CCPC

Consortium for Computational Physics and Chemistry

U.S. DEPARTMENT OF ENERGY

BIOENERGY TECHNOLOGIES OFFICE

Consortium for Computational Physics and Chemistry

Jim Parks (Oak Ridge National Laboratory)

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Denver, CO, April 3-7, 2023

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U.S. DEPARTMENT OF ENERGY

Project Overview

*Established in 2013, the **Consortium for Computational Physics and Chemistry (CCPC)** continues to evolve and adapt to advance bioenergy.*

Project Goals: Develop & apply a fundamental science-based computational toolset that ***enables & accelerates*** …

1. discovery and optimization of cost-effective catalyst materials for bioenergy applications,
2. translation of catalyst discoveries to higher technical readiness levels, and
3. cost-effective scale-up of bioenergy technologies relevant to industry.

Approach

Approach

The Consortium for Computational Physics and Chemistry (CCPC) is a Bioenergy Technologies Office (BETO) consortium composed of six national labs applying multi-scale computational science to enable bioenergy successes in other BETO consortia.

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OAK RIDGE National Laboratory

NATIONAL ENERGY TECHNOLOGY LABORATORY

Pacific Northwest NATIONAL LABORATORY

A multi-scale problem
… A multi-lab solution

Argonne NATIONAL LABORATORY

INL Idaho National Laboratory

NREL NATIONAL RENEWABLE ENERGY LABORATORY

BETO Consortia

Agile BioFoundry

ATEC

ALGAE TECHNOLOGY EDUCATIONAL CONSORTIUM

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

CO_2RUe U.S. DEPARTMENT OF ENERGY

ChemCatBio Chemical Catalysis for Bioenergy

bottle

BIOPROCESSING SEPARATIONS CONSORTIUM

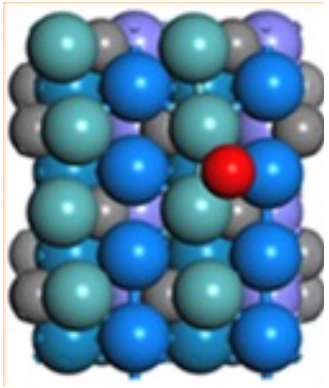
DISCOVR

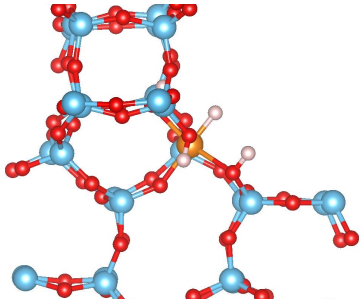
Co-Optimization of Fuels & Engines FOR TOMORROW'S ENERGY-EFFICIENT VEHICLES

Consortium for Computational Physics and Chemistry (CCPC)

A multi-scale problem… A multi-lab solution

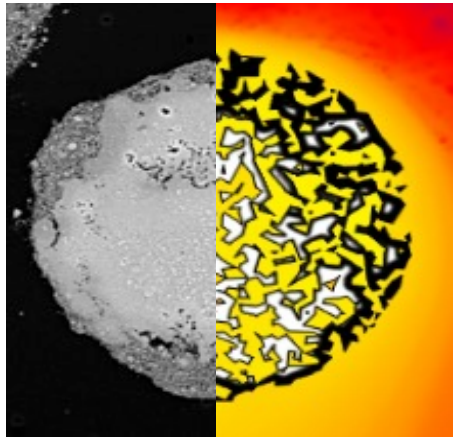
Catalysis Modeling at Atomic Scales

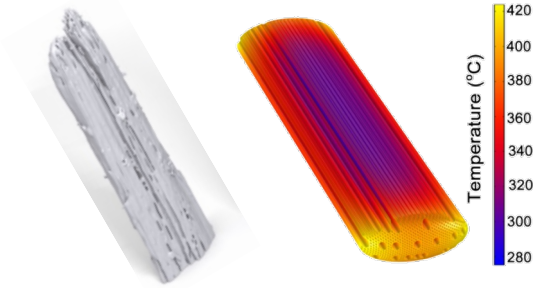




Investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists

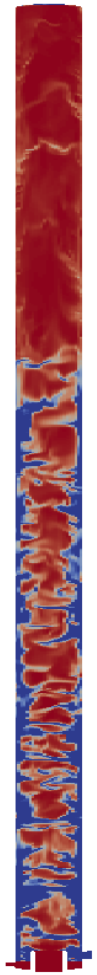
Biomass and Catalyst Particle Modeling at Meso Scales

