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An experimental and kinetic modeling study of the combustion behaviour of ammonia blended with methanol and ethanol at engine relevant conditions

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Introduction

Despite several benefits of ammonia (NH_3) as a promising carbon-free fuel, it has some barriers which hinder its effective utilization in combustion devices. These barriers include but are not limited to narrow flammability limits (16-25% by volume in air), high autoignition temperature, relatively low energy density, and pollutants. Most of these barriers can be overcome by blending ammonia with high energy density and/or high reactive fuels. Hence, co-firing NH_3 with renewable biofuels appears to be a good strategy. To this end, methanol (CH_3OH) and ethanol (C_2H_5OH) can be promising candidates to promote NH_3 combustion. These simple alcohols are long considered a clean fuel for spark ignition engines because of their high-octane rating and significantly low emission. Due to their remarkable combustion properties, they are attractive fuels to promote the combustion behaviour of ammonia.

In our previous work, we have extensively studied the blends of ammonia with the combustion promoters such as dimethyl ether (DME), dimethoxy methane (DMM), and diethyl ether (DEE) in various proportions [1,2]. Our works revealed the critical role of cross-reactions between the carbon and nitrogen family to accurately predict the combustion behaviour of the blends [2]. We found that the reactions of amino (NH_2) radicals with fuels and intermediates significantly affect the low-temperature oxidation kinetics of NH_3/oxygenate blends. Our recent theoretical work [3] demonstrated the critical importance of NH_2 reactions with CH_3OH and C_2H_5OH, particularly affecting the low temperature combustion behaviour of NH3-alcohol blends. The calculated reaction rate constants from this work have been implemented in our kinetic model to explore the blending effect of CH_3OH and C_2H_5OH on the combustion behaviour of NH_3. The main aim of this work is to develop a comprehensive kinetic model for the NH_3/CH_3OH and NH_3/C_2H_5OH blends at engine relevant conditions. The developed model has been extensively validated against the newly experimental data from this work and the available literature data for NH_3-C_1/C_2 alcohols chemical systems.

Experimental Details

Laminar flame speeds of NH_3/CH_3OH and NH_3/C_2H_5OH blends were measured using the constant volume spherical flame methodology as fully described in Halter et al. [4]. The measurement of the laminar flame speed of expanding spherical flames is obtained by using both pressure and flame radius growth, based on the hypothesis of an isentropic compression of the unburned gases following the ignition: thus, resulting in a simultaneous increase of both pressure and temperature within the vessel. Therefore, as each flame propagation is submitted to simultaneous pressure and temperature increase, the flame speed values are a function of the couple (P, T). The laminar flame speed were measured for $\chi_{CH3OH/C2H5OH}$ = 0, 25, 50 and 100% ($\chi_{CH3OH/C2H5OH} = \frac{CH3OH/C2H5OH}{NH3+CH3OH/C2H5OH}$ % (by mol)).

Ignition delay time (IDT) measurements of NH_3/ethanol blends were conducted utilizing the high- and low-pressure shock tubes described in [5,6]. The IDT were measured for χ_{C2H5OH} = 10 and 30% at 1, 10, and 20 bar and ϕ = 1.0, respectively. Additionally, simultaneous multi-species (CO, NO, and C_2H_5OH) measurements were carried out by employing the mid-IR laser absorption technique. Temperature and pressure dependence of the absorption-cross section of these species were also measured to accurately determine the species concentration in the rapidly changing thermodynamic properties of the chemical system.

Chemical Kinetic Modeling

This work is an ongoing effort aiming to build a comprehensive kinetic model for C/H/N/O chemical systems. For a few years, there has been a constant update on the theoretical rates of elementary chemistry in the ammonia sub-set. Despite this, there is still high uncertainty in ammonia sub-set chemistry. The knowledge of several important elementary reactions is still in its infancy. In several cases, the predictions of the kinetic model exhibit a significant discrepancy with the experimental data. The existing discrepancy motivated us to conduct the present study. The current kinetic model presents a major update in the ammonia kinetic model compared to all our past published models [1,7]. The new experimental data from this study and the newly available theoretical study from the literature motivated us to make a major update in the ammonia model. However, the main aim of this work is also to develop the kinetic model for NH_3/CH_3OH and NH_3/C_2H_5OH blends. The current kinetic model updates our recent modeling work characterizing the oxidation behavior of NH_3/DEE blends [2]. Several kinetic parameters have been updated in the present work following suggestions from the recently published experimental, theoretical, and modeling work. The updates were made on NH, NH_2, NH_3, N_xH_y, H_2NO, HONO, HNO_2, and HNO sub-mechanism. The cross-reactions between the nitrogen and carbon families relevant to NH_3/CH_3OH and NH_3/C_2H_5OH systems have also been included.

Results and Discussions

Figure 1 shows the laminar flame speed of NH_3/air as a function of pressure and temperature at φ = 1.0 (a) and ignition delay time of NH_3/ C_2H_5OH blends at φ = 1.0 and 20 bar (b). Fig. 1a displays the model predictions with the present work (blue solid line) and model prediction with our previous model (blue dashed lines); whereas other lines represent the model predictions using literature models. Clearly, there is a large discrepancy between different models. However, the present model performs better than all other models, and our model prediction is within the experimental uncertainty range.

Likewise, Figure 1b compares the current model predictions with the IDT experimental data. As seen, for both χ_{C2H5OH} = 10 and 30% blends, our model captured the experimental data remarkably. Black solid lines show the model predictions for neat NH_3. A small addition of C_2H_5OH (10%) can significantly shorten the IDT of NH_3. Further increase of C_2H_5OH to 20% doesn't enhance the ignition with the same magnitude.

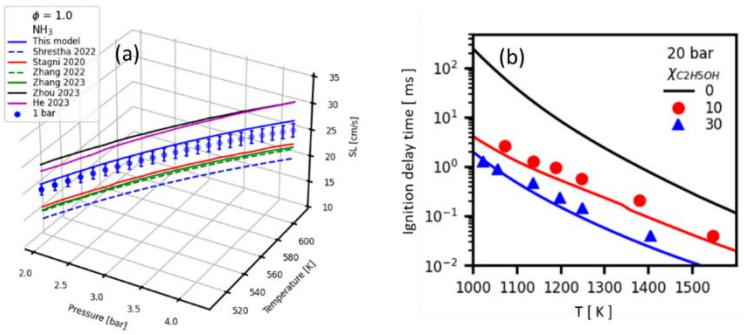

Figure 1: Laminar flame speed of ammonia/air as a function of pressure and temperature at φ = 1.0 (left) and ignition delay time of NH_3/ethanol blends (right) at φ = 1.0 and 20 bar. Symbols: present experimental work. (a): solid blue line (this model), rest (literature model). (b): lines (this model).

Conclusions

We measured the laminar flame speeds of NH_3 and its blends CH_3OH using the combustion vessel at φ = 1.0, 2 – 7 bar, 508 – 610 K for NH_3/air, 2 – 9.6 bar, 506 – 645 K, for NH_3/CH_3OH/air, and 2 – 11.3 bar, 503 – 645 K, for NH_3/C_2H_5OH/air. We found that adding CH_3OH and C_2H_5OH to NH_3 significantly enhanced the laminar flame speed of ammonia. We also determined IDTs and measured multi-species in real time for various blends of NH_3/C_2H_5OH in shock tubes over a wide range of conditions. The addition of C_2H_5OH significantly improved the reactivity of NH_3, leading to the shortening of auto-ignition timing.

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