

Effects of Equivalence Ratio, Inlet Temperature and Pressure on NO Emission for Two Stage Combustion of NH₃/H₂ Fuel Mixture

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Abstract

There is growing interest in the application of carbon-free fuel NH₃ to support future energy requirements, however combustor designs and strategies require considerable development to improve combustion characteristic and to decrease NO_x emissions for NH₃-containing fuel. In this paper, the effects of equivalence ratio, inlet temperature, and pressure on NO emission and primary laminar burning velocity are investigated for two stage combustion of 70%NH₃/30%H₂ fuel mixture by computation. The results show that primary equivalence ratio plays a more important role in NO emission at atmospheric pressure, and $\phi_{primary}=1.25$ is an optimal primary condition to reduce NO emission. The effect of pressure on NO emission is twofold: (1) inhibits NO formation in primary combustion zone by thinning primary flame thickness; (2) promotes the thermal NO formation in lean combustion zone. Additionally, no matter the primary equivalence ratio is, the NO emission can be lower than 100ppm at $\phi_{total}=0.6$, $P>0.5$ MPa. Increased inlet temperature increases laminar burning velocity dramatically, and elevated pressure reduces NO emission significantly. Hence high inlet temperature combined with pressurization can realized improved flame propagation and NO emission. NO emission less than 200ppm and primary laminar burning velocity greater than 0.2m/s can be achieved at pressurized condition for inlet temperature between 500K and 600K.

1 Introduction

Recently, in order to cope with the increasingly serious greenhouse effect, ammonia as a carbon-free fuel has attracted wide attention. Ammonia has a high hydrogen density of 17.8% [1], and having a lower boiling and condensation temperature [2] makes it easier to store and transportation. Additionally ammonia has a well-established production and distribution network, favoring it as a commercial fuel. However, it is necessary to solve defects of ammonia combustion, such as low laminar burning velocity and narrow flammability range. Burning ammonia and hydrogen blend can effectively improve the ammonia combustion characteristic. A number of studies has focused their research on the NH₃/H₂/air flame, showed this blend's possibility as a substitute fuel for practical gas turbine burner [3-6]. However, the NO_x emission is another issue for

the usage of NH₃/H₂ as a fuel. NO_x will hazard the environment, causing acid rain and photochemical pollution. The two stage combustion is proposed for reducing NO_x in NH₃/H₂ combustion [7-8]. Therefore this paper employed a chemical reacting network (CRN) [4-5] method to study the effect of total equivalence ratio, primary equivalence ratio, pressure and inlet temperature on NO concentration and primary laminar burning velocity for two stage combustion of NH₃/H₂ mixture fuel.

2 Numerical investigation

The calculation is carried out with CHEMKIN-PRO and a gas turbine burner CRN method adapted for two stage combustion is proposed. Figure 1 illustrates the CRN model. It consists of Perfectly Stirred Reactor (PSR), Plug Flow Reactor (PFR) and Partially Stirred Reactor (PaSR). The clusters from left to right present primary swirl flame zone, post flame zone, secondary air mixing zone and lean burn zone respectively. The chemical mechanism of Xiao et.al [9] containing 24 species and 91 steps agrees well with experiments for prediction of laminar burning velocity and NO emission and takes less time to calculate [10]. Therefore the Xiao's mechanism was selected for finite chemistry calculation. A fuel composition with an NH₃/H₂ volume ratio of 70%/30% was specified for the model. Here the inlet temperature were set in range of 300K-800K with an increment of 100K, the pressure condition were specified at 0.1, 0.5, 1.0, 1.5MPa. The primary equivalence ratio $\phi_{primary}$ and total equivalence ratio ϕ_{total} are varied from 1.1 to 1.3 and from 0.4 to 1 respectively. All examined conditions are summarized in Table 1.

