Kinetic Model for Single-Step Ethanol to Butene-Rich Olefin Process over Cu-Y/Beta Catalysts

Background/Objective

Direct conversion of ethanol to C_{3+} olefins for the production of sustainable aviation fuel (SAF), is a promising supplement to conventional fossil-based jet fuel. However, a comprehensive and validated kinetic model capable of describing the process at the reactor scale necessary for SAF scale-up, optimization, and techno-economic analysis is currently unavailable.

Approach

A comprehensive kinetic model for ethanol-to-butene-rich olefins over bifunctional Cu-Y/Beta catalysts was developed by:

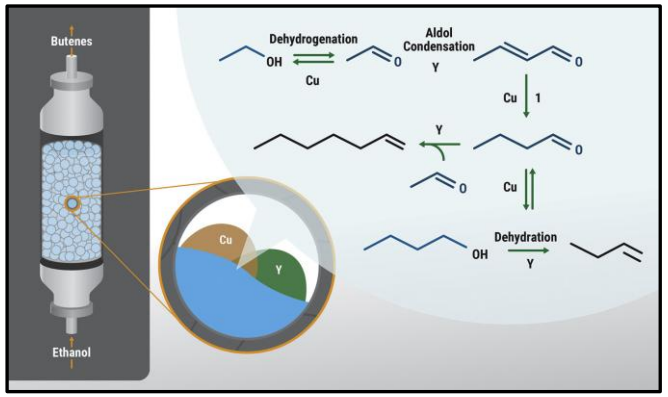
- Defining the reaction network using chemical equations and identifying the associated active sites
- Formulating the rate expressions and conducting rate analysis.

Results

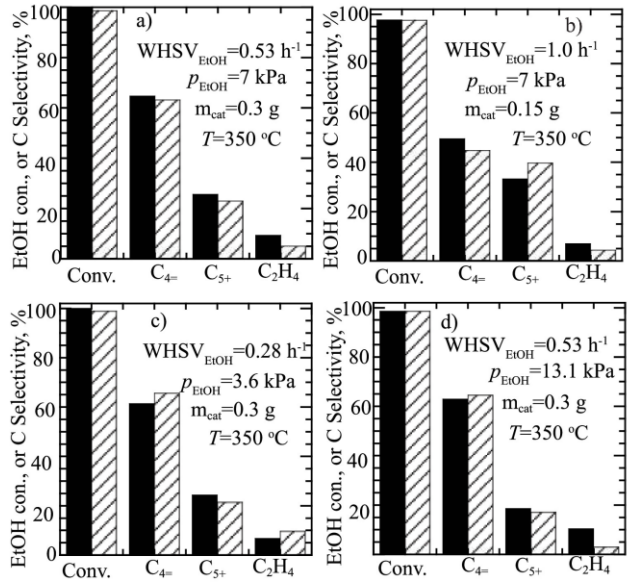
- The model captured co- and by-product formation with explicit temperature and weight hourly space velocity (WHSV) dependencies and formulated intrinsic rate expressions for bi-functional Cu-Y/Beta catalysts using the Langmuir-Hinshelwood-Hougen-Watson (LHHW) equation.
- The model was validated against lab-scale data through 2-D reactor modeling.
- A transferable framework for reactor design toward ethanol-to-SAF processes using this model was developed.

Significance/Impacts

This study presents the first intrinsic kinetic model for the single-step conversion of ethanol to butene-rich olefins over bifunctional Cu-Y/Beta catalysts, addressing a critical gap in the design and scale-up of SAF processes.



2-D reactor model and product outputs



Comparison of model-predicted ethanol conversion and carbon selectivities with experimental results

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