Study on Counterflow Premixed Flames using High Concentration Ammonia Mixed with Methane

Hua XIAO [1,2], Shini LAI [1], Agustin VALERA-MEDINA [3], Juying LI [1], Jinyuan LIU [2], Huide FU [1]*

1. College of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, 518060, China
2. Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, China
3. School of Engineering, Cardiff University, Queen's Building, Cardiff, CF24 3AA, United Kingdom

Abstract

In the present study, combustion characteristics of ammonia as an alternative fuel were evaluated computationally utilizing counterflow premixed ammonia/methane/air flames at normal temperature and pressure conditions. Investigations were carried out over a wide range of flame strain rates, fuel blend compositions and equivalence ratios. Extinction characteristic results showed that methane addition and equivalence ratio have significant impact on the extinction limits of the stretched flames. With more methane in the ammonia/methane fuel blends, the flames' sustainability to high stretch rate substantially increases. Flame structures of the stretched flames were then investigated to have a deep insight into the combustion process of the ammonia/methane premixed combustion. Results showed that temperature, heat release rate and important intermediate radicals of the flames are enhanced. However, emission analyses showed that carbon oxides and nitrogen oxide emissions all increased with methane addition. Pathway and sensitivity analyses revealed the chemistry of NOx emission characteristics of different ammonia/methane flames.

Keywords: Ammonia; Methane; Counterflow flame; Extinction limit

1   Introduction

Continued consumption of fossil fuel has been drawing great concern due to the global warming issues in recent decades. Under such background, worldwide agreements have been made to reduce the greenhouse gas emissions which require development of alternative routes to conventional fossil fuel energy. One possible alternative is to use ammonia for future energy systems, concept that has attracted considerable interest in recent years [1-4].

Ammonia is a carbon-free substance with a high hydrogen content. Just like hydrogen, ammonia is a clean energy source that produces only water and nitrogen when completely combusted. It can be used as refrigerant and neutralizer for combustion NOx emissions [5, 6]. Furthermore, as an important feedstock, ammonia is

also used for production of various nitrogen compounds such as fertilizers, nitric acid, etc. Therefore, as a versatile chemical, mature experience for ammonia has been gained in its production, handling and distribution [7]. In addition, ammonia can be produced not only from conventional fossil fuels such as coal and natural gas, but also from various renewable energy sources such as solar energy, biomass, etc. As a result, ammonia has shown good potential as a promising alternative fuel.

A number of studies have explored utilizing ammonia in combustion equipment such as internal combustion engines, gas turbines, boilers, etc [7-14]. For instance, Ryu et al. [8] developed direct injection strategies of gaseous ammonia in SI engine and proved feasible engine combustion and energy efficiency. Frigo and Gentili [9] used hydrogen as a combustion promoter to support combustion of ammonia in a SI engine. It was found that the minimum ratio hydrogen-to-ammonia is roughly 7% at full load based on the behaviour of a 4-stroke SI engine. Valera-Medina et al. performed a series of experimental and numerical studies investigating ammonia combustion characteristics in gas turbine combustors [10-12], while Kurata et al. [13] realized successful ammonia combustion gas-turbine power generation tests, which proved the potential of ammonia as gas turbine fuel. Numerous fundamental studies also have been performed in order to gain a deep insight into ammonia-based fuels combustion. Some researchers performed comprehensive experimental studies on combustion of ammonia-based fuel mixtures and proposed chemical reaction mechanism models based on careful species profiles measurements [15-18]. Some researchers studied basic laminar combustion properties for ammonia-based fuels such as flame speed, ignition delay, exhaust emissions, etc [19-22]. As for stretched flames, Lee and Kwon [23] numerically studied non-premixed ammonia/hydrogen/air flames at normal pressure condition. The effects of ammonia substitution were investigated on the extinction limits and structure of stretched flames. Colson et al. [24] studied the stretch effect of ammonia/air counterflow premixed flames. Extinction characteristics were investigated under different pressure conditions both experimentally and numerically. Choi et al. [25] experimentally studied the extinction limits, flame temperature and morphology of counterflow hydrogen-doped ammonia/air flames, demonstrating the potential of hydrogen-doped ammonia as a fuel. These fundamental studies explored basic combustion phenomena and helped to gain deep insight into the combustion process behind the use of the molecule.

