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Abstract:

Ammonia is a promising alternative fuel, which is considered to have the potential to substitute conventional fossil fuels. In the present work, auto-ignition characteristics of ammonia substitution on methane are investigated both experimentally and numerically. The auto-ignition procedure of ammonia-substituted methane/air mixtures are measured behind the reflected shock wave in a shock tube experiment system over temperatures from 1355 to 1877 K, pressure up to 5 atm and an equivalence ratio from 0.5 to 2. Numerical simulation studies using a detailed kinetics mechanism are also performed to gain a deep insight into the auto-ignition procedure of ammonia-substituted methane fuel mixtures. The established numerical model is verified with the measured auto-ignition delay time data by experiments. Then, the auto-ignition delay times are predicted under a wider range of conditions such as equivalence ratio, pressure, temperature, etc. In this way, combustion characteristics of such mixtures are investigated. It is found that adding ammonia fuel to methane will not change the autoignition delay time of methane a lot, while it can effectively benefit the reduction of carbon emissions. Finally, sensitivity analyses are performed to provide essential information for the elementary reaction sensitive to the ignition characteristics. The results present in this work can provide fundamental information for combustion application of ammonia-based fuels.

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1. Introduction

Since the Industrial Revolution, the use of fossil fuels in power generation, industry and transportation processes has produced large amounts of greenhouse gases, seriously influencing the global ecosystem. In this situation, renewable energy and alternatives to traditional fossil fuels have been considered essential ways to reduce carbon emissions. However, the intermittent and unstable features of most renewable energy sources, such as solar and wind energy, have problems such as the inefficiency and high cost of energy storage. It is still difficult for renewable energy to replace traditional fossil fuels. Therefore, developing alternative green fuels to reduce the consumption of traditional fossil fuels is a great priority [1,2].

Ammonia fuel is carbon-free, high-energy-density chemical, which has gained great interest from researchers all around the world [3–6]. It is relatively easy to achieve effective utilization in combustion applications. In previous studies, various fuels have been explored to enhance the ammonia combustion [7–12], as ammonia has relatively high resistance to ignition and low flame propagation speed. For example, Ryu et al. [7] investigated port-injection of gasoline with ammonia direct injection to promote ammonia combustion in a spark ignition (SI) engine. Combustion characteristics and emissions were

tested to develop feasible injection strategies. Valera-Medina et al. [8] investigated the combustion of the ammonia–methane fuel mixtures in a tangentially injected swirl burner of gas turbine. The flame stability and emission characteristics at different equivalence ratios were determined carefully. Okafor et al. [9] studied the physical and chemical processes of methane–ammonia fuels in a gas turbine combustion chamber. Laser diagnostics and the Fourier transform infrared gas analysis method were used to characterize the flame structure and emission of methane–ammonia–air flame. Choi et al. [10] studied the extinction limits and flame morphology of the opposed ammonia–hydrogen flames in elevated temperature conditions, experimentally and numerically. It has been shown that the blow-off limits are enhanced with the addition of hydrogen for ammonia/air flames, demonstrating the potential of hydrogen as an enhancer for ammonia/air flames. The attempts to utilize ammonia combustion have generally demonstrated promising characteristics of ammonia fuel mixtures.

To utilize ammonia more successfully, ignition properties of fuel mixture are important when it comes to understanding the fuel chemistry in detail, which can help to improve fuel application in turn [13,14]. Shu et al. [15] studied autoignition delay times of ammonia fuel over the intermediate temperature conditions of 1100–1600 K and elevated pressure of 20–40 bar. He et al. [16] studied ignition delay of ammonia/hydrogen fuel blends using rapid compression machine experiments in high-pressure conditions ranging from 20–60 bar and low-temperature conditions from 950 to 1150 K, demonstrating that hydrogen can effectively improve the reactivity. Dai et al. [17] investigated ignition delay of ammonia/methane mixtures in a rapid compression machine in elevated conditions. In the study, methane concentration varying from 0 to 50% in ammonia/methane mixtures were tested, showing promoting effects with methane addition. Yu et al. [18] studied the impact of adding ammonia on the auto-ignition delay of n-heptane at pressure of 10 and 15 bar and temperature ranging from 635 to 945 K. It was found that ignition delay time increases with the ammonia addition in the low-temperature conditions tested. Though several studies have been performed on ammonia combustion [19–22], investigations on the auto-ignition are still needed for ammonia-based fuels. The effect of ammonia addition on the auto-ignition delay of methane has not been investigated, especially under pressure conditions lower than 10 atm. Therefore, the goal of the present study is to investigate the ignition delay time of the ammonia/methane mixtures, both experimentally and numerically.

