Experimental and modeling study on ignition delay of ammonia/methane fuel

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Abstract

Ammonia mixed with methane is a potential clean fuel for engine applications toward a low carbon economy. Studies are scarce on ignition phenomenon for ammonia/methane fuels in literature. In the present study, the ignition characteristics for ammonia–methane–air mixtures have been investigated by both experimental measurements and numerical simulations. Ignition processes of a 60%ammonia/40%methane (mol%) fuel blend were investigated with shocktube experiments. Measurements of the ignition delay times were performed behind reflected shock waves for such fuel/air mixtures with different equivalence ratios of 0.5, 1, and 2, at pressures around 2 and 5 atm within the temperature range of 1369 to 1804 K. Experimental results were then compared with numerical prediction results employing detailed kinetic mechanism, which showed satisfactory agreement within most of the range of the temperatures, equivalence ratios, and pressures investigated. Within the temperature range of 1300 to 1900 K, pressure range of 1 to 10 atm, equivalence ratio range of 0.5 to 2, and methane proportion range of 0% to 50% in fuel blends, the impacts of temperature, pressure, equivalence ratio, and methane additive were simulated on the ignition delay times of the fuel blends based upon the numerical model. It was found that the improvement of ammonia/methane ignition is significant with the increase of temperature, pressure, and methane additive while it is relatively not sensitive to equivalence ratio within the studied conditions. This suggests a promising potential of such fuel blends in real engine application. In addition to the calculations, reaction sensitivity analyses were also performed to have a deep insight into the observed differences between ammonia/methane/air ignition delay times with variation of conditions.

1. Introduction

In recent decades, the high consumption rate of conventional fossil fuels has been causing crises such as high fuel price, depletion of non-renewable fuels, sever environmental pollution, global warming, etc. Under this situation, great concern has been drawn all over the world to move

to environmentally friendly renewable fuels [1-3]. Among the possible alternative fuels for future energy systems, ammonia has attracted considerable interest in recent years [4-6]. As a carbon-free substance, ammonia has a high hydrogen content of 17.8% by weight. But unlike hydrogen, which has complicated safety problems in its practical application, ammonia has an excellent record in previous industrial utilization processes [7]. Actually, ammonia is an important feedstock for production of various nitrogen compounds such as fertilizers, nitric acid, etc. It also has been used as refrigerant and neutralizer for combustion NOx emissions. Therefore, as one of the most-produced chemicals in the world, well-established networks for ammonia transportation and mature experience have been developed in its production, storage, handling and distribution. Although ammonia is mainly produced from fossil fuels such as coal and natural gas, various renewable energy sources can also be utilized for its manufacturing, such as wind energy, solar energy, biomass, etc [8]. Thus, ammonia has been considered to have good potential as alternative fuel in the near future.

In terms of utilizing ammonia in combustion equipment, pertinent studies have tested and applied ammonia in internal combustion engines [9-11], gas turbines [12-15], etc. Generally, ammonia combustion has proved to have satisfactory feasibility for potential applications. Meanwhile, in order to support the application of ammonia combustion, lots of fundamental kinetics studies also have been performed using ammonia-based fuels. For instance, Tian et al. [16] performed a comprehensive experimental and modelling study on premixed combustion of ammonia/methane/oxygen/argon mixtures. Based on the careful species profiles measurement in a McKenna burner, a comprehensive chemical mechanism was proposed for the combustion of different ammonia/methane ratio fuel mixtures. Mendiara et al. [17] studied the oxidation of ammonia in oxy-fuel combustion of methane using a flow reactor and proposed a detailed chemical kinetic mechanism based on the experimental data. Zieba et al. [18] investigated flameless jet combustion of ammonia doped with methane and found that NO_x emissions can be reduced by decreasing the methane in the fuel mixture. These and other fundamental studies explored basic combustion phenomena and helped to gain deep insight into the combustion process of ammonia-based fuels.