Although previous work has provided essential information for the utilization and understanding of ammonia combustion, more investigations are still needed. For example, in order to use ammonia with methane for practical applications such as gas turbine or IC engine, more studies including stretched flames need to be performed. In previous studies, stretch effects on flame structure and extinction limits have been investigated using a counterflow configuration [23, 26]. Therefore, the objective of the present study is to investigate the combustion characteristics of counterflow premixed flames for ammonia/methane fuel blends. Numerical simulations of a counterflow burner were performed to establish premixed flames. A series of quantitative analyses were conducted on extinction limits, flame structures, reaction kinetics, etc.

2 Numerical Modelling

Numerical modeling for the counterflow flame was performed using the CHEMKIN-Pro software, which has demonstrated satisfying accuracy in previous studies of stretched flames [24]. In the model, a one-dimensional flow is assumed based on simplifications of a three-dimensional flow, having the fluid properties as functions of the axial distance only [27]. The geometry configuration of the counterflow flame is sketched in figure 1. As can be seen, two streams from opposing nozzles impinge each other generating flat flames between the nozzles. This is an attractive configuration for flame structure studies.

Using such well-defined model, a laminar, strained and axisymmetric counterflow premixed flame can be obtained by premixed blends of fuel and oxidizer in the upper and lower nozzle. The one-dimensional simulator can be used to predict the temperature, species and velocity profiles in the flame between the nozzles. The extinction limits were then calculated through an iterative series of counterflow flame simulations. While keeping the equivalence ratio constant, by iteratively increasing nozzle flow rate until extinction, flame temperature was obtained as a function of strain rate. More details about the model can be referred to [28]. The model was then used to study the combustion properties of premixed NH_3/CH_4/air mixtures considering detailed chemistry.
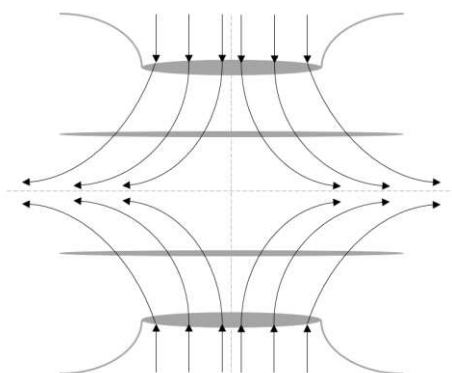

Figure 1. Schematic of counterflow burner

3 Results and Discussion

3.1 Model Verification

In order to validate feasibility of the combustion model, numerical simulation of premixed counterflow ammonia flames were firstly performed under different equivalence ratio conditions as investigated in the experimental study by Colson et al. [24]. In the experimental study, ammonia and air were premixed and then flowed through an opposed burner as described in the previous section. Outlet diameter of the burner is 10mm and distance between the outlets is 10 mm.

The Tian's mechanism [15] is a comprehensive chemical kinetic mechanism on the basis of well-designed experimental studies for premixed $NH_3/CH_4/O2/Ar$ flames. In

previous studies, the Tian's mechanism has already been tested in several ammonia flames [11, 19, 22] and has shown an outstanding performance among the widely-used kinetic mechanisms for ammonia-based fuels combustion. Specifically, the Tian's mechanism without species and elementary reactions associated with carbon atom was validated for counterflow flames of ammonia in Colson's work. Then the complete Tian's mechanism was employed in the present study for the analysis of ammonia-based fuels combustion.
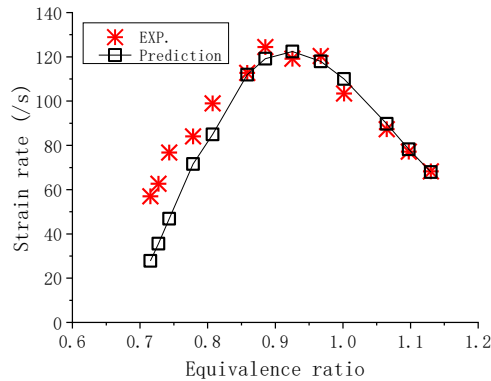

Figure 2. Calculation of strain rate at extinction of NH_3 flames. Experiments as in [24].

As shown in Fig. 2, numerical predictions of extinction limits are plotted as a function of equivalence ratio at normal temperature and pressure conditions (initial pressure of 0.1 MPa and initial temperature of 300 K), using the Tian's mechanism [15]. It can be seen that both numerical and experimental results show the same trend of extinction limits with variation of equivalence ratio conditions. The peak value of extinction strain rate is obtained at around equivalence ratio of 0.9 for such premixed ammonia/air flames. Therefore, the results can generally indicate a satisfactory agreement between experimental and numerical results within the range of experiments, though a bit higher prediction results can be observed under relatively lower equivalence ratio conditions. Thus, further studies will employ Tian's mechanism.

