrogen oxide and nitrous oxide emissions in EDM ignition was investigated and calculated by Lee et al.\[14\]. The results show that nitrogen oxide emission first increases and then decrease with the amount of ammonia replacement under fuel-rich condition, and the increase of nitrogen oxide emission is much lower than that under low-combustion conditions. The results support the use of ammonia as a carbon-free and clean addition that can reduce the emission of nitrogen oxide emissions in a fuel-rich hydrogen/air flame, thus improving the safety of hydrogen use.

To sum up, the domestic and foreign scholars have conducted many studies on the combustion of ammonia/hydrogen mixed fuel. However, at present, they mainly focus on the research on the change law of ammonia/hydrogen combustion stability limit, flame burning speed and nitrogen oxide emission under certain conditions, and lack of research on the combustion characteristics of ammonia/hydrogen mixed fuel under different working conditions. This article will focus on ammonia/hydrogen/air premixed laminar combustion, systematically studies the different initial temperature, pressure, the influence of the ratio of ammonia/hydrogen combustion characteristic.

### 2 Calculation Model

#### 2.1. Control Equation

The one-dimensional laminar premixed free-propagation flame model takes into account the effect of radiant heat loss on the flame\[15\]. The governing equations are as follows:

\[
m = \rho u A
\]

\[
m \frac{dT}{dx} - \frac{1}{C_p} \frac{d}{dx} (\lambda A \frac{dT}{dx}) + \frac{A}{C_p} \sum_{i=1}^{K} \rho Y_i C_{p,i} \frac{dT}{dx}
\]

\[+ \frac{A}{C_p} \sum_{i=1}^{K} \rho h_i W_i + \frac{A}{C_p} Q_{rad} = 0
\]

\[M \frac{dY_i}{dx} + \frac{d}{dx} (\rho A Y_i V_i) - \Lambda_{\omega} W_i = 0
\]

\[\rho = \frac{P \overline{\rho}}{RT}
\]

Where, \( \overline{\rho} \) is the average molar mass of the mixture, \( W_i \) is the molar mass of the kth substance, \( h_i \) is the enthalpy of the kth substance, \( A \) is the flame cross-section area after normalization of the cross section of the combustion reactor, \( Q_{rad} \) is the heat loss due to radiation, \( Y_i \) is the mass fraction of the kth substance, and \( C_{p,i} \) is the specific heat at constant pressure of the kth substance.

#### 2.2 Boundary Conditions

The one-dimensional laminar ammonia/hydrogen mixture and air premixed adiabatic flame were simulated by detailed chemical reaction mechanism. The model assumes that flame propagation is a steady-state, adiabatic, quasi-one-dimensional process, and assumes that the upstream of the flame is a cold boundary with a specific temperature and component mass fraction, while the downstream is a fully developed thermal boundary. The length of the computational domain is 10 cm, and the 3000~5000 grid is set in the flame reaction region. The detailed chemical reaction mechanism includes GRI3.0 mechanism, Konnov mechanism, Mei mechanism, Okafor mechanism, Otomo mechanism, et al.\[16-20\]. The calculation parameters are shown in Table 1.

<table>
<thead>
<tr>
<th>Table 1. Calculating parameter</th>
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<tr>
<td>Parameter</td>
</tr>
<tr>
<td>equivalent ratios</td>
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<tr>
<td>pressure</td>
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<td>temperature</td>
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<td>hydrogen ratio</td>
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3 Result and discussion

3.1 Comparative Study on Mechanism

Figure 1 shows the comparison of simulation results and test results of ammonia laminar combustion flame velocity at different equivalent ratios when the initial pressure is 1 bar and the initial temperature is 298 K. For specific test conditions, see Han’s research[21], where the maximum experimental error range is 1.4 cm/s, and the main source of error caused by thermocouple temperature measurement. It can be seen from the figure that the simulation results of Hadi mechanism is higher than the measured results in all equivalent ratio conditions, Konnov mechanism is lower than the measured results in most equivalent ratio conditions, Okafor mechanism and Mei mechanism are slightly higher than the measured results when rich fuel, while GRI3.0 mechanism and Otomo mechanism are closest to the measured values.

Figure 2 shows the flame velocity of laminar combustion of ammonia/hydrogen mixture with different equivalent ratios when the initial temperature is 298 K, the initial pressure is 1 bar and the hydrogen ratio is 0.25. It can be seen from the graph that with the increase of equivalent ratio, the flame velocity increases first and then decreases, reaching the maximum when equivalent ratio is 1.1. At the same time, as the temperature of the unburned gas increase, the laminar flame velocity of NH3/H2 mixture keeps increasing.