Although previous work has made a good progress in the utilization and understanding of ammonia combustion, there are still lots of issues needed to be better settled. For instance, since ammonia has a relatively low burning intensity and higher resistance to autoignition, it is usually mixed with other more reactive fuels such as hydrogen, methane and diesel to enhance combustion [19-22]. However, when the combustion promoters are added into ammonia, the properties and kinetics of a certain mixture can be quite different. As methane is a popular clean fuel widely used in engine and power industries [23, 24], some researchers have explored to use methane to enhance ammonia combustion. For instance, Valera-Medina et al. [13] experimentally studied ammonia–methane blends combustion in a generic tangential swirl burner for gas turbine use and determined the flame stability and emissions produced at different equivalence ratio and pressure conditions. Xiao et al. [20] numerically studied the characteristics of ammonia/methane premixed combustion. Kurata et al. [15] performed NH_3/CH_4/air combustion operation tests in a micro gas turbine. Okafor. et al [21] investigated the laminar burning velocity of premixed methane/ammonia/air mixtures experimentally and numerically in a wide range of conditions. Nonetheless, further studies are still needed to determine fundamental combustion properties such as ignition delay [20, 25]. From the knowledge about previous research, ignition characteristics studies on ammonia-based fuels are

quite limited [26-28], especially seldom experimental studies can be found on ammonia-methane ignition delay characteristics.

Therefore, the objective of the present study was to investigate the ignition characteristics of ammonia/methane/air mixtures. Ignition delay times were measured behind the shock tube wave with different equivalence ratios under different pressure and temperature conditions. Numerical simulations were also performed to predict the ignition delay times under a wide range of conditions informing on the reaction kinetics of the process. The results support a better understanding of the combustion characteristics of ammonia/methane fuels and promote the development of such alternative fuels in more practical use.

2. Experimental setup

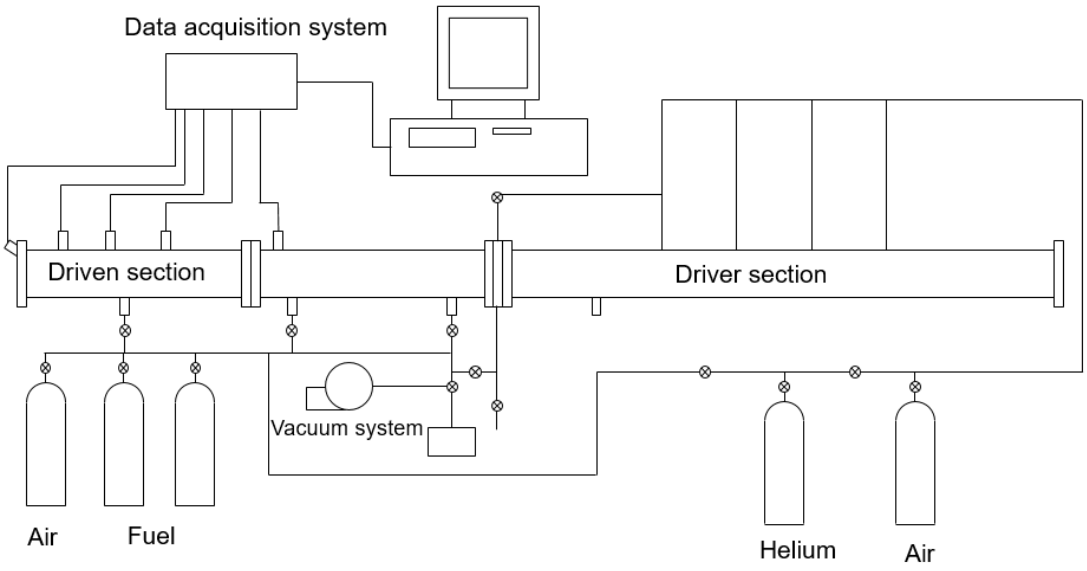

Fig. 1 Experimental setup

Experimental measurements of the ignition delay times were performed in a single-diaphragm, stainless steel shock tube. A schematic of the shock-tube device is shown in fig.1. The shock tube is divided into a driver section and a driven section with 4 m and 5.5 m in length respectively. The inner diameter of the shock tube is 100 mm and the wall thickness of the shock tube body is 17.5mm. Three PCB113B24 pressure transducers were equally installed along the driven section sidewall with a distance of 200 mm between each sensor. According to the shock wave pressure signal measurements by the sensors, incident-wave velocities can be determined at the end-wall location. Then post reflected-shock conditions were calculated using the wave speed in conjunction with shock wave relations. The pressure time history after the reflected shock wave was measured by a PCB3 located at 20 mm away from the reflection end surface. A Hamamatsu CR131 photoelectric multiplier, located in the same plane as PCB3 at the sidewall was used to record the change of OH radical self-luminous signal at the measuring point.