In the present study, auto-ignition delay times of ammonia-substituted methane fuels were analyzed. The auto-ignition delay times of ammonia-substituted methane were firstly investigated using shock tube experiments under pressures of 2 and 5 atm, temperature from 1355 to 1877 K and equivalence ratio from 0.5 to 2. Numerical simulations were also performed with detailed chemical mechanisms to analyze auto-ignition characteristics under different temperature, pressure, equivalence ratio and ammonia fuel substitution rates. The obtained results can serve as a basis for promoting ammonia as potential alternative fuel to conventional fossil fuels.

2. Experimental Setup and Numerical Analysis

The experiments of the auto-ignition were conducted in a stainless-steel single-diaphragm shock tube device, of which a detailed setup description can be found in [23]. The schematic of the shock tube is illustrated in Figure 1. Briefly, this shock tube consists of a driver section and pneumatically driven sections with lengths of 4 m and 5.5 m, respectively, which are cylindrical steel pipes of high temperature resistant. The inner diameter of the shock tube is 100 mm and the thickness of the wall is 17.5 mm. Along the sidewall of the driven section, three pressure sensors were installed equally, with 200 mm between each other in distance.

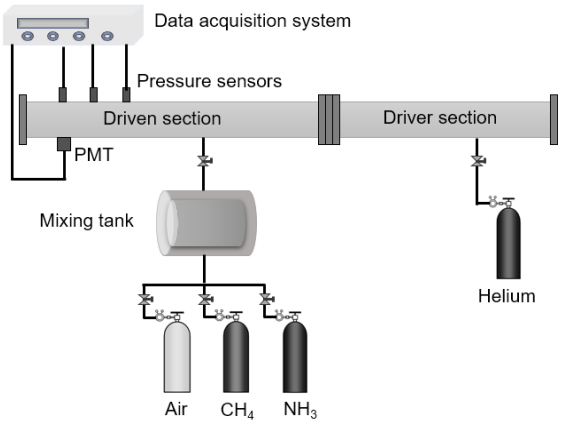

Figure 1. Experimental setup.

According to the measured signal of shock wave pressure, incident-wave speeds can be determined at the tail end of the driven section. Then, the ignition temperature and pressure conditions of post reflected-shock can be calculated using the incident-wave speed in combination with shock wave relations. The profile of pressure respective to time for the reflected shock wave was recorded by a sensor placed at 20 mm away from the end surface. A photoelectric multiplier was placed at the same location as the sensor on the sidewall to measure the profile of the luminous signal. In the experiments, gas mixtures were passed to the mixing tank and rested for at least 1 h to ensure homogeneity through diffusion processes. Figure 2 illustrates typical pressure and luminous signal profiles respective to time for an auto-ignition experiment under pressure of 5 atm. The ignition delay time is defined as the time interval between the arrival of the reflected shock wave at the position of pressure sensor and the time when the ignition occurs [23]. Additionally, the moment of auto-ignition is defined as the intersection of lines drawn along the maximum rate of change of PMT signal curve and the horizontal baseline. In the shock tube experiments, auto-ignition delay times of ammonia-substituted methane were investigated under post-reflected-shock pressures of 2 and 5 atm. As shown in Table 1, a fuel mixture of 10% ammonia and 90% methane is used and the air concentrations are determined by equivalence ratios from 0.5–2.

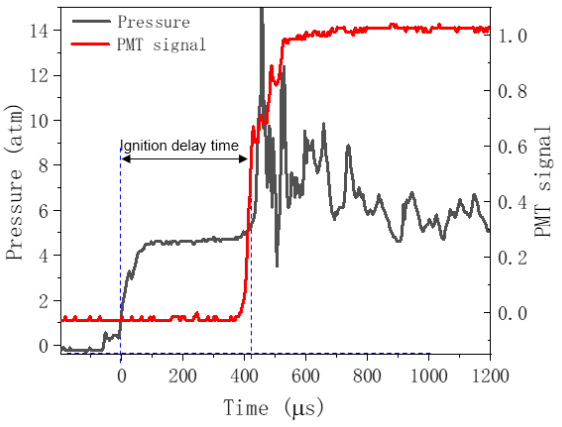

Figure 2. Determination of auto-ignition delay time for ammonia–methane/air.

Table 1. Test methane–ammonia–air mixtures investigated in present study.

