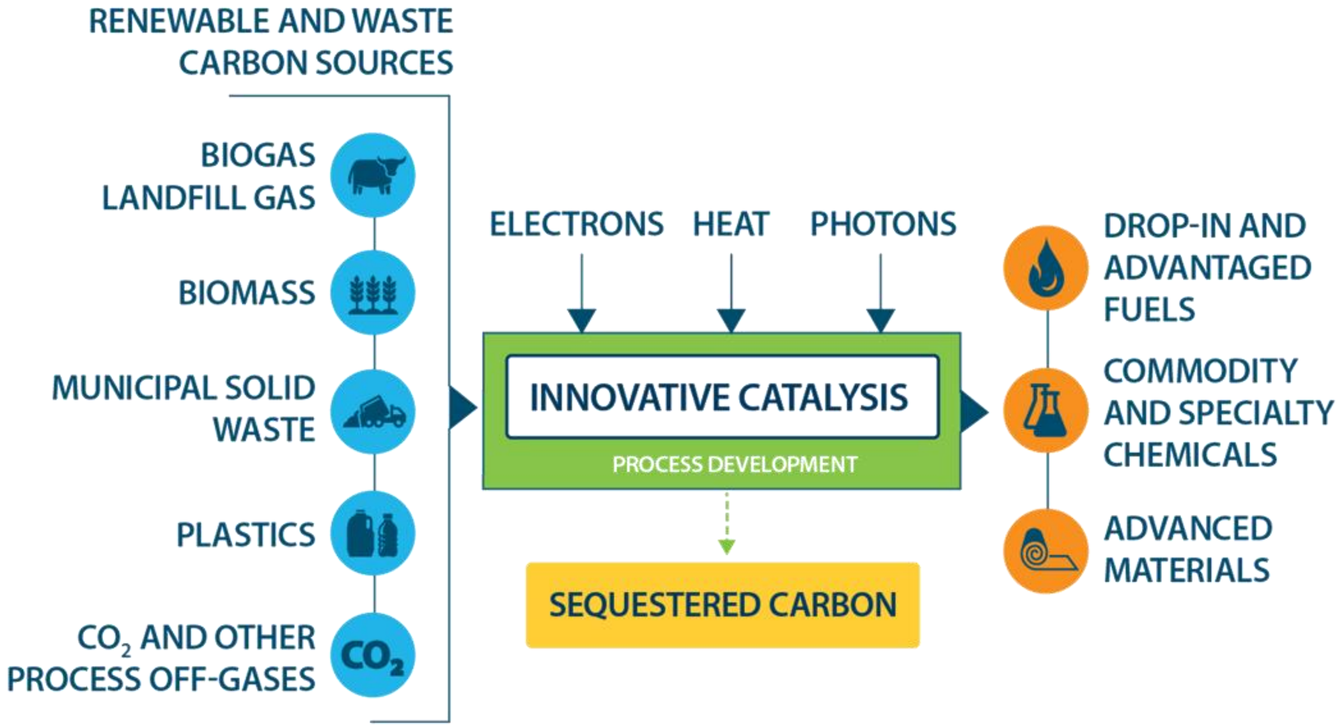
Catalytic Carbon Transformation Platform

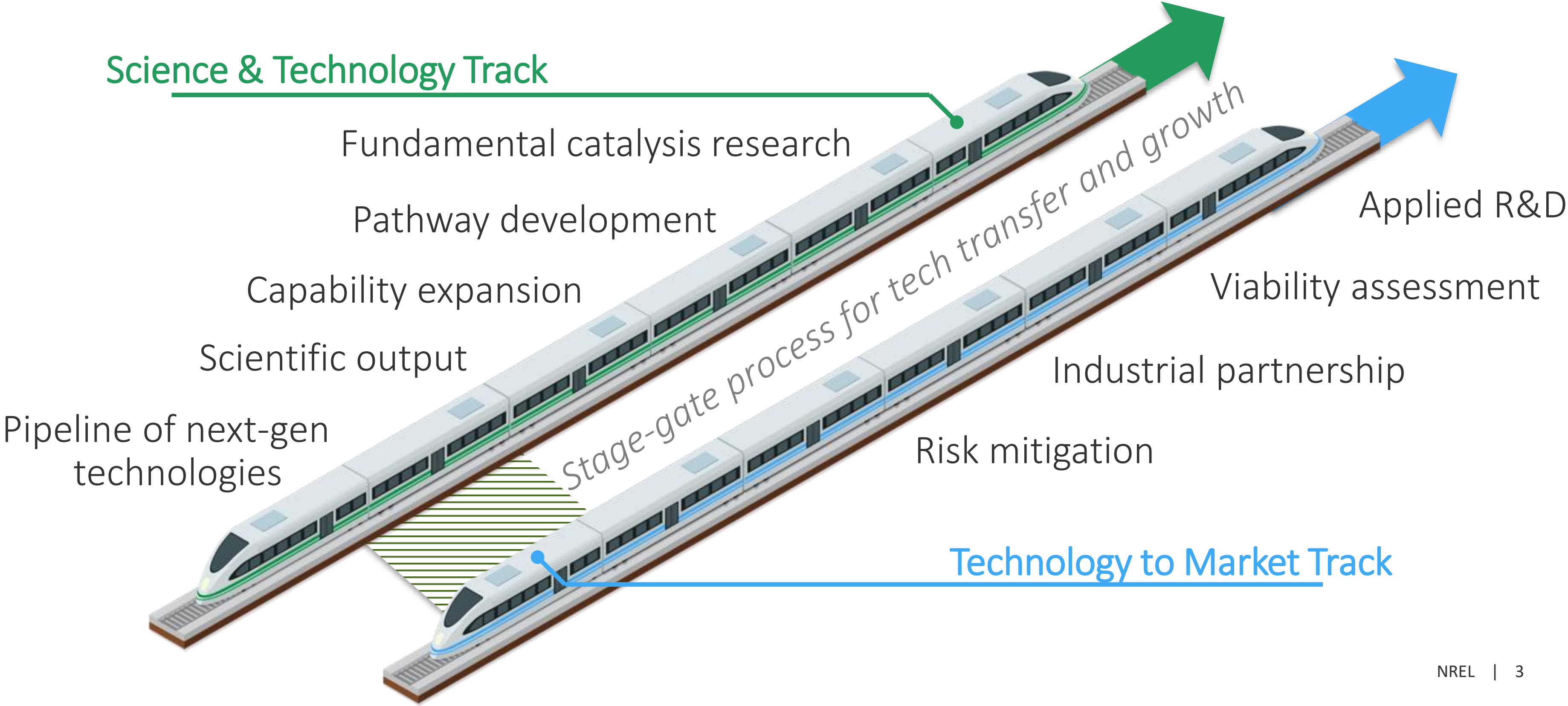
Driving Catalysis Innovation

Our goal is to innovate, develop, de-risk, and integrate catalytic technologies for the production of energy-dense biofuels and renewable chemicals



An R&D Pipeline to Enable BETO’s Transportation Strategy

A harmonized portfolio that spans TRLs to enable industry to achieve strategic production goals



MULTI-SCALE THERMAL DECONSTRUTION

- Ability to perform pyrolysis and gasification
- Feedstock flexible
- Entrained Flow and Fluid Bed Reactor technologies available
- Grams to tens of kilograms biomass per hour throughput
- Solid, liquid, and gas feeds possible

