Energy 126 (2017) 796–809

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Numerical study on laminar burning velocity and ignition delay time of ammonia flame with hydrogen addition

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ARTICLE INFO

Article history:
Received 7 April 2016
Received in revised form
11 January 2017
Accepted 17 March 2017
Available online 20 March 2017

Keywords:
Laminar burning velocity
Ignition delay time
Ammonia flame
Hydrogen addition

ABSTRACT

This study focuses on the application of NH_3 as a carbon-free alternative fuel in internal combustion devices. The two key parameters for fuel combustion, namely, laminar burning velocity and ignition delay time of the NH_3 flame at various H_2 blending levels, are numerically investigated. Results show that the selected modified Dagaut-Kéromnès mechanism is acceptable and repeatable for calculating the burning velocity and ignition delay time of NH_3-air flame at various H_2 addition conditions. H_2 addition increases the reactivity of NH_3 combustion at all conditions and enhances the burning velocity. This enhancement is mainly due to chemical effect caused by the reduction in chemical activation energy and the transport effect resulting from the high mobility of H_2. Furthermore, an increase in pressure and H_2 addition ratios can significantly decrease the ignition delay time of NH_3 mixtures and promote NH_3 ignition. The enhancement of H_2 addition on NH_3 ignition and laminar burning velocity is mainly attributed to the contribution of the three following reactions: $O + H_2 = OH + H$, $H + O_2 = OH + O$, and $H_2 + OH = H_2O + H$. These reactions can significantly increase the concentration of free radicals and accelerate the peak of radicals.

1. Introduction

In recent decades, the study of alternative and clean fuels has attracted increasing attention with the depletion of fossil fuels and strengthening of pollutant emission regulations [1,2]. One of the prospective alternative fuels is NH_3 [3]. NH_3 is recognized as one of the most promising alternative fuels demonstrating the following favorable properties: (a) free of CO_2, SO_x, and soot emission because no carbon is present in this fuel [3–5]; (b) synthesized from fossil fuels (e.g., petroleum, coal, and natural gas), or renewable sources (such as wind, solar, hydropower, and biomass) [5–7]; and (c) easily and economically stored and transported in the liquid phase in large quantities via NH_3 tanks, trucks, ships and pipelines [5–7]. Therefore, NH_3 has become a key alternative fuel candidate. NH_3 has been utilized in specific energy devices, such as industry gas turbines and gas engines operated at high pressure and temperature [8,9].

As a fundamental property for fuel combustion in practical energy devices, laminar burning velocity is determined by the combined properties of diffusivity, exothermicity, and reactivity of a fuel. The laminar burning velocity is a key parameter to describe flame stabilization, extinction limits, flame structures, and velocity [10–12]. Unfortunately, the burning velocity of NH_3 is usually low around 5–13 cm/s [6,7,13]. This low value obstructs its application in specific energy devices. NH_3 combustion at various conditions, such as dual fuel with H_2 [7,14–18] and CH_4 [19–21]with high burning velocity, preheating condition [9,22,23] from exhaust heat, and O_2-enriched condition [24,25], has been investigated to improve the laminar burning velocity of NH_3. Lee et al. [16] investigated the burning velocity and emission characteristics of NH_3 with H_2 addition ratio from 0% to 50%. They found that the laminar burning velocity substantially increases with H_2 addition, and low NO_x formation occurs at fuel-rich conditions. Li et al. [17] experimentally studied the combustion characteristics and NO_x formation of NH_3–H_2 combustion with H_2 ratio from 33.3% to

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http://dx.doi.org/10.1016/j.energy.2017.03.085
0360-5442/

60.0%. The laminar burning velocity improved to a favorable level, similar to CH_4; whereas NO_x emission should be further treated when NH_3 is used as a fuel. The laminar burning velocities of pure NH_3 combustion at preheating and O_2-enriched conditions have also been studied by Li et al. [23,25]. Preheating temperature and O_2 enrichment positively affect the laminar burning velocity of NH_3 because of the high reaction rate and free radical formations. Furthermore, NO reacts with NH_x radicals and leads to low NO formation. Reducing NO emission in NH_3-air combustion is also observed.

Ignition delay time is another key property for fuel combustion in practical energy devices. It is a significant validation parameter in the development of chemical kinetics. The ignition delay time directly determines the ignition of fuel in practical energy devices. The fuel ignition process is recognized as zero-dimensional and homogeneous in a standard shock tube measurement facility. For NH_3 combustion, the ignition temperature and ignition energy of NH_3 are high and limit the application of NH_3 as a practical fuel. Therefore, the studies on the ignition characteristics of NH_3 and the enhancement of NH_3 ignition are necessary. Many studies [26–32] on application of NH_3 in compression-ignition and spark-ignition engines have been reported. However, previous experiments showed shortage with poor ignition property of NH_3. Additionally, little work has been conducted on the ignition delay time of NH_3 [33] and enhancement of NH_3 ignition. However, the fundamental key properties of NH_3, such as burning velocity, auto-ignition temperature, and minimum ignition energy are far apart with H_2, methanol, and gasoline as shown in Table 1 [30,31]. The burning velocity of NH_3 is only approximately 0.42% of H_2 (3.51 m/s), and the minimum ignition energy is 4440 times of H_2 (0.0018 mJ). By mixing with H_2, it is possible for NH_3 to present promising properties at suitable H_2 addition ratios. Furthermore, the kinetic of NH_3 combustion at various H_2 addition conditions remains also unclear and needs further investigation. Thus, studies on the laminar burning velocity and ignition delay time of NH_3 combustion are still rare and worthwhile.