No.	CH_4	NH_3	Air	Equivalence Ratio (φ)	Temperature	Pressure
1	4.77%	0.53%	94.70%	0.5	1415–1813 K	2 atm
2	9.06%	1.01%	89.93%	1.0	1665–1877 K	2 atm
3	16.47%	1.83%	81.70%	2.0	1479–1559 K	2 atm
4	4.77%	0.53%	94.70%	0.5	1390–1712 K	5 atm
5	9.06%	1.01%	89.93%	1.0	1375–1643 K	5 atm
6	16.47%	1.83%	81.70%	2.0	1355–1709 K	5 atm

The closed homogeneous reactor model in CHEMKIN-PRO [24] was used to simulate the auto-ignition procedure of ammonia-substituted methane fuels used in the present experiments, as shown in Table 1. The equivalence ratio (φ) is defined as the ratio of the actual fuel/air ratio to the stoichiometric fuel/air ratio. As a zero-dimensional model, numerical simulations using a detailed kinetics mechanism were performed to help gain a deep insight into auto-ignition delay effectively and with low computational cost. Furthermore, the auto-ignition delay times of ammonia-substituted methane fuel mixtures can be predicted under wide variation of conditions such as pressure, temperature, equivalence ratio, etc. In this way, combustion characteristics of such mixtures can be investigated.

Detailed description of the chemical reaction mechanism for the auto-ignition process is essential for understanding details of the ignition delay phenomenon [25–30]. In relevant studies, a variety of kinetics mechanism models have been proposed for ammonia combustion chemistry. However, kinetics models for combustion of ammonia-substituted methane fuels are scarce. The present work chooses a kinetics model by Tian et al. [26] for auto-ignition simulation of ammonia-substituted methane/air blends. The Tian's kinetics model contains more than 700 elementary reactions and 84 species, which was established for premixed combustion of ammonia–methane under stoichiometric conditions. The model has been used in several studies of ammonia combustion [31,32], demonstrating satisfying performance in numerical prediction work specifically for auto-ignition delay studies. Thus, the Tian's kinetics model was employed in the numerical simulation of auto-ignition for ammonia-substituted methane fuel blends.

3. Results and Discussion

3.1. Validation of the Model

In the present work, the auto-ignition delay time (τ) of the fuel mixture of 10%NH_3/90%CH_4 was tested at an initial pressure of 2 and 5 atm and temperature ranging from 1355 to 1817 K, with an equivalence ratio (φ) of 0.5 to 2, and the results are shown in Figure 3a–c. According to the figures, the increased pressure can promote the auto-ignition process using the ammonia-substituted methane mixture under the temperature and equivalence ratio tested in the experiments. The error can be due to the non-ideal conditions of measurement of the auto-ignition delay time. According to Figure 3a–c, the initial temperature of the mixture has a significant impact on promoting the auto-ignition process. Generally, under higher initial temperature conditions, the auto-ignition delay time is shorter. From the experimental data in the figure, there is a similar linear relationship between the auto-ignition delay time logarithm of the tested fuel mixture and the inverse of the initial temperature. To verify the numerical model, auto-ignition simulations were conducted under the same conditions as in the experimental work.