3.2 Extinction limits

As extinction strain rates for ammonia flames are relatively low, adding other fuels such as methane can have the potential to improve the combustible range of ammonia, which will help to enhance the performance of practical combustion devices when using ammonia. Therefore, to investigate the combustion stability limit characteristics for fuel mixtures of methane and ammonia, numerical simulations of counterflow premixed flames were performed in the present study.
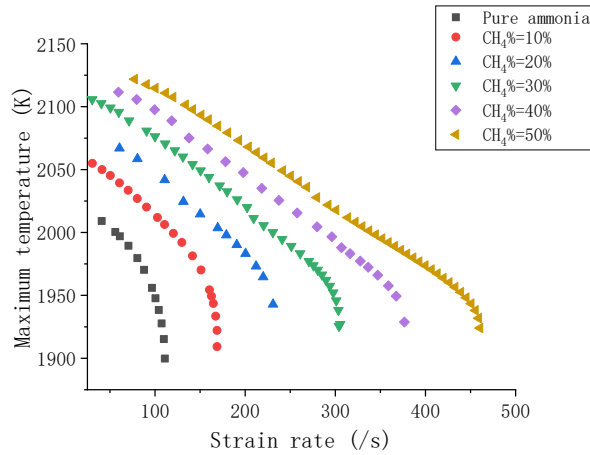
Figure 3. Maximum temperature as a function of strain rate for NH_3/CH_4 flames at STP (ambient pressure of 1atm, initial temperature of 300K) and equivalence ratio of 1.0.

Figure 3 shows the maximum temperature as a function of strain rate for different CH_4 concentration (0~50% in fuel blends) added NH_3/air premixed flames under atmospheric pressure and temperature and stoichiometric conditions. Decreasing trends can be observed for maximum temperatures with the increase of strain rate for all the different NH_3/CH_4 fuel blends. The reason is mainly attributed to shorter residence time for reactions under higher strain rate conditions, as corresponding to higher burner outlet velocities. Blow off limits are reached when the strain rates are high enough, indicating the effect of flame stretch leading to insufficient reaction time for reactants.

It also can be seen from Fig. 3 that from pure ammonia to 50% methane (mole fraction), all maximum temperatures increase with the increase of strain rate. However, as observed, the sensitivities to flame stretch are quite different between cases: the maximum temperature tends to decrease more sharply with increasing strain rate for higher ammonia content fuel blends. Another phenomenon that can be observed is that the maximum temperature and extinction stain rate are both enhanced with more methane addition in fuel mixtures. The reason is mainly due to the higher reactivity of methane, which plays a positive impact on the survival of such NH_3/CH_4/air flames.
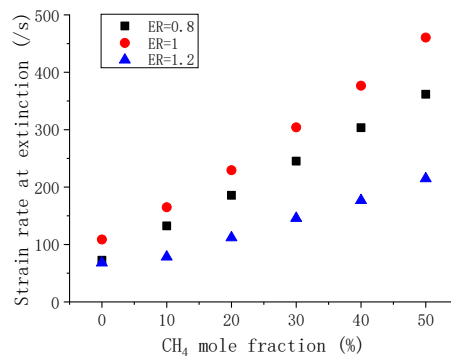

Figure 4. Strain rate at extinction as a function of CH_4 fraction in NH_3/CH_4 fuel blends.

