EFFECT OF NANOSECOND PLASMA DISCHARGE ON IGNITION DELAY TIME OF AMMONIA/AIR MIXTURE

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Abstract

Plasma-assisted ignition and combustion is now a very attractive subject due to its numerous applications in the fields of transportation and power generation using zero-carbon fuels. Plasma discharge can improve combustion by producing a high number of chemically active particles that influence the chemical process. This numerical study investigated the effect of nanosecond plasma discharge on ignition delay time (IDT) of ammonia/air mixture at low and intermediate temperatures (850 - 1100 K) under atmospheric pressure. Employing ZDPlasKin and CHEMKIN codes, coupled with a validated kinetic mechanism, the study aims to assess the combustion enhancement of ammonia by plasma. The results showed that using the 20 pulses plasma discharge, the IDT was reduced from 210.55 s to 3.01 s and the flame temperature increased from 2388.5 K to 2433.1 K at an initial temperature of 850 K and pressure of 1 atm.

Introduction

Among the various greenhouse gases, carbon dioxide (CO_2) emitted from the combustion of fossil fuels is identified as the primary contributor to this global warming trend [1]. Recognizing the urgency of addressing climate change, many countries globally are adopting substantial measures to transit towards cleaner and more sustainable energy sources [2, 3]. Ammonia (NH_3) emerges as a promising solution to address aspects of the impending energy crisis. It has gained considerable attention as a carbon-free fuel and hydrogen carrier. In addition, ammonia enjoys well-established storage and transportation infrastructures, rendering the long-term storage and transport of ammonia a cost-effective solution [4]. While ammonia offers numerous advantages, there are several challenges that must be addressed before its direct utilization in combustion devices like compression ignition (CI) and spark ignition (SI) engines. These challenges include high resistance to autoignition (with an octane number around 130) [5], a narrow flammability range, slow flame speed, NOx emission, and a high latent heat of vaporization. Recent review articles [6,7], contemplate ammonia as a prospective future fuel, acknowledging the need to navigate and resolve these challenges for its effective integration. Identifying ammonia as a potential future fuel necessitates a comprehensive understanding of its oxidation processes.

The ignition delay time (IDT) stands out as a crucial characteristic in the combustion of fuels within practical energy devices. In the context of NH_3 combustion, it's noteworthy that the high ignition temperature and ignition energy of NH_3 pose limitations on its practical application as a fuel. Therefore, investigating the ignition characteristics of NH_3 and exploring methods to enhance NH_3 ignition is necessary. The present study specifically addresses this challenge by utilizing non-equilibrium plasma. Because plasma discharge has the potential to enhance ignition by generating chemically active particles that influence chemical reaction mechanisms that dominate the ignition process. This numerical investigation focuses on the impact of nanosecond plasma discharge on the IDT of ammonia/air mixtures at low and intermediate temperatures (850-1100 K) under atmospheric pressure.

Numerical Methodology

Numerical modeling has been performed by coupling a zero-dimensional plasma kinetic model (ZDPlasKin) [8] and the chemical kinetic model (CHEMKIN) [9]. ZDPlasKin was used to analyze the nanosecond repetitive pulse discharge and CHEMKIN was used to predict the IDT. The plasma enhancement ignition process is divided into discharge and ignition phases due to the significant difference in the time scales of the two phases. The discharge phase is characterized by the transfer of energy and the activation of neutral particles. A significant number of active particles are created during the plasma discharge phase such as NH_2, NH, H, O, O_3, and OH which are delivered as the active species into the ignition process of the NH_3/air mixture in the ignition stage, simulating the whole process of plasma-enhanced ammonia ignition. Simulations of plasma discharges are performed using the validated Plasma Kinetic Mechanism [11] and modified Mei's ammonia combustion mechanism [12]. Mei's ammonia combustion mechanism is selected because it can accurately capture the laminar flame speeds (S_L) and IDT [12,13] within the experimental uncertainties. Furthermore, the Mei mechanism was discovered to better predict NO than other mechanisms [14]. The rate constants of significant reactions are modified from recent experimental, numerical, and review studies for better performance at low and intermediate temperatures, and O_3 sub-mechanism reactions from ZH Wang et al. [15] are added to the base mechanism. The general methodology can be summarized in Figure 1 using the numerical procedure flowchart.