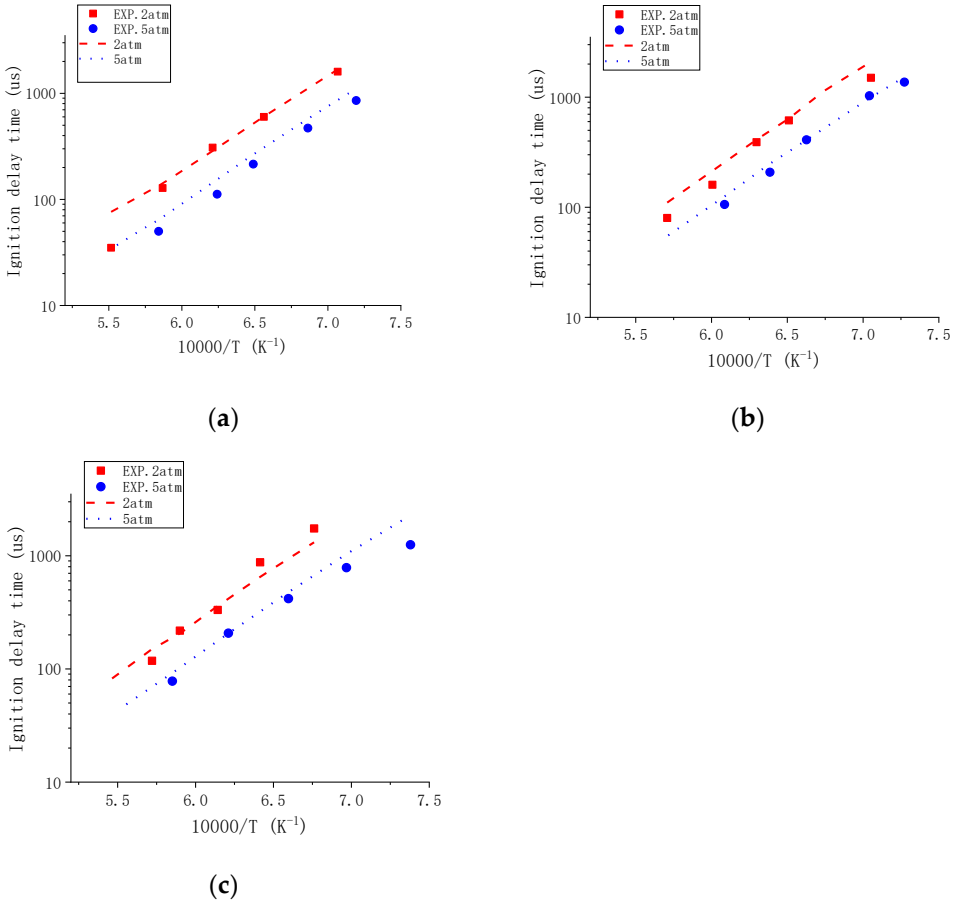

Figure 3. Auto-ignition delay time of the NH_3 substituted CH_4/air mixtures at equivalence ratio (φ) of (**a**) 0.5, (**b**) 1, (**c**) 2.

Figure 3a–c shows the comparison between the experimental results of the ammonia-substituted methane mixture and numerical results under the same conditions. It can be found from all three figures that there are overall good agreements between the experimental and numerical data, although some deviation in high-temperature conditions can be observed, especially under 2 atm conditions. The figures also indicate that the numerical model predicts better performance in the relatively lower-temperature range, while in the high-temperature regions, the auto-ignition delay time is predicted with relatively larger error. Additionally, the reaction mechanism used in this work can also lead to the deviation. As also found in other relevant studies [15,16], good agreements between the simulations and measurements are usually found for autoignition delay time region of 100–1000 μs. Although the general trend of the auto-ignition delay time with the pressure can be well predicted by numerical simulations, more work on refining the reaction mechanism is still needed. The average relative error of the ignition delay time at all simulated conditions is 23.2%.

3.2. Effect of Pressure

To analyze the effect of different pressure conditions on auto-ignition, the auto-ignition delay times are predicted at different pressure conditions by the verified numerical model. The 10%NH_3/90%CH_4 mixture is simulated under the pressure conditions ranging from 1 to 20 atm, as shown in Figure 4a–c. In the numerical simulation process, the model used is a closed homogeneous reactor, so it is assumed that the studied auto-ignition process is mainly determined by the chemical reaction kinetics. Therefore, the auto-ignition characteristics can be studied based on the detailed reaction kinetic model. The exponential

increases can be found in auto-ignition delay time with the temperature reduction under all the pressure and equivalence ratio conditions.

