

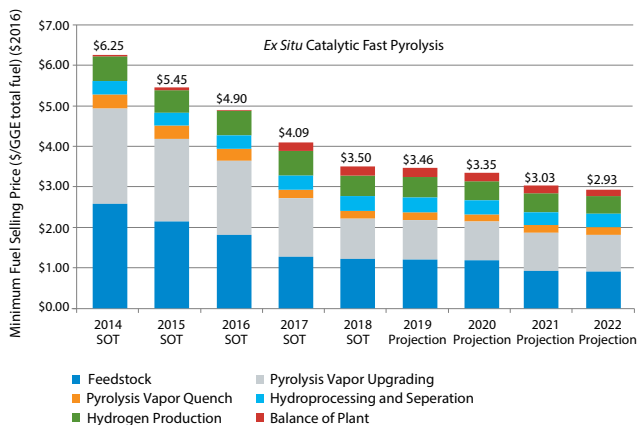
## NREL'S CAPABILITIES IN TECHNO-ECONOMIC AND SUSTAINABILITY ANALYSES FOR THERMAL AND CATALYTIC CONVERSION OF BIOMASS AND WASTE FEEDSTOCKS



### CORE CAPABILITIES AND APPLICATIONS

Our analysis team integrates experimental results with detailed process models to estimate conversion costs.

- Offer rigorous process modeling using best-in-class industrially relevant tools
- Provide leading-edge custom expertise developed for biomass and waste conversion research
- Guide research and development (R&D) towards the most impactful areas for cost reduction and quantify associated research metrics
- Reduce cost of R&D and accelerate technology advancement through predictive capabilities
- Quantify sustainability impacts of scale-up implementation of new technologies
- Quantify the relevance of lab-scale research in future industrial contexts.



Top Photo: An NREL engineer works on a target model for commercial scale cellulosic biofuel production. Photo by Dennis Schroeder, NREL 30263

#### RIGOROUS PROCESS SIMULATIONS AND HEAT INTEGRATION

Conceptual process simulations with detailed heat integration help predict process outputs and quantify inside battery limit versus outside battery limit costs based on current research results and future projections.

#### ECONOMICS BASED ON PROCESS SIMULATIONS

Economics tied to detailed process simulations provide a rigorous and consistent basis for cost estimation, identification of key economic drivers, and comparison across technologies.

#### INTEGRATION OF EXPERIMENTAL AND ANALYTICAL DATA

Integration of experimental and analytical data in process simulations helps improve the models and provide accurate and constructive feedback for the research.

#### PREDICTIVE KINETIC, REACTOR, PHASE EQUILIBRIUM, AND REFINERY MODELS

Predictive models help optimize operating conditions, process recycles, and separations in integrated conceptual designs, without costly lab reconfigurations and experiments.

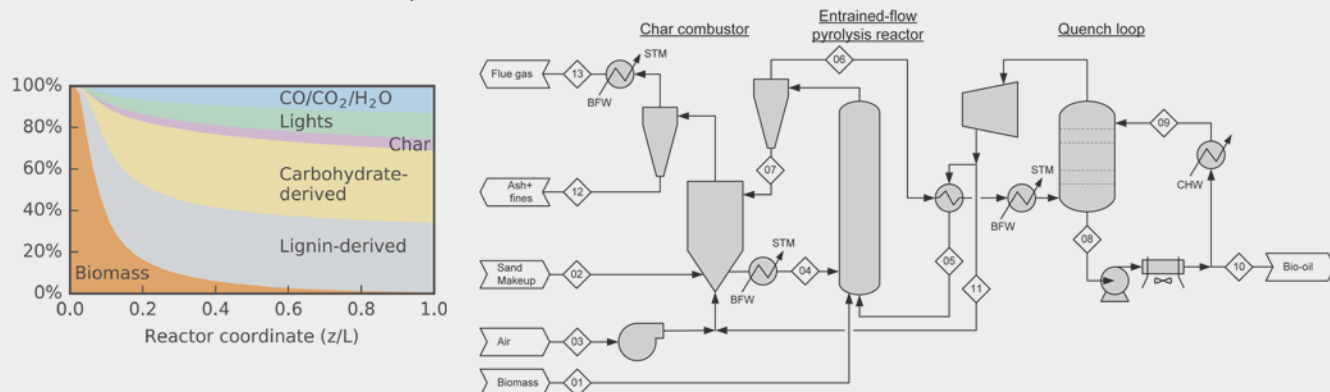
#### SUSTAINABILITY ANALYSIS

The NREL analysis team quantifies process greenhouse gas emissions, water use, and other environmental impacts relevant to meeting regulatory mandates such as the Renewable Fuel Standard and the Low Carbon Fuel Standard Program.

# RECENT SUCCESSES

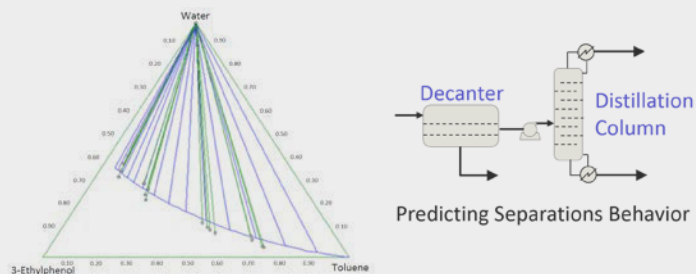
## DETAILED REACTOR MODELING IN PROCESS SIMULATIONS:

NREL successfully integrated a fast pyrolysis reactor model with reaction kinetics and one-dimensional fluid dynamics into a process simulation. This integration will enhance our predictive modeling capabilities for catalytic fast pyrolysis processes as reaction kinetics are established for catalytic materials.



## PHASE EQUILIBRIUM AND SEPARATIONS:

Collaboration with the National Institute of Standards and Technology has led to predictive phase equilibrium models and associated experimental validation, which enables modeling of separations for less-studied biomass-derived molecules without having to perform a significant number of experiments.



## Highlighted Publications

A. Dutta, et al. "Conceptual Process Design and Techno-Economic Assessment of *Ex Situ* Catalytic Fast Pyrolysis of Biomass: A Fixed Bed Reactor Implementation Scenario for Future Feasibility." *Topics in Catalysis*. DOI: 10.1007/s11244-015-0500-z.

A. Dutta, et al. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels: Thermochemical Research Pathways with In Situ and Ex Situ Upgrading of Fast Pyrolysis Vapors*. nrel.gov/docs/fy15osti/62455.pdf.

E. Tan, et al. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons via Indirect Liquefaction: Thermochemical Research Pathway to High-Octane Gasoline Blendstock Through Methanol/Dimethyl Ether Intermediates*. nrel.gov/docs/fy15osti/62402.pdf.

D. Humbird, et al. "One-Dimensional Biomass Fast Pyrolysis Model with Reaction Kinetics Integrated in an Aspen Plus Biorefinery Process Model." *ACS Sustainable Chem. Eng.* DOI: 10.1021/acssuschemeng.6b02809.

M.B. Griffin, et al. "Driving Towards Cost-Competitive Biofuels through Catalytic Fast Pyrolysis by Rethinking Catalyst Selection and Reactor Configuration." *Energy and Environmental Science*. DOI: 10.1039/C8EE01872C.

## Find Out More

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