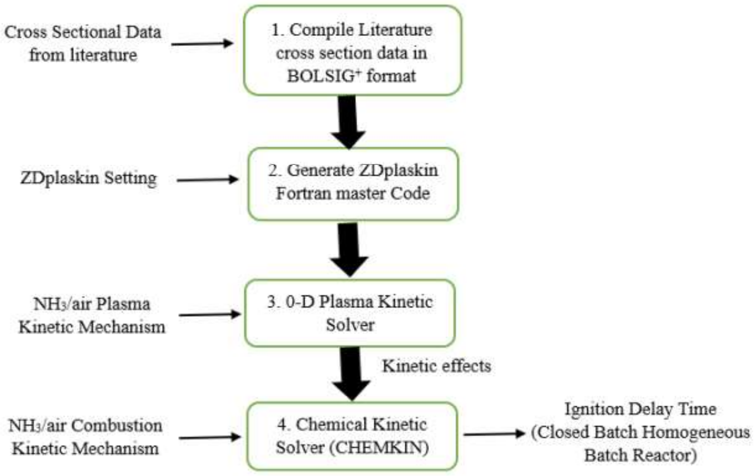

Figure 1. A detailed diagram of the numerical modeling approach with integration of ZDPlasKin and CHEMKIN

Validation

To assess the validity of the updated reaction mechanism used in this investigation, a validation analysis was performed by comparing experimental [16] and numerical data [17-19]. To investigate the IDT of the NH_3/air mixture, different mechanisms were employed in numerical simulations using CHEMKIN [9]. In this study, IDT is defined as the time when the temperature gradient reaches its maximum and the Closed Homogeneous Batch Reactor module was employed to calculate the IDT. Figure 2 highlights that present, Stagni et al. [17] and Han et al. [18] mechanisms have good agreement with the IDT experimental values. However, the mechanisms proposed by Okafor et al. [19] tend to slightly overestimate the experimental values under current conditions.

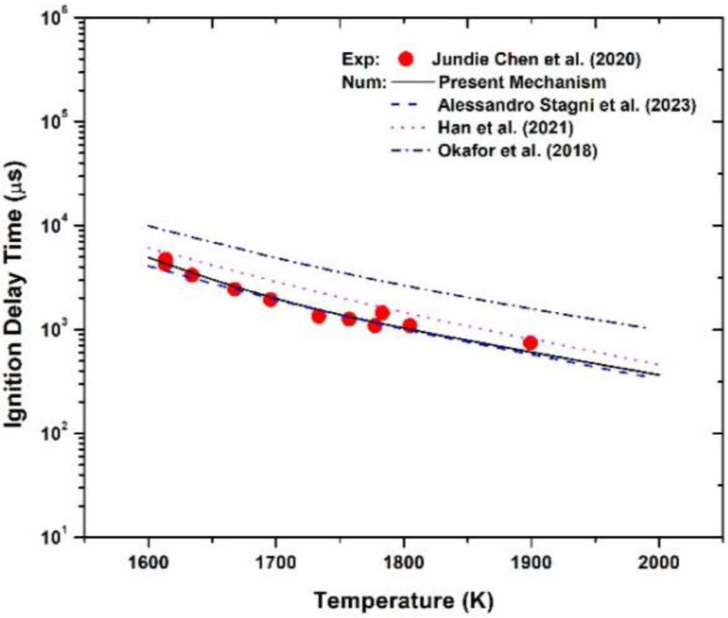

Figure 2. IDTs of $0.04375NH_3/0.03281O_2/0.92344Ar$ mixture as a function of temperature at a pressure of 1.2 atm and $\phi = 1.0$. Symbols represent the experiment data, and lines depict the simulated results of the current and prior models.

Results

The current analysis was conducted to investigate the effect of initial temperature and plasma discharge with 20 sequential pulses by keeping the E/N 180Td constant on IDT and flame temperature of NH_3/air mixture in the range of low and intermediate temperature (850 - 1100 K) under atmospheric pressure. During the plasma discharge active particles (O, H, OH, NH, NH_2, and O_3) presented in Table 1 are generated due to ionization, excitation, dissociation reactions, and recombination of electron-ion reactions.

