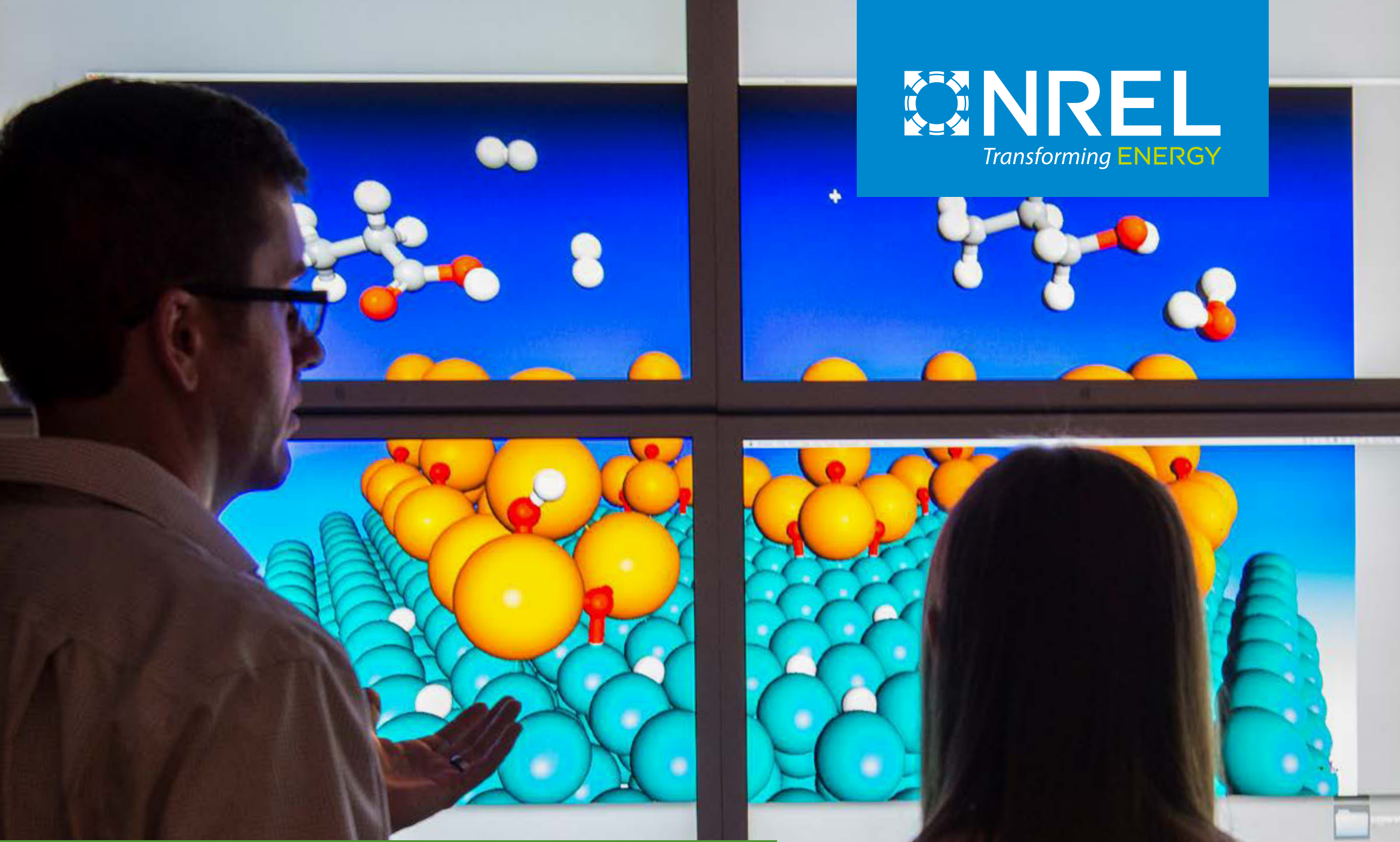


Driving Catalysis Innovation for Tomorrow's Feedstocks

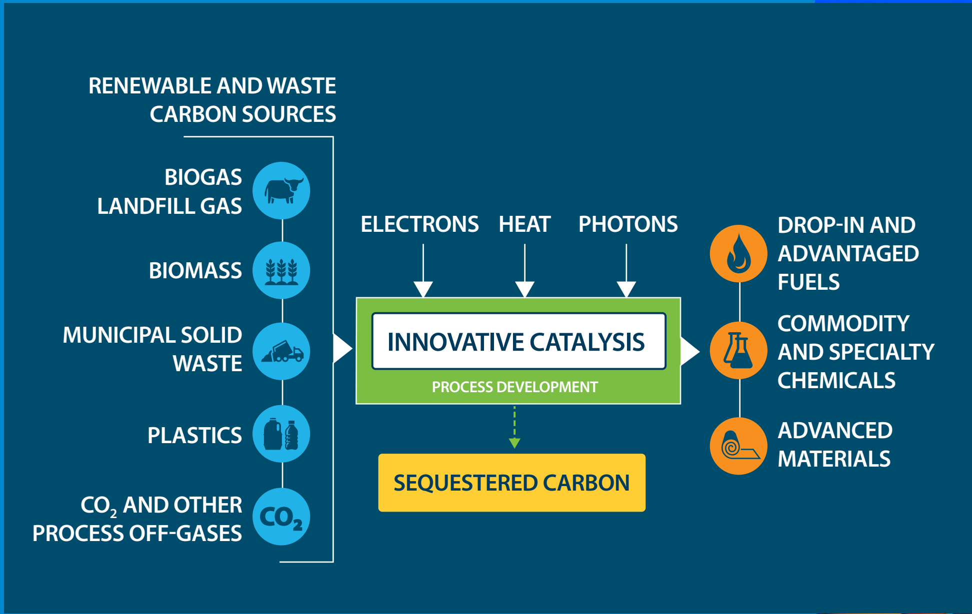
Overview of NREL's Catalytic Carbon Transformation Platform

OUR GOAL

Lead innovation in the catalytic conversion of renewable and waste carbon sources

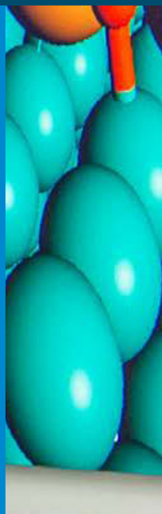
The U.S. Department of Energy's National Renewable Energy Laboratory (NREL) performs cutting-edge research and development (R&D) to advance innovative and cost-effective solutions that move the production of renewable fuels, products, chemicals, and energy to market.

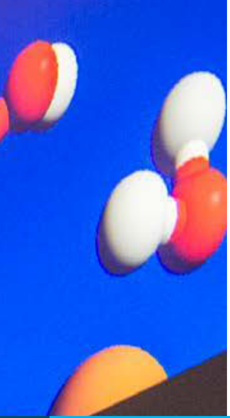
From thermal deconstruction and catalytic upgrading to computational modeling and *operando* catalyst characterization, NREL is pioneering the way to a sustainable future through carbon recycling, where captured carbon in biomass and waste sources can be converted back into advanced materials, commodity and specialty chemicals, and drop-in and advantaged fuels, ***all enabled by catalysis***.



On an annual basis, the United States currently emits ~6 billion tons of carbon dioxide (CO_2), generates over 35 million tons of carbon-rich plastics with 75% of those plastics being landfilled after use, and has the potential to sustainably produce over 1 billion tons of non-food biomass. This creates a vast opportunity to utilize renewable and waste carbon sources as feedstocks for our energy- and products-driven economy.

To accelerate innovation, NREL researchers collaborate closely with industry, academia, and government partners to address critical technology risks across length and time scales through foundational science. We believe that only through hypothesis-driven R&D coupled with rich multidisciplinary collaboration can global-scale challenges be overcome.





OUR APPROACH

Our technical approach is based on three core principles:

1) **Understanding the fundamental relationships that govern a process enables transformative breakthroughs in technology development**
2) **Transitioning technologies from discovery to the cusp of commercialization requires integrated catalysis and process R&D that bridges the gap between foundational science and applied engineering**
3) **Driving R&D from the bottom up through fundamental science and the top down with techno-economic analysis and life cycle assessment accelerates technology advancement.**

Aligned with these principles, NREL's staged, multiscale evaluation approach improves research efficiency and reduces cost. Our catalytic carbon transformation platform links foundational science with applied engineering by executing catalysis and process R&D across multiple scales, ranging from lab scale (mg) to pilot scale (kg).

