

Using Ammonia as an Alternative Fuel: Effects of Ammonia Substitution on Methane/Air Counterflow Premixed Flames

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Abstract:

As a promising green fuel, ammonia can be used as an alternative to traditional fossil fuels. In this study, the effect of ammonia substitution on methane/air counterflow premixed flames was evaluated numerically at standard temperature and pressure conditions. The methane-ammonia-air counterflow flames were modelled within a wide range of ammonia mole fractions, equivalence ratio conditions and flame stretch rates. Extinction limits calculation has quantified the stable burning range and determined the reduction of combustible range of different ammonia-substituted methane fuel blends. With increasing ammonia mole fractions in the methane/ammonia fuel blends, combustion stability limits of the flames tend to decrease. Flame structure analysis reveals the detailed development of the stretched premixed flames. It showed no remarkable reduction of temperature in the methane/ammonia flames. Emission analysis of ammonia-substituted methane/air flames showed considerable reduction of CO₂ emissions compared with the methane/air flames, while moderate reduction of combustible range is found. It was also found that nitrogen oxides emissions tend to increase with ammonia substitution. Finally, sensitivity analyses help to gain a deep insight into the NO_x chemistry of different methane/ammonia fuel blends.

Keywords: *Alternative fuel, Ammonia, Methane, Combustion.*

I. INTRODUCTION

Ammonia has recently been considered as a potential carbon free chemical for supplying energy and storing hydrogen generated by renewables, therefore ammonia based fuel is a field gaining significant interest [1]. It is much easier and cheaper to store and transport compared to liquid hydrogen [2]. Ammonia also has an established large capacity storage and distribution network with a long history of handling experience. In this situation, utilizing ammonia as a green fuel has already shown great potential in lots of applications in recent years [3-8]. However, because of the problems such as relatively low flame

propagation speed and high ignition resistance, the promotion of ammonia combustion is of much concern when used in combustion energy systems.

In previous studies, lots of investigations have been performed on ammonia combustion applications cofired with different fuels including internal combustion engines, gas turbine engines, etc [3-7]. For instance, Reiter et al. [4] investigated the application of ammonia fuel in CI diesel engine by using ammonia to replace biodiesel, achieving energy replacement as high as 95%. Frigo et al. [5] demonstrated hydrogen can be used to enhance ammonia combustion performance in a SI engine. Grannell et al. [6] used ammonia and gasoline in a SI engine, achieving knock-free operation at higher loads than gasoline. Valera-Medina et al. [7] studied swirl burners using ammonia/methane combustion for gas turbine engines. These studies have generally demonstrated the acceptable performance of dual-fuel strategy using ammonia in engine applications. However, more work is still needed to further optimize the performance such as higher combustion efficiency and lower exhaust emissions.

To further promote the application of ammonia-based fuels, understand the fundamental combustion process is essential. For instance, to achieve optimal operation of the combustion process for ammonia-based fuels, it is essential to know the basic combustion features of the fuel mixtures such as flame propagation, auto-ignition, extinction limit, etc [9-11]. Thus, fundamental studies on ammonia combustion are a field gaining significant interest in recent years. As for premixed combustion of ammonia-based fuels, studies have mainly been carried out for spherical flames using combustion bomb and counterflow flames using opposed flow burner. For instance, Lee et al. [12] studied partial ammonia substitution of hydrogen fuels by using counterflow non-premixed flames for ammonia and hydrogen. It was found ammonia can significantly improve the safety of hydrogen. Ku et al. [13] explored combustion characteristics of methane/ammonia fuel blends and confirmed the feasibility of ammonia as a clean fuel to reduce carbon dioxide emissions, in which reasonable burning conditions were determined experimentally and numerically. Choi et al. [14] experimentally investigated extinction limits of the counterflow non-premixed methane/hydrogen flames at elevated temperature conditions. It was demonstrated hydrogen addition can improve the reactivity and ignition of ammonia. Colson et al. [11] studied the stretch rate at extinction of premixed ammonia/air flames and investigated the impact of pressure on the extinction characteristics. It was found in the research that compared with ammonia/air flames the extinction stretch rate is relatively low for ammonia/air flames. It was also found that the increase of pressure can increase extinction stretch rate a lot for ammonia/air flames. Therefore, the effect of ammonia substitution needs to be studied on the basic characteristics of extinction limits. However, earlier studies mainly investigated ammonia /hydrogen/air flames and the non-premixed methane-added ammonia flames. As natural gas is a widely used clean fuel, it is necessary to explore fundamental features of the premixed ammonia-substituted methane/air flames, of which the main component is methane.

Based on the aforementioned considerations, in this study ammonia substitutions on methane were investigated numerically in stretched premixed methane/ammonia/air flames. Fundamental extinction limits of ammonia-substituted methane/air flames are firstly studied to quantify the reasonable burning range. Flame structure of counterflow premixed flames are then studied to understand the extinction

mechanism. Studies on emission characteristics and mechanism are also carried out to investigate the effect of ammonia substitution.