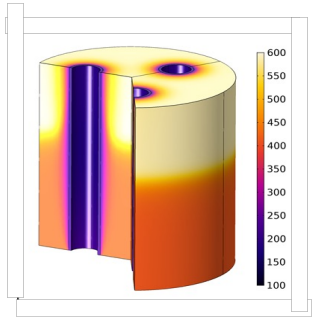


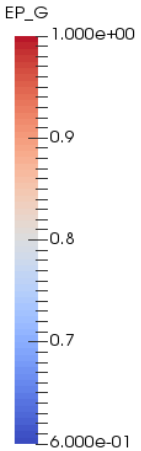


Understanding mass transport of reactants/products, reaction kinetics, and coking and deactivation processes

Conversion Modeling at Reactor Scales

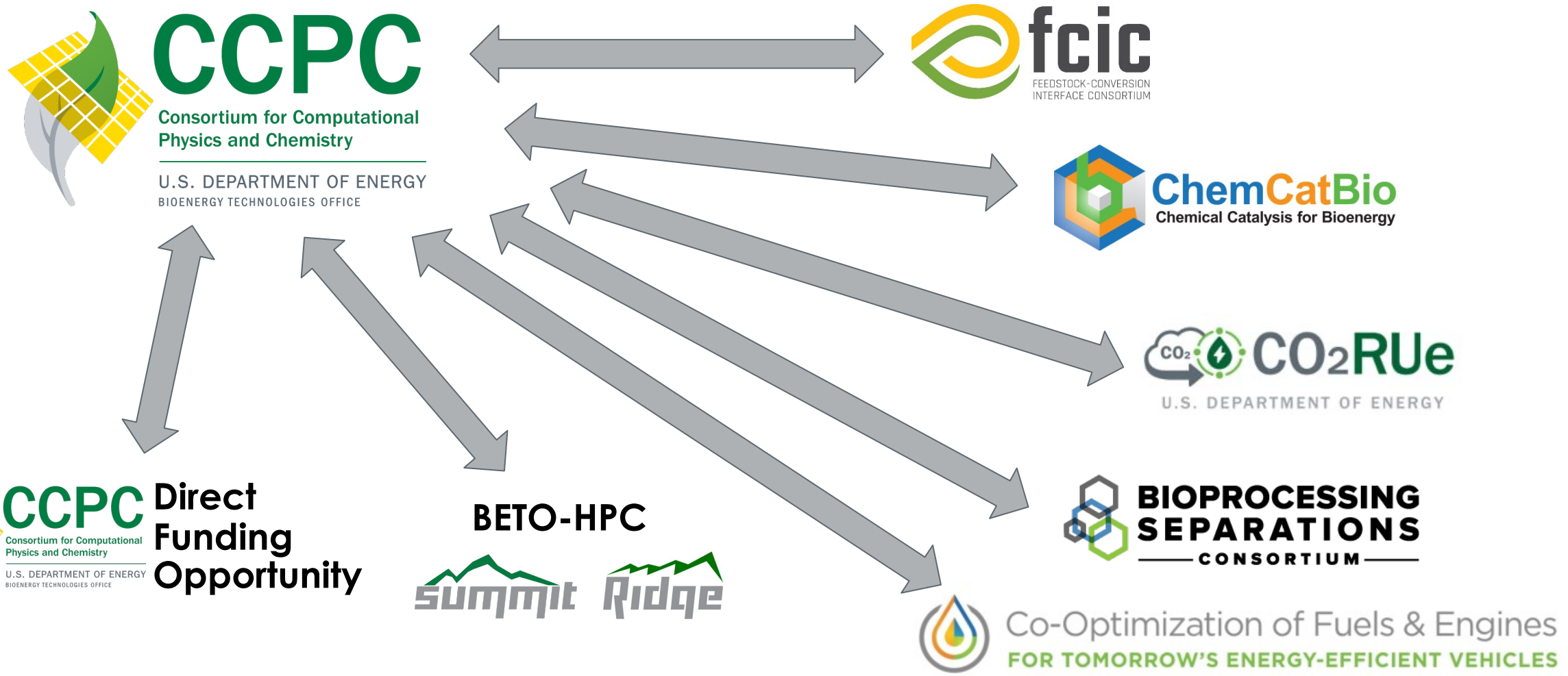




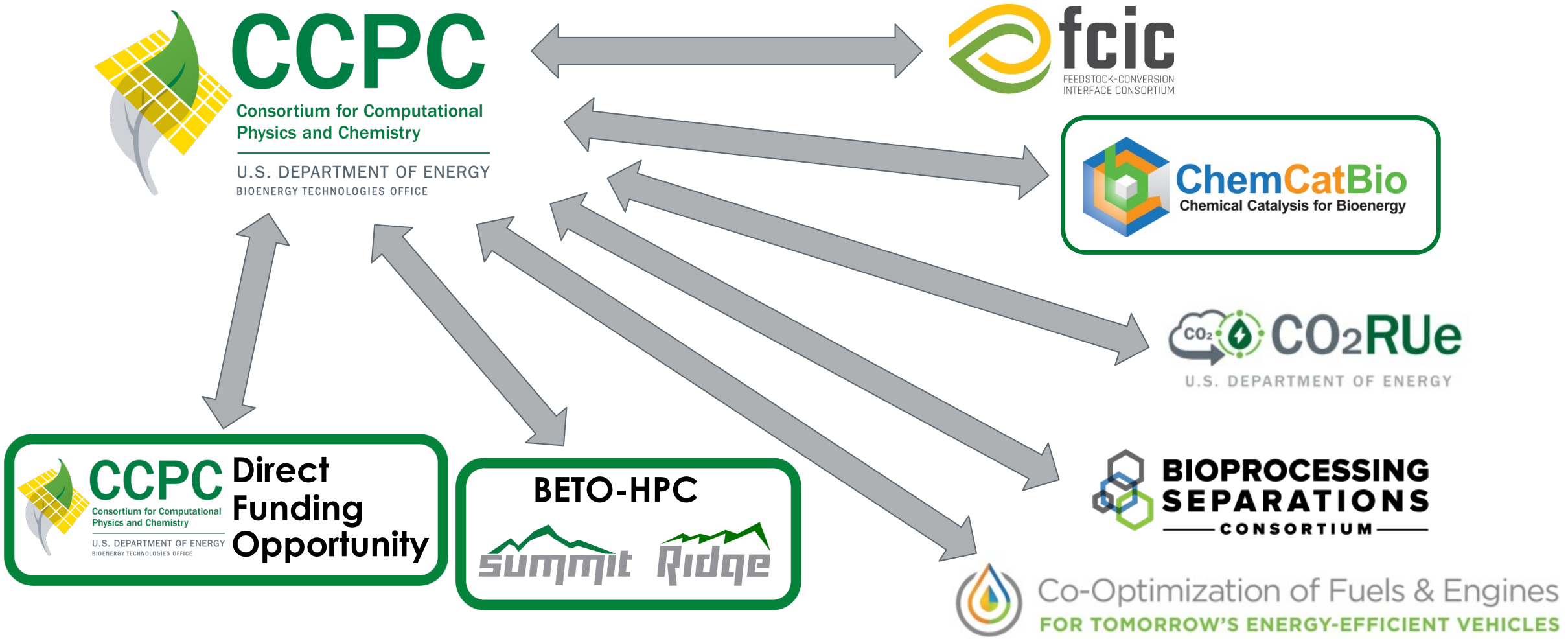


Determining optimal process conditions for maximum yield and enabling scale-up of biomass conversion and catalytic upgrading reactors