3.2 Research on influencing factors of ammonia/hydrogen combustion characteristics

Figure 3 shows the variation of laminar flame velocity with equivalent ratio when the initial pressure is 1 bar and the initial temperature is 298 K. It can be seen from the above study that the current reaction mechanisms have certain limitations, and not all of them can be applied to the combustion simulation of ammonia/hydrogen mixture.
raising the temperature of the unburned gas helps to increase the combustion velocity of the NH3/H2 mixture.

Figure 5 shows the variation of the maximum combustion temperature with equivalent ratio when the initial pressure is 1 bar and the unburned gas temperature is 298K. It can be seen from the diagram that the maximum combustion temperature first increases and then decreases with the increase of equivalent ratio. And the maximum combustion temperature does not appear under a certain equivalent ratio, but varies with the hydrogen ratio. At the same time, it can also be seen from the figure that the maximum combustion temperature increases with the increase of hydrogen ratio, so that the maximum combustion temperature can be increased by mixing hydrogen in ammonia fuel.

Figure 6 shows the variation law of the maximum combustion temperature with equivalent ratio when initial pressure is 1 bar and hydrogen ratio is 0.3. It can be seen from the figure that the maximum combustion temperature first increases and then decreases with the increase of equivalent ratio. However, when the initial temperature is different, the position of the extremum is different, and the position of the extremum moves backward with the increase of the temperature. At the same time, it can also be found from the figure that the maximum combustion temperature increases with the increase of the initial temperature.

Figure 7 shows the change law of NO molar fraction with equivalent ratio when the initial pressure is 1 bar and the initial temperature is 298K. It can be seen from the figure that the NO mole fraction gradually decreases with the increase of equivalent ratio. At the same time, the molar fraction of NO increases with the increase of hydrogen ratio. This is mainly because the combustion temperature keeps increasing with the increase of hydrogen ratio. Therefore, adding hydrogen to ammonia will lead to the deterioration of NO emission. However, it can be seen from the graph that when the equivalent ratio is greater than 1.2, although there are differences in the molar fraction of NO caused by the different hydrogen ratio, the difference is gradually decreasing.

Figure 8 shows the variation of NO molar fraction with equivalent ratio when the initial pressure is 1 bar and the hydrogen ratio is 0.3. It can be seen from the diagram that the molar fraction of NO decreases with the increase of equivalent ratio. At the same time, the molar fraction of NO also increased with the increase of the initial temperature, mainly because the increase of the initial temperature led to the increase of the maximum combustion temperature, which leads to the increase of the molar fraction of NO.
Figure 10 shows the change trend of the maximum combustion temperature of ammonia/hydrogen laminar premixed combustion with the initial pressure when the initial temperature is 298 K and the hydrogen ratio in the mixture is 0.3. As can be seen from the diagram, the maximum combustion temperature gradually increases with the increase of initial pressure, but the amplitude of increase gradually decreases with the increase of initial pressure. At the same time, it can be seen from figure 5 and figure 6 that the maximum combustion temperature decreases first and then increases with the increase of equivalent ratio.

Figure 11 shows the change law of NO molar fraction of ammonia/hydrogen laminar premixed combustion product with initial pressure when the initial temperature is 298 K and hydrogen ratio is 0.3. It can be seen from the graph that the molar fraction of NO decreases with the increase of initial pressure, and the range of reduction decreases with the increase of initial pressure. At the same time, it can be seen from figure 5 and figure 6 that the molar fraction of NO decreases with the increase of equivalent ratio.

4. Conclusion

Ammonia/hydrogen premixed laminar combustion is studied in this paper. The detailed chemical reaction mechanism suitable for ammonia/hydrogen premixed laminar combustion was obtained by comparing the flame velocity simulation with the experimental results. Based on this mechanism, the combustion and emission characteristics of ammonia/hydrogen premixed laminar combustion are studied. The main conclusions are as follows.

With the increase of equivalent ratio, the flame velocity of ammonia hydrogen laminar flow first increases and then decreases, however, with the increase of hydrogen ratio and initial temperature in ammonia/hydrogen mixed fuel, the laminar flame velocity also presents a law of first increasing and then decreasing, and the maximum value occurs when the equivalent ratio is 1.1. The laminar flame velocity and NO molar fraction of ammonia/hydrogen combustion decrease with the increase of initial pressure, while the maximum combustion temperature increases with the increase of initial pressure. The emission of NO from ammonia/hydrogen combustion products decreases gradually with the increase of equivalent ratio, and the emission of NO increases with the increase of hydrogen ratio and initial temperature. With the increase of the equivalent ratio, the maximum temperature of ammonia/hydrogen combustion first increases and then decreases. However, when the maximum temperature reaches the extreme value, the equivalent ratio increases with the increase of hydrogen ratio. At the same time, with the increase of hydrogen ratio and initial temperature in ammonia/hydrogen mixed fuel, the maximum combustion temperature presents a law of first increasing and then decreasing.

Acknowledgments

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References