Understanding deconstruction across scales

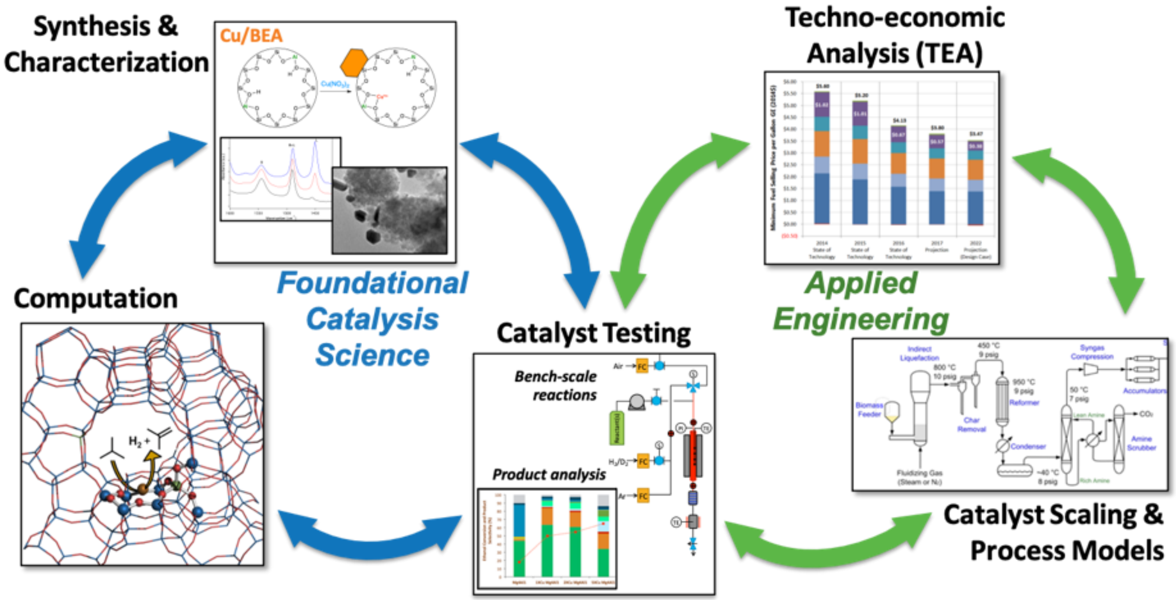
Fundamental studies of thermochemical reactions and kinetics

Rapid evaluation of emerging process technologies

Evaluation of long-term process and equipment performance

Catalytic Upgrading that Spans Multiple Scales

Linking foundational science and applied engineering to develop and evaluate catalysts for synthesis of fuels and chemicals



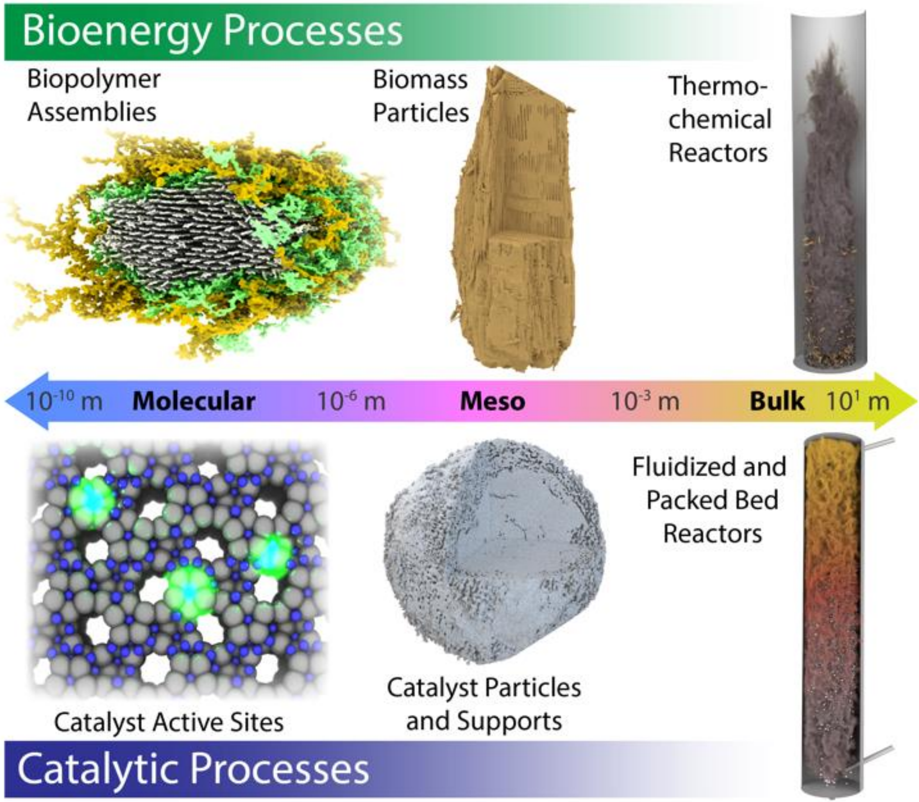
Integrated Testing

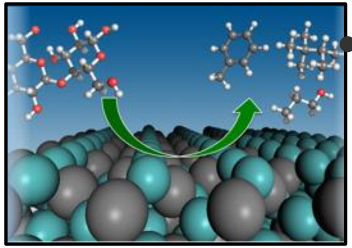
- ***Feed stream flexibility*** – Biomass and waste (e.g., CO_2) streams from stand-alone or coupled operation with upstream deconstruction systems (hybrid processing)
- ***Diverse Configurations*** – Riser/CFB, fluid bed, and packed bed reactor technologies (1g – 100kg_{cat} scale)
- CFD models of reactors provide fundamental insight into operations
- Evaluation of co-processing strategies

ChemCatBio Consortium

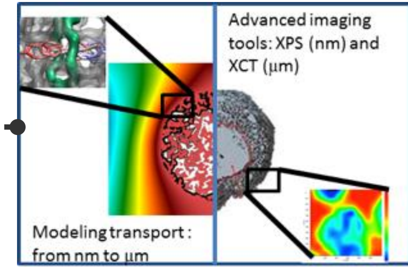
A Multiscale Approach to Computational Modeling

Reliable predictive models may greatly de-risk scaleup and deployment of pathway technologies

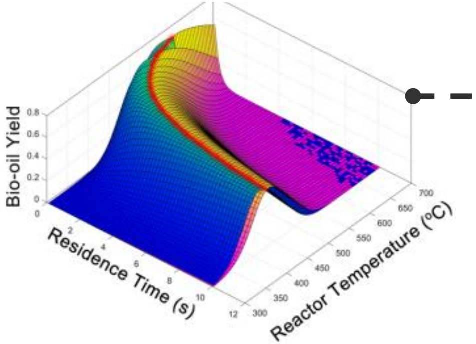




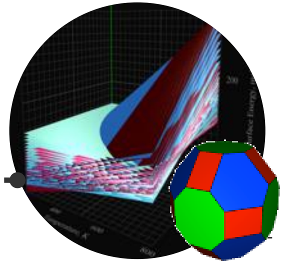
Molecular transformations over catalysts to inform compositional design



Structurally accurate particle simulations to explore mass transport and structural design