Our team couples this approach with overarching enabling efforts in feedstock analysis, comprehensive process stream characterization, computational modeling from atomic scale to process scale, integrated scale-up, and world-class techno-economic analysis and life cycle assessment.

Driven by energy inputs from electrons, heat, and photons, advancements in catalysis enable the transformation of renewable and waste carbon sources into fuels, chemicals, and materials while generating carbon-negative opportunities through CO_2 sequestration and solid carbon products.

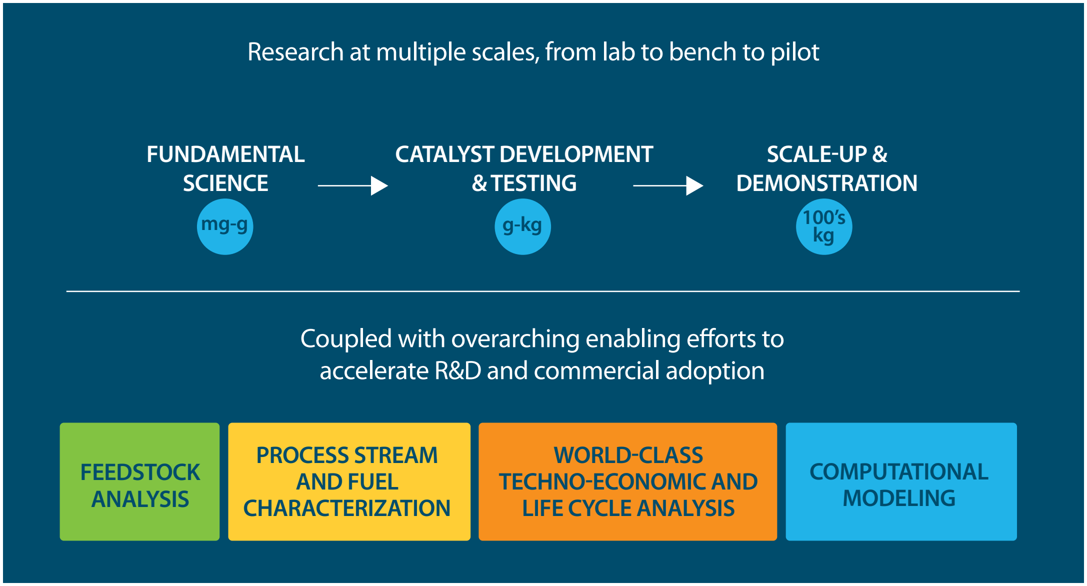


Photo by Dennis Schroeder, NREL 52765

MULTISCALE **THERMAL DECONSTRUCTION**

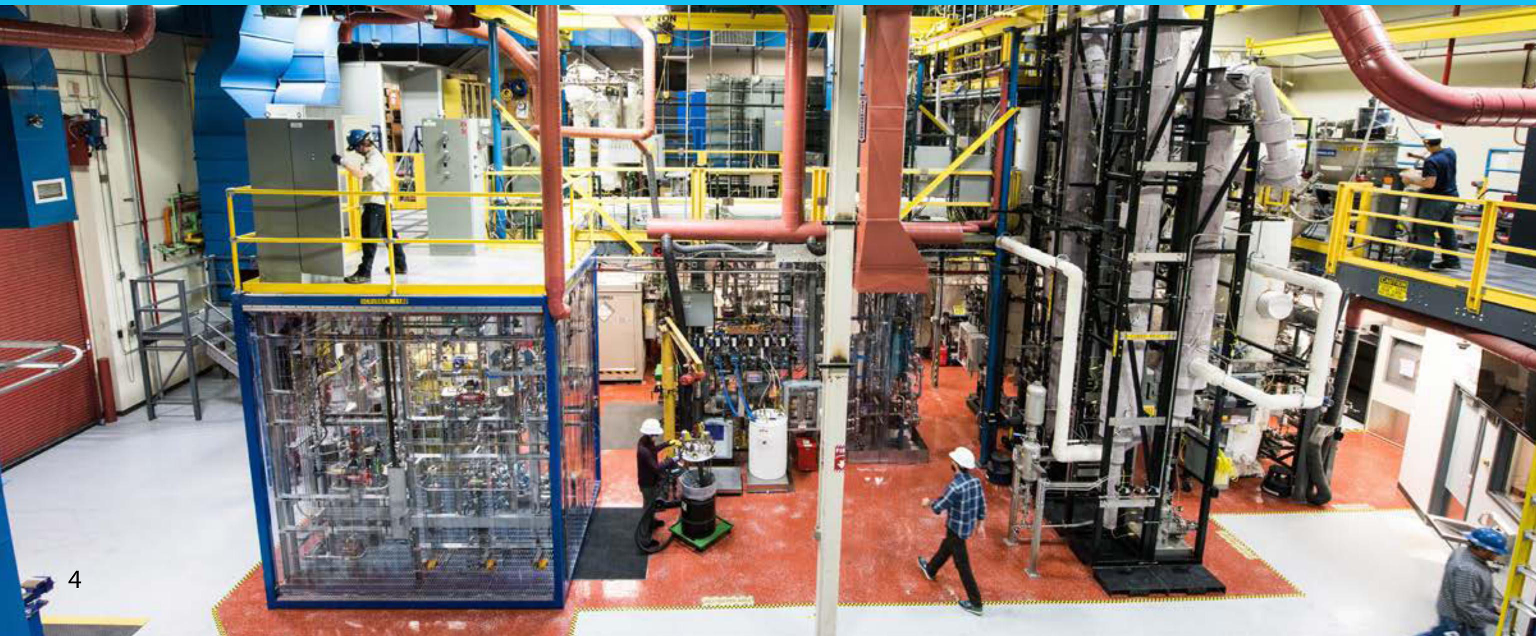
NREL researchers gain a better understanding of the thermal deconstruction of carbon-rich renewable and waste feedstocks across scales by (1) performing fundamental studies of thermochemical reactions and kinetics, (2) rapidly evaluating emerging process technologies, and (3) assessing long-term process and equipment performance.

NREL works with our partners to design flexible research systems that include extensive instrumentation for thorough process characterization, enabling the identification and mitigation of commercialization risks associated with operability and scale-up.