The CCPC Enables and Accelerates R&D Across BETO



The CCPC Enables and Accelerates R&D Across BETO



CCPC Timeline: Continued Evolution to Meet Needs

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FY13

Original logo in 2013

Computational Pyrolysis Consortium Began

FY14

Accomplishment
Identified aldol pathway preference (vs.alkyl) for reduction coke formation

FY15

Accomplishment
Sub-models used in commercial software (CSFMB©)

FY16

Go/No-Go Stage Passed
Pyrolysis and catalysis outcomes on track

Accomplishment
Demonstrated ability to predict pyrolysis oil yield as function of feedstock size and shape

ChemCatBio Launched
with CCPC, ACSC, and CCM enabling projects

ChemCatBio
Chemical Catalysis for Bioenergy

FY17

Accomplishment
Surface Phase Explorer tool released to public

Accomplishment
Tech transfer of biomass feedstock model assists Forest Concepts to convey product value to customers

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

FY18

Go/No-Go Passed
Kinetics application

Accomplishment
Modeling outcomes provided critical input into Catalytic Fast Pyrolysis decisions

FY19

New Task Structure implemented to align with BETO Verification Pathways

New AOP includes kinetics focus, new tools, & more connections

FY20

BETO-HPC Launched
Dedicated BETO High-Performance Computing

summit

FY21

3 DFO Projects Launch

forestconcepts
Catalyxx
PYRAN The 5-Carbon Company

FY22

CO2 Utilization
Seed projects show modeling needs

FY23

Redefined as **Consortium for Computational Physics and Chemistry (CCPC)** with expanded focus on catalysis

Peer Review Guidance
Interactions with Bioprocessing Separations Consortium initiated

BIOPROCESSING SEPARATIONS CONSORTIUM

Our CCPC Team: Bioenergy *and* Computational Experts


Rajeev Assary (ANL)


Canan Karakaya (ORNL)


Yidong Xia (INL)


Mal Soon Lee (PNNL)

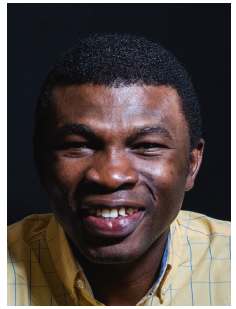

Greg Collinge (PNNL)


Paul Humble (PNNL)


Peter Ciesielski (NREL)


Carrie Farberow (NREL)


Michelle Nolen
(Colorado School of Mines)


Femi Oyedeji (ORNL)


Huamin Wang (PNNL)


Hieu Doan (ANL)


Bruce Adkins (ORNL)


Yupeng Xu (NETL)


Mehrdad Shahnam (NETL)


Subhodeep Banerjee (NETL)


Jim Parks (ORNL)

Thanks as well to former team members: Bill Rogers (NETL), Gavin Wiggins (ORNL), Zach Mills (ORNL), and Brennan Pecha (NREL)