Reactor-scale simulations to determine scale-up transfer functions

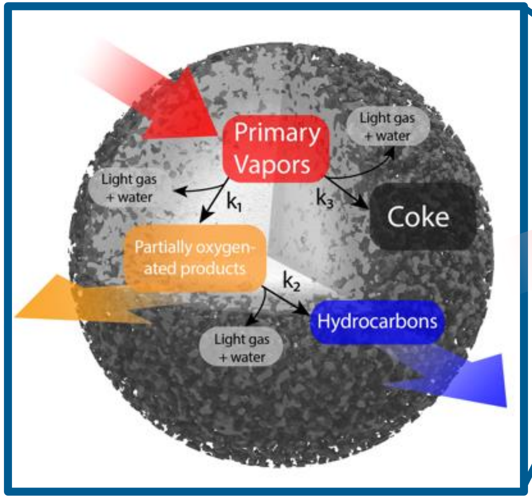


Tool development to facilitate knowledge transfer between modeling and experiment

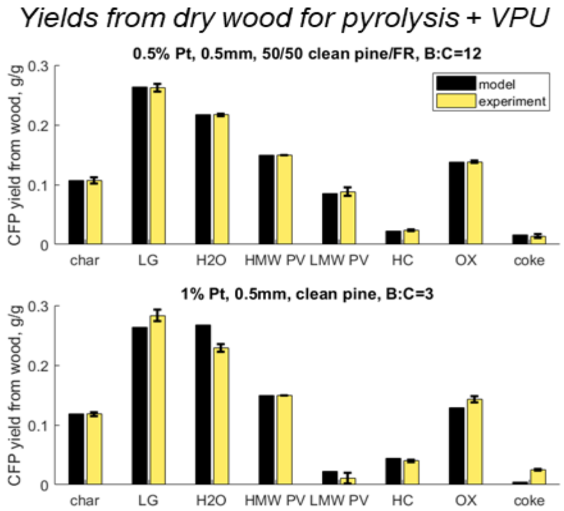
Ciesielski, et al. "Bridging Scales in Bioenergy and Catalysis: A Review of Mesoscale Modeling Applications, Methods, and Future Directions." Energy & Fuels, **2021**, 35, 18, 14382.

Mesoscale Catalyst Performance Modeling

Mesoscale model incorporates intraparticle transport and catalyst deactivation



Reactor scale models capture bulk transport behavior and provide predictions of product yields and catalyst activity lifetime to guide scaleup efforts



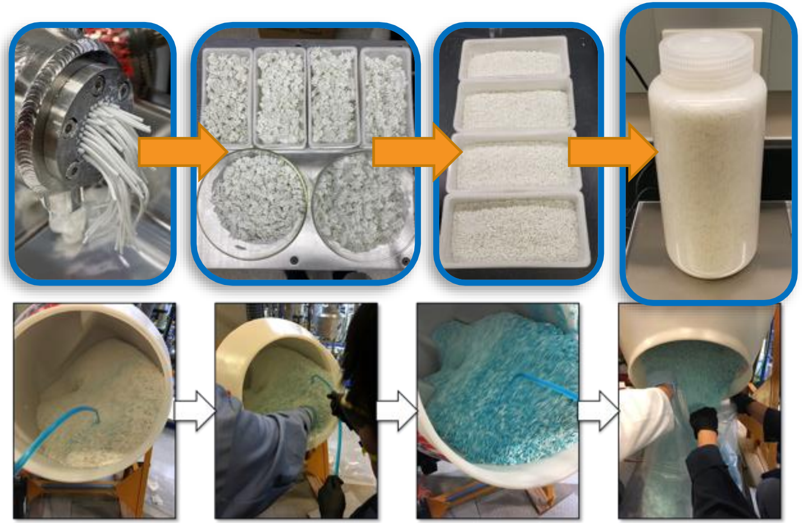
- Meso/reactor scale simulations were validated against multiple experiments performed at NREL and found to be highly accurate across the range of operating conditions tested.
- The kinetic parameters obtained from the model were used to investigate scaleup of the technology and identified and quantified several potential risks associated with catalyst regeneration.

Pecha, et al. and Ciesielski, P. N. "Ex situ upgrading of pyrolysis vapors over $PtTiO_2$: extraction of apparent kinetics via hierarchical transport modeling." Reaction Chemistry & Engineering, 2021.

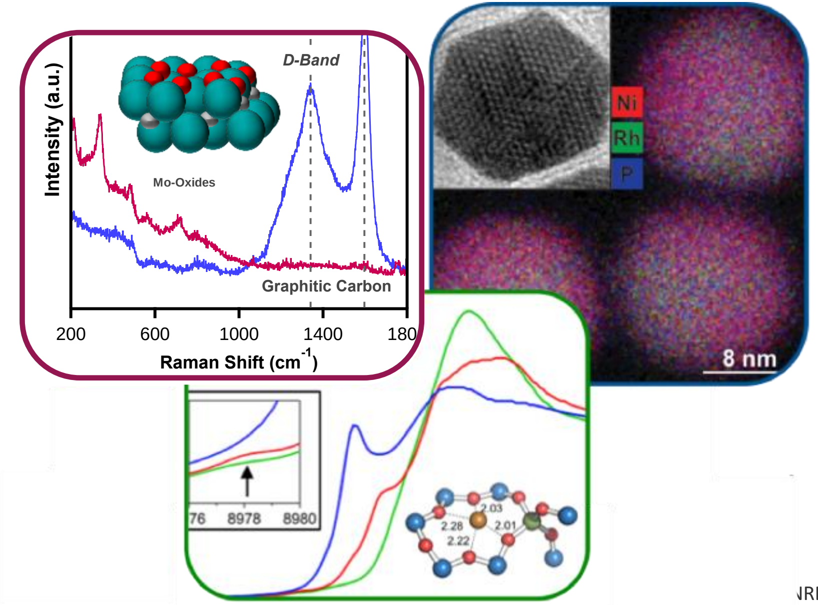
Engineered Catalyst Production and Characterization

Overcoming process scale-up challenges by coupling scaled catalyst production with comprehensive catalyst characterization and multi-scale evaluation

Demonstrated capability and expertise in catalyst production in engineered forms



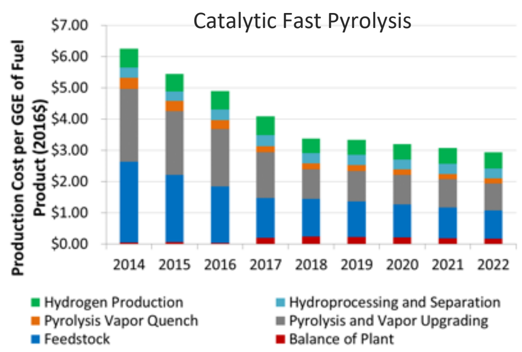
Demonstrated capability and expertise in advanced in-situ/in-operando catalyst characterization



REDUCING COST AND GHG EMISSIONS

Guiding research and development through techno-economic analysis (TEA) and life-cycle assessment (LCA)

Targeting cost reduction through TEA



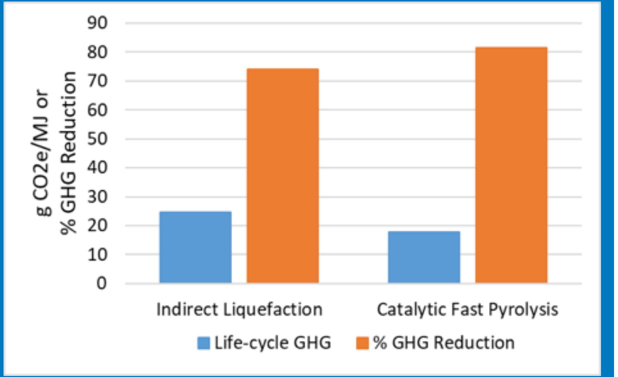
Economics based on process simulations

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 feedback for R&D.