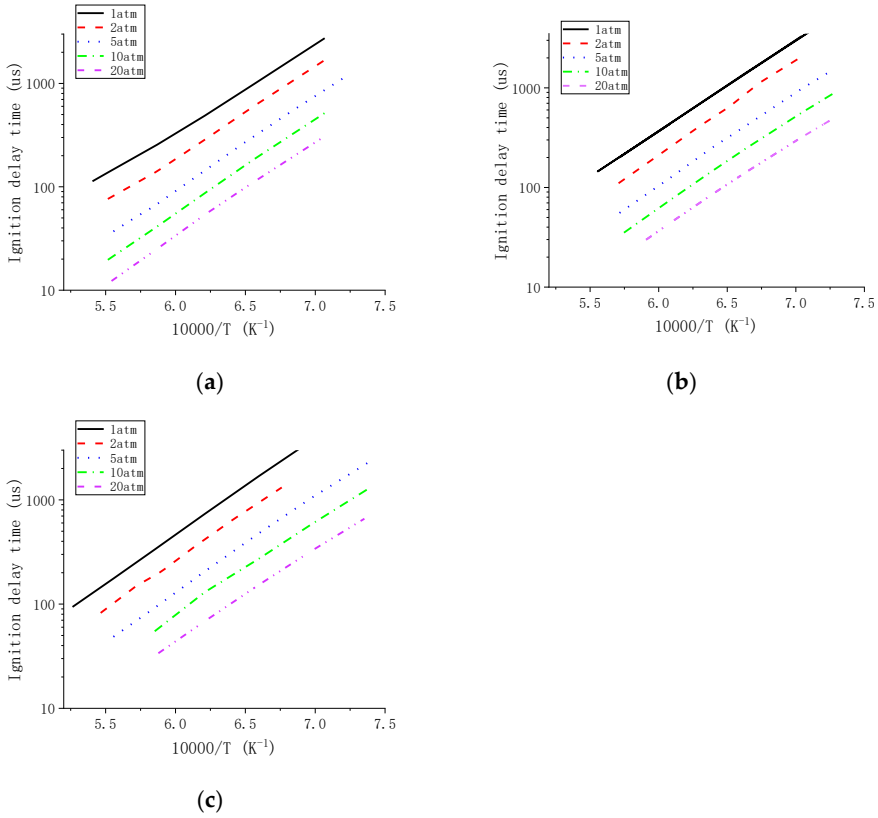

Figure 4. Effect of pressure on the auto-ignition delay time of the NH_3 substituted CH_4/air mixtures at X_{NH3} = 10% and equivalence ratio (φ) of (**a**) 0.5, (**b**) 1, (**c**) 2.

As can be seen from Figure 4a–c, the auto-ignition delay time decreases significantly with increasing pressure of the mixed fuel at different temperature and equivalence ratio conditions. Such a phenomenon is mainly because the rise in pressure will lead to higher reactant concentration. The reaction rates will elevate when reactant concentration becomes higher. The rates of the reduction of the auto-ignition delay time with pressure are very close at both low-pressure and high-pressure conditions. For instance, at temperature of 1610 K and equivalence ratio of 0.5, the auto-ignition delay time value of 2 atm is around 1.7 times lower than that of 1 atm, and the value of 5 atm is also around 1.7 times lower than that of 10 atm. The findings suggest that the auto-ignition delay time of this type of ammonia-substituted fuel is similarly sensitive to pressure at low- and high-pressure conditions.

3.3. Effect of Equivalence Ratio

The equivalence ratio (φ) is the ratio of the actual fuel/air ratio to the stoichiometric fuel/air ratio. The equivalence ratio has great significance in combustion studies of ammonia-substituted methane fuel. To understand the effect of the equivalence ratio on ammonia-substituted fuel mixture, the auto-ignition delay times under different equivalence ratio conditions are simulated, as shown in Figure 5a–c.

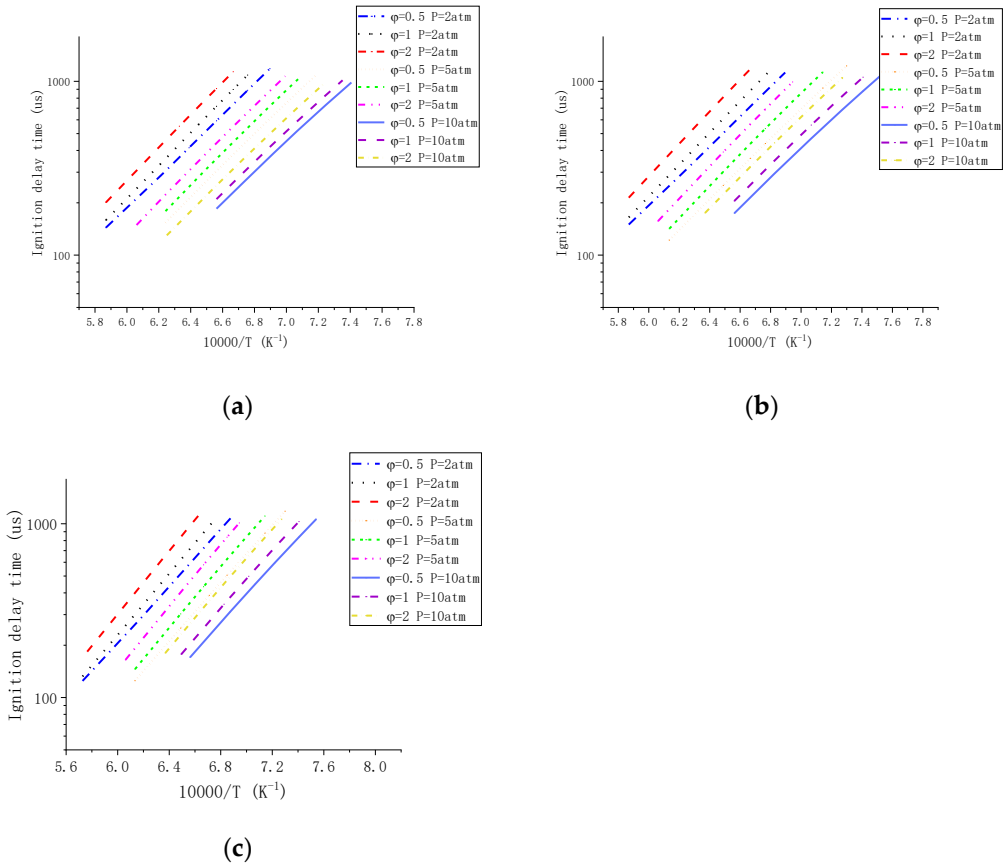

Figure 5. Effect of equivalence ratio (φ) on auto-ignition delay time at (**a**) X_{NH3} = 10%, (**b**) X_{NH3} = 30%, (**c**) X_{NH3} = 50%.