Table 1. Production of species with 20 sequential pulses of plasma discharge in NH_3/air mixture at, E/N = 180Td, P = 1 atm, $\phi = 1.0$ with PRF = 50 kHz used in the CHEMKIN.

Temperature K	Maximum mole fraction of species					
	O	H	OH	NH	NH_2	O_3
850	0.00306	0.00331	0.00127	0.000383	0.00392	2.07513E-5
900	0.00267	0.00283	0.00109	0.000328	0.00336	1.45403E-5
950	0.00230	0.00239	0.000934	0.000278	0.00285	1.01764E-5
1000	0.00198	0.00204	0.000803	0.000237	0.00243	7.09373E-6
1050	0.00170	0.00173	0.000685	0.000201	0.00207	4.87725E-6
1100	0.00145	0.00146	0.000581	0.000170	0.00175	3.25817E-6

The results showed that using the 20 pulses plasma discharge, the IDT was reduced from 210.55 s to 3.01 s and the flame temperature increased from 2388.5 K to 2433.1 K at an initial temperature of 850 K as shown in Figure 2. The ignition delay time of the combustion under the plasma case is significantly shorter and the flame temperature higher than that of the case without plasma, indicating that the excitation of the plasma promotes the reaction and provides new reaction pathways in boosting low-temperature NH_3 ignition.

It can be seen in the NH_3/air mixture, that the initial temperature has a significant influence on the IDT without a plasma case. As the initial temperature increases, the IDT decreases significantly. When the initial temperature increases from 850 K to 1100 K, the ignition delay time is reduced from 210.55 s to 0.36 s and the flame temperature gradually increases from 2388.5 K to 2514.1 K. In the case of plasma, the initial temperature has an insignificant impact on the NH_3/air mixture. The IDT decreases gradually as the initial temperature increases, but the difference is not as significant as that for the case without plasma. As the initial temperature increases from 850 K to 1100 K, the IDT decreases from 3.01 s to 0.038 s and flame temperature increases from 2433.1 K to 2531.5 K.

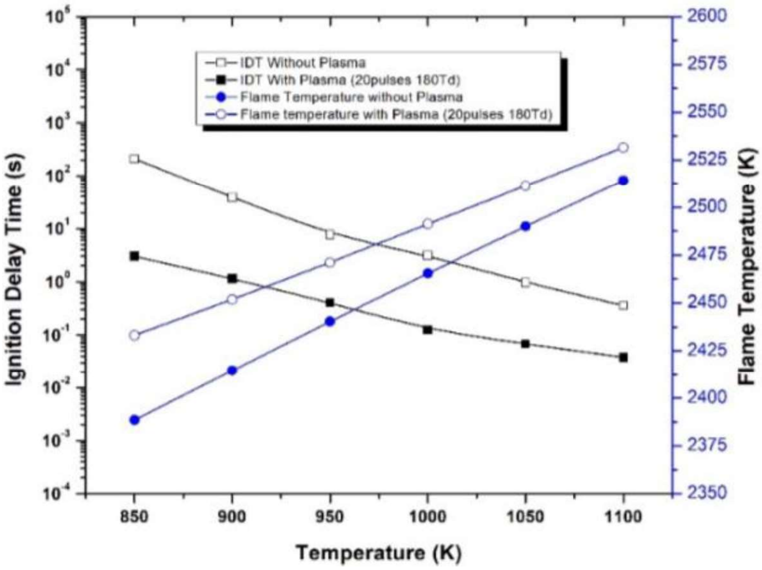

Figure 2. IDT and flame temperature without and with 20 sequential pulses of plasma discharge in NH_3/air mixture at, $E/N = 180$Td, $P = 1$ atm, $\phi = 1.0$ with PRF = 50 kHz.

Conclusion

This numerical investigation focuses on the impact of nanosecond plasma discharge on the IDT of an ammonia/air mixture for low and intermediate temperatures (850 - 1100 K) under atmospheric pressure. The results revealed the IDT of the ammonia combustion under the plasma case is significantly shorter and the flame temperature higher than that of the case without plasma. Employing a 20 pulses plasma discharge, the IDT was reduced from 210.55 s to 3.01 s and the flame temperature increased from 2388.4 K to 2433.1 K at an initial temperature of 850 K.

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