Thanks to BETO TMs Trevor Smith, Sonia Hammache, and Kevin Craig

Collaboration is a Key to Success

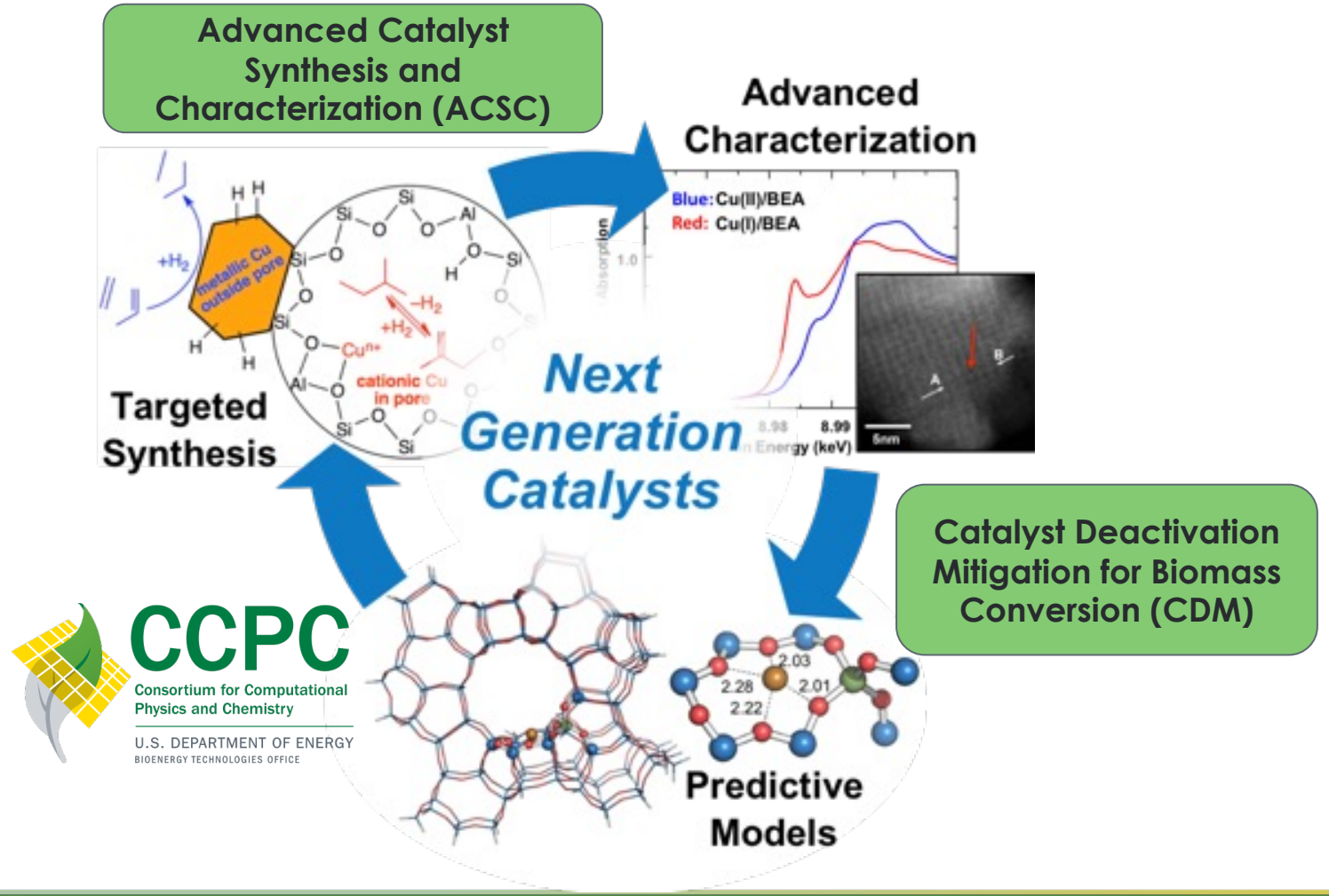
Recent CCPC meeting hosted by ORNL in January 2023

Progress & Outcomes: ChemCatBio

CCPC+ACSC+CDM = ChemCatBio Accelerated Catalyst Development

ChemCatBio
Chemical Catalysis for Bioenergy

Accelerated catalyst and process development cycle



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BIOENERGY TECHNOLOGIES OFFICE

ChemCatBio Pathway Projects

- **C1 Upgrading** (Gasification)
- **C2+ Upgrading** (Biochem-EtOH)
- **CUBI** (Biochem)
- **Catalytic Fast Pyrolysis (CFP)**
- **CO2 Utilization**
- **DataHub**