II. NUMERICAL METHOD

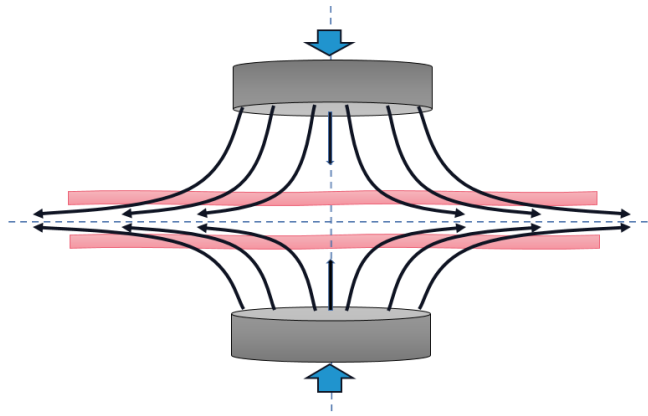


Fig 1: Schematic of the counterflow flame

Numerical simulation was performed using methods similar to previous work [15]. As shown in Fig 1, the counterflow, axisymmetric premixed flames are stabilized on both sides of the stagnation plane with two streams from opposite nozzles, which is a typical configuration for fundamental flame studies. Premixed counterflow flames were numerically modelled by using the CHEMKIN package [16], which has proved good performance in prediction of stretched flames [11]. In the model by assuming a linear relation between radial velocity and radial coordinate, the two-dimensional flow analysis is simplified so that fluid fields are considered as only functions of the axial distance. As the dynamics of the configuration is well defined, the configuration of counterflow premixed flames was used to represent one-dimensional, strained, laminar flame jets in the present study. Such one-dimensional simulator will be used to calculate parameters such as temperature, species of the flame. Extinction stretch rates can be calculated by initially establishing a premixed counterflow and then increasing stretch rate up until extinction occurs. Then temperature of the flames can be described as a function of stretch rate. Distance between the outlets is 10 mm and diameter of the outlets is 10mm. More details about the numerical model can be found in [17].

Simulation of counterflow premixed methane/ammonia/air flames was carried out with detailed chemical mechanism of Tian et al. [18]. The Tian mechanism was established based on detailed experimental study of CH_4/NH_3 premixed combustion, containing 701 reactions among 84 species. The mechanism has been verified in different ammonia flame studies and demonstrating a satisfying precision among the recent developed ammonia chemical mechanisms [19-21]. Therefore, the complete mechanism of Tian et al. was employed to perform numerical calculation on counterflow premixed flames of ammonia/methane fuels over a wide range of conditions in this study. All the simulations are conducted with the mechanism of Tian et al. and ammonia mole fraction varying from 0-50% in methane/ammonia fuel blends at standard temperature of 298 K and atmospheric pressure conditions.

III. RESULTS AND DISCUSSION

3.1 Extinction Limits

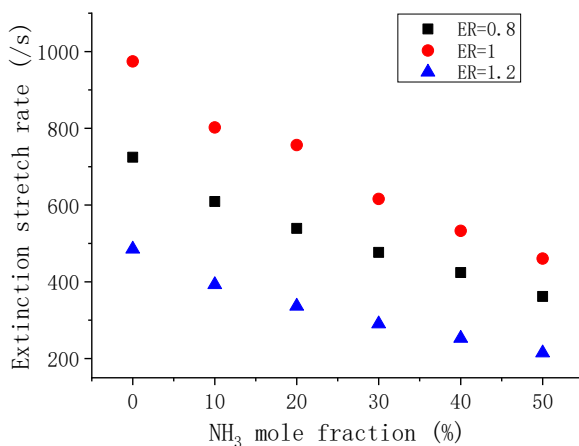


Fig 2: Extinction limits as function of ammonia mole fraction for counterflow premixed methane/ammonia/air flames at different equivalence ratios.

Extinction limits were calculated in order to illustrate the impact of ammonia substitution in counterflow premixed methane/ammonia/air flames under different equivalence ratio conditions as shown in Fig 2. As illustrated, at different equivalence ratio conditions, significant decreasing tendencies of extinction limit are observed with ammonia mole fraction increasing in fuel blends. It is because the reactivity of methane/ammonia/air become lower as ammonia added. Though ammonia has much lower reactivity than methane, the combustion can be sustained at all the ammonia concentrations studied. This can indicate that ammonia substitution of methane is possible for CO₂ reduction in combustion application. In Fig 2 it is also shown that at different equivalence ratio conditions, the extinction limits variation is also significantly different. The extinction limit for stoichiometric mixture is relatively much higher than the other two equivalence ratio conditions, indicating equivalence ratio also has big influence on extinction features of methane/ammonia/air counterflow flames.

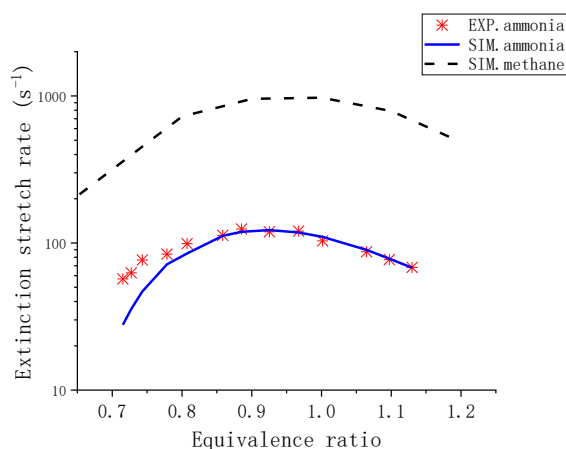


Fig 3: Extinction limits of premixed ammonia/air and methane/air flames as a function of equivalence ratio. Experiments as in [11].