To investigate the effect of fuel composition on extinction characteristics for ammonia-based stretched flames, numerical calculations were performed for counterflow premixed NH_3/CH_4 flames with different CH_4 mole fractions. In Fig. 4, strain rate at extinction is plotted as a function of CH_4 mole fraction in NH_3/CH_4 blends at three different equivalence ratios (ER =0.8, 1.0, 1.2). It can be seen that from pure ammonia to CH_4 mole fraction of 50% extinction strain rate increases almost linearly with the increase of CH_4 fraction in the fuel blends. The increase rate of the strain rate at extinction is relatively higher at stoichiometric conditions than under fuel lean or fuel rich conditions. Although pure ammonia can be used in such stretched flames, the extinction limits are much lower than CH_4 added into the fuel blend. For instance, the strain rate at extinction for pure ammonia fuel is only 60/s while it reaches near 1000/s for NH_3/CH_4 fuel blend with 50% CH_4 mole fraction. The reason for such increasing extinction limit is due to methane's higher reactivity compared with ammonia. Actually, a 10% of CH_4 in the fuel blend remarkably increases extinction strain rate, e.g. 60/s to 100/s at stoichiometric condition. This characteristic supports the feasibility of NH_3/CH_4 as a fuel to substitute conventional methane fuels, as significant CO_2 reduction can be expected while maintaining good flame stability properties.
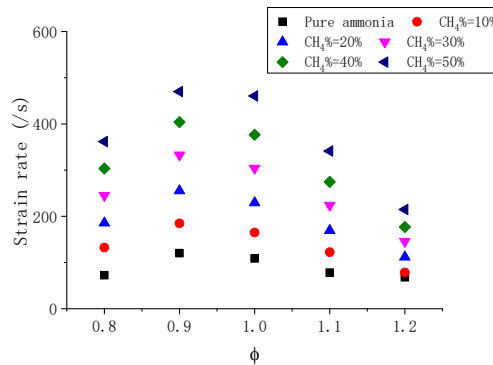

Figure 5. Stretch rate at extinction for various equivalence ratios of NH_3/CH_4 flames

Since equivalence ratio is an essential factor that defines various characteristics of premixed combustion, a numerical simulation was performed to study the effect of equivalence ratio on the counterflow premixed NH_3/CH_4 flames. Figure 5 illustrates the effect of equivalence ratio on extinction limits of the counterflow premixed NH_3/CH_4/air flames. With equivalence ratio ranging from 0.8 to 1.2 at different CH_4 mole fractions in NH_3/CH_4 fuel blends, the stain rates at extinction all increase first and then decrease under fuel rich regimes. The peak value is presented at the equivalence ratio around 0.9. For different equivalence ratios, all extinction strain rates increase with more CH_4 addition and around the peak point the increase is more remarkable. From the results, it is suggested that a bit fuel lean conditions can lead to extension of combustion stability range, which will also have advantage in emission reduction as more completed combustion is achieved under such conditions.

3.3 Flame structure

Flame structure analyses were performed to understand the effect of methane addition in ammonia combustion. As shown in Fig. 7~20, prediction results of different methane mole fractions in NH_3/CH_4 fuel mixtures are presented at an ER=1 and strain rates of 60 at STP. Profiles of selected species were derived from numerical simulations to capture more details in the reaction zone of the counterflow premixed NH_3/CH_4 flames.
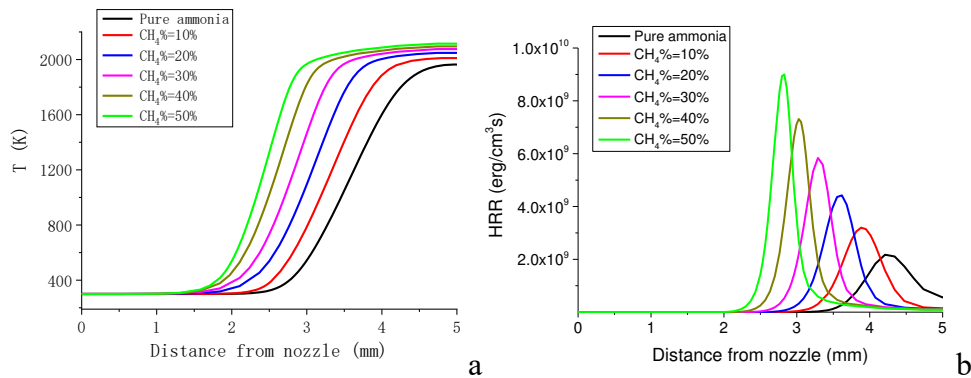