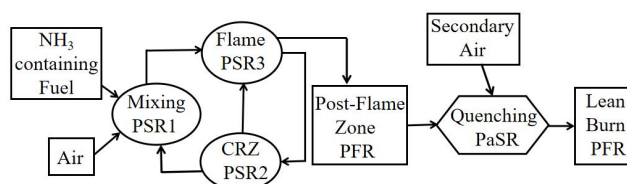


Figure 1:1D Chemical Reactor Network schematic.

Composition (Volume Fraction)	70%NH ₃ /30%H ₂
Fuel Mass Flow Rate (g/s)	1.388
ϕ_{primary}	1.10, 1.15, 1.20, 1.25, 1.30
ϕ_{total}	0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0
Inlet Temperature T_i (K)	300, 400, 500, 600, 700, 800
Pressure (MPa)	0.1, 0.5, 1.0, 1.5
2nd Air Temperature (K)	300

Table 1: Examined condition.

3 Results and Discussion

3.1 Effect of Equivalence Ratio

Figure 2 shows the effects of total equivalence ratio and primary equivalence ratio on NO concentration at $T_i=300\text{K}$ and $P=0.1\text{MPa}$. The rightmost points stand for the states without secondary airflow. Secondary airflow cause the reduction of NO emission except for $\phi_{\text{primary}}=1.3$. The reduction of NO with the decrease of total equivalence ratio is mainly due to the dilution of secondary air flow. There also exists NO formation in lean combustion zone, especially obvious for $\phi_{\text{primary}}=1.3$. NO formation exceeding the dilution of secondary airflow cause the increase of NO mole fraction for two stage combustion of $\phi_{\text{primary}}=1.3$. The increase of primary equivalence between 1.1 and 1.25 decreases NO concentration, and slows down the variation of NO mole fraction with total equivalence ratio. The dilution of secondary airflow is limited, the NO emission is mainly determined by primary flame. Therefore primary equivalence ratio exerts greater importance in effectively NO reduction than total equivalence ratio. And $\phi_{\text{primary}}=1.25$ is recommend as the most feasible one for effectively reducing NO emission at atmospheric pressure and $T_i=300\text{K}$.

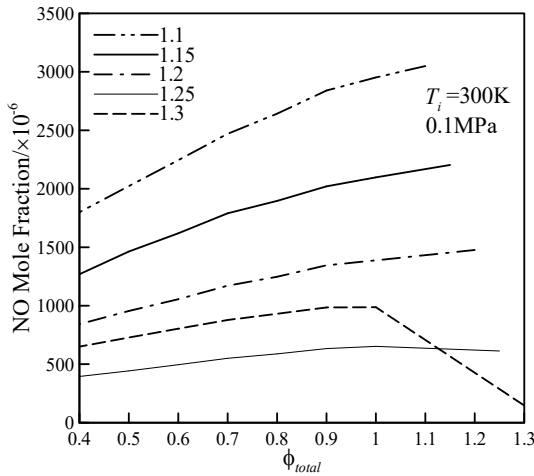


Figure 2: NO emission against total equivalence ratio with different primary equivalence ratio.

However laminar burning velocity of NH₃/H₂ fuel mixture decrease monotonously with the increase of equivalence ratio

for single stage combustion at rich condition, for $\phi=1.25$, the laminar burning velocity is about 0.19m/s at atmospheric pressure and higher pressure lowers the laminar burning velocity[10]. The low laminar burning velocity tends to blow the flame out. Meanwhile pressure is an important parameter for NO emission reduction in single stage combustion, elevated pressure can conduce NO reduction significantly, as shown in [10]. Therefore, the effect of inlet temperature on primary laminar burning velocity at different pressure condition for $\phi_{\text{primary}}=1.25$ is studied, as shown in figure 3. It is noticed that pressure around 0.8MPa, ammonia can be condensed at room temperature so that laminar burning velocity are calculated in the range of 400-800K at $P=1.0, 1.5\text{MPa}$. No matter whether the pressure is high or low, primary laminar burning velocity increases with inlet temperature dramatically. Moreover, the increase of inlet temperature intensifies the increase rate of primary laminar burning velocity. The effect of pressurization on primary laminar burning velocity is less significant than inlet temperature. It's also worth noting that the laminar burning velocity shouldn't be too large, otherwise it will cause a flashback. Hence NH₃/H₂ fuel mixture can be burned at a reasonable high inlet temperature and elevated pressure to improve laminar burning velocity and reduce NO emission for single stage combustion. But the effects of inlet temperature and pressure on NO emission of two stage combustion have not been studied yet, so the parametric studies of inlet temperature and pressure on NO mole fraction are shown below.