We can process biomass and waste streams (such as plastics) in solid, liquid, and gas phases from independent or coupled operations with upstream deconstruction systems, including hybrid biological-thermochemical processing. To that end, our facilities can provide a test-bed for industry partners to evaluate their technologies.

Transforming Thermal Biomass Deconstruction Products into Valuable Products

Our 3,500-square-foot pilot-scale facility, the Thermal and Catalytic Process Development Unit (TCPDU), is feedstock flexible, can operate in gasification or pyrolysis modes at solid feed rates up to tens of kilograms per hour, and can incorporate skid-mounted units from partners. Our dedicated operations staff are facility experts and maintain stringent safety standards, resulting in high-quality operations and data. *Photo by Dennis Schroeder, NREL 48566*

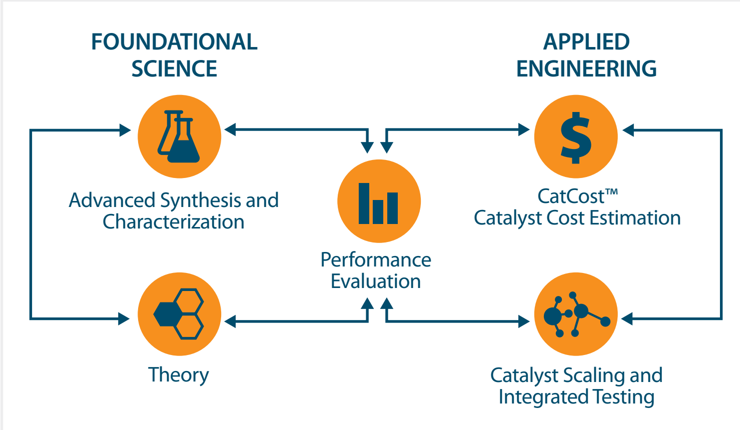


INFORMED **CATALYST DESIGN** COUPLED WITH **MULTISCALE EVALUATION**

The centerpiece for our catalyst development approach is performance evaluation. This ranges from microscale intrinsic kinetic experiments to integrated testing with real biomass and waste streams in industrially relevant reactors.

