**Effect of CH₄, Pressure, and Initial Temperature on the Laminar Flame Speed of an NH₃—Air Mixture**

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**ABSTRACT:** Ammonia (NH₃) is not only expected to be used as a hydrogen energy carrier but also expected to become a carbon-free fuel. Methane (CH₄) can be used as a combustion enhancer for improving the combustion intensity of NH₃. In addition, it is important to understand the flame characteristics of NH₃—air at elevated pressures and temperatures. The laminar flame speed of NH₃—CH₄—air is numerically investigated, where the mole fraction of CH₄ ranges from 0 to 50% in binary fuels and the pressure and initial temperature are up to 10 atm and 1000 K, respectively. The calculated value from the Okafor mechanism is in excellent agreement with experimental data. The CH₄ in the fuel affects the flame speed by changing the main species of free radicals in the flame; the high pressure not only increases the rate-limiting reaction rate in the flame but also reduces the amount of H, O, and OH radicals in the flame, so as to restrain the propagation of the flame. At a higher initial temperature, the faster flame speed is mainly due to the higher adiabatic flame temperature. The laminar flame speed correlation equation has a consistent trend with the simulation results, though with a slight underestimation at higher pressures and temperatures. It is a more effective way to calculate the laminar flame speeds of NH₃—air for a given pressure and temperature.

**INTRODUCTION**

Ammonia has a high hydrogen density (17.7% by weight), boiling point, and condensation temperature, similar to propane, and is easier to store and transport than hydrogen, so it is a promising carbon-free hydrogen carrier. As one of the most produced chemicals in the world, it has more than 100 years of mass production history and has a complete production and distribution network. In addition, ammonia can be produced from different sources of energy, such as wind energy, biomass energy, nuclear energy, etc., which means that it is a promising green future fuel and may not produce carbon dioxide. However, its narrower flammability range, comparably low laminar flame velocity and flame temperature, slightly hinders its technical application, which is about 5 times lower than that of CH₄—air under stoichiometric conditions at 298 K and 0.10 MPa.¹⁻⁵

To successfully use ammonia combustion in practical applications, it is necessary to have an in-depth understanding of the basic combustion characteristics of ammonia fuel. Laminar flame speed is an important and well-defined characteristic of combustible mixtures: it indicates the reactivity, diffusivity, and exothermicity of the mixture. Therefore, an accurate understanding of the laminar flame speed is essential for the study of combustion characteristics and equipment design. For the development of burners for these new fuels, it is important to accurately predict their laminar flame speed. On the other hand, it is one of the most important overall properties of a fuel, which can be used to describe many premixed flame phenomena, and it is a size parameter to be considered in the design of high-energy industrial systems such as internal combustion engines and gas turbines. In fact, this physical and chemical property of combustible mixtures significantly affects the heat release rate, that is, flame stabilization. Its importance makes it the main goal for dynamic mechanism verification.⁶⁻⁹ Laminar burning velocity at elevated pressures and temperatures is also the fundamental parameter in premixed combustion. It can be used to validate the chemical reaction mechanisms and is of practical importance in the design and optimization of internal combustion engines, and empirical correlations based on the laminar flame speed of the mixture of fuels and oxidations at elevated pressures and initial temperatures are often required.¹⁰⁻¹¹

As one of the most common gaseous fuels, the research of laminar burning velocity of CH₄ is of great interest in the community. Chu et al.¹² measured the laminar burning velocity of methane, and the effects of equivalence ratio and N₂ doping on it were numerically analyzed. The laminar flame speeds of

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NH3–air premixed flames have been investigated by Han et al., Li et al., and Hayakawa et al. According to their results, the laminar flame speed of NH3–air premixed flames is lower than that of hydrocarbon flames, such as CH4–air flames and H2–air flames, and decreases with an increase in the initial pressure. To improve the lower combustion intensity of ammonia, the addition of methane has been considered. A mixture of ammonia and hydrocarbons may produce a low carbon fuel with a higher flame speed than ammonia. This mixture therefore offers the potential to improve the combustion characteristics of ammonia and to reduce carbon dioxide emissions from hydrocarbon combustion.

