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Study on premixed combustion characteristics of co-firing ammonia/methane fuels

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ABSTRACT

Ammonia is believed to eventually play an important role in substituting conventional fossil fuels for future energy systems. In this study, to gain a deep insight into the combustion properties of co-firing ammonia/methane fuel blends for the power and steel industry, a detailed chemical-kinetics mechanism model was developed for comprehensively modelling ammonia/methane fuels combustion. Characteristics of ignition delay time, unstretched laminar flame speed and NO, CO_2 and CO emissions in the exhaust gas were obtained over a wide range of equivalence ratios and ammonia fractions. High NO emissions will be a main problem as CO and CO_2 emissions tend to drop when adding ammonia into methane. To gain a further understanding of the effect of ammonia substituting methane for combustion use, analyses of laminar premixed flame structures were performed. The impact of ammonia substitution was illustrated by analysing relevant specific radicals. Furthermore, to study the combustion characteristics of ammonia/methane under more practical conditions, effects of engine relevant conditions (elevated pressure and initial temperature) were also studied. Results indicate that pressure has a more prominent effect than initial temperature and there is a good potential that unwanted emissions can be reduced significantly under industrial conditions.

1. Introduction

To deal with the contradiction between environment detrimental and human development, a low-carbon economy concept is regarded as the future choice of economic development via moderate and sustainable energy consumption, low greenhouse gas emissions and low pollution [1]. Recently, ammonia, which is a carbon free chemical, is receiving attention as an alternative fuel in the context of an ever increasing energy demand and concerns about global warming [2,3]. Just like hydrogen, ammonia can act as a potential enabler of a low-carbon economy, but without issues associated with hydrogen storage and distribution which are currently still tough barriers to the widespread use of hydrogen [4,5]. Since ammonia is widely used as an agricultural fertilizer, refrigeration liquid, and in industrial processes (e.g. steelmaking), knowledge on its production, delivery, storage, handling and distribution through existing infrastructures reaches more than a century of expertise. Moreover, ammonia has the added attraction that it can also be sold on international markets making it a very versatile and hence attractive commodity. Also, ammonia can be produced from different energy sources such as wind power, biomass, nuclear energy, etc., which means it is a promising green future fuel potentially yielding no carbon dioxide.

Thus, due to the potentially beneficial aspects of utilizing ammonia as a fuel, progress on the use of NH_3 to replace high intensive CO_2 production fuels is a main priority for groups working on this area [6–8]. However, previous studies also show that to achieve satisfying performance in combustion facilities, there are still considerable challenges for ammonia to be solved, e.g. toxicity, corrosion to container materials, narrow flammability range, high resistance to ignition, low burning velocity, etc. In order to improve ammonia combustion rate for successful applications combustion promoters have been proposed to be co-fired with ammonia. Some fundamental flame studies investigated the effect of burning ammonia/hydrogen fuel mixtures with deep insight into combustion chemical kinetics [4,9–11]. Some internal combustion engine studies tested different fuels for ammonia combustion implementation into practical transportation applications, such as hydrogen [2,8], gasoline [6,12], diesel [13,14], DME [15], etc. Some

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favourable results in IC engines studies indicate a good potential to use ammonia mixtures for practical power systems.

Furthermore, to apply ammonia into similarly responsive but larger power generators to meet local demands, the use of "green" ammonia in gas turbines for power generation is another promising proposition. Valera-Medina et al. [16–18] experimentally tested and numerically analysed ammonia/methane blends in a laboratory scale swirl combustor and suggested low swirl and different injection strategies to optimize gas turbine power generation. Kurata et al. [19] studied NH_3–CH_4–air combustion gas turbine power generation systems at various power outputs and suggested that mixed CH_4 improves the low-combustion intensity of NH_3 and effectively enhances the flame stability in the gas-turbine combustors. As a potential "substitute of natural gas", ammonia is more easily transportable than LNG. Furthermore, ammonia/methane blends could be used not only from green ammonia sources, but also from by-product ammonia obtained from industrial processes. Thus, ammonia substitution could support peak-hour energy consumption requirements with fuel cost reduction. For instance, an immediate beneficiary of this blend could be steelworks companies that produce ammonia as a by-product of coke oven gas cleaning [20,21]. More recently, a new research program "Power to Ammonia" has initiated in the Netherlands looking into potentially turning gas-fired power plants into 'super batteries' [22]. Initial tests will focus on co-firing ammonia with methane in order to determine fuel blends that cause the lowest impact on gas turbine systems in order to reduce retrofitting costs in currently running facilities. Actually, with ammonia co-firing, reduced CO_2 emissions in these projects can be achieved due to lower carbon content of the fuels. Base on the situations above, in this research ammonia/methane blends are appraised to be used to improve the performance of ammonia combustion and at the same time to use ammonia to substitute some conventional fossil fuels - natural gas as well, of which methane is the main ingredient.