Quantifying sustainability impacts through LCA



Sustainability analysis

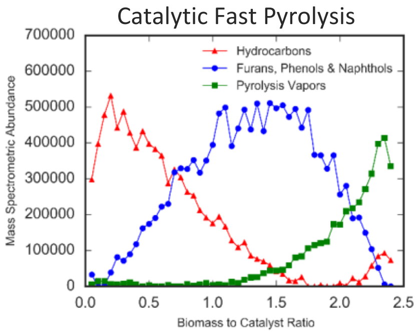
Quantifies process greenhouse gas emissions, water use, and other environmental impacts relevant to meeting regulatory mandates such as the Renewable Fuel Standard and Low Carbon Fuel Standard.

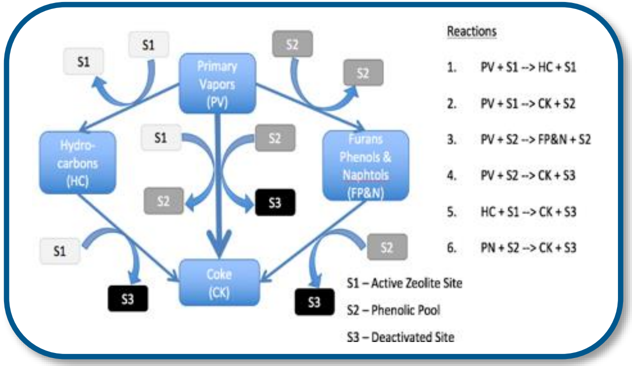
Assess impacts of scale-up implementation

Evaluation of process emissions at commercial scale provides an assessment of deployed impact in future industrial context

Informing Scale-up

Development of reactor-agnostic catalytic kinetic models, coupled with world-class process modeling, provides guidance for scale-up





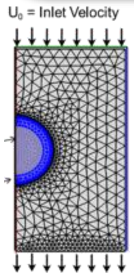
	Reaction	Rate Constant @500 °C [m³/(mol.s)]
1	PV + S1 → HC + S1	139.262
2	PV + S1 → CK + S2	40.876
3	PV + S2 → FP&N + S2	1.158
4	PV + S2 → CK + S3	69.79
5	HC + S2 → CK + S3	2.751
6	PN + S2 -> CK + S3	0.024

- Species
- Experimental Yields

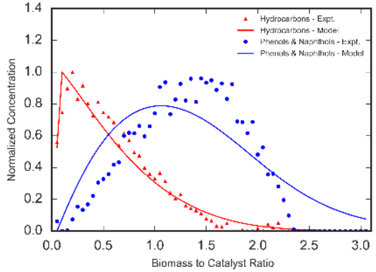
- Porosities
- Diffusivities
- Architecture
- Reaction Scheme

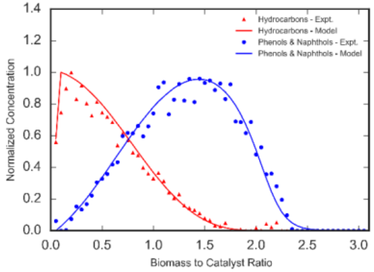
Initial Guess

- Kinetic Rate Parameters



COMSOL





Fminsearch Optimization Routine

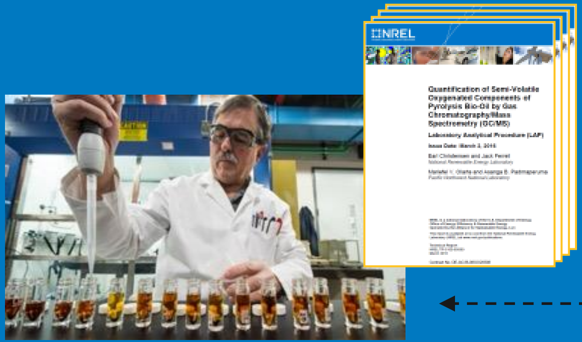
Matlab-COMSOL LiveLink

Separating site-specific chemical kinetics from particle and reactor-scale mass transport (physics) enables the kinetics to be applicable at any catalyst size and reactor scale

EXTENSIVE IN-HOUSE ANALYTICS

Enabling process evaluation through comprehensive stream characterization

Unparalleled Expertise



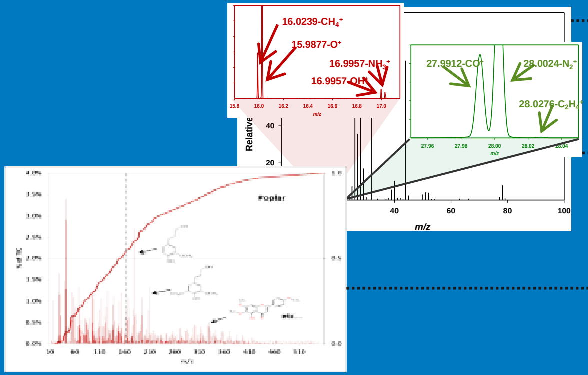
First ASTM Method for pyrolysis oil analysis (E3146)

The first ASTM method for measuring carbonyl content of pyrolysis oil was developed in part by NREL

NREL develops Laboratory Analytical Procedures

Over a dozen LAPs for biomass, liquid/gas intermediates, and end product compositions have been developed and distributed by NREL researchers

Specialized Analytical Systems



- ***Molecular Beam Mass Spectrometry***

  NREL is home to 4 molecular beam mass spectrometers (deployable)

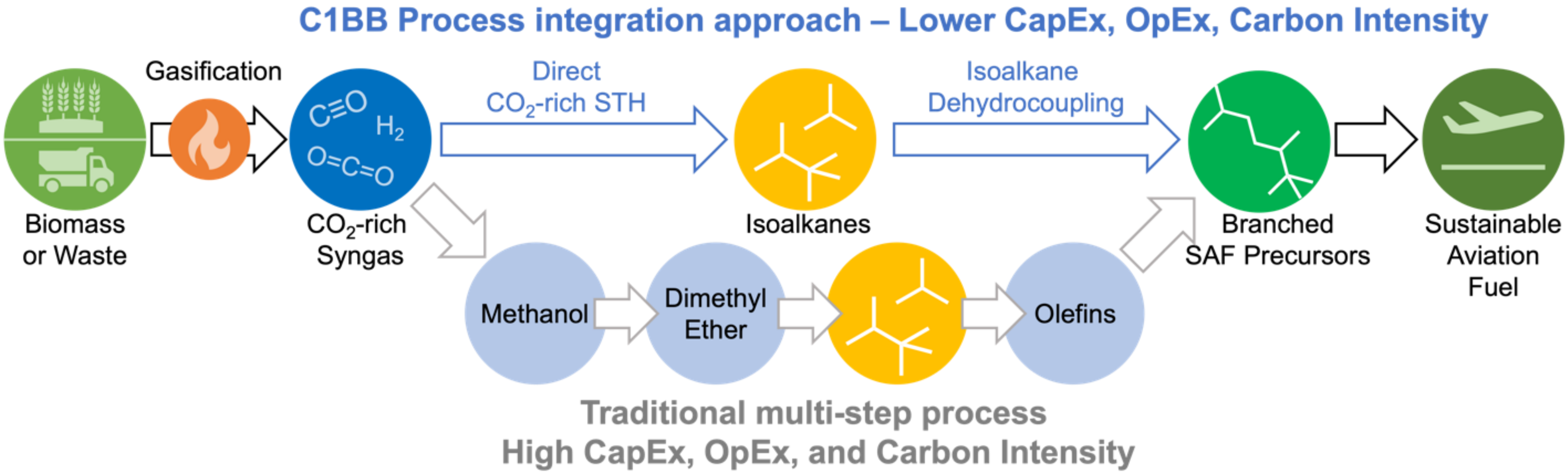
- ***High Temperature Gas Chromatography***