Some studies on detailed mechanisms of NH3–CH4 oxidation have been conducted previously. Tian et al. studied a series of low-pressure premixed NH3–CH4–O2–Ar flames to determine the influence of different NH3–CH4 molar ratios and proposed the chemical mechanism of ammonia–methane premixed combustion based on the Skreiberg mechanism. In this study, only stoichiometric conditions were studied, and ammonia was still added to the fuel mixture as a minor component. The Gas Research Institute released the latest version of the GRI-Mech 3.0 methane combustion mechanism in 2005, which contains 53 species and 325 chemical reactions. This mechanism has been verified in the combustion of ammonia-doped methane. Although Tian’s mechanism and the GRI-Mech 3.0 mechanism have been greatly developed recently and have been increasingly used in the current literature, there is little or no experimental verification of laminar flame speed. Of particular interest in the current work is the laminar flame speed of an NH3–CH4–air mixture. The mechanism proposed by Okafor et al. is based on the detailed reaction mechanism GRI-Mech 3.0, which adds some important ammonia oxidation chemistry in Tian’s mechanism. The laminar flame speed of CH4–air and CH4–NH3–air was measured under ambient pressure and temperature, and the mole fraction of NH3 in fuels is about 50%. The results show that the simulated values are very close to the experimental data. For this reason, the Okafor mechanism was selected in this work.

However, most of the previous studies only focused on the addition of a small amount of ammonia in methane and rarely performed a comprehensive analysis of the different combustion characteristics under various conditions with ammonia as the main fuel. In addition, limited studies were reported on the laminar flame speed and on the understanding of combustion characteristics of the NH3–air flames at elevated pressures and temperatures. Therefore, the objective of this study is to analyze the effects of CH4 substitution, pressure, and initial temperature on the laminar flame speed of ammonia–air through numerical simulations with a detailed chemical reaction mechanism established by Okafor to expand the understanding of the characteristics of ammonia premixed flames. On the basis of numerical calculation data, the empirical formulas for the laminar flame speed of an NH3–air flame at elevated pressures and temperatures were correlated.

## COMPUTATIONAL METHOD

In this study, to obtain the laminar flame speed, the flame structure, and radical profiles of the NH3–CH4–air mixture under different conditions and the detailed NH3–CH4–air combustion mechanism, the Okafor mechanism was used. Furthermore, an unstretched, adiabatic, and freely propagating planar flame was employed using CHEMKIN software to solve the steady-state mass, species, and energy conservation equations. In addition, mesh gradient and mesh curvature are set to 0.01, and the maximum number of grid points was maintained at 1500 to ensure the convergence of the calculation under high mesh accuracy. The computational domain of the laminar flame of NH3–CH4–air was fixed from 0 to 5 cm. To reduce the computational cost and reduce the difficulty of convergence in the calculation, the average method was used to calculate the diffusion coefficient of the mixture during the simulation. The convection term in the simulation was discretized by adopting the windward difference method.

## RESULTS AND DISCUSSION

**Effect of CH4 Mole Fraction in Fuel on the Flame Speed of an NH3–CH4–Air Mixture.** Figure 1 shows the functional relationship between the flame speed of NH3–air and the equivalence ratio under normal temperature and pressure conditions (NTP, T = 300 K, P = 1 atm), where the equivalence ratio ranges from 0.7 to 1.4. The solid lines represent the calculated values obtained by three different chemical reaction mechanisms, and the scattered points represent the corresponding experimental values in the open literature.

As shown in Figure 1, the flame speed of NH3–air is very low, and the maximum flame propagation velocity is only 6–9 cm/s; the corresponding equivalence ratio is about 1.1 of that on the fuel-rich side. Comparing the numerical results of the three reaction mechanisms, it is found that the Tian mechanism overestimates the flame propagation velocity of NH3–air and the GRI-mech 3.0 mechanism may slightly underestimate the flame propagation velocity under some equivalence ratios, such as $\phi = 1$ and $\phi = 1.1$. In contrast, the results from the Okafor mechanism can be more consistent with the experimental data and accurately capture the flame speed of NH3–air.

