Kinetic study on the influence of blending ethanol and dimethyl ether on the combustion behavior of ammonia

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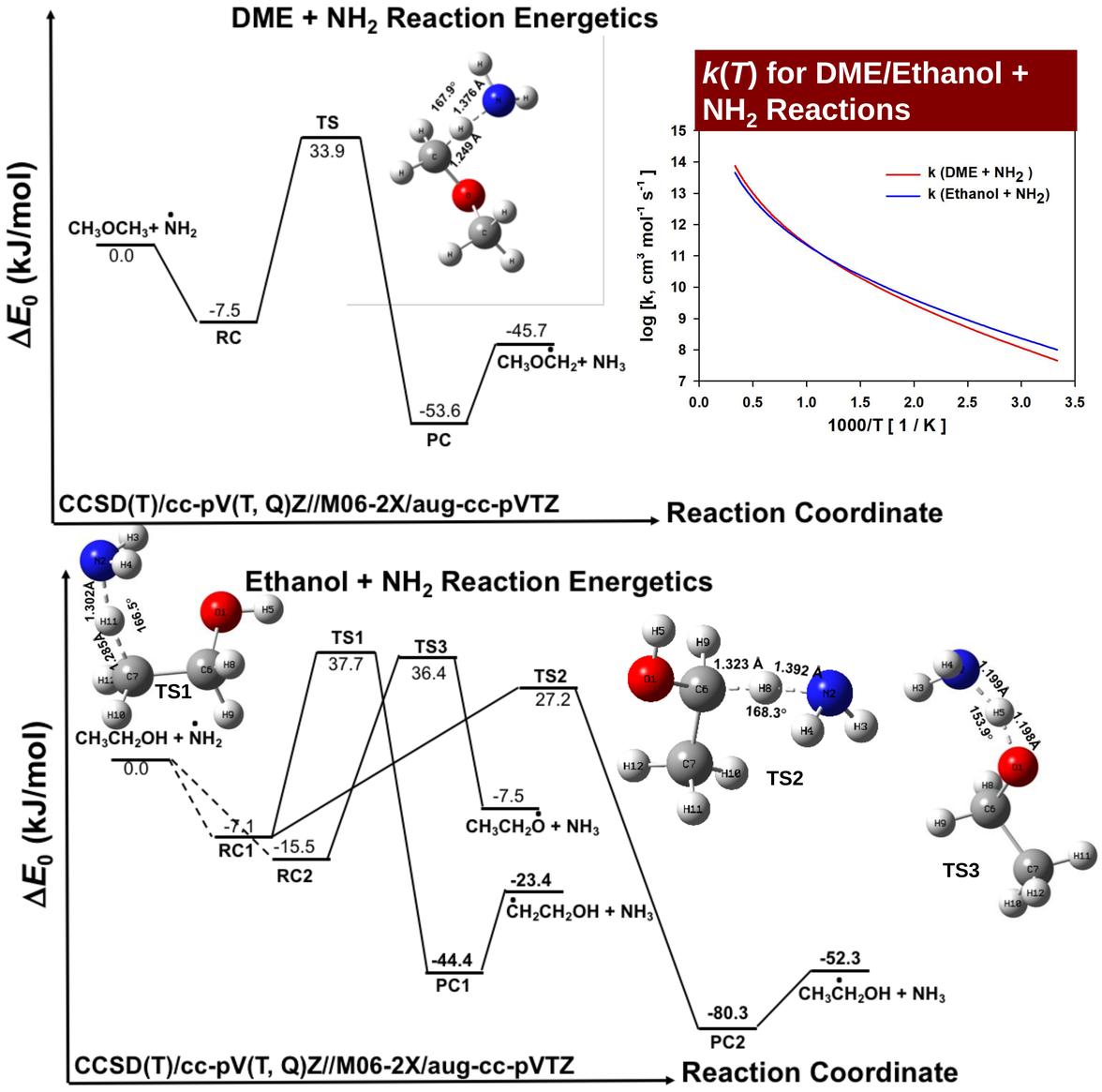
INTRODUCTION