  Provides nitrogen and sulfur heteroatom speciation on high temperature process streams

- ***High-Resolution Pyroprobe MS***

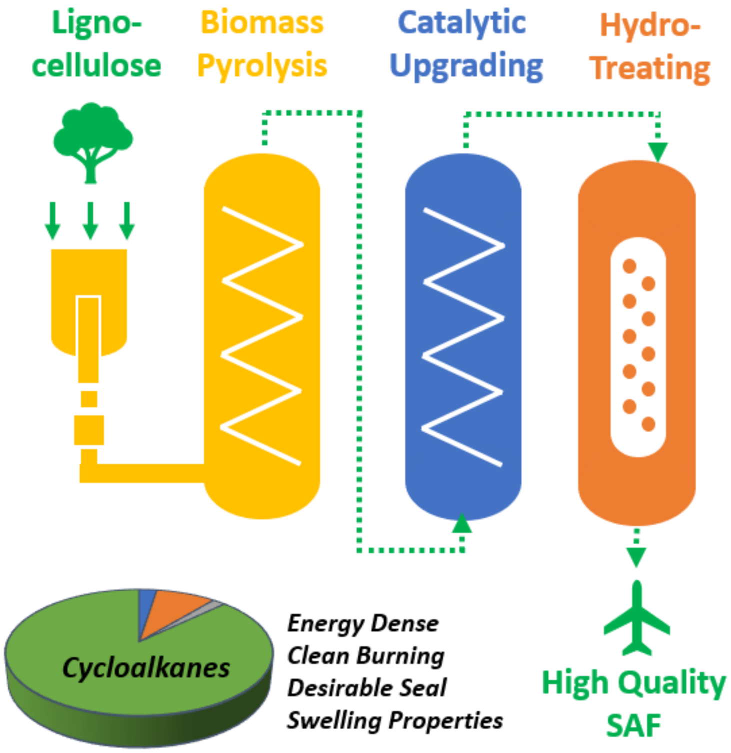
  Provides rapid evaluation of product speciation in real-time

SAF Pathway: Direct CO_2-rich STH



- Developing the **centerpiece technology** for direct syngas-to-hydrocarbons (STH)
- **Hydrocarbon SAF precursor product** using NREL's Cu/BEA zeolite catalyst
- **Comparable activity and selectivity in 1-step** compared to 3-steps
- Co-convert CO_2 with syngas to **increase overall carbon efficiency**
- Process concept translates to a variety of hydrocarbon synthesis catalysts to **target specific SAF components** (e.g,. iso-paraffins, cyclics)

SAF Pathway: Catalytic Pyrolysis and Hydrotreating



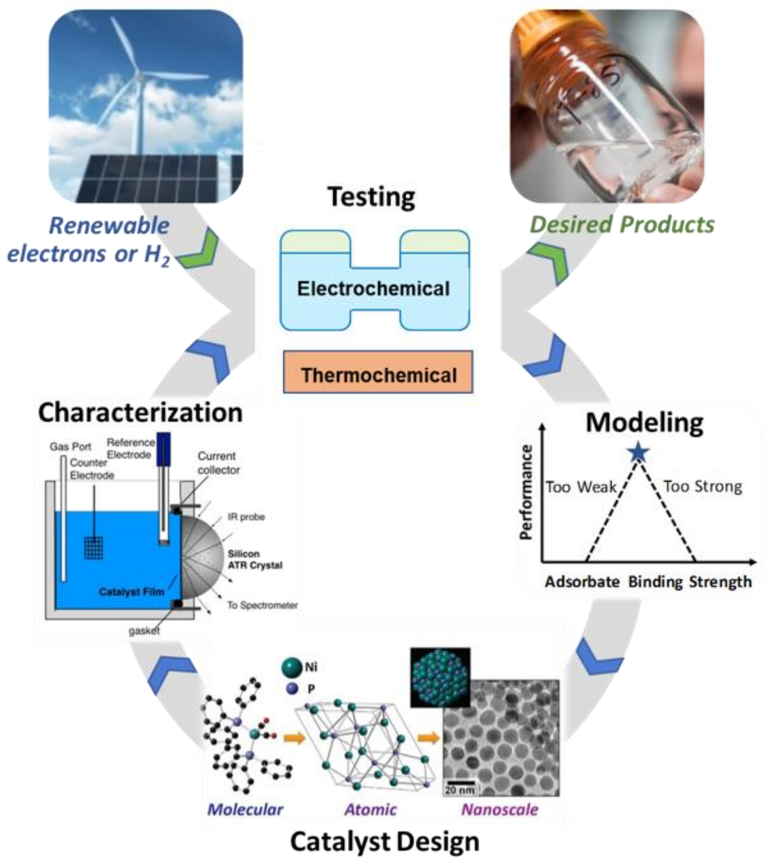
	Density, g/cm³	LHV, MJ/kg	Flash Point, °C	Freeze Point, °C
ASTM D4054	775-840	>42.8	>38	max -40
CFP + HT SAF	**834**	**43.0**	**50**	**<-70**

- Demonstrated end-to-end conversion of woody biomass to SAF
- > 90% selectivity to cycloalkanes
  - Major component of Jet A
  - Difficult via HEFA or FT routes
  - May replace aromatics for seal swelling properties of existing engines

CATALYTIC CO_2 UTILIZATION

- Thermocatalytic and electrocatalytic conversion strategies
- Leveraging low-cost electricity and abundance of CO_2 from biorefineries
- Catalyst evaluation using continuous-feed, industrially-relevant systems
- Combined experimental and modeling approach

Developing advanced catalytic materials to enable CO_2 utilization technologies



Cutting-Edge Facilities Lead to Innovation

Davison Circulating Riser Reactor Laboratory

- Refinery-like (FCC) upgrading capabilities with a pyrolyzer on the front end
- Allows for vapor phase upgrading, catalytic fast pyrolysis and refinery integration experiments at process-relevant scale and conditions

Fuel Synthesis Catalysis Laboratory

- Highly controlled lab-scale catalyst testing capabilities
- Enables catalyst development, intrinsic kinetic measurements, durability testing, and surface chemistry evaluation

De-risking Innovation through Public-Private Partnerships

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

RTI INTERNATIONAL

Chevron

gevo

PHILLIPS 66

DOW

VELOCYS®

the Wonderful company

ENSYN

Enerkem

JM Johnson Matthey
Inspiring science, enhancing life

BIG OX ENERGY

ExxonMobil
Energy lives here™

LanzaTech

BR PETROBRAS

FORGE NANO

ALD nanosolutions

Vertimass
Transformative fungible biofuels.

twelve

ALDER FUELS

Thanks for your attention!