In Figure 5a, with the increasing equivalence ratio, the auto-ignition delay time of the mixture fuel is slightly longer, which is also consistent with the experimental results presented in the previous section. Although the change in the equivalence ratio can affect the auto-ignition delay time, the effect is much smaller compared with other factors, such as pressure and temperature. For example, at temperature of 1500 K and pressure of 5 atm, when the equivalence ratio increases from 0.5 to 2, the auto-ignition delay time increases only about 1.5 times. Such phenomenon is consistent with the observation of previous literature [15,21]. This is mainly attributed to the chemical nature of autoignition process of the mixture, which mainly depends on factors such as reactant concentration, temperature and pressure. Moreover, it is suggested from the figures that the equivalence ratio has a bit more impact on the auto-ignition delay time in fuel rich than in lean conditions. However, as the impact of the equivalence ratio on the auto-ignition delay time is usually rather complex, the trend of auto-ignition delay time under different equivalence ratio conditions was only preliminarily analyzed. The differences in different auto-ignition processes still need to be explored in practical engineering applications.

Figure 5b,c show the effect of different equivalence ratios on auto-ignition delay time at NH_3 = 30% and NH_3 = 50%, respectively. Generally, at the 50% and 30% of ammonia fraction conditions, the auto-ignition delay time characteristics are still consistent with the numerical results at NH_3 = 10%. With the increasing equivalence ratio, the auto-ignition delay time of the fuel mixture slightly changes, indicating less effect than the other factors, such as temperature and pressure.

3.4. Effect of Ammonia-Substituted Methane Fuel Blends Composition

Figure 6a–c show the numerical results of the auto-ignition delay time for the fuel mixture of NH_3 substituted CH_4 with different NH_3 concentrations. According to the

figures, under all the conditions studied, the auto-ignition delay time of NH_3 substituted CH_4 fuels increases exponentially with the decrease in temperature. It has been shown that adding a small amount of ammonia fuel to methane will prolong the auto-ignition time; however, the effect is insignificant. This phenomenon indicates that ammonia fuel can suppress the auto-ignition performance of methane. Additionally, quite a small difference is observed in the auto-ignition delay times of different ammonia concentrations in fuel mixtures. To better explain the effect of ammonia substitution, the auto-ignition delay times are plotted against ammonia mole fraction in fuel mixtures, as shown in Figure 7.