Figure 2 shows the functional relationship between the flame speed and the equivalence ratio of mixtures with different NH3–CH4 ratios. The solid lines and solid points represent the calculated values obtained by the Okafor mechanism, while the hollow scattered points represent the experimental values.
in the existing literature. \( X_{\text{NH}_3} \) is defined as the mole fraction of \( \text{NH}_3 \) in the \( \text{NH}_3-\text{CH}_4 \) binary fuel, which is expressed as

\[
X_{\text{NH}_3} = \frac{n_{\text{NH}_3}}{n_{\text{NH}_3} + n_{\text{CH}_4}}
\]

(1)

where \( n_{\text{NH}_3} \) and \( n_{\text{CH}_4} \) represent the amount of substance of \( \text{NH}_3 \) and \( \text{CH}_4 \), respectively.

The hollow red circle represents experimental data of the heat fraction of \( \text{NH}_3 \) in the \( \text{NH}_3-\text{CH}_4 \) binary fuel, \( E_{\text{NH}_3} = 60\% \)\(^{23} \) (the mole fraction of \( \text{NH}_3 \) is about 52\%), and the hollow blue triangle represents experimental data\(^{13} \) of the mole fraction of \( \text{NH}_3 \) which is 80\% in the \( \text{NH}_3-\text{CH}_4 \) binary fuel. It can be seen from Figure 2 that the addition of \( \text{NH}_3 \) can significantly reduce the flame speed of the blend fuel, and the equivalence ratio corresponding to the peak flame speed seems to change slightly with the composition of the fuel, ranging from 1 to 1.1 in the fuel-rich region. The higher concentration of radicals in the flame front leads to the maximum flame speed at the rich side, \( \phi > 1 \).\(^{32} \) In addition, the calculated values of \( X_{\text{NH}_3} = 80\% \) are almost in good agreement with the experimental data.

Figure 3 shows the adiabatic flame temperature as a function of the equivalent ratio at different mole fractions of \( \text{NH}_3 \). The numerical results in Figure 3 are all obtained by the Okafor mechanism. As can be seen from Figure 3, with the increase of the proportion of \( \text{NH}_3 \) in the fuel, the adiabatic flame temperature decreases significantly, which is similar to the change of the flame speed. This also indicates that temperature has a great influence on the flame speed. After further comparison with Figure 2, it is found that the equivalent ratio corresponding to the peak value of the adiabatic flame temperature is \( \phi = 1.0 \) at all \( \text{NH}_3 \) proportions and does not change with it unlike the flame propagation speed. This difference seems to indicate that the flame propagation speed of \( \text{NH}_3-\text{CH}_4-\text{air} \) is not only affected by temperature but also by chemical reactions in the flame.

A sensitivity analysis for \( S_1 \) was carried out to identify the elementary reactions that affected the flame speed the most. The effects of the main branching reaction and termination reactions on the flow rate were evaluated. Figure 4 shows the analysis results of the sensitivity of chemical reactions to the flow rate under different \( \text{NH}_3 \) mole fractions. The reaction with a positive sensitivity coefficient indicates that this kind of reaction can promote flame propagation, which is called the acceleration reaction; on the contrary, the reaction with a negative sensitivity coefficient indicates that this kind of reaction can inhibit flame propagation, which is called the rate-limiting reaction. It can be found from Figure 4 that the sensitivity coefficient of R39 is the highest in different \( X_{\text{NH}_3} \) flames, which indicates that chain branching R39 has the most positive effect on flame propagation. In the \( X_{\text{NH}_3} = 50\% \) flame, almost all of the accelerated reactions, except for R257, are associated with free radicals containing carbon elements, such as \( \text{CH}_3 \), CO, and HCO free radicals; R53 is the rate-limiting reaction with the highest negative sensitivity coefficient. In the flame of \( X_{\text{NH}_3} = 80\% \), the acceleration reaction containing carbon free radicals is only R122, the sensitivity coefficient decreases obviously, and the most important rate-limiting reaction is also transformed from R53 to R273. For a pure ammonia flame with \( X_{\text{NH}_3} = 100\% \), R271 is the accelerated reaction with the second highest sensitivity coefficient and R273 is the rate-limiting reaction with the highest negative sensitivity coefficient, which indicates that the HNO radical has an important effect on the flame propagation velocity in a pure \( \text{NH}_3 \) flame.