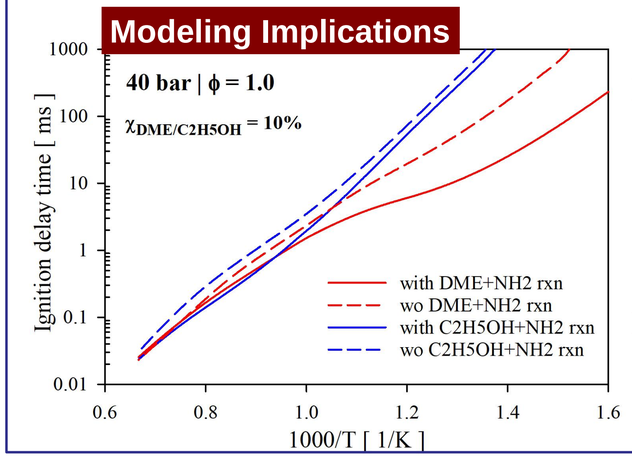
- Over the past few years, ammonia has caught attention for its effective use in combustion devices to mitigate global warming.
- Blending NH_3 with high reactivity fuels can overcome some of the inherent challenges of pure NH_3 combustion. Therefore, we carried out a comparative study on the blending effects of ethanol (C_2H_5OH) and dimethyl ether (DME, CH_3OCH_3) on NH_3 combustion. These oxygenates are isomeric fuels, and can be produced from biomass.
- Here, we present a kinetic modeling study aiming to characterize the combustion behavior of NH_3 blended with DME and ethanol.

THEORY AND MODELING

- The kinetics of NH_2 radicals reactions with DME and Ethanol were investigated using *ab*-initio/statistical rate theory calculations.
- The potential energy surfaces were mapped out at the CCSD(T)/cc-pV(T, Q)Z//M06-2X//aug-cc-pVTZ level of theory.
- Rate coefficients were calculated using conventional TST theory, then incorporated into our recently published kinetic model [1].



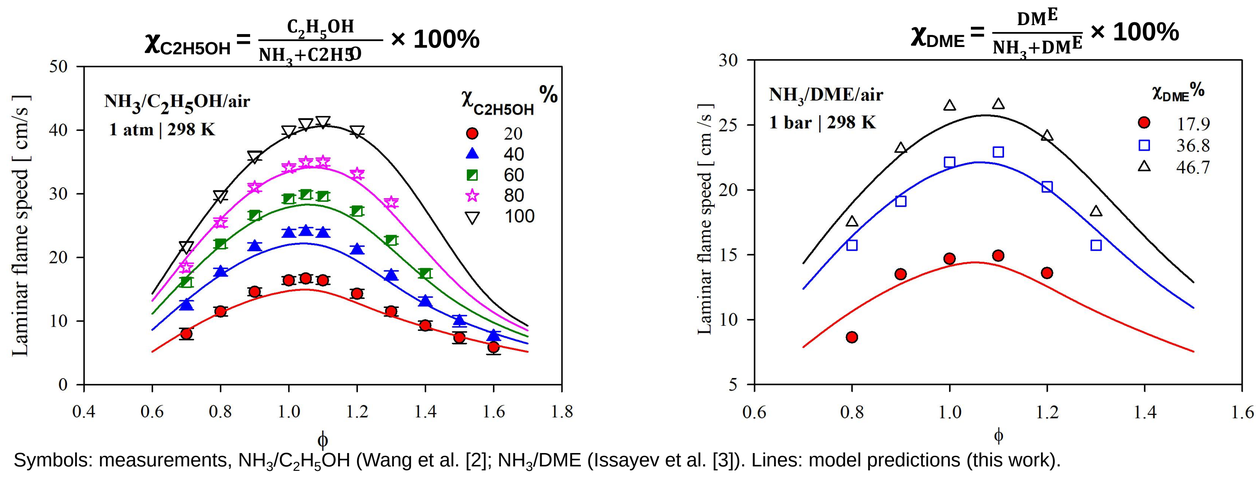
Modeling Implications



- As seen, the reactions of NH_2 with ethanol and DME significantly impact the ignition delay times of the blends of these fuels with ammonia.
- The reaction shows higher sensitivity for low-temperature oxidation kinetics of the fuel blends.