Coupling advanced catalyst synthesis and characterization and computational modeling with multiscale performance evaluation enables development of structure-function relationships. We use this foundational knowledge to achieve predictive capabilities toward the design of next-generation catalysts.

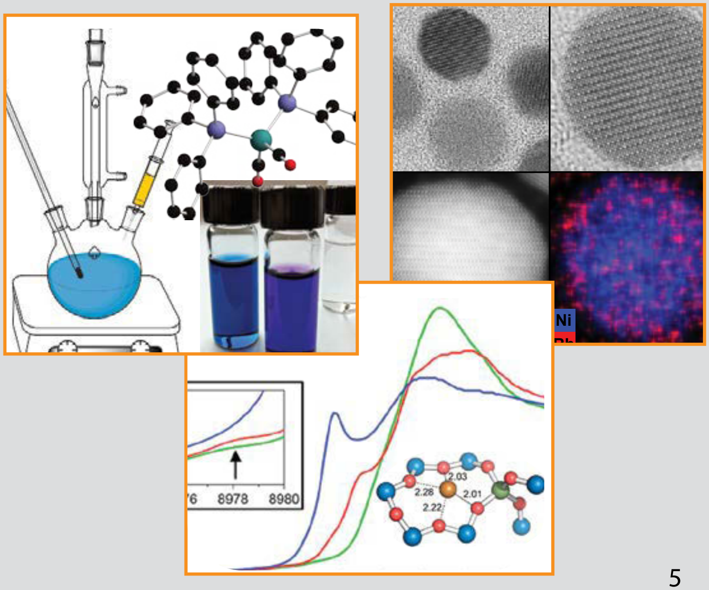
To assess commercial relevance of these next-generation catalysts, we have established in-house capabilities for catalyst cost estimation through our publicly available CatCost™ tool (catcost.chemcatbio.org) and for catalyst scale-up (1–10 kg).

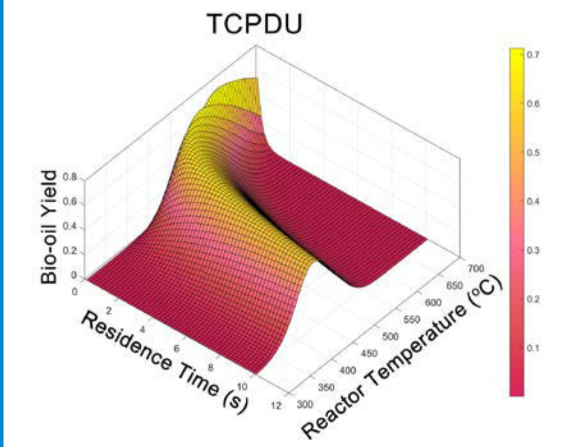


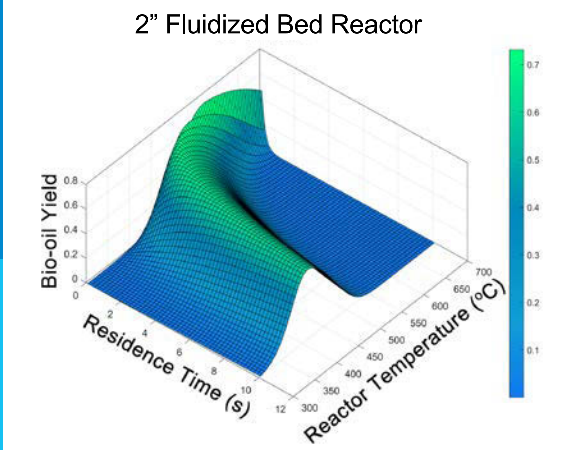
Our integrated approach couples foundational science and applied engineering to accelerate the catalyst-process development cycle.