Figure 6. Temperature profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

Figure 6a shows the temperature distribution along the burner outlets. As can be observed, not only the maximum temperature but also the temperature along the reaction zone are higher with more CH_4 mole faction. The flames move toward the nozzle as temperature increases along the distance from nozzle, becoming sharper with more CH_4 mole faction. Such an obvious difference in flame temperature profiles is due to the stronger reactivity of CH_4 than NH_3. As can be illustrated in Fig. 6b, the origin of different temperature distribution can be attributed to the behavior of combustion heat release. With more CH_4 mole faction the maximum heat release rate increases leading to the sharper slope of temperature profiles for higher CH_4 concentration mixtures, Fig. 6a. The peak location for heat release rate profiles explains the flame behavior, denoting how the flame moves toward the nozzle with more CH_4, Fig. 6a.
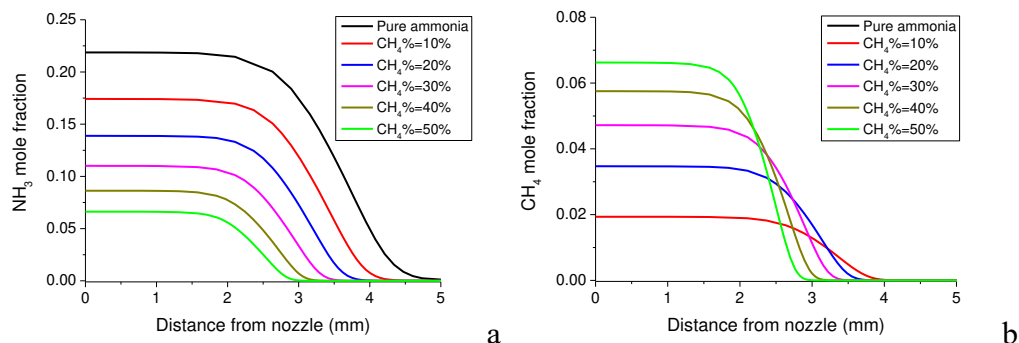

Figure 7. NH_3 and CH_4 profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

The fuel mole fraction profiles of NH_3 and CH_4 with various CH_4 fractions in fuel

mixtures are presented in Fig. 7. In Fig. 7a, NH_3 starts to be consumed at the position about 1.5 mm from the nozzle outlet and it is consumed completely at about 3 mm from the nozzle outlet for pure ammonia fuel. These positions move upstream with CH_4 mole fraction increasing in NH_3/CH_4 fuel blends.

Figure 7b shows the profiles of CH_4 mole fraction in the counterflow flames. Compared with ammonia profiles in Fig. 7a, CH_4 profiles are quite different with the CH_4 mole fraction variation in NH_3/CH_4 fuel mixtures. As CH_4 mole fraction increases from 0 to 50%, the consumption rate of CH_4 becomes much higher and the CH_4 profiles also tends to move upstream. This is mainly due to the reactivity of CH_4 which is higher than NH_3, thus leading to much higher burning velocities.
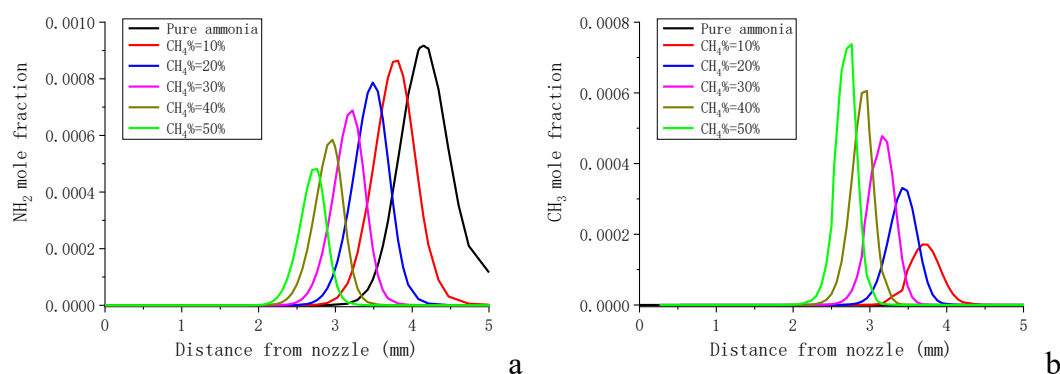

a   b

Figure 8. NH_2 and CH_3 profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

The radial NH_2 is essential in ammonia's oxidation. As shown in Fig. 8, NH_2 is produced in the same areas of reaction as those of ammonia consumption. Through rate of production analyses, key reactions related to NH_3 consumption can be identified, such as $NH_3 +OH<=>NH_2 + H_2O$, $NH_3+H<=>NH_2 + H_2$，$NH_3 + O<=>NH_2 + OH$. These H-abstraction reactions suggest NH_2 is a main product of ammonia's first step decomposition. Also, the production rate analyses show that $NH_3 +OH<=>NH_2 + H_2O$ plays a prominent role in the heat release corresponding to the characteristics of heat release rate and temperature profiles.

