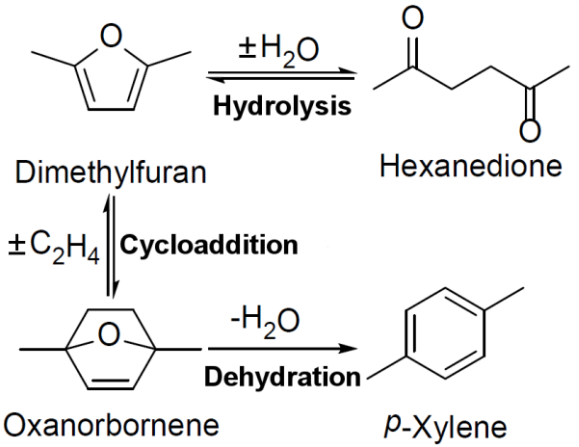
Kinetic Regimes in the Production of Renewable *p*-Xylene

Scientific Achievement

Experiments and hybrid multiscale models for the production of *p*-xylene from DMF and ethylene indicate two regimes vs. acid site concentration and reveal the mechanism for tandem Lewis/Brønsted catalyzed reactions.

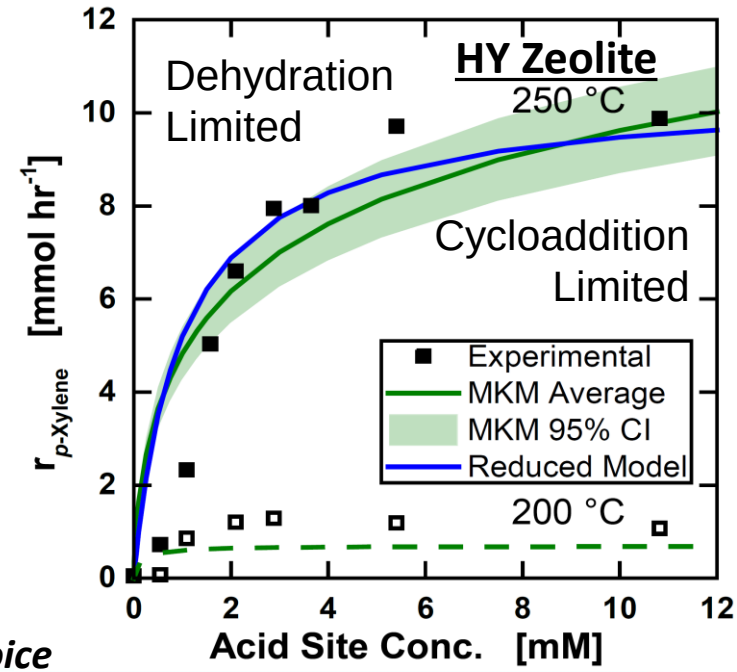


Significance and Impact

- ***p*-xylene is a target molecule for plastics manufacturing.**
- ***p*-xylene production transitions from being dehydration- to cycloaddition-limited as catalyst loading increases.**
- **Our work is the first to demonstrate multiple kinetic regimes for tandem reactions.**

Research Details

- Kinetic experiments indicate two regimes despite cycloaddition having a higher energy barrier.
- Embedded cluster ONIOM and microkinetic calculations were performed and reduced models were developed.
- Experimental and modeling production rates, reaction orders, and activation energies are in good agreement.



Patet *et al.* **ACS Catal. 2015**, DOI: 10.1021/cs5020783. ***ACS Editors' Choice***

U.S. DEPARTMENT OF ENERGY | Office of Science

Work was performed at the Universities of Minnesota, Massachusetts and Delaware by the group of Dauenhauer, Fan, Caratzoulas and Vlachos