This study are aims to evaluate the kinetic models of NH_3 combustion, investigate the laminar burning velocity at various H_2 addition ratios (up to 90%), calculate the ignition delay time of NH_3 flames at various conditions, and discuss the effect of H_2 addition on the chain reaction mechanism, laminar burning velocity. The results will be used to provide a fundamental database and a favorable method for the enhancement of NH_3 combustion in practical energy devices.

2. Numerical simulations

The laminar burning velocity is simulated by a freely propagating adiabatic, premixed, laminar flame speed calculation model [34] in CHEMKIN 4.0. The hybrid time–integration/Newton-iteration technique with adaptive meshes and mixture–averaged transport parameters is applied to solve the steady–state mass, species and energy conservation equations of the flames; this technique has been described in detail in previous studies [22,23,25]. The inlet gas molar fractions for laminar burning velocity calculation at various H_2 addition ratios are summarized in Tables S1–S6 in Appendix A1. Estimated values for the initial, intermediate and production fractions along with temperature profiles are set before the simulations. The final solution is obtained at adaptive grid control based on the solution gradient and curvature (GRAD and CURV) set as 0.01 and 0.05, respectively. These values are sufficiently accurate for our results. The burning velocity is calculated with Soret effect using multicomponent transport method in CHEMKIN [34], which is shown as following equation based on Metghalchi and Kech power-low relation [25,35]:

$$S_u = S_{u0}\left(\frac{T_u}{T_0}\right)^{\alpha}\left(\frac{p}{p_0}\right)^{\beta}$$

where S_u is the laminar burning velocity (cm/s), T_u and p is the unburned temperature (K) and pressure (atm), S_{u0}, α, and $\beta$are constants, and the subscript 0 represents the standard state.

The ignition delay time is calculated using CHEMKIN package. A homogeneous charge compression-ignition model is selected for the simulations. A wide range of engine related conditions is investigated with pressure from 1.4 atm to 30 atm, temperature from 1500 K to 2500 K, and equivalence ratio from 0.5 to 2.0. The calculated ignition delay time of τ_{NH_2} and τ_{OH} is defined as the time interval between zero to the maximum molar fraction of NH_2, and OH radical. The ignition process is calculated by constraining pressure and solving the energy equation. The end ignition time is set as 0.5 s, which is quite enough for the ignition process. The initial temperature and pressure, along with the inlet gas composition, are set at the beginning of simulations. The inlet gas compositions for calculating the ignition delay time of NH_3 flames at various H_2 addition ratios are summarized in Table S7 in Appendix A2.

Three mechanisms are employed in this research, namely, modified Dagaut–Kéromnès (DK) mechanism [36,37], Millar–Bowman (MB) mechanism [38], and Reductive Konnov (RE) mechanism [39]. There are 43 species and 271 elementary reactions containing 40 elementary reactions for H_2/CO chemistry from Kéromnès [37] in the DK mechanism. The replacement of H_2/CO chemistry from Kéromnès is proved to improve the prediction for the ignition delay time and laminar burning velocity of NH3 for involving mixture with H_2 and O_2. The DK mechanism can simulate the oxidation of NH_3, H_2, and carbon monoxide at elevated temperature and pressure conditions. The MB mechanism is a C4 kinetic model (including 58 species and 255 elementary reactions) in which the NH_3 oxidation reaction developed by Sandia National Laboratories and Stanford University is considered, which has confirmed to be a significant mechanism for NH_3 oxidation process during hydrocarbon combustion. The RE mechanism is a NH_3/H_2 kinetic model with 19 species and 80 elementary reactions established by the Université Catholique de Louvain. The RE mechanism was developed from reduction of Konnov mechanism, those small

Table 1
Fundamental key properties of various fuels [30,31].

Items	Ammonia	Hydrogen	Methanol	Gasoline
Lower heating value/MJ/kg	18.8	120.1	19.7	44.5
Lower heating value/MJ/L	11.3	8.5	15.5	29.7
Laminar burning velocity/m/s	0.015	3.51	0.50	0.58
Flammability limits, gas in air/vol%	15–28	4.7–75	6–36	0.6–8
Auto-ignition temperature/°C	651	571	470	230
Minimum ignition energy/mJ	8.0	0.0018	0.14	0.14
Density, 25 °C, 1 atm/g/L	0.703	0.082	787	740