NREL
NATIONAL RENEWABLE ENERGY LABORATORY

NATIONAL
BIOENERGY CENTER

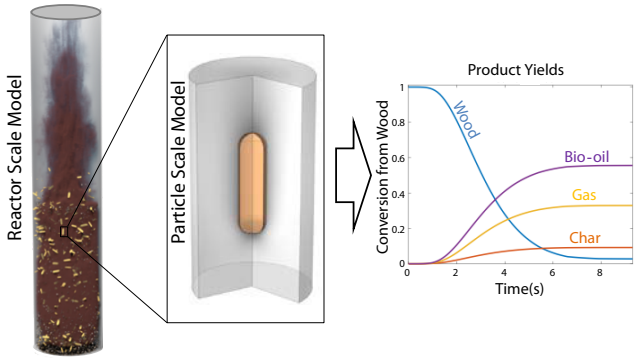
NREL'S CAPABILITIES IN **MODELING AND SIMULATION OF THERMAL AND CATALYTIC CONVERSION PROCESSES**

CORE CAPABILITIES AND APPLICATIONS

From molecular-scale chemistry to process-scale operations, NREL's thermal and catalytic simulation and modeling team strives to integrate experimental and computational capabilities that address the complexities of real biomass and waste streams, enabling development of renewable energy technologies.

NREL's modeling team works together with experimental teams to simulate and predict the behavior of materials and systems across multiple lengths and timescales. NREL's modeling helps our partners make informed decisions about their specific conversion process.

Integrated Multiscale Fluid Bed Pyrolysis Model



Feedstock-specific particle simulations used to predict pyrolysis oil yields in a fluidized bed reactor.

Top Photo: NREL researchers investigate catalyst stability and activity in the Biomass Surface Characterization Lab. *Photo by Dennis Schroeder, NREL 52765*

UNDERSTANDING CATALYST REACTIVITY

NREL's modeling team utilizes quantum mechanics, molecular dynamics, and computational fluid dynamics to understand the activity and properties of catalysts and other functional materials. Our simulations provide information on reaction kinetics and mechanisms, poisoning and deactivation, and heat/mass/momentum transport phenomena.

PREDICTING PERFORMANCE

Integrating across modeling scales from atomistic-kinetics, microstructurally accurate particle models, and reactor-scale flow simulations, NREL's modeling team develops experimentally validated models using fundamental principles to predict process performance (e.g., yields) based on system operating conditions and feedstock attributes.

OPTIMIZING DESIGN AND OPERATIONS

Our modeling team provides its partners with actionable information that guides the design of new materials (compositional and structural), enables optimization of operating conditions, and guides scale-up from lab to commercial, all while reducing the time and cost of discovery.

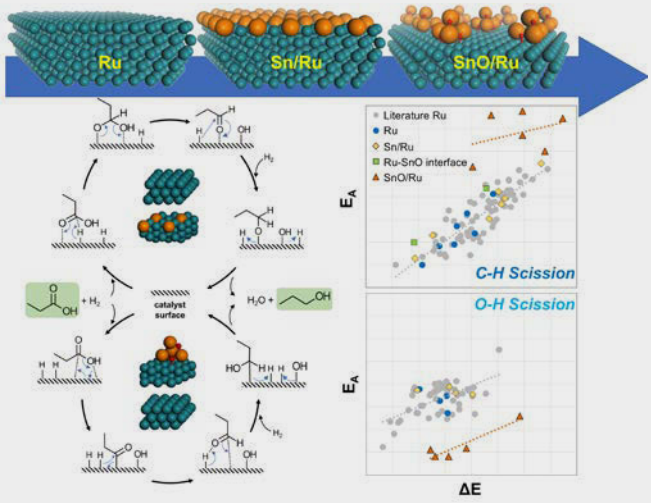
Let Us Accelerate Your Discovery

Whether you're performing basic research and development or scaling your technology to pilot and beyond, the NREL thermal and catalytic simulation and modeling team is ready to support your technology development today.

RECENT SUCCESSES

DESIGN OF INVERSE BIMETALLIC CATALYSTS USING COMPUTATIONAL MODELING

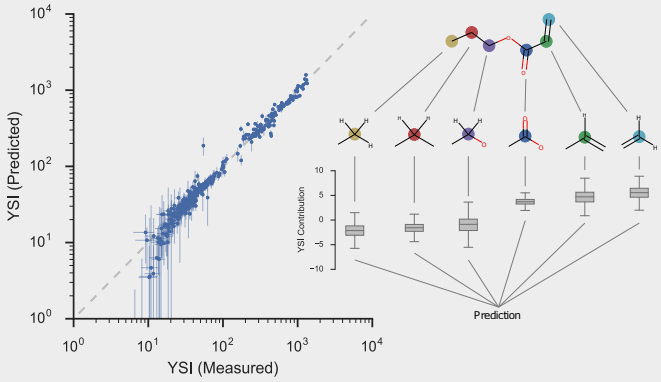
The design of inverse bimetallic catalysts for selective hydrogenation is an emerging frontier for NREL's catalyst development teams. Density functional theory models—built based on spectroscopic evidence and catalytic testing—identified eactivity of individual phases and were able to provide guidance for optimal catalyst design targets.



Computational modeling assessed metal-oxide interfaces and alloying for selective hydrogenation of propionic acid.

DEVELOPING NEW TOOLS TO PREDICT FUEL PROPERTIES

The NREL modeling team has developed a rapid screening tool based on machine learning and Bayesian regression tools to determine fuel properties from molecular structure, enabling experimental groups to focus resources on the best opportunities to meet industry requirements for new performance-advantaged fuels.



Group contribution method for estimating the yield sooting index.

Highlighted Publications

D.R. Vardon, et al. "Ru-Sn/AC for the Aqueous-Phase Reduction of Succinic Acid to 1,4-Butanediol under Continuous Process Conditions." *ACS Catal*. DOI: 10.1021/acscatal.7b02015.

P.N. Ciesielski, et al. "Advancing Catalytic Fast Pyrolysis through Integrated Multiscale Modeling and Experimentation: Challenges, Progress, and Perspectives." *WIREs Energy Environ*. DOI: 10.1002/wene.297.

D.D. Das, et al. "Measuring and Predicting Sooting Tendencies of Oxygenates, Alkanes, Alkenes, Cycloalkanes, and Aromatics on a Unified cale." *Comb. Flame*. DOI: 10.1016/j.combustflam .2017.12.005.

Find Out More

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