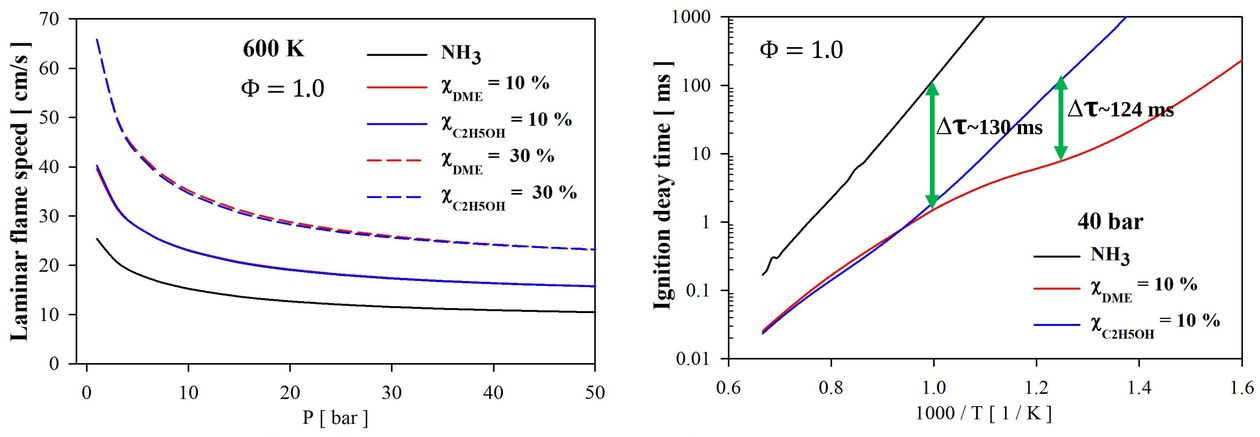
RESULTS AND DISCUSSION

Model Validation



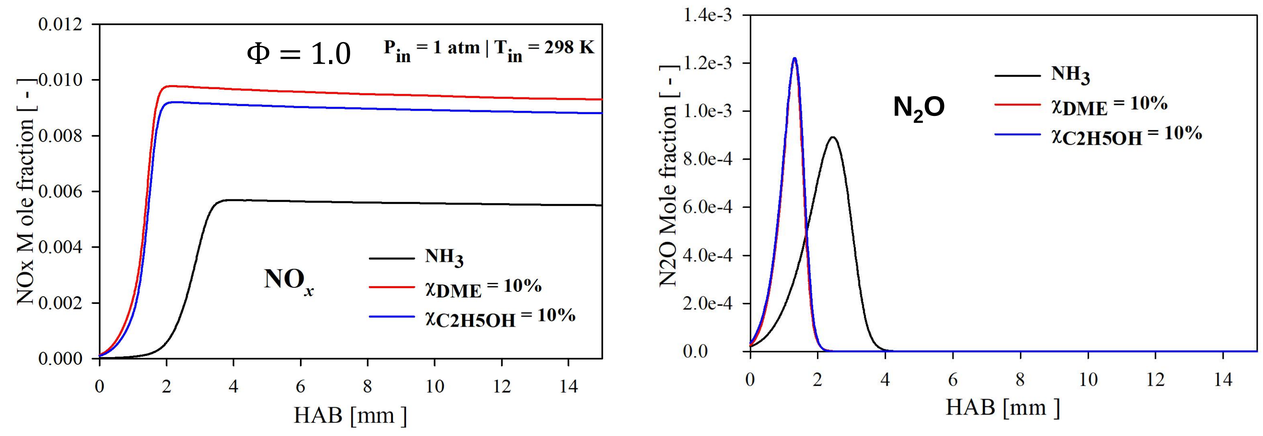
Symbols: measurements, NH_3/C_2H_5OH (Wang et al. [2]; NH_3/DME (Issayev et al. [3]). Lines: model predictions (this work).

Blending Effect Comparison Between C_2H_5OH and DME in NH_3



- Both DME and C_2H_5OH enhance the laminar flame speed of NH_3 equally.
- DME shows a more promising enhancement effect at low temperatures than C_2H_5OH for a given blend in NH_3.

NO_x Formation in Flames



- For the blends, NO_x formation was significantly increased compared to neat NH_3, which can be attributed to the reactive OH and H species increase.

CONCLUSIONS

- The reactions of NH_2 radicals with C_2H_5OH and DME were investigated using the *ab*-initio/TST method. This reaction plays a significant role to reliably predict the ignition behavior of NH_3 in C_2H_5OH and/or DME.
- A detailed kinetic model was developed, which remarkably captured the available literature data of ammonia blended with DME and C_2H_5OH.
- Both ethanol and DME enhance the laminar flame speed of NH_3 with equal propensity. However, NH_3 blended with DME is far more reactive than ethanol at low temperatures.
- For the blends, NO_x formation was found to increase.

References

[1] Shrestha et al., A detailed chemical insights into the kinetics of diethyl ether enhancing ammonia combustion and the importance of NOx recycling mechanism, Fuel Communications 10 (2022) 100051.

[2] Wang et al., Experimental and kinetic study on the laminar burning velocities of NH3 mixing with CH3OH and C2H5OH in premixed flames, Combust. Flame. 229 (2021) 111392

[3] Issayev et al., Ignition delay time and laminar flame speed measurements of ammonia blended with dimethyl ether: A promising low carbon fuel blend, Renew. Energy. 181 (2022) 1353–1370