Fig 3 shows extinction limits of both methane/air and ammonia/air flames against equivalence ratio at standard temperature and pressure conditions (pressure of 1 atm and temperature of 298 K). The experimental data from Colson [11] were employed to illustrate the particular combustion characteristics of ammonia. As can be observed, methane and ammonia show generally the same shape of extinction limits as a function of equivalence ratio. The maximum values of the peak shapes occur at around 0.9 of equivalence ratio for both methane/air and ammonia/air flames. However, as shown in the figure, the maximum value of extinction limit for ammonia flame is only about 100 s⁻¹, which is much lower than that of methane. The simulation results by using Tian's mechanism have showed a good performance comparing with experimental data, indicating the same variation trend of extinction limits against equivalence ratio condition. However, relatively large deviations are observed at fuel lean conditions especially in the range of equivalence ratio smaller than 0.8. This can suggest that the mechanism still needs optimization for such conditions in future. Therefore, the simulation study in the present work will mainly focus on the range of equivalence ratio higher than 0.8, as generally satisfactory agreement with experimental data is shown using the mechanism.

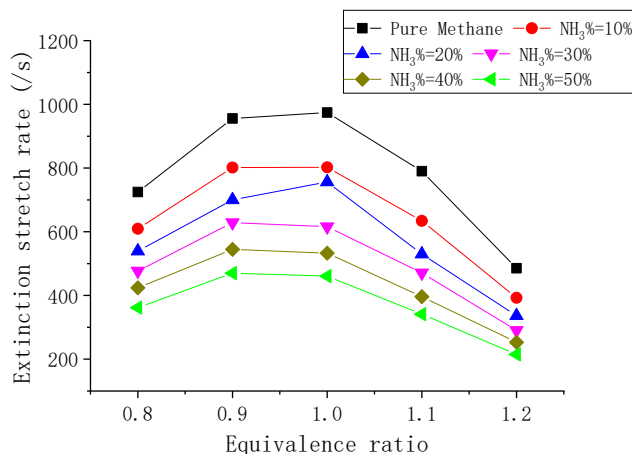


Fig 4: Extinction limits as function of equivalence ratio for counterflow premixed methane/ammonia/air flames.

Fig 4 depicts the extinction limit as function of equivalence ratio with different NH₃ concentrations in CH₄/NH₃ fuel mixtures. For all the CH₄/NH₃ fuel mixtures, extinction stretch rates firstly increase and then decrease within the equivalence ratio range investigated. What's more, the maximum extinction stretched rates all emerge between equivalence ratios of 0.9 and 1 for different fuel mixtures. As plotted in the figure, extinction limit always decreases with more ammonia substitution in fuel mixtures for a fixed equivalence ratio. Because ammonia has relatively lower reactivity than methane, the flame becomes weaker with more NH₃ substitution, leading to narrower stable combustion range. The impact of NH₃ substitution on combustion stability range tends to be more remarkable near the stoichiometric condition. As shown in the figure, fuel lean condition is more favorable for combustion stability. Under such fuel lean conditions combustion is also more completed, which will have advantages in emission reduction.

3.2 Flame Structure

To gain a deep understanding on the effect of NH₃ substitution on the CH₄/NH₃ counterflow flames, detailed flame structure is essential information for understanding the difference in extinction characteristics of CH₄/NH₃ combustion. Therefore, numerical simulation were performed with the detailed chemical mechanism of Tian to analyze the structures of CH₄/NH₃ counterflow premixed flames. As shown in Fig 5~12, profiles of temperature and some important species in premixed CH₄/NH₃ flames are plotted for different ammonia-substituted fuel blends at stoichiometric condition and standard temperature and pressure conditions.

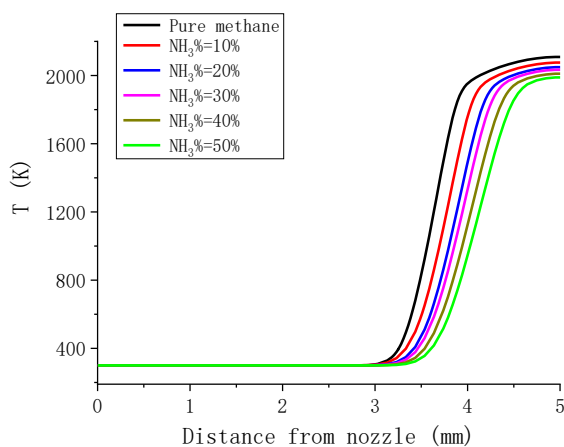


Fig 5: Temperature profiles for counterflow premixed CH₄/NH₃/air flames at stretch rate of 200 s⁻¹