The results of the sensitivity analysis shown in Figure 4 indicate that the flame speed is largely dependent on the amount of \( \text{H}, \text{O}, \text{and OH radicals in the flame} \). Figure 5a–c shows the axial distributions of \( \text{H}, \text{O}, \text{and OH radicals in different} \( X_{\text{NH}_3} \) flames. It can be seen that the addition of \( \text{NH}_3 \) reduces the concentration of the three kinds of free radicals in the flame, and in contrast, OH radicals have the least decreasing trend. Figure 5d–f shows the detailed flame structures of different \( X_{\text{NH}_3} \) flames. The mole fraction of the ordinate adopts a logarithmic coordinate form with a base of 10. The proportion of \( \text{NH}_3 \) in the fuel has a significant influence on the species in the flame. In the flame with \( X_{\text{NH}_3} = 50\% \), because of more \( \text{CH}_4 \) in the fuel, higher mole fractions of CO and \( \text{CH}_3 \) radicals are present. There is a significant decrease in the amount of \( \text{CH}_3 \) radicals in the flames of \( X_{\text{NH}_3} = 80\% \) and \( X_{\text{NH}_3} = 100\% \); however, with the increase of \( \text{NH}_3 \) in

![Figure 2](image-url) **Figure 2.** Laminar flame speed for \( \text{NH}_3-\text{CH}_4-\text{air} \) at various equivalence ratios.

![Figure 3](image-url) **Figure 3.** Adiabatic flame temperature for \( \text{NH}_3-\text{CH}_4-\text{air} \) at various equivalence ratios.
the fuel, NH, NH₂, and N₂O radicals begin to increase notably. In addition, there is only a slight change in the number of other free radicals.

Figure 6a,b shows the net reaction rates of the accelerated reactions in the NH₃−CH₄−air flame, and Figure 6c shows the net reaction rates of the rate-limiting reactions. Solid lines, dashed lines, and short dashed lines are used to distinguish the flames of different X_{NH₃}. The reaction rate curves corresponding to X_{NH₃} = 50% are shown in the solid lines in Figure 6. As can be seen from Figure 6a,b, among all of the acceleration reactions, R39 has the fastest reaction rate, followed by R102, R100, and R169, and R122 and R257 have the slowest reaction rates. The H radicals in the flame were mainly generated from the reaction between CO, HCO, and other radicals. The reaction rate curves of X_{NH₃} = 80% correspond to the dashed lines in the figure; the reaction rate of R39 is much lower than that of X_{NH₃} = 50%. In addition, the reaction rate of R122 is slightly lower than that of R257. The promoting effect of CH₃ radicals on flame propagation is weakened, and NNH and HNO radicals become the main source of H radicals in the flame. The short dashed lines are used to distinguish the reaction rates at X_{NH₃} = 100%; the reaction rate of R39 further declines. The extremely slow reaction rates of R90, R227, and R257 can hardly promote flame propagation.

Figure 6c shows the reaction rate of rate-limiting reactions in different X_{NH₃} flames. In the X_{NH₃} = 50% flame, R246 and R273 have the highest reaction rates, followed by R53 and R36. The NH₂ radicals in the flame are oxidized by O radicals to form HNO radicals and then further reacted with H radicals, which reduced the amount of H radicals and terminated the propagation of the chain. In addition, CH₃ radicals are involved in both the rate-limiting reaction R53 and the accelerated reaction R100; however, the reaction rate of R53 is only 1/2 of that of R100, indicating that CH₃ radicals are more likely to participate in the accelerated reactions. Compared with other reactions, the reaction rate of R36 is the lowest and has the least effect on restraining the flame speed. In the flame of X_{NH₃} = 80%, the main rate-limiting reactions are R245, R273, and R265. NH₂ and HNO radicals together consume H radicals in the flame. NNH radicals react with O₂ and compete with the decomposition of NNH in R260, which inhibits the formation of H radicals. In the flame of X_{NH₃} = 100%, the net reaction rate of the chain termination reaction R256 is very low and has little effect on flame propagation.