Similarly, CH_3 is an important intermediate in the oxidation of CH_4. As shown in Fig. 8b, increasing CH_4 produces higher concentration of CH_3. In counterflow flames, CH_4 is firstly decomposed through H-abstraction reactions such as $CH_4 +OH<=>CH_3+H_2O$ and $CH_4+ H<=>CH_3+H_2$. Then related reactions such as $CH_3+O<=>H+CH_2O$, $CH_3+H+M<=>CH_4+M$, $CH_3 +O\Rightarrow H+H_2+CO$ act as main contributors to heat release in methane oxidation chemistry. Compared with NH_3 relevant reactions, these CH_3 elementary reactions contribute more in the heat release of the NH_3/CH_4 counterflow flames, which helps to explain the difference between NH_3 and CH_4 mole fraction profiles in Fig. 7.
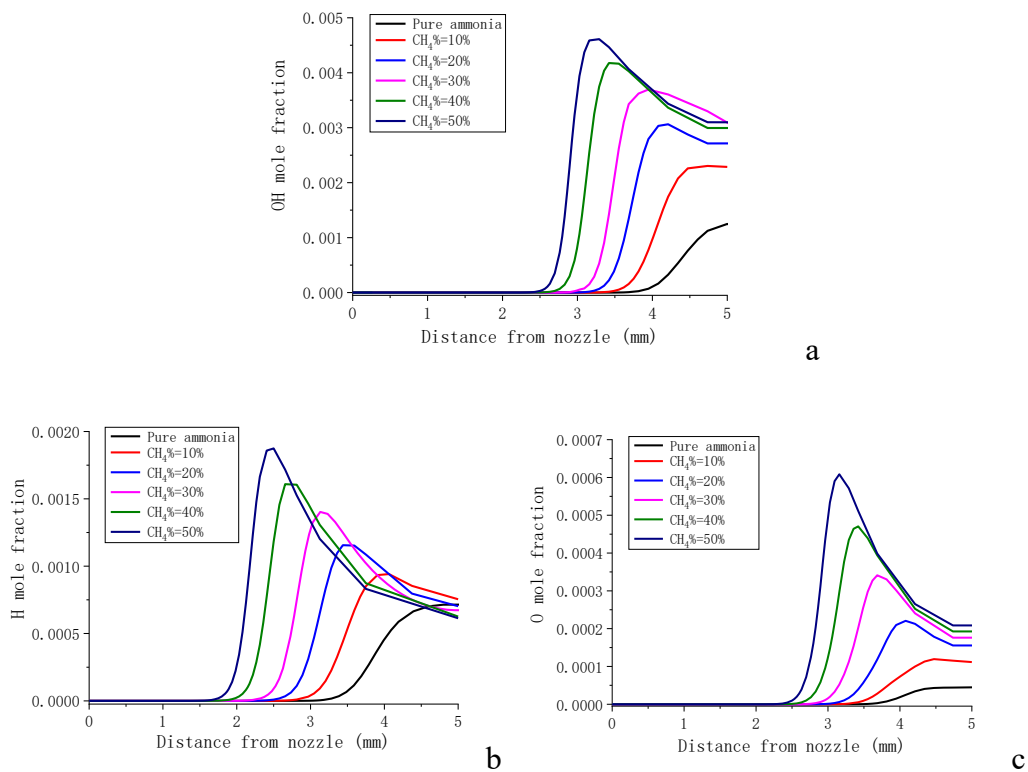
Figure 9. OH profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