Ammonia-methane/air mixtures tested in the present study are presented in table 1. The mole ratio of ammonia to methane is 60%/40%, which is a feasible ammonia-based fuel blend for stable combustion as investigated in Valera-Medina et al. [13]. Three equivalence ratios, 0.5, 1, 2 werew selected to represent fuel lean to fuel rich conditions. Pressure conditions around 2 atm and 5 atm were investigated in the experiment. The ignition delay time is defined as the time interval between

the arrival of the reflected shock wave at PCB3 position and the time when the ignition occurs, which is defined as the intersection of lines drawn along the maximum rate of change of OH self-luminous intensity signal curve and the horizontal baseline. Fig. 2 shows a typical pressure curve and the moment of auto-ignition [29], which illustrate the definition of ignition delay period.

Table 1 Test gas composition investigated in the shock tube, in % volume

Mixture	NH_3 (%)	CH_4 (%)	Air (%)	ER
1	4.65	3.10	92.25	0.5
2	8.63	5.75	85.62	1
3	15.09	10.06	74.85	2

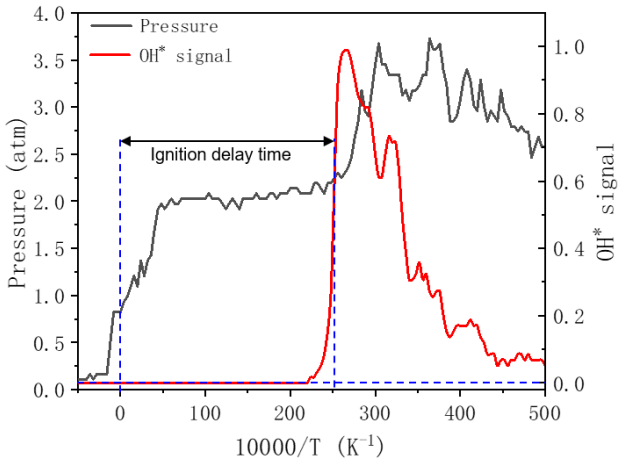

Fig. 2 Determination of the ignition delay time for ammonia-methane/air mixture

3. Numerical model

Numerical simulations of ignition delay times provide gain a deeper insight into autoignition parameters, detailed kinetics, etc. In the present study, a zero-dimensional model of a closed homogeneous reactor in CHEMKIN-PRO [30] was employed to predict the auto-ignition phenomena of ammonia-methane/air mixtures in the shock tube experiments [31]. Moreover, the ignition delay times of ammonia/methane fuel blends were also calculated under a wider range of pressures, temperatures, and equivalence ratios to investigate combustion characteristics of such mixtures.

As chemical kinetics play an important role in the ignition process, detailed chemical-kinetics reaction mechanisms can explain more details of auto-ignition phenomena [32, 33]. In previous studies, there are already a number of reaction mechanisms developed for ammonia combustion, however mechanisms specifically for ammonia/methane fuels combustion are still limited. In the present simulation study, the reaction mechanism by Tian et al. was used for auto-ignition modeling of ammonia-methane/air mixtures. The Tian mechanism contains 701 reactions among 84 species, which was developed for ammonia/methane premixed combustion under low pressure conditions. It has been widely tested in ammonia combustion studies [34, 35], showing good accuracy in simulations especially modelling ignition delay times [36]. Therefore, in the present study, the Tian mechanism was employed to perform numerical investigation on auto-ignition of ammonia/methane

fuels over a wide range of conditions. Pressures were set at 1, 2, 5 and 10 atmospheres using inlet conditions similar to those of the experimental campaigns.

As methane concentration in the NH_3/CH_4 fuel blends can have an important impact on the auto-ignition characteristics of such fuels, numerical simulations of the ignition delay times were also performed for different mole fractions of methane in the NH_3/CH_4 fuel blends. Further analyses were conducted using different ammonia-methane blends by increasing the concentration of methane up to 50% (mol). Temperature impacts were also analyzed in a range between 1300 and 1900 K.

4. Results and discussion

4.1 Effect of Pressure

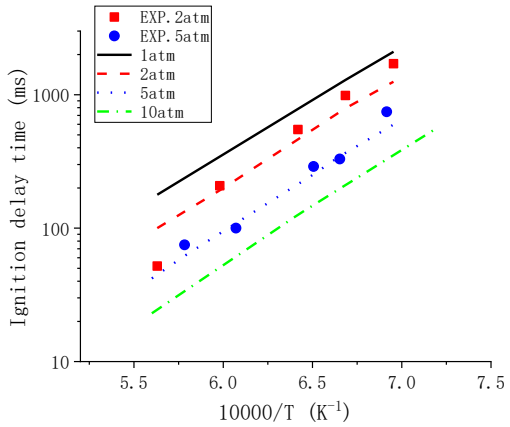

Fig. 3 Effect of pressure on the ignition delay time of the NH_3/CH_4/air mixtures at ER= 0.5