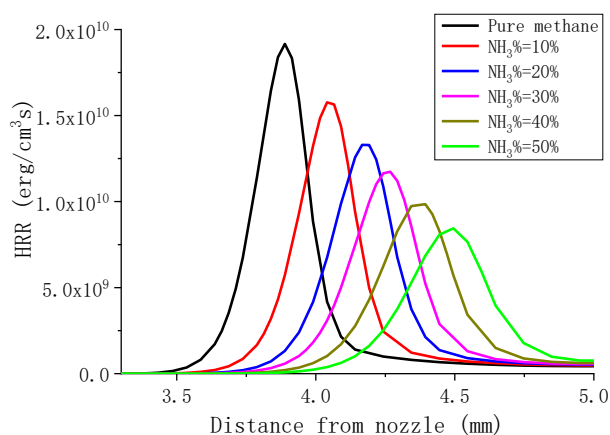


Fig 6: Heat release rate distribution for counterflow premixed CH₄/NH₃/air flames at stretch rate of 200 s⁻¹

Fig 5 shows the temperature profiles as a function of distance from nozzle in counterflow premixed CH₄/NH₃ flames. It can be observed that with more ammonia substitution in CH₄/NH₃ mixtures, temperature profiles become lower compared with that of pure methane flame. However, the temperature reduction extent is not remarkable with ammonia substitution up to 50%, as the maximum temperature drops from 2103K to 1988K. It indicates that using ammonia to substitute methane can lead to small amount of flame temperature change while large amount of carbon emission reduction. It also can be indicated that with ammonia concentration increasing in fuel mixtures, the flames move towards the stagnation plane with more smooth slopes of the temperature profiles. Such difference in temperature distribution is attributed to different behavior of heat release in the flames, as shown in Fig 6. It is illustrated that with more ammonia concentration in fuel blends, the maximum value of heat release rate decreases obviously corresponding to the decrease in temperature with ammonia substitution in Fig 5.

Positions of the maximum heat release move downstream with more ammonia substitution, which is due to lower flame speed of ammonia than methane.

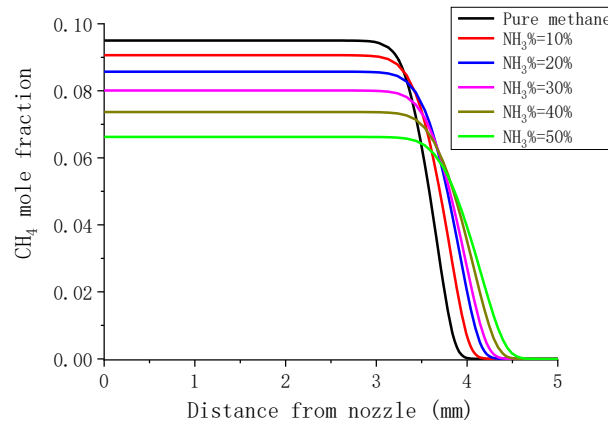


Fig 7: Mole fraction profiles of CH₄ at stretch rate of 200 s⁻¹

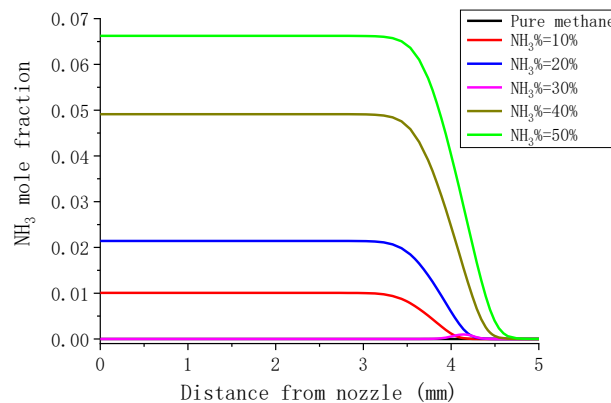


Fig. 8: Mole fraction profiles of NH₃ at stretch rate of 200 s⁻¹

Fig 7 and Fig 8 depict the profiles of CH₄ and NH₃ concentrations along the distance from nozzle in counterflow premixed CH₄/NH₃ flames. As plotted in Fig 8, for pure CH₄ flame, the fuel concentration starts to change at around 3 mm from outlet of the nozzle and it completely reacted at around 4 mm from the nozzle. The positions tend to shift downstream with the effect of ammonia substitution as can be observed, resulting from the lower flame speed of ammonia. What's more, within the ammonia mole fraction range in fuel mixtures (0 to 50%), change in consumption rate of CH₄ is not remarkable as can be observed.

Fig 8 illustrates the impact of ammonia substitution on the ammonia profiles in the CH₄/NH₃ flames. Compared with the CH₄ profiles in Fig 7, significant change in the behavior of NH₃ consumption can be

observed. With more substitution fraction of ammonia for methane, the consumption rate becomes higher for ammonia and the reaction zone of the species moves towards the stagnation plane of the counterflow flames. Such phenomenon is attributed to the higher reactivity of CH_4 , which will compete with NH_3 in oxidation reactions related to NH_3 consumption.