Effect of Pressure and Initial Temperature on the Laminar Flame Speed of NH₃−Air. Figure 7 shows the effect of pressure and initial temperature on the laminar flame speed of NH₃−air in the pressure range from 1 to 10 atm and...
initial temperature range from 300 to 500 K under stoichiometric conditions ($\phi = 1$). It is suggested that elevated pressure has a slightly adverse impact on flame propagation due to a more stable tendency with an increase of pressure, while the effect of promotion of flame speed is enhanced by higher initial temperatures.

Figure 8 shows the results of sensitivity analysis of the NH$_3$–air flame propagation velocity under different pressures. For the acceleration reactions, the sensitivity coefficient of R39 is the highest, and the sensitivity coefficients are relatively reduced with the increase of pressure. In addition, R257, R271, and R91 also have relatively high sensitivity coefficients, of which the sensitivity coefficient of R91 increases significantly with the increase of pressure. For rate-limiting reactions in the flame, R273 has the highest negative sensitivity under low pressure, while the reaction with the highest negative sensitivity coefficient under elevated pressures transformed to R88. The effect of three-body reaction R36 on the flame propagation velocity is only observed under high pressure. Figure 9 shows the mole fractions of H, O, and OH radicals and the detailed flame structures in the flame under different pressures. The increase of pressure will significantly reduce the
amounts of H, O, and OH free radicals in the flame and make the flame surface and reaction zone move toward the unburned mixtures. However, the pressure has a nonlinear relationship with the amount of radicals and the distance of flame movement. As shown in Figure 9d−f, the significant decrease in the concentrations of H, O, and OH free radicals is the main reason for the lower flame propagation velocity under high pressure. In some radicals containing the N element, NH and HNO radicals, a downward trend with the increase of pressure is also observed; only the NO₂ radical increases with the increase of pressure. In addition, there is no significant change in the amount of other radicals.

The sensitivity analysis results are shown in Figures 8 and 10, which depict the net reaction rates of all rate-limiting and acceleration reactions under different pressures. Figure 10a,b shows the net reaction rates of the accelerated reactions, and Figure 10c shows the reaction rates of the rate-limiting reactions. The solid lines, dashed lines, and short dashed lines represent the conditions under the pressures of 1, 3, and 5 atm, respectively. The illustration is a local magnification to show the reaction rate curves under 1 atm more clearly. It can be seen that the increase of pressure greatly increases the reaction rates in the flame. Through the reaction rates of the accelerated reactions shown in 10(b), it can be seen that the third-body reaction R271 has the fastest reaction rate, and the HNO radical decomposes into a H radical under the impact of the third body. Second, R91 and R257 have the second highest reaction rates, while R91 is more sensitive to pressure than R257. Specifically, at an atmospheric pressure of 1 atm, the reaction rate of R91 is slightly lower than that of R257;
however, when the pressure is up to 5 atm, the reaction rate of R91 has almost increased to twice that of R257, which indicates that the HO2 radical is an important source of OH radicals under high-pressure conditions. It can be seen from

Figure 10. Net reaction rates of acceleration reactions (a, b) and rate-limiting reactions (c) under different pressures.