The above analyses show that consumption of the fuel is mainly through H-abstraction reaction in which NH_3 and CH_4 are attacked by radicals such as OH, H, O, etc. Figure 9 shows the mole fraction profiles of OH, H and O in the counterflow premixed NH_3/CH_4 flames with different CH_4 mole fractions. With more CH_4 in the blends, an obvious increase can be observed in maximum mole fraction of all the three radicals and all their peak positions, which move upstream. These trends are consistent with the heat release rate profiles in Fig. 6, as these radicals act as significant promoters in the heat release process. The behavior of these highly active radicals indicate enhanced combustion intensities with the increase of CH_4 mole fraction.
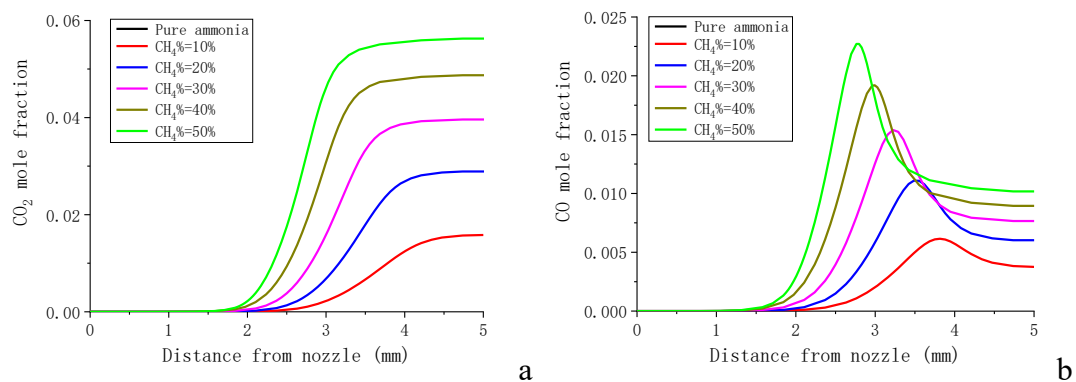
3.4 Emission analyses

Figure 10. Carbon emission profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

As the major carbonaceous products of the NH_3/CH_4 flames, CO_2 and CO species mole fraction profiles are illustrated in Fig. 10. In Fig. 10a, the maximum concentration of CO_2 increases obviously as CH_4 mole fraction in NH_3/CH_4 increases. Comparing the increase rates of CO_2 profiles, it can be found that the formation of CO_2 is much faster when CH_4 concentration is higher. This is consistent with the trend that higher temperature will be observed with more CH_4 mole fraction in the fuel mixture, indicating faster reaction rates of CH_4.

CO mole fraction shows peak-shaped profiles for the NH_3/CH_4, Fig. 12b. Both the maximum mole fraction and the maximum concentration show an increasing trend as the fuel mixture varies from pure ammonia to 50% CH_4. The results show that adding methane into ammonia fuels can significantly increase carbon oxides emissions as more carbon atoms are introduced into fuel mixture, indicating that relatively lower CH_4 mole fraction in the fuel mixture is preferred for better carbon emission reduction effects.
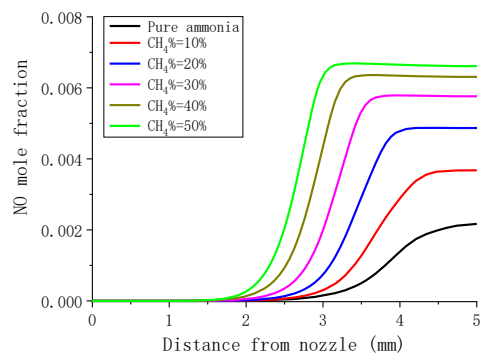

Figure 11. NO profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

As the main species of NOx emissions, the mole fraction profiles of NO are plotted at various CH_4 mole fractions, Fig. 11. The same as CO_2, with increasing mole fraction of CH_4 in NH_3/CH_4 fuel mixture, the NO concentration becomes higher. With increasing CH_4 in NH_3/CH_4 fuel mixture, it can be observed that the profile shifts upstream and the formation of NOx also becomes faster. It is interesting to notice that the formation of NO in the flames tend to be promoted with more CH_4 added.

