Reaction pathway analysis of plasma-assisted fuel reforming (PAFR) with ammonia/air mixtures

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Abstract: In this work, we perform reaction pathway analysis of plasma-assisted fuel reforming (PAFR) with ammonia/air mixtures. The model incorporates detailed energy branching mechanisms to simulate the interaction of plasma discharges with the ammonia/air mixture, highlighting the influence of plasma on fuel reforming (hydrogen), radical species generation, and potential to enhance combustion processes.

1. Introduction

Non-equilibrium plasma-based igniters can be easily integrated into modern gas turbines and internal combustion (IC) engines, promoting localized volumetric ignition kernel development through both thermal and chemical assistance [1]. Unlike traditional ignition systems, plasma igniters enable faster, more reliable ignition under lean or high-pressure conditions, which are critical for improving fuel efficiency and reducing emissions [2]. A key advantage of plasma-assisted combustion (PAC) lies in its ability to generate radical species and intermediate reactants that lower the ignition energy threshold. These radicals accelerate chemical reactions, thereby enhancing flame stability and extending the operability of engines to extreme conditions [3]. This study focuses on developing 0D and phenomenological modelling to investigate plasma-

This study focuses on developing 0D and 2D phenomenological modelling to investigate plasma-assisted fuel reforming (PAFR) with ammonia/air mixtures, aiming to elucidate the role of ammonia and radical species in enhancing combustion.

2. Methods

To analyze the reaction pathways of plasma-assisted fuel reforming (PAFR) with ammonia/air mixtures, we use our in-house 0D NRPD code [1] by conducting 0D plasma discharges at 800 K. By solving the species number density evolution and gas energy equations, we obtain power density functions for electrons, gas molecules, and ions, providing detailed insights into the evolution of chemical species, energy deposition, and vibrational energy transfer processes during the plasma discharge. These results enable the identification of key reforming pathways and the quantification of plasma parameter impacts on the fuel reforming process.

3. Results and Discussion

Fig. 1 shows path flux analyses to understand the consumption of NH3 during the plasma discharge and ignition. The deposited energy is $0.05~\mathrm{J/cm^3}$ at two values of E/N: 0 and 150 Td (1 Td = $10^{-17}~\mathrm{V~cm^2}$). Specifically, we observe that the pathway from NH2 to NH is more dominant at 150 Td, facilitated by the electric field influence, which enhances the decomposition of NH2 into NH. We will also observe the effects of E/N on reaction pathways of reactants, products, and radicals under different sets of initial conditions.

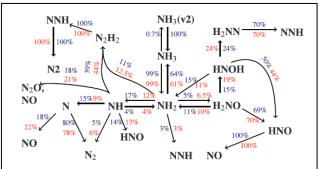


Fig. 1. NH3 consumption with NH3/air mixtures under nanosecond thermal energy deposition in a constant volume 0D reactor with two values of E/N: 0 (red) and 150 (blue) [1].

4. Conclusion

This study demonstrates the effectiveness of 0D and 2D phenomenological modeling in analyzing plasma-assisted fuel reforming (PAFR) with ammonia/air mixtures. By employing our in-house NRPD code, we identified key reaction pathways and the significant influence of the electric field (E/N) on the decomposition of NH3 and the formation of radicals. The findings highlight the critical role of plasma parameters in enhancing chemical reactivity, providing valuable insights for optimizing PAFR systems under varying operational conditions.

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References

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