Figure 11. Sensitivity coefficients of chemical reactions for the flow rate under different initial temperatures.
the reaction rate of the rate-limiting reaction shown in 10(c) that the reaction rate of R273 is the highest at low pressure. However, with the increase of pressure, there is a dramatic increase in the reaction rates of R36 and R88. Especially at the pressure up to 5 atm, the reaction rate of R88 has exceeded that of R257. The third-body reaction R36 has a very strong consumption of H free radicals under high pressure. HO2 radicals consume the amount of OH radicals in the flame by...
chain-terminated reaction R88, thus inhibiting the propagation of the flame. Figure 11 shows the analysis results of the sensitivity of chemical reactions to the NH$_3$–air flame propagation velocity at different initial temperatures. The main acceleration reactions are R39, R271, and R257, and the rate-limiting reactions are R273 and R265; the sensitivity coefficients of almost all reactions do not change significantly with the increase of the initial temperature. Figure 12 shows the mole fractions of H, O, and OH radicals and the detailed flame structure in the flame at different initial temperatures. An increase in the initial temperature causes the flame to move slightly toward the unburned mixture, and the amount of major radicals in the flame increases, but the structure of the flame does not change significantly. According to the sensitivity analysis results shown in Figure 11, the reaction rates of accelerated reactions and rate-limiting reactions in the flame at different initial temperatures are plotted in Figure 13. Figure 13a,b shows the reaction rates of the accelerated reactions, and Figure 13c shows the reaction rates of the rate-limiting reactions. The solid lines, dashed lines, and short dashed lines represent the flames with initial temperatures of 300, 400, and 500 K, respectively. Among the accelerated reactions, R39, R260, and R271 have the fastest reaction rates. Among the rate-limiting reactions, the three fastest reaction rates are shown by R245, R265, and R273. In addition, it can be found that with the increase of the initial temperature, there is almost no change in the growth rate of all of the reactions, which indicates that the initial temperature may mainly lead to the increase of the adiabatic flame temperature, thus further improving the flame propagation speed.

Correlation of Laminar Flame Speed at Elevated Pressures and Temperatures for an NH$_3$–Air Flame. As shown in Figure 14, there seems to be some kind of functional relationship between $S_L$ and pressure or initial temperature. As shown in Figure 14, the flame speed $S_L$ shows a nonlinear decreasing trend with the increase of pressure, while with the increase of initial temperature, it shows a nonlinear increasing trend. For this situation, two models were selected for the fitting of $S_L$ at different pressures and temperatures: allometric and exponential models. The equations of fitting curves relative to pressure are

$$S_L(P) = 6.64025P^{-0.28368}, \quad (T_{in} = 300\, K, \, 1\, atm \leq P \leq 10\, atm)$$

(2)

Figure 14. Laminar flame speed at various initial temperatures (a) and pressures (b).

Figure 15. Exponents $\alpha_T$ (a) and $\beta_P$ (b) for stoichiometric NH$_3$–air flames.
\[ S_l(P) = 4.4042 \exp\left(\frac{P}{3.14303}\right) + 3.28811 \]

\[ (T_{in} = 300 \text{ K}, 1 \text{ atm} \leq P \leq 10 \text{ atm}) \]  \hspace{1cm} (3)

and those of the fitting curves relative to temperature are

\[ S_l(T_{in}) = 4.63309 + 6.60142 \times 10^{-9} T_{in}^{3.0844}, \]

\[ (P = 1 \text{ atm}, 300 \text{ K} \leq T_{in} \leq 1000 \text{ K}) \]  \hspace{1cm} (4)

\[ S_l(T_{in}) = 6.61719 \exp\left(\frac{T_{in}}{331.97629}\right) - 10.36819 \]

\[ (P = 1 \text{ atm}, 300 \text{ K} \leq T_{in} \leq 1000 \text{ K}) \]  \hspace{1cm} (5)

Figure 14 shows that eqs 2–5 can perfectly capture the \( S_l \) of an NH\(_3\)–air stoichiometric flame under ambient pressure and temperature.

The influence of temperature and pressure on laminar flame speed \( S_l \) can be correlated through the following empirical expression\(^{11}\)

\[ \frac{S_l}{S_{l,0}} = \left(\frac{T_{in}}{T_0}\right)^{\alpha_T} \left(\frac{P}{P_0}\right)^{\beta_P} \]

where subscript 0 represents the reference condition, that is, \( T_0 = 300 \text{ K} \) and \( P_0 = 1 \text{ atm} \). Exponents \( \alpha_T \) and \( \beta_P \) are the temperature- and pressure-dependent parameters, respectively. The stoichiometric laminar flame speed under reference conditions, \( S_{l,0} \), is 6.566 cm/s.