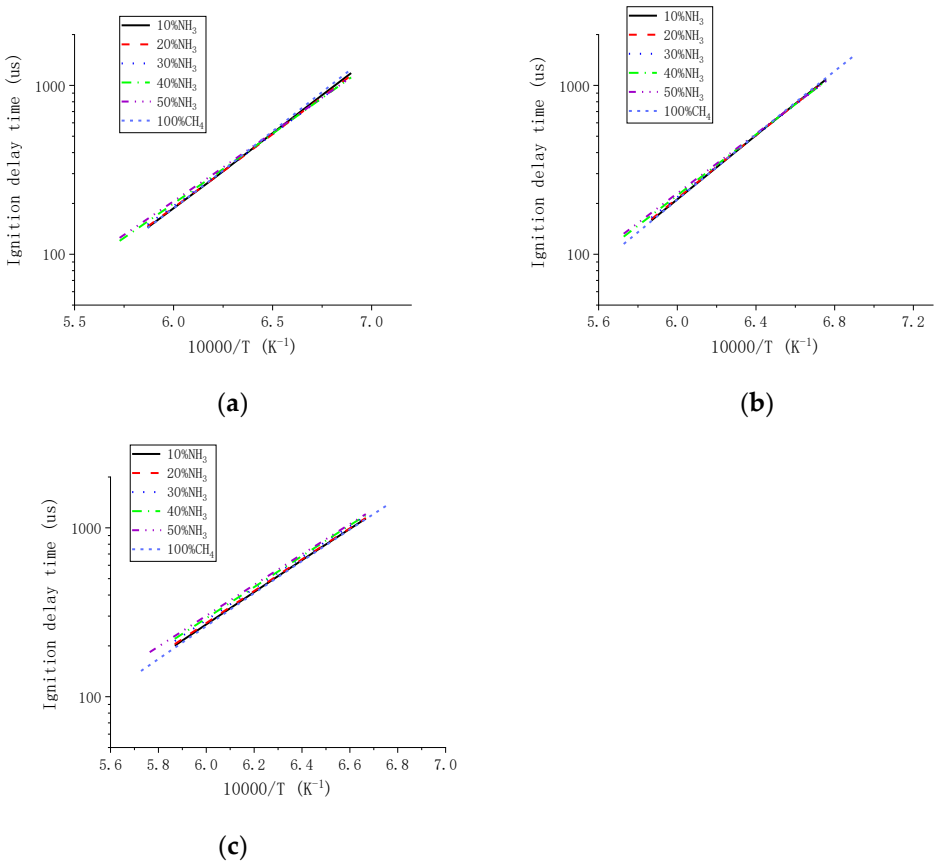

Figure 6. Effect of X_{NH3} on the auto-ignition delay time of NH_3 substituted CH_4 fuel blends at pressure of 2 atm and equivalence ratio (φ) of (**a**) 0.5, (**b**) 1, (**c**) 2.

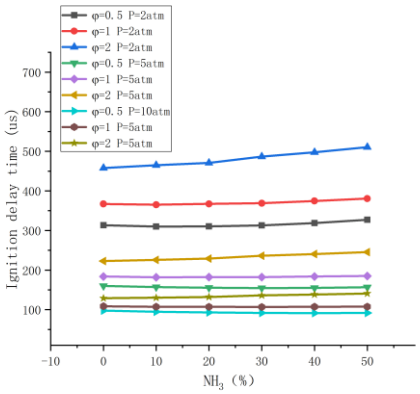

Figure 7. Auto-ignition delay time as a function of NH_3 concentration in fuel mixture.

In Figure 7, when the concentration of the ammonia fuel varies from 0% to 50%, the corresponding auto-ignition delay time does not change significantly with the increase in

the ammonia fuel concentration. The auto-ignition delay time is significantly reduced from low- to high-pressure conditions, indicating that increasing the auto-ignition pressure while increasing the NH_3 content can be a choice for the good auto-ignition delay characteristic. Therefore, using ammonia fuel to substitute methane fuel has relatively little impact on the auto-ignition delay time, whilst it will effectively reduce the carbon emissions, which indicates good potential in energy saving and emission reduction.

3.5. Sensitivity Analysis

To gain a deep understanding of the auto-ignition delay of the simulation results of NH_3-substituted CH_4 mixture under different working conditions, sensitivity analyses of OH radicals are conducted. Sensitivity analysis is used to quantitatively determine the dependence of a solution on certain parameters that appear in a model's definition. See the "raw" first-order sensitivity coefficient matrices:

$$S = \frac{\partial \phi}{\partial \alpha} \tag{1}$$

where S is the sensitivity coefficient matrix, ϕ is the dependent variable vector (e.g., temperature, mass fractions, surface composition), α is the parameter vector (e.g., reaction rate constants).

The sensitivity coefficients are calculated by the CHEMKIN program. When the sensitivity coefficient for a reaction is positive, it is indicated that increasing the rate of this reaction will lead to a higher species production rate. In contrast, negative sensitivity coefficient for a reaction indicates that increasing the rate of this reaction will lead to a lower production rate of a radical. The important reactions can be identified from the numerical results of the OH sensitivity analyses. Figures 8–10 show the sensitivity analyses of pure CH_4, 10%NH_3/90%CH_4, and 30%NH_3/70%CH_4, respectively. The values are normalized to the range of -1 to +1. A positive sensitivity coefficient indicates auto-ignition delay time is reduced with pre-exponent factor increase, suggesting the reaction promotes the auto-ignition.

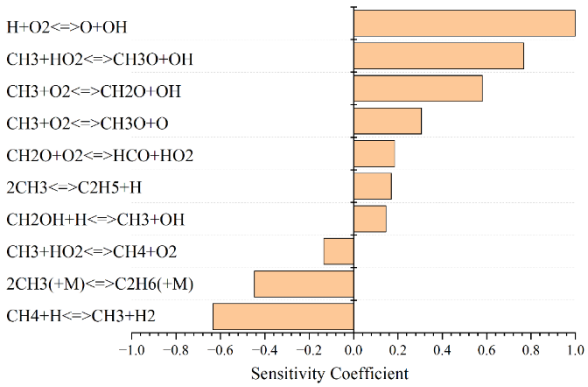

Figure 8. Sensitivity analysis for pure CH_4 blend at equivalence ratio (φ) of 1.0, p = 2 atm, T = 1550 K.