To successfully utilize ammonia/methane combustion for practical application, it is essential to have a deep understanding on the characteristics of fundamental combustion properties of methane/ammonia fuel mixtures. There is a considerable amount of studies investigating ammonia-based flames experimentally and numerically [23–28]. For instance, Lindstedt et al. [26] conducted detailed chemistry modelling for ammonia oxidation and verified the mechanism in flat laminar premixed flames. Skreiberg et al. [27] studied the oxidation of ammonia in the presence of H_2, CO, and CH_4 below 1400 K under fuel-rich conditions. A detailed chemical kinetic model was established and validated against flow reactor measurements. Tian et al. [23] studied a series of premixed NH_3/CH_4/O_2/Ar flames at low pressure to identify the effect of different mole ratio of NH_3/CH_4 and also proposed a chemical mechanism based on the Skreiberg mechanism for premixed combustion of ammonia/methane. In this study only the stoichiometric conditions were investigated and the ammonia was still added in the fuel mixtures as the minor ingredient. Recently, the Tian mechanism was tested in several ammonia combustion studies [29–31] showing good performance. Mathieu and Petersen [28] investigated the ammonia oxidation in shock-tube experiments over a wide range of temperatures, pressures (up to 30 atm) and equivalence ratios. Specifically, in this study new ignition delay time measurements were used to provide data for ammonia oxidation under engine relevant conditions (e.g. pressure above 10 atm) which before then remained fairly unexplored. However, previously most of the relevant studies only have investigated small amounts of ammonia addition into methane and rarely comprehensively analysed the different combustion properties under a wide range of conditions regarding ammonia as main fuel.

Therefore, the objective of this study is to analyse the effects of ammonia substitution on ammonia/methane flames through numerical simulations with a proper detailed chemical reaction mechanism in order to help find the way and feasibility of implementing ammonia as a primary fuel. In the present study, properties such as autoignition, flame propagation, flame temperature and emissions concentration have been analysed to extend the knowledge of premixed ammonia/methane flame characteristics.

2. Methodology

2.1. Ignition delay times modelling

Autoignition is a fundamental phenomenon of premixed combustion studies, which is the spontaneous and homogeneous ignition of the fuel-air mixture. Therefore the ignition delay time, representing the time for a mixture to reach autoignition, is an essential property for premixed combustion, which is highly dependent on the reactivity of a mixture. Numerical prediction of ignition delay times is helpful in understanding autoignition parameters, detailed kinetics and reduction of detailed mechanisms. In practice, as an important well-known validation technology, computational prediction of ignition delay times is usually compared with shock-tube experiments [32,33]. In the present study, ignition delay times were modelled with a closed homogeneous reactor in Cantera [34]. The ignition delay times are extracted as the time corresponding to the steepest rate of OH generation [28]. The model is calculated at constant volume and adiabatic conditions. In the simulation, the ammonia and oxidiser mixtures are highly diluted to minimize effects of viscosity, heat transfer and non-equilibrium as performed in shock-tube experimental conditions [35]. The numerical work was carried out under the same conditions as in the experimental work performed by Mathieu et al. [28].

2.2. Freely propagating laminar flame modelling

In this study, a one dimensional premixed freely propagating flame model has been employed to study the premixed combustion of NH_3/CH_4 fuel blends. Numerical simulations were performed using the computational code of premixed flame from Cantera [34] for the modelling of laminar flames. The steady state mass, energy and species equations were solved with adaptive meshes and mixture-averaged transport parameters to get quick convergence to an accurate solution. This freely propagating flame model can provide analysis of unstretched flame speed, reaction rates, radical concentrations, sensitivity analyses, etc., as used in previous studies [31,36]. In the model, flame speed of the freely propagating flame is calculated based on a point of reference which is a fixed position on the flame. The laminar flame speed is defined as the inlet velocity that keeps the flame to stay in a fixed position. Then an eigenvalue can be obtained as flame speed from the solution method. More details of the well-established conservation equations for the one-dimensional laminar flame and the solution strategy can be referred to the Cantera's theory. In the present study, numerical simulations were conducted similarly to the experimental conditions in [25] firstly to verify the model in terms of laminar flame speed of NH_3/CH_4 mixtures. The validated model can be used to study other different parameters, e.g. the maximum temperature in the flames was extracted as the adiabatic flame temperature. Then the validated model was used to study the characteristics of NH_3/CH_4 mixtures under different conditions.