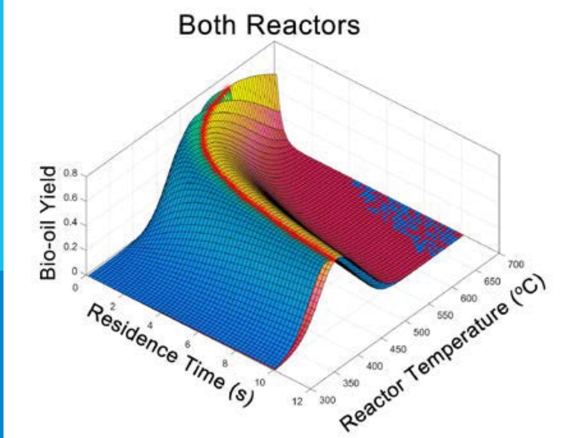
Informed Catalyst Design through Foundational Science

NREL's method is to achieve a foundational understanding of the governing relationships between catalyst composition/structure and performance. To accomplish this, we utilize comprehensive *in situ* and *operando* characterization of catalysts to inform computational models, and then combine those models with intrinsic performance measurements to develop reaction mechanisms and determine structure-function relationships. Guided by these underlying relationships, we implement innovative synthetic strategies to access targeted catalyst formulations and functionalities.









MULTISCALE **COMPUTATIONAL MODELING**

NREL's simulation and modeling team strives to integrate experimental and computational capabilities to address the complexities of real biomass and waste streams. We probe molecular transformations over catalysts to inform compositional design, perform structurally accurate particle simulations to explore mass transport and structural design, and construct reactor-scale simulations to determine scale-up transfer functions.

Predicting Performance and Optimizing Design

By leveraging NREL's nearly 8-petaflop high-performance computing facility—known as Eagle—we model conversion technologies from atoms to reactors, and study the interactions between solids, liquids, and gases. Integrating across modeling scales, NREL develops experimentally validated models using fundamental principles to predict process performance.

Combining modeling and experimentation enables optimization of performance across reactor scales and types.

REDUCING COST AND GREENHOUSE GAS EMISSIONS

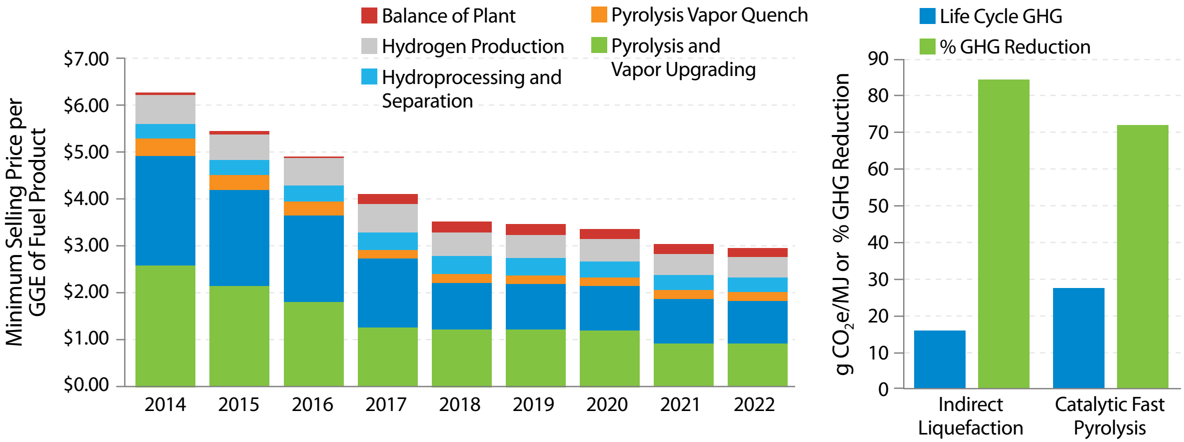
NREL performs world-class techno-economic and life cycle analyses to help guide R&D toward the most impactful areas for cost reduction and to quantify sustainability impacts such as greenhouse gas emissions.

Our modeled process economics are directly connected to detailed process simulations that integrate experimental and analytical data. This approach provides a rigorous and consistent basis for cost estimation, identification of key economic drivers, and comparison across technologies.

Through life cycle analysis, we can provide insight into the potential for a specific technology to meet regulatory mandates and be eligible for credits, which represents a critical consideration for market adoption of emerging technologies connected to carbon recycling.