Figure 15 shows the variations of \( \alpha_T \) and \( \beta_P \) for the stoichiometric NH\(_3\)–air flames. The variations of \( \alpha_T \) and \( \beta_P \) are given by the following equations

\[ \beta_P = \ln\left(\frac{S_l}{S_{l,0}}\right) / \ln\left(\frac{P}{P_0}\right) \]

\[ (7) \]

\[ \alpha_T = \ln\left(\frac{S_l}{S_{l,0}}\right) / \ln\left(\frac{T_{in}}{T_0}\right) \]

\[ (8) \]

where \( \alpha_T \) and \( \beta_P \) are obtained at the pressure of 1 atm and initial temperature of 300 K, respectively.

It can be seen from Figure 14 that \( \beta_P \) is decreased with the increase of pressure and \( \alpha_T \) is increased with the increase of the initial temperature, while the relationship is still nonlinear for them. Hence, \( \beta_P \) and \( \alpha_T \) are correlated as

\[ \beta_P = 0.06214 + 8.27745 \times 10^{-4} \exp\left(\frac{P}{4.94125}\right) - 0.29461 \]

\[ (9) \]

\[ \alpha_T = 0.53047 T_{in}^{0.22041} \]

To validate eq 6, Figure 14 gives the comparison of the results calculated using CHEMKIN and eq 6 under at pressures and temperatures. The results of eq 6 and CHEMKIN are in good agreement of tendency. However, the data calculated by eq 6 gradually underestimates the \( S_l \) under elevated pressures and temperatures. For this reason, there is a need to further improve eq 6 for a more accurate prediction of \( S_l \) of NH\(_3\)–air flames at various pressures and temperatures.

**CONCLUSIONS**

In this paper, the flame propagation velocities of NH\(_3\)–CH\(_4\)–air with different fuel components and at different pressures and initial temperatures are calculated using the CHEMKIN software package. The sensitivity analysis of flame speed is carried out by a numerical method, and the detailed flame structures and reaction rate distributions under different conditions are also plotted. The effects of the mole fraction of CH\(_4\), pressure, and initial temperature on the flame propagation velocity are also investigated. On the basis of numerical results, the mathematical fitting of the empirical correlation formula for the flame speed of NH\(_3\)–air under high temperatures and pressures is carried out. The main results are summarized as follows.

The simulated results by the Okafor mechanism\(^{23}\) are in good agreement with the experimental data. As the equivalence ratio increases, the laminar flame speed increases in the case of the lean fuel mixture and decreases in the case of the rich fuel mixture. The maximum laminar flame speed is obtained at an equivalent ratio of 1.1.

The flame speed is largely dependent on the amount of H, O, and OH radicals and the reaction rate of R39 in the flame. The higher proportion of CH\(_4\) in the fuel can increase the mole fraction of H, O, and OH radicals and reaction rates in the flame to further increase the flame speed of the mixtures. The amount of CH\(_4\) has an obvious effect on the structure of the combustion flame. In the flame with lower X\(_{NH_3}\), CO and HCO radicals mainly play a role in promoting flame propagation, HNO and NH\(_3\) radicals inhibit flame propagation, and CH\(_3\) radicals participate in the promotion and inhibition of flame at the same time. In the high X\(_{NH_3}\), flame, NH\(_2\), NNH, and HNO radicals almost simultaneously participate in the production and consumption of H radicals.

The increase of pressure will lead to a significant decrease of H, O, OH, and other radicals in the flame, which is the main reason for the decrease of the NH\(_3\)–air flame speed under high pressure; only NO\(_2\) radicals tend to increase with pressurization. HO\(_2\) is an important radical, and the generation and consumption of OH in flames have a strong correlation with the reaction path of HO\(_2\) radicals. Compared with other reactions, the huge increase of the rate-limiting reaction R88 leads to a further decrease of the flame speed under elevated pressures. The increase of the initial temperature has little effect on the increase in the range of all reaction rates; for this reason, the increase of the flame speed may simply be related to the increased adiabatic flame.

The fitting equations of laminar flame speed are in good agreement with the simulated results with the CHEMKIN package,\(^{33}\) even though higher underestimation of the \( S_l \) under elevated pressure and temperature is observed. Using these equations, the laminar flame speed can be calculated for a given initial pressure and temperature.

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Notes
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