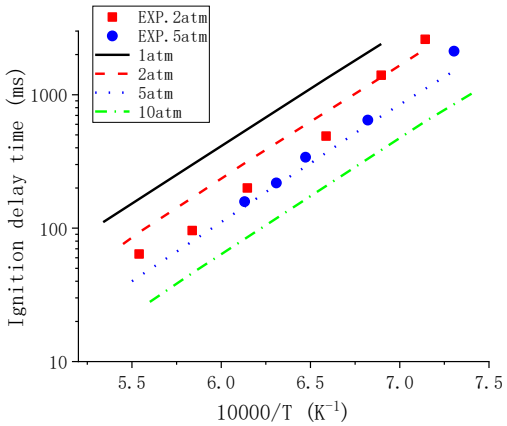

Fig. 4 Effect of pressure on the ignition delay time of the NH_3/CH_4/air mixture at ER= 1

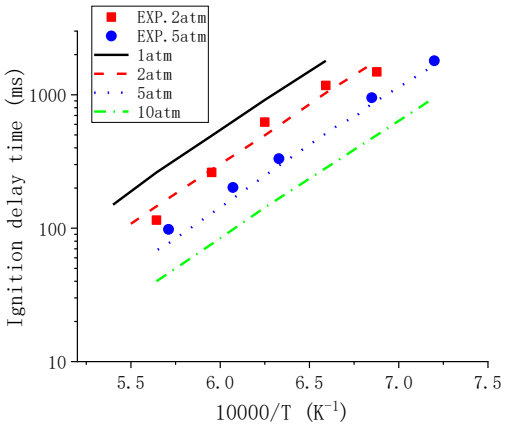

Fig. 5 Effect of pressure on the ignition delay time of the NH_3/CH_4/air mixture at ER= 2

Experimental results of the ignition delay times for 60%NH_3/40%CH_4 fuel blend are obtained under the initial pressure conditions of 2 atm and 5atm, initial temperature between 1300K- 1900K and equivalence ratios of 0.5-2 as shown in Fig. 3~5. For such fuel blend, an obvious promoting effect of pressure on auto-ignition can be observed under all the temperature and equivalence ratio conditions investigated. To validate the auto-ignition model, numerical simulations were performed with the Tian mechanism at the same conditions as those of experimental works. General good agreement can be observed between experimental data and simulation results though relatively bigger deviation can be found at pressure of 2atm under stoichiometric conditions in fig. 4. Through numerical simulation, tendencies of the ignition delay times with initial temperature and pressure are well captured, which indicates the numerical model with the selected detailed reaction mechanism is suitable for the ignition delay time calculation of NH_3/CH_4 fuel blends.

By using the established numerical model, the ignition delay times of different pressure conditions were predicted to further investigate the effect of pressure on auto-ignition process. As shown in fig. 3~5, simulation results of 60%NH_3/40%CH_4 in mole fraction at 1-10atm were obtained under different equivalence ratio conditions. In the figures, significant decrease in the ignition delay time can be observed with the increase of pressure for such fuel blend. From fuel lean to fuel rich conditions, the difference of equivalence ratio doesn't tend to change the dependencies of pressure and temperature for the ignition delay time. While it can be observed that the decrease rate of ignition delay time is close at both lower pressure conditions and elevated pressure conditions. For instance, the factor between the ignition delay times obtained at 1atm and 2atm is about 1.75 at 1550 K and ER=0.5, and a similar factor of 1.71 is found from 5atm to 10atm. This suggests that the auto-ignition processes are sensitive to pressure under both normal and elevated pressure conditions for such ammonia-based fuels.

4.2 Effect of equivalence ratio

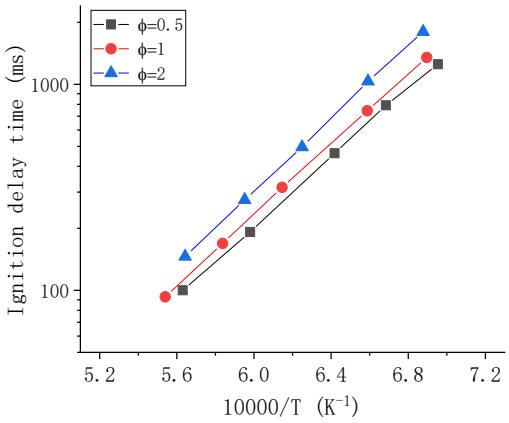

Fig. 6 Effect of equivalence ratio on the ignition delay time of the NH_3/CH_4/air mixtures at pressure of 2 atm.