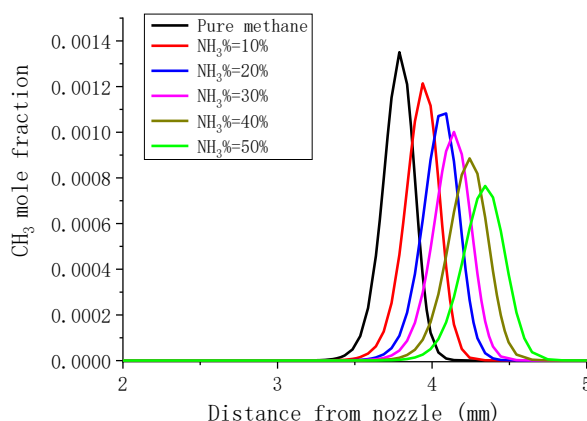


Fig 9: Mole fraction profiles of CH_3 at stretch rate of 200 s^{-1}

Fig 9 depicts the species profile of CH_3 in counterflow premixed $\text{CH}_4/\text{NH}_3/\text{air}$ flames at stoichiometric conditions. As more ammonia substitutes methane in the fuel mixture, value of CH_3 concentration peak decreases notably and the position moves downstream. Compared with Fig 7, CH_3 is generated in the areas corresponding to the reaction zones of methane consumption. Rate of production analysis of CH_4 shows that methyl radical is the product of the early steps of methane decomposition through the reactions of CH_4 with OH , H and O . H-abstraction reactions such as $\text{CH}_4 + \text{H} \rightleftharpoons \text{CH}_3 + \text{H}_2$, $\text{CH}_4 + \text{OH} \rightleftharpoons \text{CH}_3 + \text{H}_2\text{O}$ and $\text{CH}_4 + \text{O} \rightleftharpoons \text{CH}_3 + \text{OH}$ are identified as the key reactions in the first step NH_3 oxidation. Then CH_3 is converted to CH_2 mainly by reacting with OH , etc.

Fig 10 depicts the species profile of NH_2 in counterflow premixed $\text{CH}_4/\text{NH}_3/\text{air}$ flames at stoichiometric conditions. With increasing NH_3 substitution for CH_4 in the fuel mixture, NH_2 concentration increases remarkably and moves downstream. Compared with Fig 9, NH_2 is generated in the areas of ammonia consumption. Rate of production analysis of NH_2 shows NH_3 decomposition is mainly initiated through H-abstraction reactions such as $\text{NH}_3 + \text{OH} \rightleftharpoons \text{NH}_2 + \text{H}_2\text{O}$, $\text{NH}_3 + \text{O} \rightleftharpoons \text{NH}_2 + \text{OH}$, $\text{NH}_3 + \text{H} \rightleftharpoons \text{NH}_2 + \text{H}_2$. These key elementary reactions in the first step of NH_3 oxidation will compete with methane oxidation reactions, which explains the characteristics of methane and ammonia consumption profiles in Fig 7 and Fig 8.