Targeting Cost Reduction and Quantifying Sustainability Impacts

NREL's analysis team has broad expertise in modeling processes for conversion of renewable and waste carbon sources. Our combined techno-economic and life cycle analyses, leveraging best-in-class industrially relevant tools, can provide a starting point for evaluating market-competitiveness and assessing deployed impact in a future industrial context.



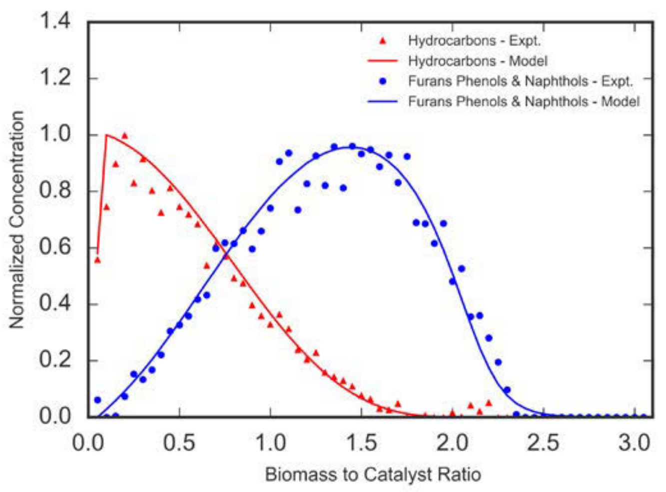
GGE = gasoline gallon equivalent; GHG = greenhouse gas

Techno-economic analysis and life cycle assessment serves as a guide for R&D as well as a benchmark for technology comparison in both current and future scenarios. *Complete life cycle assessment conducted in collaboration with Argonne National Laboratory and Idaho National Laboratory; data sourced from https://doi.org/10.2172/1499023*.

INFORMING **SCALE-UP**

Understanding the fundamentals of process scale-up for complex reaction systems accelerates technology transition from discovery to commercialization by informing reactor system design and process optimization.

Our scientists and engineers integrate their work across scales to bridge the gap between foundational science and applied engineering, with the end goal of establishing intrinsic scaling relationships for emerging technologies under real-world operating conditions. By coupling the development of reactor-agnostic catalytic kinetic models with world-class process modeling, our team provides guidance for the scale-up of carbon conversion technologies.



Rigorous experimental measurements of product evolution and catalyst deactivation enable the extraction of intrinsic kinetic parameters, leading to validated reaction schemes that can be used to guide scale-up and process optimization.

Guiding Scale-Up by Understanding Intrinsic Chemical Kinetics, Reaction Mechanisms, and Catalyst Deactivation

Catalyst deactivation is a common problem during the conversion of renewable and waste carbon sources, and the rate of deactivation is dictated by several interdependent factors, which span broad length and time scales.

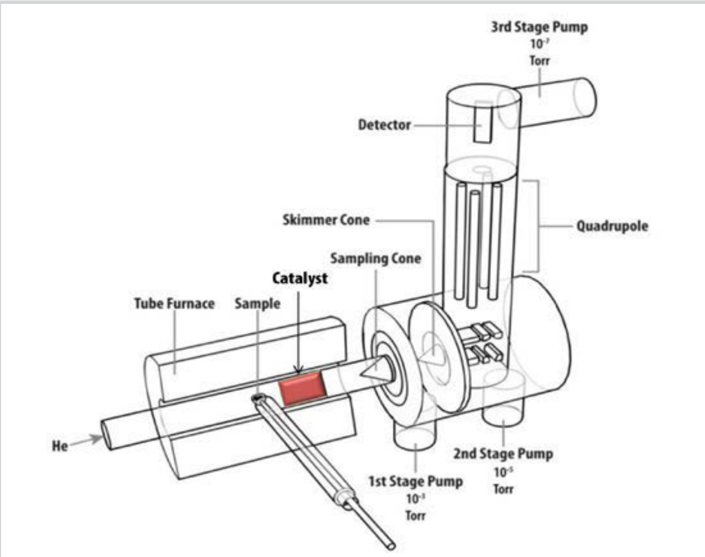
To address this challenge, we utilize a modeling framework that consists of meso-scale particle simulations that are uniquely suited to bridge across these scales by incorporating chemical reaction kinetics, transport phenomena, reactor conditions, and hierarchical catalyst geometries. Coupled with experimental validation, our approach enables the reaction kinetics to be applicable at any catalyst size and reactor scale.