In order to better understand the effect of equivalence ratio on the NH_3/CH_4 fuel blend, simulation studies were performed for a number of equivalence ratio conditions, Figs. 6 and 7. Although small differences of the ignition delay time can be observed, the variability is quite small compared to the factors of pressure and temperature. Moreover, at both pressure conditions, effect of equivalence ratio on the ignition delay time tends to be more moderate at fuel rich conditions than fuel lean conditions. Such tendencies indicate that in the practical gas turbine engine applications, the difference in ignition process caused by equivalence ratio is relatively less complicated to handle and a promising trend for the use of rich ammonia blends.

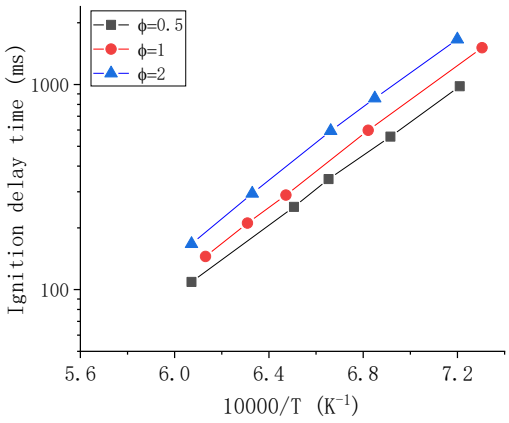

Fig. 7 Effect of equivalence ratio on the ignition delay time of the NH_3/CH_4/air mixture at pressure of 5 atm.

4.3 Effect of ammonia/methane fuel blends composition

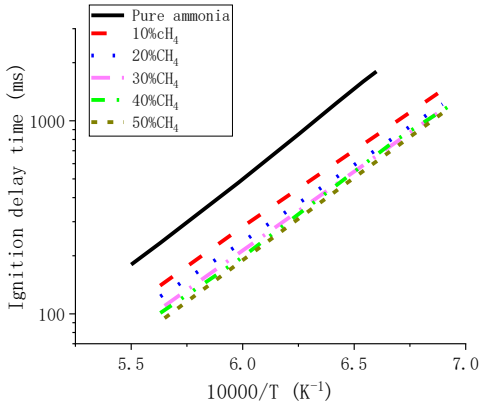

Fig. 8 Effect of CH_4 concentration on the ignition delay time of NH_3/CH_4 fuel blends at ER=0.5 and 2 atm.

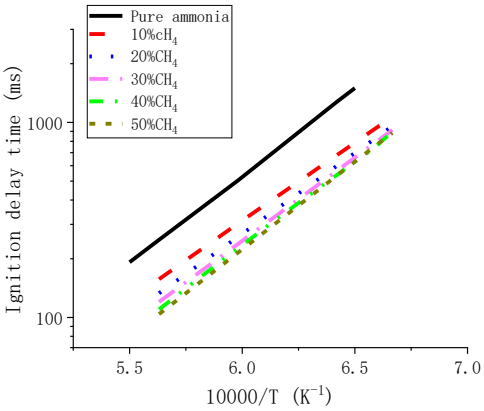

Fig. 9 Effect of CH_4 concentration on the ignition delay time of NH_3/CH_4 fuel blends at ER=1 and 2 atm.

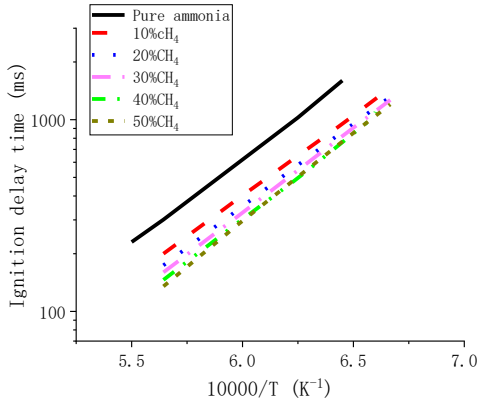

Fig. 10 Effect of CH_4 concentration on the ignition delay time of NH_3/CH_4 fuel blends at ER=2 and 2 atm.