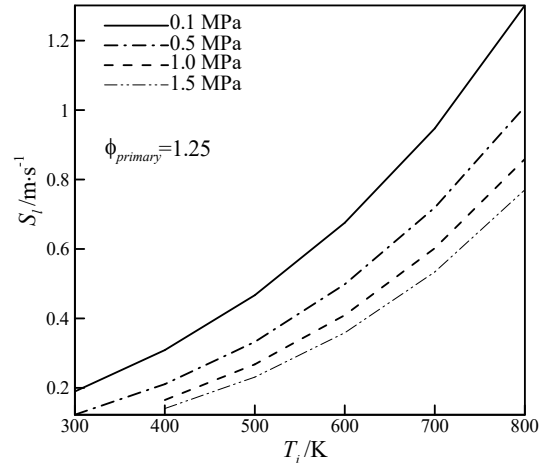


Figure 3: Primary laminar burning velocity as a function of inlet temperature at different pressure

Figure 4 shows mole fraction against total equivalence ratio with increased pressures. Note that the primary equivalence ratios fixed to $\phi_{\text{primary}}=1.1, 1.25$ respectively and inlet temperature is constant at 400K. It can be seen that except for $P=0.1\text{MPa}$, NO mole fraction at the pressurized conditions appears a peak at the total equivalence ratio equaling to 0.9. A small amount of secondary air promotes the NO formation of lean combustion significantly at pressurized condition. As increasing secondary airflow further, NO mole fraction decreases. The effect of pressure on NO emission for two stage combustion can be divided into two parts: (1) the increased pressure inhibits the formation of NO in primary flame zone; and (2) NO formation is more active in the lean combustion zone for evaluated pressure. Pressurization thins the primary flame thickness, just as figure 5 shown. NO formation is greatly sensitive to OH radicals [11] gathered in flame zone. Decreased flame thickness with increased pressure reduces the zone of NO formation, and as a result NO mole fraction is diminished. In addition, figure 5 can also explain that in spite

of the similar flame thicknesses for two primary equivalence ratios, the higher flame temperature promotes the formation of thermal NO at $\phi_{primary} = 1.1$. According to the analysis of absolute rate of production NO in lean combustion zone, the formation of NO is mainly through thermal NO formation $O+N_2 \rightleftharpoons NO+N$, $N+O_2 \rightleftharpoons NO+O$, and $N+OH \rightleftharpoons NO+H$. Figure 6 shows increased pressure increases the temperature in lean combustion zone, so enhances the formation of NO. The inhibition effect of pressure on NO formation in primary combustion zone dominates the NO emission for slightly rich primary equivalence ratio. As for richer primary equivalence ratio, the influence of pressure in lean combustion zone plays a more important role, causing NO mole fraction even higher for pressurized conditions at $\phi_{total}=0.9$. Hence combined with pressure effect in two combustion zones, NO emission can be lower than 100ppm at $\phi_{total}=0.6$, $P>0.5MPa$, regardless of the rich primary equivalence ratio.