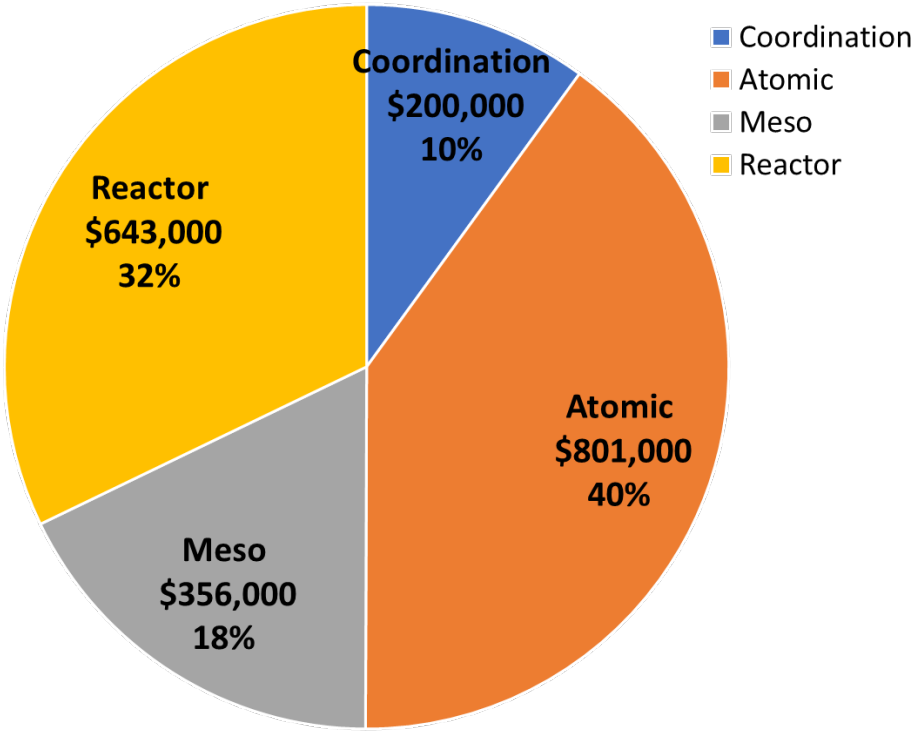
Atomic-Meso-Reactor Allocation Adjusted to ChemCatBio Priorities

ChemCatBio
Chemical Catalysis for Bioenergy

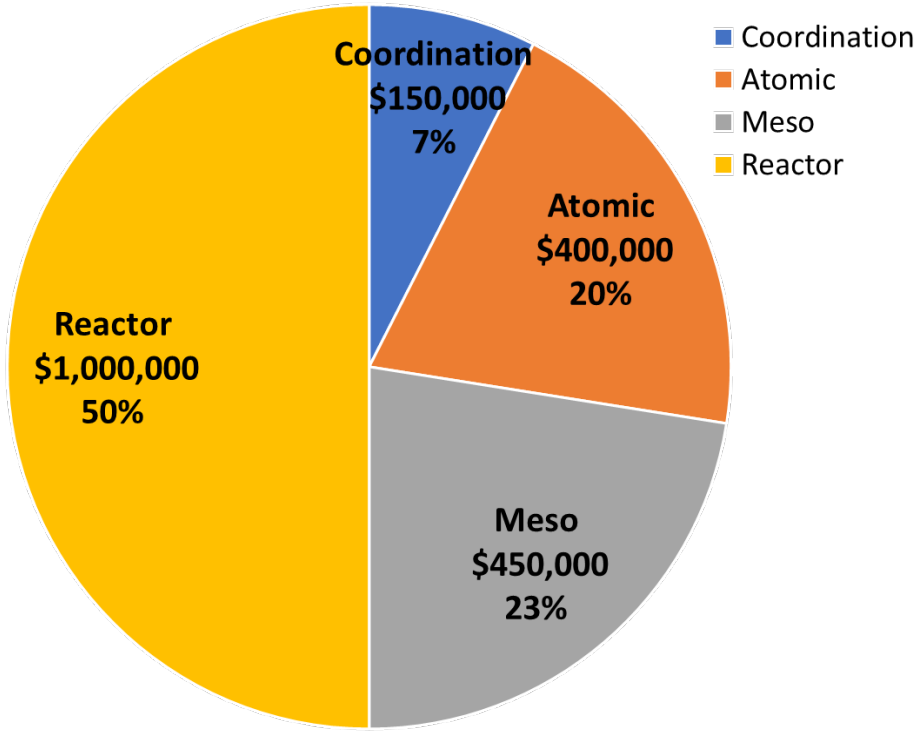
FY23-FY25 ChemCatBio Directions

- Shift to Engineered Catalysts
- Move to Higher Technology Readiness Levels
- Process Scale Up