Figures 8-10 illustrate the effect of different NH_3/CH_4 fuel blend compositions on the ignition delay time of NH_3/CH_4/air mixtures. Within the equivalence ratio of the studied conditions, for all the different NH_3/CH_4 fuel blends the ignition delay times have shown the same tendencies of evolution with temperature. Considerable reduction in ignition delay time can be observed when

methane is added into ammonia indicating a promoting effect of methane on ammonia ignition. However, it is worth noting that obvious difference of the ignition delay time reduction can be observed between different methane concentrations in the fuel blends.

To better illustrate this phenomenon, the ignition delay times are also plotted as a function of CH_4 mole fraction in CH_4/NH_3 fuel blends as shown in fig. 11. At both pressures of 2 atm and 5 atm, the ignition delay times drop sharply from pure ammonia to 10%CH_4 in NH_3/CH_4 fuel blend whilst from 10% to 50% of CH_4 reduction of the ignition delay times is relatively much slighter with methane addition. This suggests that the ignition delay time is more sensitive to CH_4 addition when at low CH_4 concentration conditions.

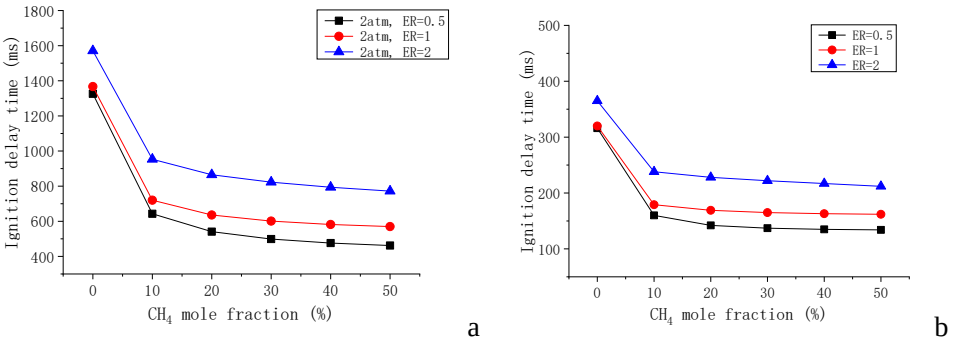

Fig. 11 Ignition delay time as a function of CH_4 mole fraction in NH_3/CH_4 fuel blends at T=1550K (a) 2atm (b) 10atm

4.4 Sensitivity analysis of the kinetic mechanism

To further elucidate the differences in ignition delay times obtained from simulation results for NH_3/CH_4/air mixtures under different conditions, sensitivity analyses were performed on OH radical at various equivalence ratios, pressures and methane mole fractions in the fuel blends. In previous studies, OH has been identified as the crucial radical of which sensitivity analysis can provide quite similar result to that of ignition delay time. Hence, as shown in fig. 12~17, under selected conditions essential reactions have been identified for NH_3/CH_4 auto-ignition from the simulation results of OH sensitivity analysis.

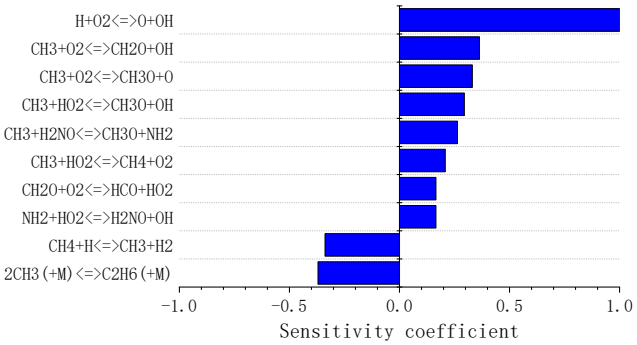

Fig. 12 Normalized sensitivity analysis on OH for 60%NH_3/40%CH_4 fuel blend at ER=0.5, p=2atm, T=1550K.

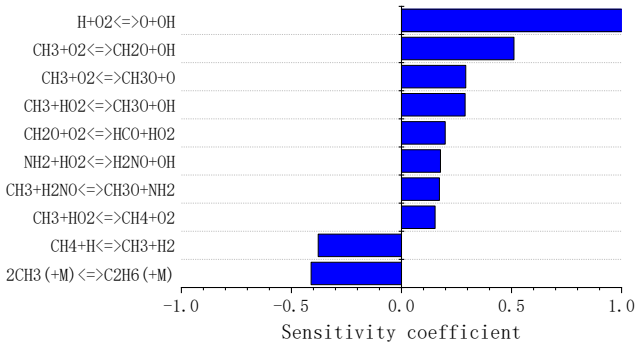

Fig. 13 Normalized sensitivity analysis on OH for 60%NH_3/40%CH_4 fuel blend at ER=1, p=2atm, T=1550K.