As NOx emissions are an essential issue in combustion of ammonia-based fuels, pathway analyses were conducted to gain a deep insight of the NOx chemistry. Figure 12 shows the path of NOx formation in the flame of 60%NH_3/40%CH_4 at stoichiometric condition and strain rate of 60/s. It can be seen that the main precursors of NO are HNO, NH_2 and CH_3. Besides, H_2CN and N_2H_3 produced from CH_3 also have prominent effects on NO formation. As CH_3 is the product of initial steps of CH_4 oxidation, these results explain how the NOx increasing behavior of the counterflow premixed NH_3/CH_4 flames occur, Fig. 11.
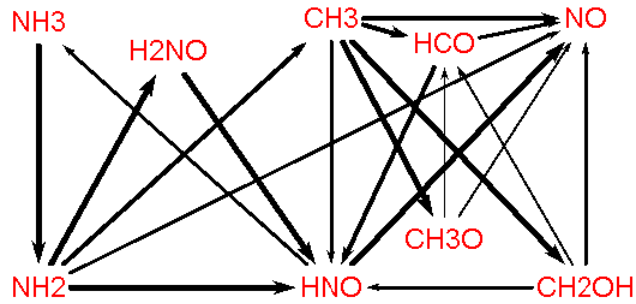
Figure 12. NO formation pathway in counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)
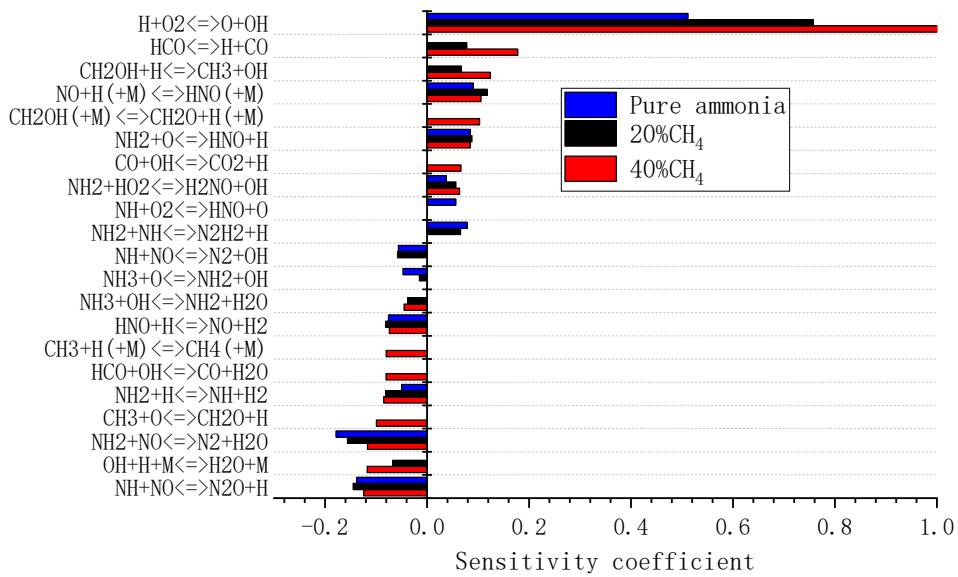

Figure 13. NO profiles for counterflow premixed NH_3/CH_4 flames (strain rate of 60 /s and ER =1 at STP)

Sensitivity analyses have also been performed to identify important reactions which have prominent impact on NOx conversion. As shown in Fig. 13, sensitivity analysis results are presented for pure ammonia, $80\%NH_3/20\%CH_4$ and $60\%NH_3/40\%CH_4$ fuel blends at stoichiometric condition and strain rate of 60/s. From the sensitivity analysis results, noticeable differences can be seen between flames of different fuel compositions. In all these cases, $H + O_2 <=> O + OH$ and $NH_2 + O <=> HNO + H$ are the two most-promoting reactions while $NH_2 + NO = N_2 + H_2O$ and $NH + NO <=> N_2O + H$ are the most-inhibiting reactions. Although the predominant role of these reactions in the NOx chemistry does not change for the different flames investigated, different sensitivity coefficients can be still observed. For the most sensitive reactions an increase of CH_4 mole fraction in the NH_3/CH_4 fuel mixture, higher sensitivity coefficients are exhibited, indicating higher promoting or inhibiting effect of these reactions. It also can be seen that NO species doesn't show high sensitivity to hydrocarbon/amine reactions as none of them are shown in the figure.

4 Conclusions

In the present study, characteristics of stretched premixed flames for methane/ammonia fuels were investigated under atmospheric pressure and temperature conditions. Over a wide range of flame strain rates, fuel blend compositions and equivalence ratios, counterflow premixed ammonia/methane/air flames were simulated using the Tian mechanism.

The extinguish strain rate tends to be much higher with more methane added into the fuel blends, implying that methane addition will help sustain higher flame stretch effects and therefore promote the combustion stability of ammonia fuel. Flame structure analyses showed that the temperature, heat release rate and important intermediate radicals' concentration of these flames are enhanced. Emission analyses indicated that within the studied conditions CO_2, CO and NO emissions in the flame have all increased with methane addition in ammonia for the counterflow flame configuration, suggesting more investigations are needed to reduce NOx emission for stretched flames. Further pathways and sensitivity analyses revealed the difference in reaction mechanism for NOx emission characteristics in such ammonia/methane flames.

Acknowledgement

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