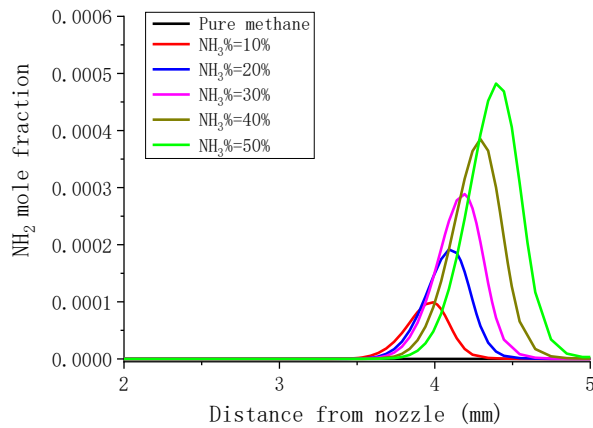


Fig 10: Mole fraction profiles of NH_2 at stretch rate of 200 s⁻¹

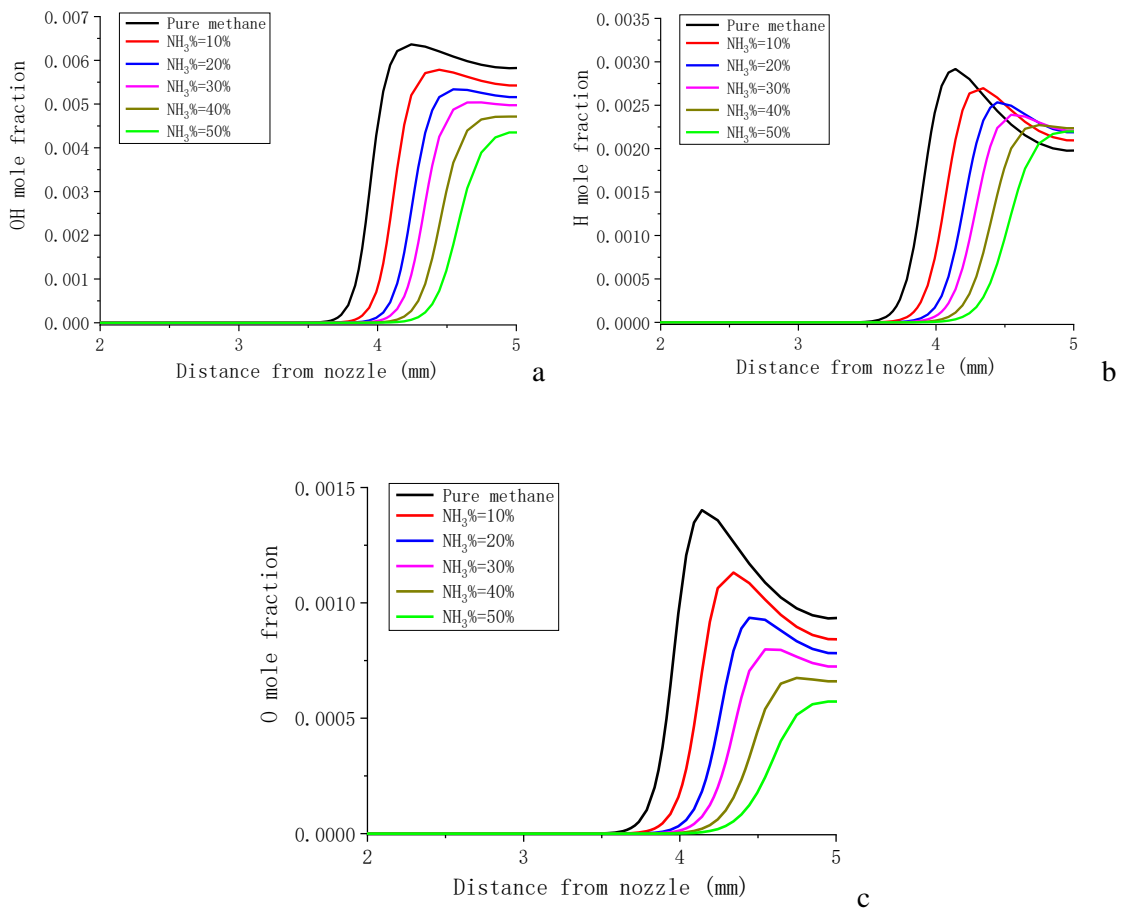


Fig 11: Mole fraction profiles of OH, H and O at stretch rate of 200 s⁻¹

The above flame structure analysis shows that the first H dissociation from the fuel is highly relevant to the intermediate species such as OH, H and O. Therefore, prediction results are presented in Fig 11 for

distribution of OH, H and O radicals in NH_3/CH_4 premixed flames. As ammonia concentration increases in the fuel mixture, obvious reduction in concentration can be observed for all the three light radicals as a result of the relatively low reactivity of ammonia compared with methane. As expected, the peak positions of the three radicals also shift to stagnation plane side with ammonia substitution. Compared with Fig 5 and Fig 6, the behavior of the radicals is consistent with the temperature and heat release decrease in the reaction zone of ammonia/methane flames. Such consistence is because the radicals play significant promoting roles in the heat release and these active radicals suggest combustion intensities reductions with ammonia substitution in fuel mixtures.

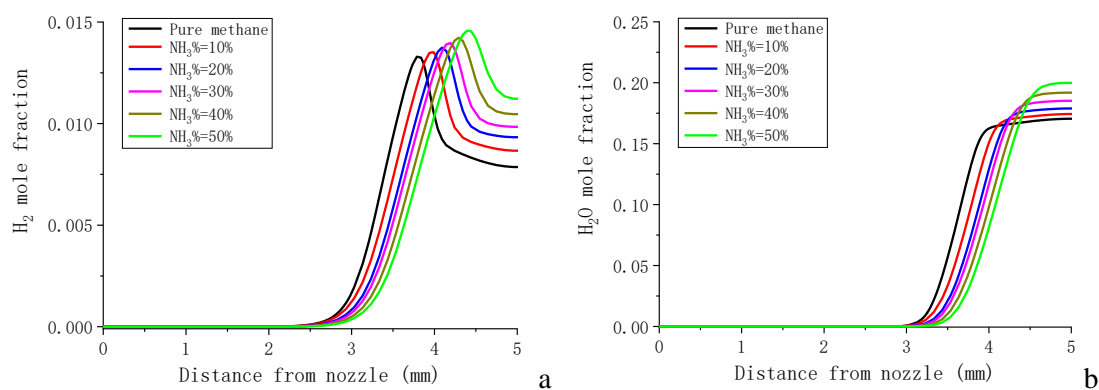


Fig 12: Mole fraction profiles of H₂ and H₂O at stretch rate of 200 s⁻¹

Fig 12 depicts the distribution of H₂ and H₂O in the $\text{CH}_4/\text{NH}_3/\text{air}$ flames. In Fig 12a, H₂ shows peak-shaped profiles in all the investigated ammonia-substituted flames. It is suggested that value of the H₂ profile peak increases with increasing ammonia concentration in fuel mixtures and the position moves downstream. As a typical of intermediate species, the increasing trend of H₂ concentration indicate the fuel mixture need to be combusted more completely with ammonia substitution. For H₂O, as a major product of premixed $\text{CH}_4/\text{NH}_3/\text{air}$ combustion, the mole fraction profiles tend to move downstream and the equilibrium value become higher with increasing ammonia substitution in fuel mixture. This phenomenon mainly results from the reduction of the CO₂ product for replacement of CH₄ with NH₃ in fuel mixtures.