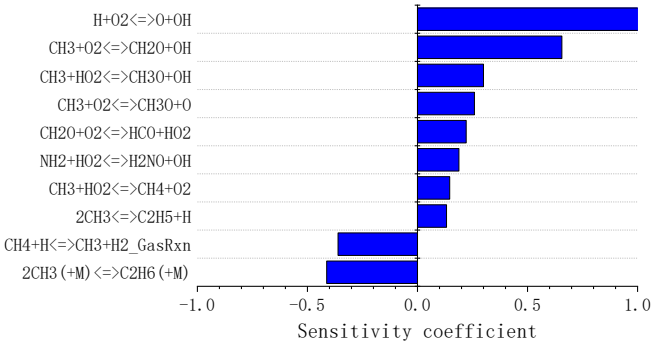

Fig. 14 Normalized sensitivity analysis on OH for 60%NH_3/40%CH_4 fuel blend at ER=2, p=2atm, T=1550K.

Figures 12-14 show the sensitivity analysis results under different equivalence ratio conditions for 60%NH_3/40%CH_4 fuel blend at 2atm and 1550K. In all the three figures, the most important elementary reactions are the same. Moreover, under all the equivalence ratio conditions H+O2<=>O+OH and CH3+O2<=>CH2O+OH play the most promoting reaction while 2CH3(+M)<=>C2H6(+M) and CH_4+H<=>CH3+H2 are the most inhibiting reactions. These results can explain the small difference of the ignition delay time between different equivalence ratio conditions in section 4.2. It is also worth noting that with the increase of equivalence ratio, the reaction CH3+O2<=>CH2O+OH becomes more sensitive in the results, corresponding to the slight increase of ignition delay time from fuel lean to fuel rich conditions.

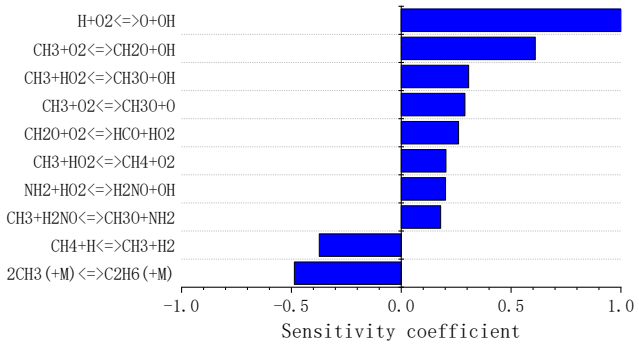

Fig. 15 Normalized sensitivity analysis on OH for 60%NH_3/40%CH_4 fuel blend at ER=0.5, p=5atm, T=1550K.

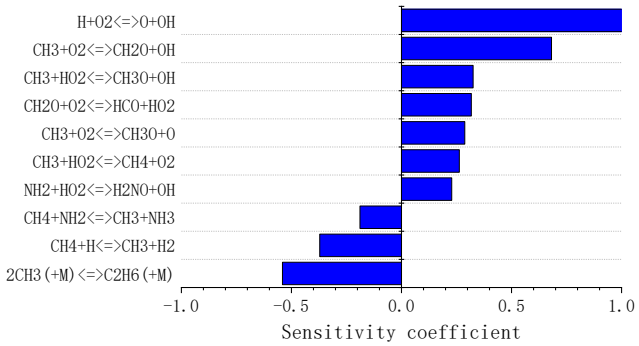

Fig. 16 Normalized sensitivity analysis on OH for 60%NH_3/40%CH_4 fuel blend at ER=0.5, p=10atm, T=1550K.

Figures 15 and 16 show the sensitivity analysis results under the pressure of 5atm and 10atm for 60%NH_3/40%CH_4 at 1550K and equivalence ratio of 1. Comparing fig. 15 and 16 with fig. 13, it can be identified that with the variation of high pressure conditions, most of the sensitive reaction are the same. Under all the pressure conditions, the most promoting reactions H+O2<=>O+OH and CH3+O2<=>CH2O+OH and the most inhibiting reactions 2CH3(+M)<=>C2H6(+M) and CH_4+H<=>CH3+H2 are the ones driving most of the reactivity of OH. However, with the increase of pressure condition, the inhibiting reaction 2CH3(+M)<=>C2H6(+M) becomes more prominent as observed. Another noticeable difference is the inhibiting reaction CH_4+NH2<=>CH3+NH3 which plays an important role under elevated pressure conditions, implying higher sensitivity of ignition process towards the interactions between ammonia and hydrocarbon species with the increase of pressure.