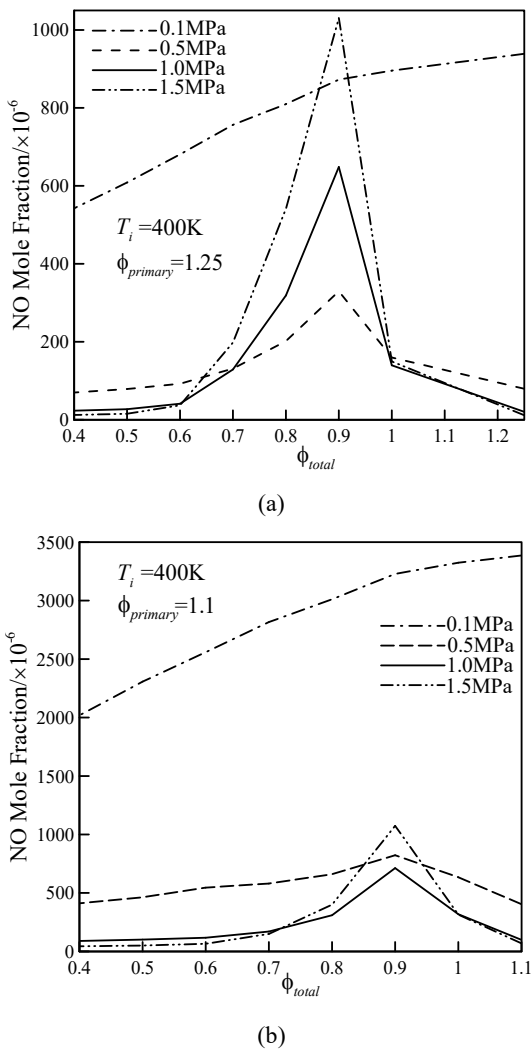


Figure 4: NO mole fraction against total equivalence ratio with increased pressure at $\phi_{primary} = 1.15$ (a); $\phi_{primary} = 1.3$ (b)

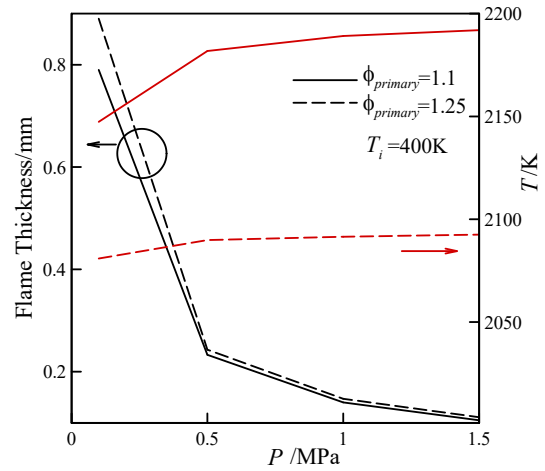


Figure 5: Variations of flame thickness and flame temperature with pressure in primary combustion zone

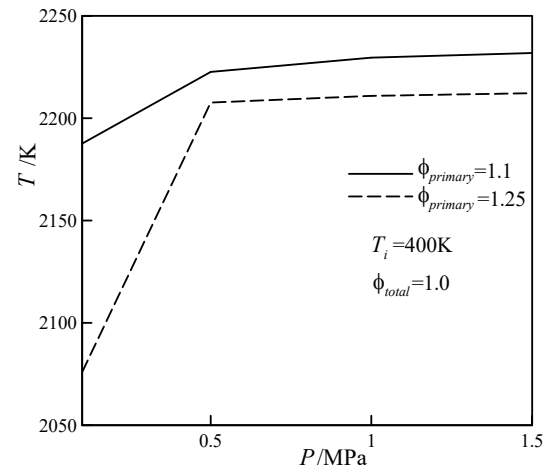


Figure 6: Flame temperature against pressure with different primary equivalence ratio

The effects of inlet temperature on NO concentration with different pressure are shown in figure 7. The condition of $\phi_{primary} = 0.9$ and $\phi_{total} = 0.6$ is taken as the example on account of its low NO emission at all pressure. The NO mole fraction increases with the increase of inlet temperature in range of 400K-800K. Figure 8 shows increased inlet temperature increases primary flame temperature and decreases primary flame thickness. The effect of flame temperature and flame thickness on NO formation is opposite, and competition of the two effect causes the variation of NO emission. And elevated pressure significantly reduces NO concentration. The variation of NO concentration with inlet temperature slows down most at $P = 0.5MPa$ due to dramatic decrease of flame thickness with increased pressure. Comparing the reduction of flame thickness between $P = 0.1MPa$ and $P = 0.5MPa$, the variation of flame thickness at $P = 0.5MPa$, 1.0MPa, 1.5MPa is really small, as figure 5 shown. Therefore it's feasible to burn NH_3/H_2 fuel mixture at a higher inlet temperature and pressurized condition for two stage combustion to yield larger laminar burning velocity and lower NO emission. For example, NO emission less than 200ppm and laminar burning velocity greater than 0.2m/s can be achieved at pressurized condition for inlet temperature between 500K and 600K.