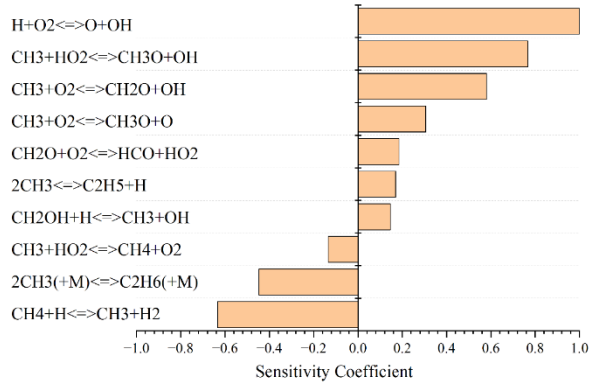

Figure 9. Sensitivity analysis for 10%NH_3/90%CH_4 at equivalence ratio (φ) of 1.0, p = 2 atm, T = 1550 K.

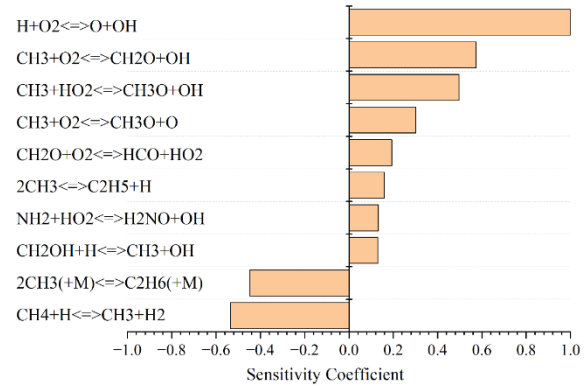

Figure 10. Sensitivity analysis for 30%NH_3/70%CH_4 at equivalence ratio (φ) of 1.0, p = 2 atm, T = 1550 K.

It is shown that the elementary reactions H + O_2 <=> O + OH and CH_4 + H <=> CH_3 + H_2 are the top predominantly sensitive reactions promoting and inhibiting the auto-ignition of the mixture. Chain-branching reactions CH_3 + HO_2 <=> CH_3O + OH and CH_3 + O_2 <=> CH_2O + OH have also played important roles as promoting reactions. The difference is that with the increase in ammonia concentration, the promoting effect of reaction CH_3 + HO_2 <=> CH_3O + OH gradually decreases, while the relative sensitivity of CH_3 + O_2 <=> CH_2O + OH increases obviously. For instance, about a 30% increase in the relative sensitivity can be observed when comparing 30%NH_3 with 10%NH_3 fuel mixtures.

Moreover, only in the case of ammonia concentration of 30% in fuel mixture, nitrogen-containing reaction NH_2 + H_2O <=> H_2NO + OH ranks in the 10 most sensitive reactions, which explains the relatively small influence of ignition delay time on ammonia substitution on methane. It also can be noticed that CH_4 + OH <=> CH_3 + H_2O shows a slightly inhibitory effect on auto-ignition at low-ammonia conditions, while it is not among the top dominant reactions in the case of ammonia concentration of 30%. It suggests that with the increase in ammonia concentration, the effect of methane can be reduced slightly.

4. Conclusions

To date, the effect of ammonia addition on the auto-ignition delay of methane has not been reported in the shock-tube literature, especially under the pressure and temperature conditions investigated in the present study. In the present work, auto-ignition characteristics of ammonia-substituted methane fuels are studied experimentally and numerically over temperatures from 1300 to 1900 K, pressure up to 20 atm and an equivalence ratio from 0.5 to 2. Comparisons between the measured auto-ignition delay time data and model prediction illustrate generally good performance of Tian's kinetics model. Under

the temperature and equivalence ratio conditions tested in this work, it is shown that the increased pressure can promote the auto-ignition process of the ammonia-substituted methane mixture. Additionally, the temperature has a great impact on promoting the auto-ignition. It is found that adding small proportion of ammonia fuel to methane will not change the auto-ignition delay time of methane a lot, while it can effectively reduce the carbon emissions, which indicates the good potential of using such fuels in practical applications. Sensitivity analysis studies have shown that the most sensitive reactions are H + O_2 <=> O + OH, CH_3 + O_2 <=> C_2H_6 (+M) and CH_4 + H <=> CH_3 + H_2, at different ammonia concentrations in fuel mixture. The results of auto-ignition delay time characteristics and chemical mechanism obtained in this work can provide fundamental data and guidance for future application of ammonia substitution on methane fuels.

Author Contributions: Conceptualization, H.X. and A.C.; methodology, H.X. and Y.G.; software, H.X. and X.D.; formal analysis, L.Z., X.D., J.L. and W.Y.; writing—original draft preparation, H.X. and Y.G.; writing—review and editing, M.Z. and A.C.; visualization. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data presented in this study are available on request from the corresponding author. The data are not publicly available due to privacy.

Conflicts of Interest: The authors declare no conflict of interest.

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