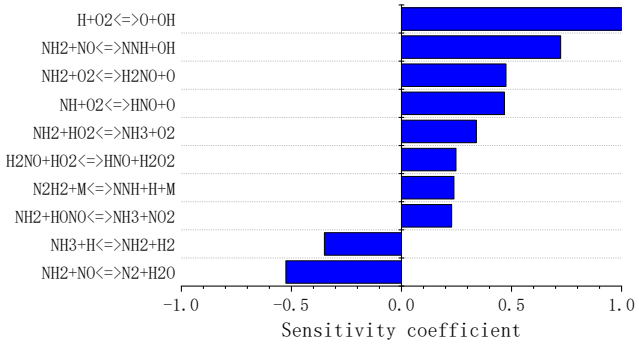

Fig. 17 Normalized sensitivity analysis on OH for pure NH_3 fuel at ER=0.5, p=2atm, T=1550K.

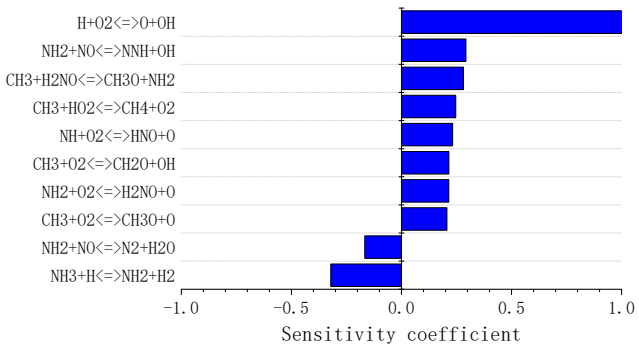

Fig. 18 Normalized sensitivity analysis on OH for 90%NH_3/10%CH_4 fuel blend at ER=0.5, p=2atm, T=1550K.

Finally, Figs. 17 and 18 show the sensitivity analysis of pure ammonia and 90% NH_3/10%CH_4 in mole fraction respectively. Compared with Fig. 13, the variation of CH_4 concentrations in NH_3/CH_4 fuel blends leads to quite different sensitivity analysis results. Although the promoting reaction H+O2<=>O+OH plays the most prominent role in all the three cases, the most inhibiting reactions are NH_3+H<=>NH2+H2 and NH2+NO<=>N2+H2O at low methane concentrations (pure ammonia and 10%CH_4 in fuel blend) while 2CH3(+M)<=>C2H6(+M) and CH_4+H<=>CH3+H2 become the most inhibiting ones at 40%CH_4 concentration. Also the second most promoting reaction changes from NH2+NO<=>NNH+OH at low methane concentration to CH3+O2<=>CH2O+OH at high methane concentration conditions. Such sensitivity results indicate the more prominent role of hydrocarbon species with more methane added into fuel blends, which is consistent with the reduction of the ignition delay time phenomenon along with methane addition shown in section 4.3.

5. Conclusions

In the present study, experimental measurements and numerical simulations of ammonia/ methane/air ignition were performed to explore the characteristics of utilizing ammonia/methane as a fuel blend for combustion energy systems.

An extensive set of experimental measurements were performed for the ignition delay times of 60%NH_3/ 40%CH_4 fuel blend at high temperatures up to 1800K and pressures up to 5 atm in a shock tube device. Significant reduction of the ignition delay time was observed with an increase in initial temperature and mixture pressure.

Numerical modelling using Tian mechanism has been validated with the experimental data measured in this study, which generally showed satisfactory within the range of equivalence ratios, temperatures, and pressure conditions investigated.

Further calculations using the validated model show that both mixture pressure and methane fraction in fuel blends have significant impact on the ammonia/methane fuel blends ignition process while less sensitivity is found on equivalence ratio. The significant promoting effect of pressure and methane addition on the ignition process suggests the feasibility of ammonia/methane fuels application under engine relevant conditions. Further studies of chemical kinetics for higher pressures are needed.

The sensitivity analyses showed that the ignition delay is most sensitive to the reactions H+O2<=>O+OH, promoting the ammonia consumption by forming OH radicals, while at higher methane concentrations hydrocarbon radicals such as CH3 play a more crucial role in the process. Moreover, the variation of most-sensitive reactions explains the characteristics of the ignition delay times under different initial conditions.

Acknowledgement

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