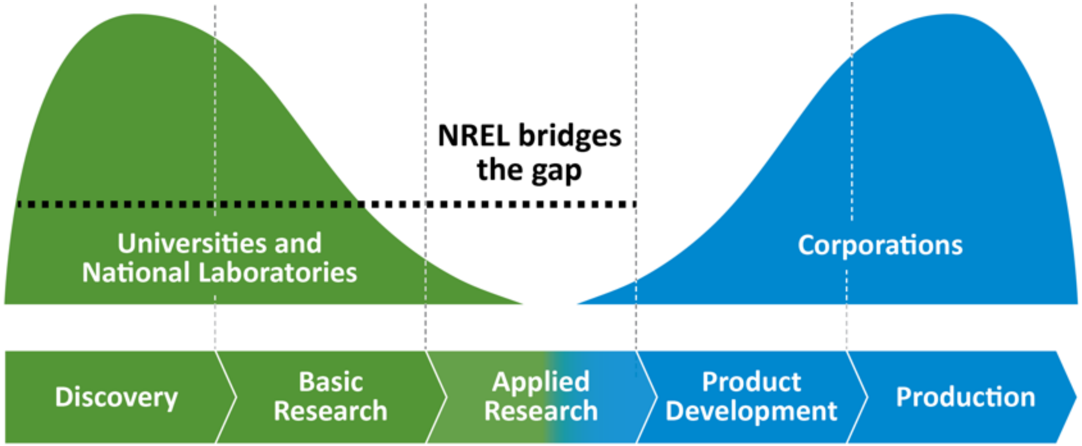
www.nrel.gov

Value of Partnering with the National Labs

Partnership Advantages for Cleantech Startups:

- **Patenting activity of cleantech startups increases by 73 percent** with every additional governmental technology alliance
- **Private financing deals increase by 155 percent** for every additional license from a government organization

C. Doblinger, K. Surana, L. D. Anadon, *Research Policy 48, 6, 1458*.



Working with Us

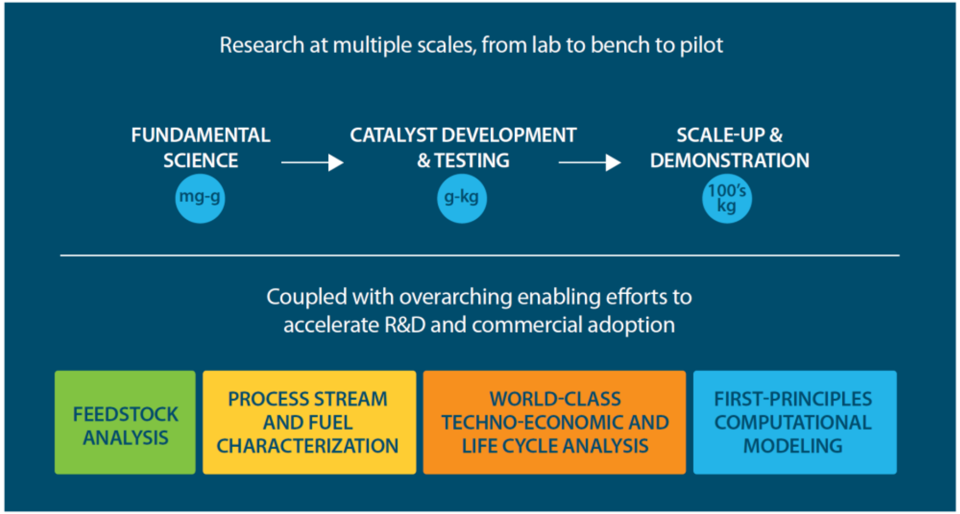
Various mechanisms exist for working with our Catalytic Carbon Transformation Platform

Agreement	Purpose	Benefits	Requirements
Cooperative R&D Agreement (CRADA)	Collaborate and share results of jointly conducted R&D	**Collaborate:** Leverage research efforts and funding by NREL & partner **Inventions:** NREL & partner may own respective inventions **Confidentiality:** Generated information can be protected for up to 5 years. Partners proprietary information can be protected. **License:** Partner has option to negotiate license to NREL subject inventions	• Substantial U.S. manufacturing requirements for CRADA IP • 90-day advance payment • Government use license • Signature approval by DOE
Funds-In Agreement (FIA)	Allows NREL to perform mission-related, reimbursable work	**Access:** Highly specialized or unique DOE facilities, services, or technical expertise **Inventions:** IP ownership subject to project parameters **Confidentiality:** Generated information treated as proprietary when marked; partner's proprietary information can be protected	• U.S. Preference: Partners agree there will be no exclusive third party license unless manufactured substantially in US • 90-day advance payment • Government use license • Approval by DOE required
Agreements for Commercializing Technology (ACT)	Allows NREL to perform mission-related, reimbursable work	**Access:** Highly specialized or unique DOE facilities, services, or technical expertise **Flexibility:** Negotiable agreement terms, provided DOE required IP provisions and disclaimer are used **Optional:** Limited government R&D license	• U.S. Preference: Partners agree there will be no exclusive third party license unless manufactured substantially in US • Pricing structure differs from other agreements • Approval required by DOE
Technical Services Agreement (TSA)	Allows NREL to perform mission-related, reimbursable work	**Access:** Highly specialized or unique DOE facilities, services, or technical expertise **Confidentiality:** Generated information treated as proprietary when marked; partner's proprietary information can be protected **Easy:** Quick to execute for projects that meet certain parameters **Efficient:** Ideal for consulting, testing, and evaluation	• Terms non-negotiable • Less than $250k and 3 y • Not intended to develop project generated IP • 90-day advance payment • Typically pre-approved by DOE
Funding Opportunity Announcement (FOA)	Industry, university, and labs team to pursue DOE R&D projects	**Access:** Provides DOE funding and national lab expertise on R&D projects of strategic interest to industry **Inventions:** NREL & partner may own respective inventions **Confidentiality:** Generated information treated as proprietary when marked; partner's proprietary information can be protected **License:** Subject Inventions are generally made available to industrial partners	• Often requires industrial cost share • U.S. Preference: Partners agree there will be no exclusive third party license unless manufactured substantially in US • Substantial U.S. manufacturing requirements for IP • 90-day advance payment • Government use license

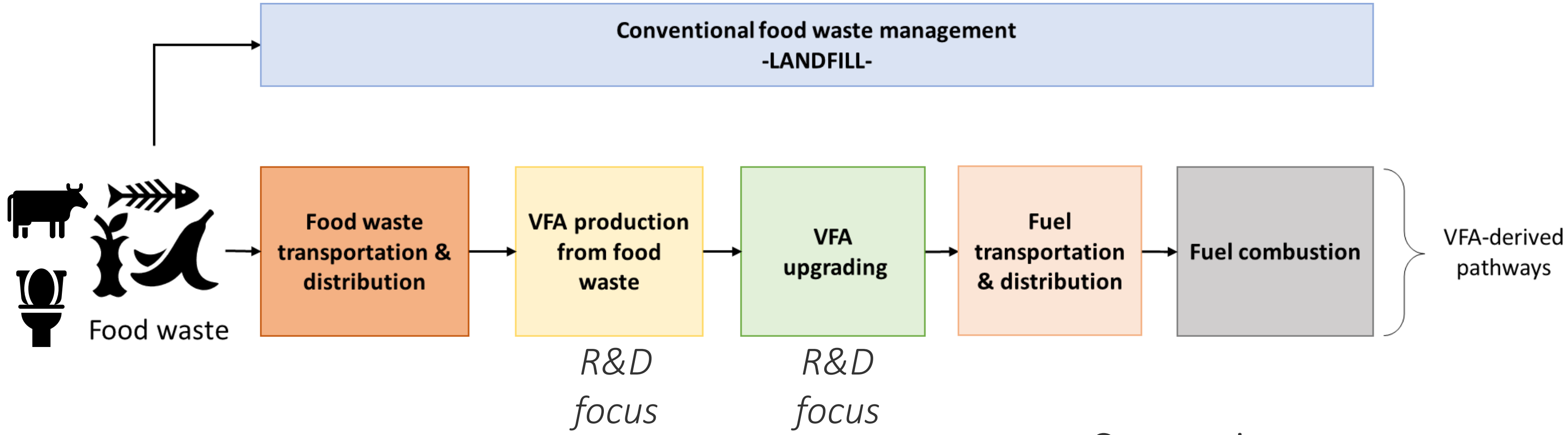
Contact: Fred Baddour, Frederick.Baddour@nrel.gov