3.3 Emission Analyses

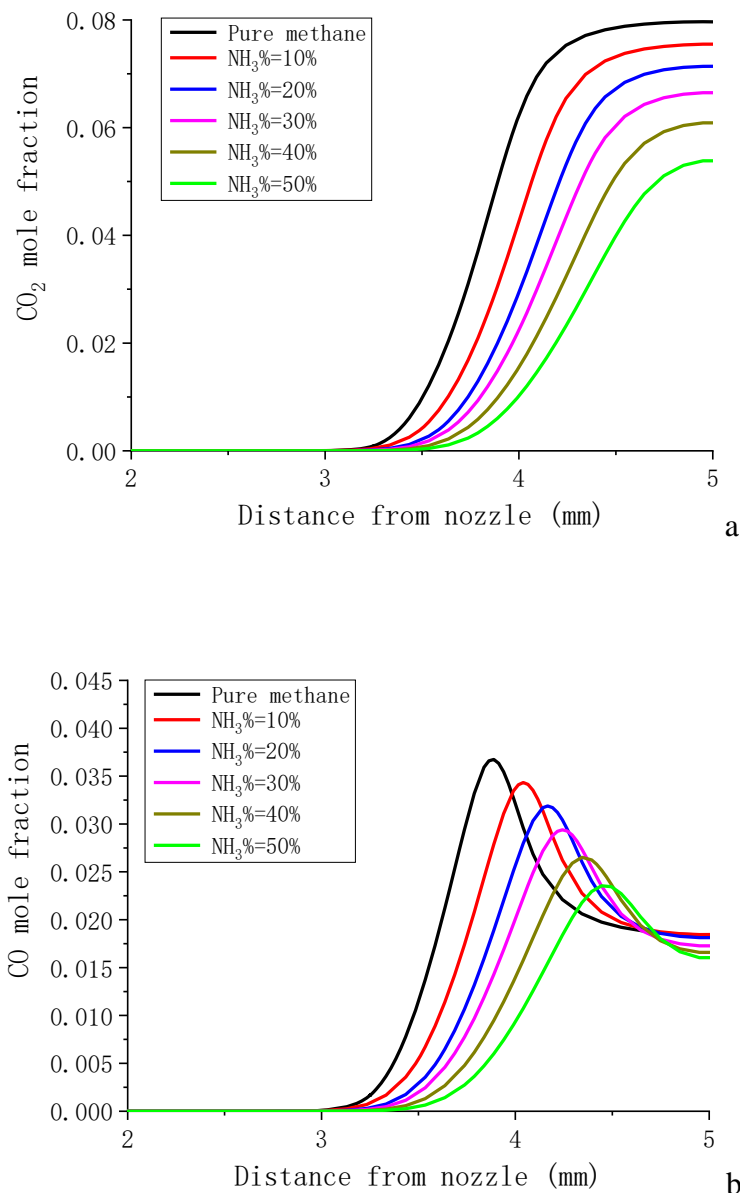


Fig 13: Mole fraction profiles of CO₂ and CO at stretch rate of 200 s⁻¹

Fig 13 shows the profiles of the major carbonaceous product CO₂ and CO against distance from nozzle for the CH₄/NH₃/air flames. In Fig 13a, as expected, significant reduction of CO₂ concentration can be observed with increasing ammonia substitution in fuel mixtures. A detailed look at the slope of CO₂ production profiles shows that the formation of CO₂ becomes slower with higher ammonia concentration. This is attributed to the relatively lower reactivity of ammonia leading to lower temperature with higher

ammonia concentration in fuel mixtures, suggesting slower combustion reaction of CH_4 . Fig 13b depicts peak-shaped profiles of CO for all the $\text{CH}_4/\text{NH}_3/\text{air}$ flames studied. Both the peak value and the equilibrium value of CO concentration show a decreasing trend as the fuel blends vary from methane to 50% ammonia in fuel mixture. The positions of the peaks move downstream with ammonia substitution. Such results indicate that substitution of ammonia for methane fuels can considerably decrease carbon emissions as more carbon atoms are replaced in fuel blend, suggesting higher ammonia substitution in fuel mixture is an efficient way for better carbon emission reduction effect.