EXTENSIVE **IN-HOUSE ANALYTICS**

Unparalleled in the industry is NREL's expertise in developing lab analytical procedures for comprehensive characterization of complex process streams, including biomass, liquid/gas intermediates, and end-product compositions. Our team established the first ASTM method for chemical characterization of biomass pyrolysis oil. Through our deep expertise and access to leading-edge analytical equipment, we provide end-to-end process characterization that is critical for informed decision-making.

Take Advantage of Our Specialized Analytical Systems

NREL is home to state-of-the-art equipment, including six (four stationary and two deployable) molecular beam mass spectrometers that can sample complex, corrosive process streams at temperature and provide a "fingerprint" of their composition. Our high-temperature gas chromatography system provides nitrogen and sulfur heteroatom speciation on high-temperature process streams.



Molecular beam mass spectrometry provides real-time, continuous monitoring and direct sampling from harsh environments, enabling on-line assessment of catalyst and process performance. *Photo by Dennis Schroeder, 17382 NREL*

CUTTING-EDGE FACILITIES LEAD TO INNOVATION

Our Davison Circulating Riser Reactor Laboratory employs refinery-like fluid catalytic cracking upgrading capabilities with a pyrolyzer on the front end and allows for vapor phase upgrading, catalytic fast pyrolysis, and refinery integration experiments at process-relevant scale and conditions.

The Fuel Synthesis Catalysis Laboratory offers highly controlled lab-scale catalyst testing capabilities, enabling catalyst development, intrinsic kinetic measurements, durability testing, and surface chemistry evaluation.

NREL engineers evaluate bio-oil co-processing using the 2,000-square-foot Davison Circulating Riser Reactor Laboratory. *Photo by Dennis Schroeder, NREL 33048*

The Fuel Synthesis Catalysis Laboratory is a newly renovated 1,120-square-foot laboratory space that houses six semi-automated reactor systems with online gas chromatography product analysis. *Photo by Dennis Schroeder, NREL 51117*

WORKING WITH US

Leverage NREL expertise and capabilities by joining us in a public-private partnership to drive catalysis innovation for tomorrow's feedstocks.

Only through hypothesis-driven R&D coupled with rich multidisciplinary collaboration can global-scale challenges be overcome. Contact us to get started.

Cooperative Research and Development Agreements (CRADA)

NREL uses CRADAs when a partner and the lab intend to collaborate on a project. It protects a company's and NREL's existing intellectual property, and allows the company to negotiate for an exclusive field-of-use license to subject inventions that arise during CRADA execution.

Funds-In Agreement (FIA)

With a strategic partnership project (SPP), a nonfederal entity pays NREL to conduct a research-oriented project. This version of the nonfederal SPP has no agreement value limit and has intellectual property provisions which address inventions.

Agreements for Commercializing Technology (ACT)

NREL uses ACTs when a partner seeks highly specialized or technical services to complete a project. An ACT agreement also authorizes participating contractor-operated labs, such as NREL, to partner with businesses using more flexible terms that are aligned with industry practice.

Technical Services Agreement (TSA)

A TSA is suitable for projects $500,000 or less in value, up to three years in duration, and funded entirely by the sponsor for services, which would not be expected to result in any inventions. A TSA cannot be used for agreements with federal agencies. It has been preapproved by the U.S. Department of Energy, which means that terms cannot be changed.

Funding Opportunity Announcement (FOA)

A FOA may be open to one or more institution types, including industry, university, and national labs to pursue U.S. Department of Energy R&D projects. FOAs are discretionary grants or cooperative agreements, usually as a result of a competition for funds.

FIND OUT MORE

For more information and collaboration opportunities, contact:

Josh Schaidle, Joshua.Schaidle@nrel.gov

or visit: **www.nrel.gov/catalysisforcarbon**

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NREL Transforming ENERGY

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