CCPC-ChemCatBio Budget: FY22



CCPC-ChemCatBio Budget: FY23



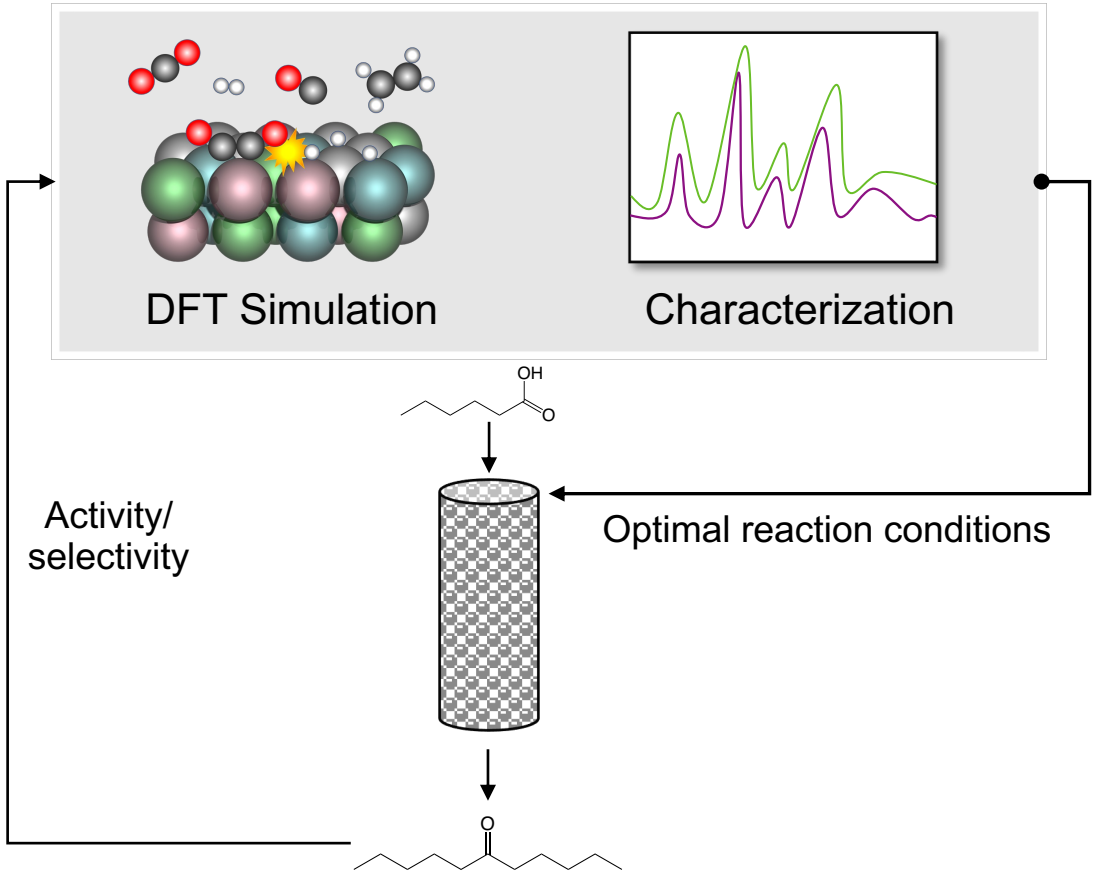
Optimizing Conversion of Volatile Fatty Acids to Sustainable Aviation Fuel

ChemCatBio
Chemical Catalysis for Bioenergy

CUBI (Biochem)	CCPC Atomic

- Catalytic ketonization of hexanoic acid to 6-undecanone on zirconia catalysts with acid/base site pairs
- As part of conversion of Volatile Fatty Acids (VFA) to Sustainable Aviation Fuels (SAF)