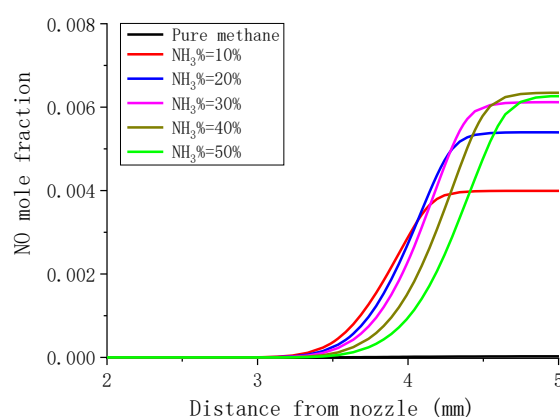


Fig 14: Mole fraction profiles of NO at stretch rate of 200 s-1

As the major nitrogenous pollutant in premixed $\text{CH}_4/\text{NH}_3/\text{air}$ flames, profiles of NO concentration are plotted in Fig 14. As can be observed, significant increase of NO emissions is produced with ammonia substitution in fuel blends. This is mainly because of the more nitrogen atoms added into fuel blend leading to more fuel-bond NO emission with increasing ammonia concentration in fuel mixture. Thus, as a N-containing fuel, ammonia will cause higher nitric oxide emission when used to substitute methane in real devices though it is also expected to considerably reduce CO_2 .

To gain a deep insight into NO_x formation mechanisms, it is helpful to perform sensitivity analyses for counterflow $\text{CH}_4/\text{NH}_3/\text{air}$ premixed flames. In Fig 15, sensitivity analysis of NO formation has been performed for pure methane, 10% $\text{NH}_3/90\%\text{CH}_4$ and 50% $\text{NH}_3/50\%\text{CH}_4$ fuel mixtures, which can help to identify important species and reactions having prominent impact on NO_x conversion. The sensitivity analysis results for NO formation show remarkable differences between different ammonia/methane fuel mixtures. It can be identified that $\text{H}+\text{O}_2\rightleftharpoons\text{O}+\text{OH}$ plays an important role in NO formation in all cases, i. It is the most-promoting reaction for ammonia-substituted methane cases and the third promoting reactions for pure methane. Elementary reactions $\text{NH}_2+\text{NO}\rightleftharpoons\text{N}_2+\text{H}_2\text{O}$, $\text{NH}_2+\text{NO}\rightleftharpoons\text{NNH}+\text{OH}$ and $\text{NH}+\text{NO}\rightleftharpoons\text{N}_2\text{O}+\text{H}$ play prominent roles as inhibiting reactions for ammonia-substituted methane fuel mixtures whilst $\text{CH}_3+\text{O}\rightleftharpoons\text{CH}_2\text{O}+\text{H}$ is the most-inhibiting reaction for pure methane and 10%ammonia-substituted cases. The results have shown that the predominant reactions in NO_x sub-chemistry haven't changed in the ammonia-substituted methane flames, while significant difference can be found comparing

ammonia-substituted flames with pure methane flame. Also, in the ammonia-substituted flames none of hydrocarbon/amine reactions plays a key role in NO formation as shown in the figure.

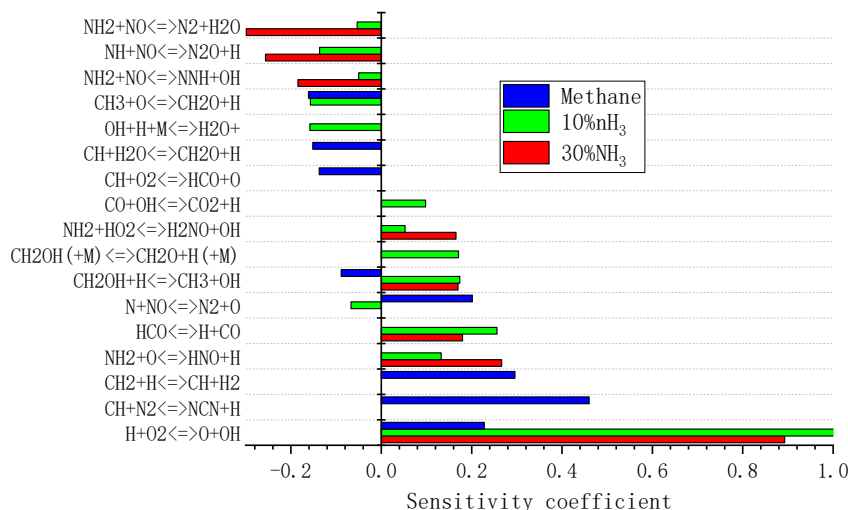


Fig 15: Normalized sensitivity analysis of NO on ammonia/methane/air flames

IV. CONCLUSION

In this study, impacts of ammonia substitution on methane/air counterflow premixed flames were investigated numerically within a wide range of flame stretch rates, fuel compositions and equivalence ratio conditions. The major conclusions can be summarized as follows.

With more ammonia substitution in methane/air flames, extinction limits tend to become lower at different equivalence ratio conditions. A bit fuel lean condition is more favorable for combustion stability.

Flame structures analyses showed that the temperature profile doesn't drop remarkably while concentration of important intermediate radicals decreases with more ammonia substitution in fuel mixtures.

Emission analysis showed that carbon dioxide emissions decrease significantly supporting methane/ammonia as a low-carbon fuel.

As an important issue in ammonia combustion, NO emission was found to increase with more ammonia in fuel mixture in the flames, indicating more studies are needed in future on NO_x emission reduction for such stretched flames.

ACKNOWLEDGEMENTS

This work was supported by the University Scientific Research Project of Guangzhou Education Bureau (grant number 202032786).

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