

Numerical Modeling of n-Hexane Hydropyrolysis with an Optimized Kinetic Mechanism in a Rotating Gliding Arc Reactor

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Abstract: This study explores hydrogen plasma pyrolysis for n-hexane cracking. An optimized kinetic mechanism was developed to estimate the chemical conversion and selectivity in n-hexane hydropyrolysis. This simple and accurate reaction mechanism was incorporated into CFD analysis. The results show gas mixing and feed injection strategies are key factors for improving the conversion and maximizing the C2 monomer production.

1. Introduction

As the effects of climate change become increasingly severe, the urgency for reducing carbon emissions has never been greater. In most petrochemical processes, hydrocarbon pyrolysis depends on fossil fuels for heat source. To address this challenge, the electrification of heat supply using renewable energy sources has emerged as a key strategy for decarbonization. Therefore, plasma technology can be a promising solution[1]. It can efficiently convert electrical energy into high-temperature heat required for pyrolysis.

2. Methods

A mixture of hydrogen and Argon was used as the plasma gas to suppress solid carbon formation and improve heat transfer by promoting uniform temperature distribution. n-Hexane, commonly used as a surrogate for naphtha, was employed as the feedstock for the plasma cracking process. To model and optimize the operating conditions, we developed an in-house chemical reaction mechanism and performed CFD analysis. The reaction mechanism includes a total of 130 reactions, optimized to reduce the computational cost.

3. Results and Discussion

Our mechanism, generated using the Reaction Mechanism Generator (RMG) [2] for n-Hexane hydropyrolysis, was validated through comparisons with experimental data [2] and simulation results obtained with the existing chemical kinetics mechanisms. As shown in Fig.1, our mechanism aligns well with the experimental results, particularly demonstrating high accuracy for our target product, ethylene.

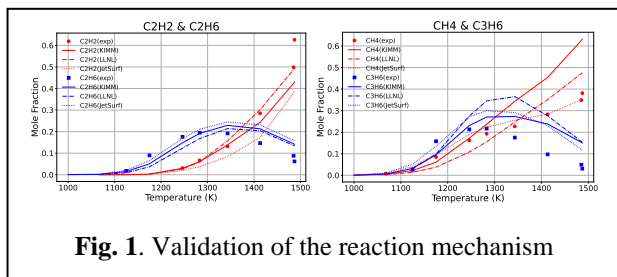


Fig. 1. Validation of the reaction mechanism

Next, we conducted a CFD simulation to evaluate the conversion rate variations based on the feed injection location. Figure 2 illustrates the variation in reactant inlet locations, with one case positioned at the reactor wall and the other at the reactor center. This difference can be attributed to the degree of mixing with the reactant and the plasma discharge gas. The findings suggest that mixing plays a crucial role in determining the conversion rate.

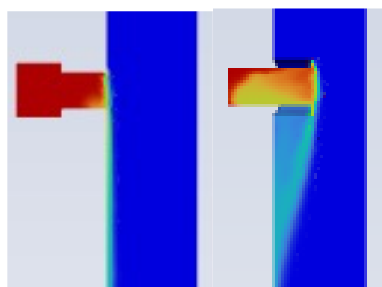


Fig. 2. CFD simulation results for n-hexane conversion based on reactant inlet location (wall(left) vs. center(right))

4. Conclusion

In this study, numerical analysis was conducted to determine the optimal conditions for maximizing the conversion rate of n-hexane and selectivity of the target product, ethylene. The results showed that efficient mixing of the plasma discharge gas with the reactants inside the reactor is significant for enhancing pyrolysis efficiency.

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References

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