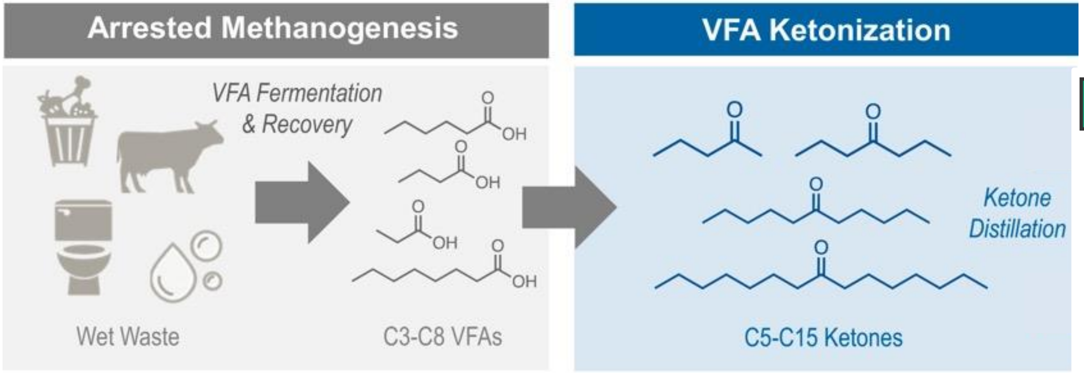
An approach based on 3 core principles

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

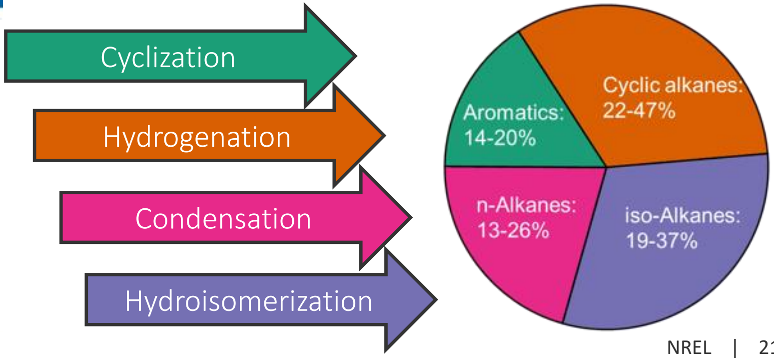


SAF Pathway: Upgrading of Biological Intermediates



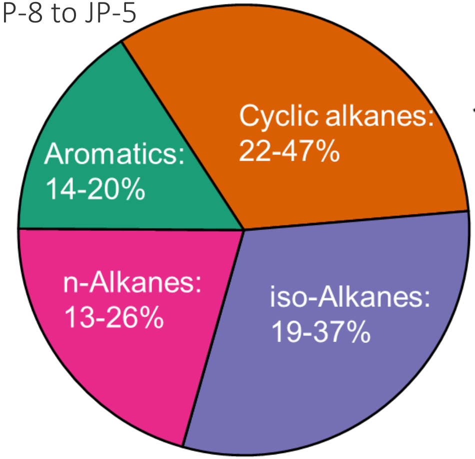


Conversion strategy targeting (Jet A POSF 10325)

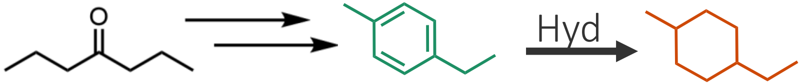


SAF Pathway: Upgrading of Biological Intermediates

Composition range:
JP-8 to JP-5

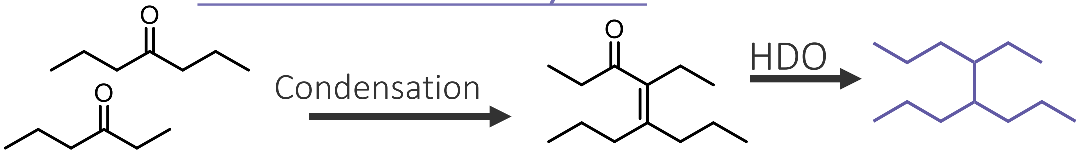


Ketone cyclization



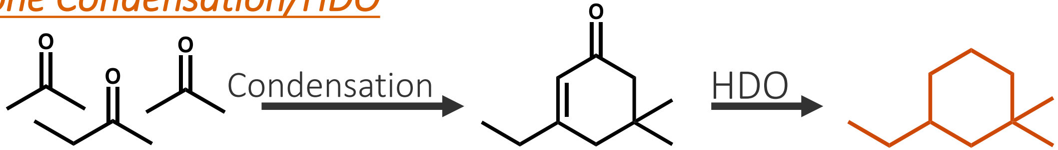
T=350°C, H/ZSM-5 (Si/Al=40), P=1 atm, WHSV=1 hr^{-1}