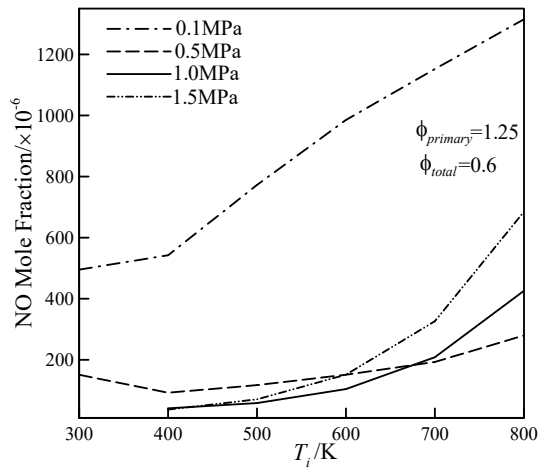


Figure 7: NO Mole Fraction against inlet temperature with different pressure

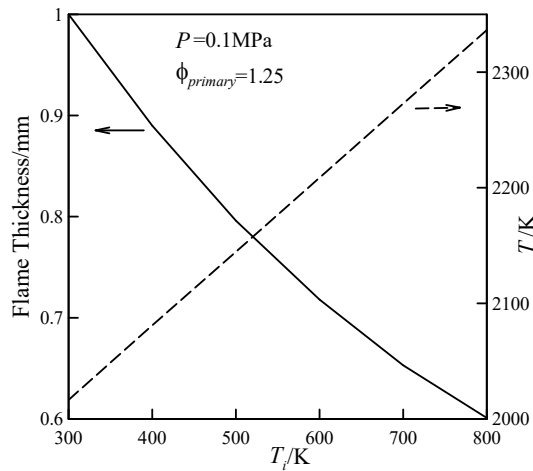


Figure 8: Variations of flame thickness and flame temperature with inlet temperature in primary combustion zone

4 Conclusions

The effects of equivalence ratio, inlet temperature and pressure on NO Emission and laminar burning velocity for two stage combustion are investigated by computations. Results are summarized as followings.

The variations of NO mole fraction with primary equivalence ratio and total equivalence ratio reveal that primary equivalence ratio plays a more important role in NO emission at atmospheric pressure and $\phi_{primary}=1.25$ is the most effective one to reduce NO emission. As pressure elevating, NO concentrations at different primary equivalence ratios show different trend with pressure. The effect of pressure can be divided into: (1) inhibits NO formation in primary combustion zone by thinning primary flame thickness; and (2) promotes the thermal NO formation in lean combustion zone. Therefore combined with pressure effect in two combustion zones, no matter the primary equivalence ratio is, the NO emission can be lower than 100ppm at $\phi_{total}=0.6$, $P>0.5\text{MPa}$.

The comparison of the effect of inlet temperature and pressure on laminar burning velocity demonstrates that the increase of laminar burning velocity with the increase of inlet temperature is more significant than the reduction effect of pressure.

Furthermore increased pressure reduces NO emission remarkably, and a low NO concentration can also be realized even at a high inlet temperature for pressurization. Hence the high inlet temperature and pressurization condition is feasible to both improve flame propagation and NO emission of NH_3/H_2 fuel mixture. NO emission less than 200ppm and laminar burning velocity greater than 0.2m/s can be achieved at pressurized condition for inlet temperature between 500K and 600K.

5 Acknowledgment

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