Ketone Condensation/HDO



T=190-200°C, Niobic acid, P=1 atm, 6-8 h batch

Ketone Condensation/HDO



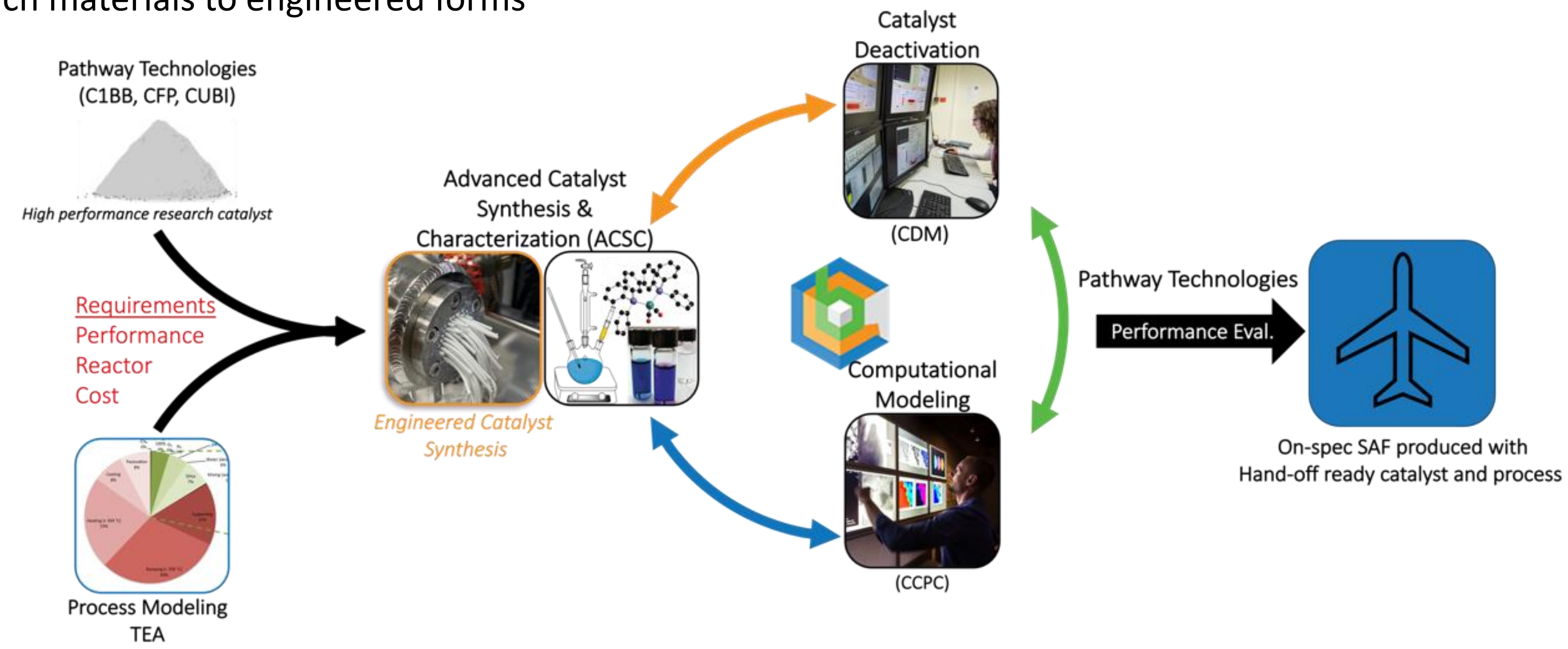
T=190-200°C, Niobic acid, P=1 atm, 6-8 hour batch reaction

Ketone HDO

T=345°C, Pt/Al_2O_3, P_{H2}=35 bar, WHSV=3 hr^{-1}

Engineered Catalyst Forms to Address the "Valley of Death"

Catalyst forming capabilities enable pathway technologies to **evaluate the catalytic performance of realistic** engineered catalysts and **develop a fundamental understanding of the impact** of transitioning from powdered research materials to engineered forms



Addressing the non-trivial transition from research to engineered catalysts forms and reduces the risk of commercialization

Comprehensive Characterization Capabilities to Accelerate Deployment

Demonstrated a 4x reduction in time between characterization of a baseline catalyst and **development of a next-gen catalyst** with increased performance

ChemCatBio — Chemical Catalysis for Bioenergy

Founded ChemCatBio — FY17

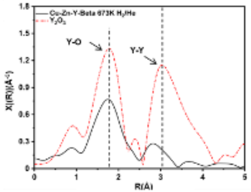
Initiated ACSC

Argonne National Laboratory · NREL · Oak Ridge National Laboratory

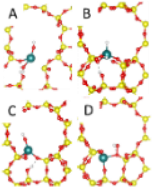
FY18 Q1 — Initiated C2-ACSC collaboration

FY18 Q1 — Developed baseline Cu-Zn-Hf/BEA with 62% C_{3+} olefin selectivity

Q2 — Identified ionic Cu as active site for hydrogenation and Y to minimize dehydration

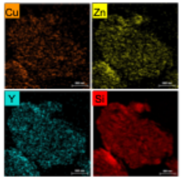


Q4 — Developed Cu-Zn-Y/BEA catalyst



CCPC — Consortium for Computational Physics and Chemistry

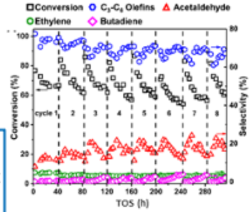
FY19 Q1 — Identified isolated Cu, Zn, and Y sites in working catalyst



Q2 — Developed predictive model based on isolated sites

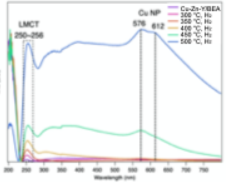
Q2 — Determined that minimization of Al sites and alternative Lewis acid sites can increase olefin selectivity

Q3 — Demonstrated 89% C_{3+} olefin selectivity by synthetic optimization based on single site identification and support impact



Q4 — Demonstrated 300 h TOS

Q4 — Identified Cu sintering at extended TOS



FY20 Q3 — Technology licensed

FY21 Q1 — Identified Cu redispersion during regeneration

Q4 — Optimize regeneration

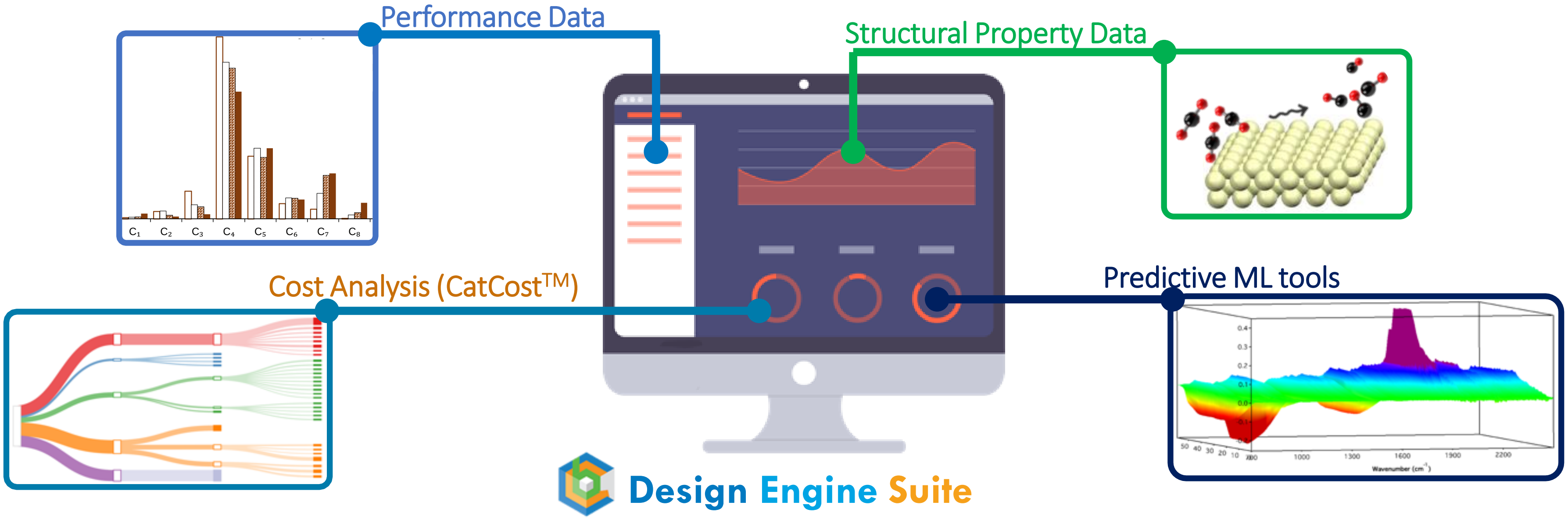
● **Catalyst development** — 1.75 years

● **Durability and regeneration** — 1.75 year

● **Technology maturation** — 2.75 years

Catalyst Design Engine

To support and accelerate catalysis RD&D by addressing barriers with a suite of predictive analytical tools



Integrating database technology from **Databhub**, cost estimation from **CatCost** at the **frontier of machine learning** to transform catalyst design and deployment