- CCPC Toolset Applied:
  - Atomistic scale modeling (periodic DFT) for elucidating reaction mechanisms, effect of CO_2, water on rate determining steps.
  - Theory and experimental characterization for identifying key reaction intermediates
- Impact and Relevance:
  - Determination of optimal reaction conditions for enhanced catalytic activity and selectivity



H. Doan, R. Assary (ANL, CCPC), J. Miller (CCB, NREL)

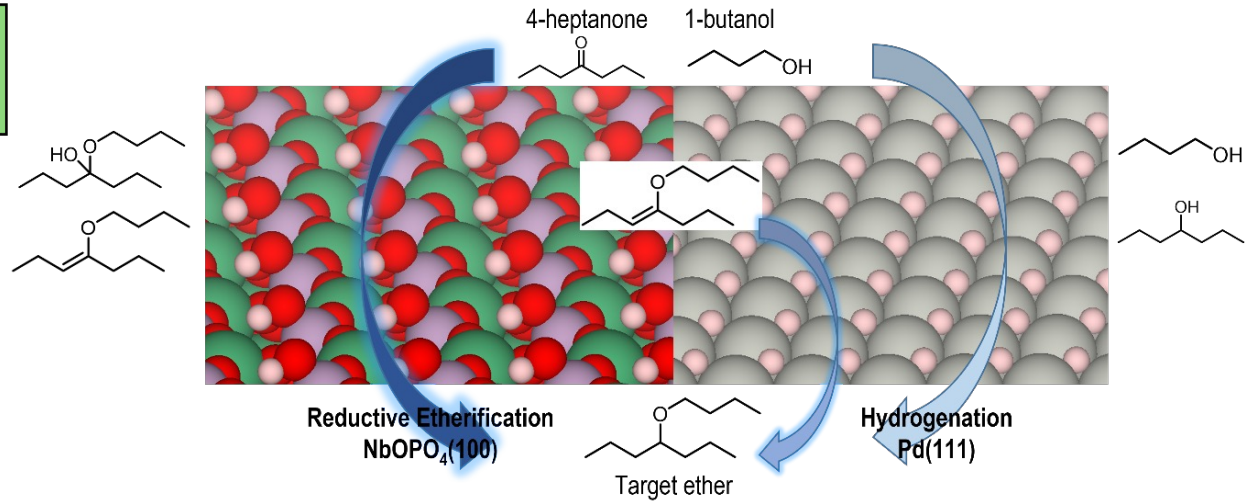
Mechanisms for Reductive Etherification On Pd/$NbOPO_4$ Catalysts

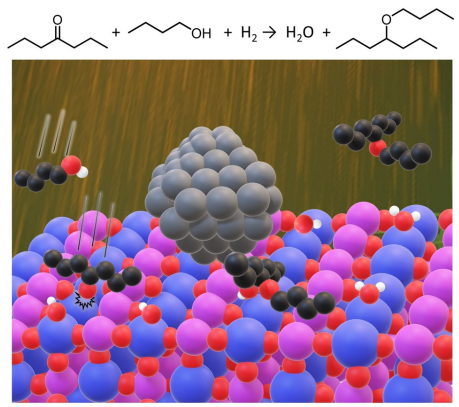
ChemCatBio
Chemical Catalysis for Bioenergy

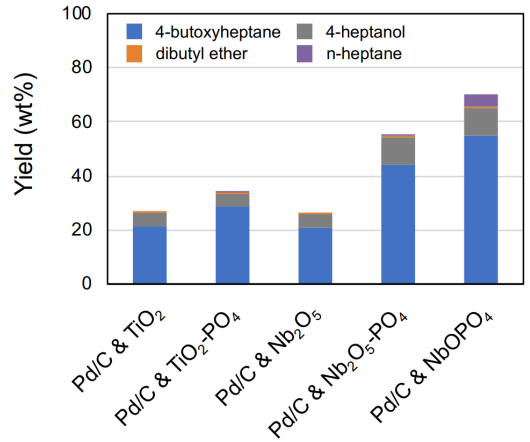
CUBI (Biochem)	CCPC Atomic

- Elucidated reaction mechanism of reductive etherification of n-butanol and 4-heptanone on Pd/$NbOPO_4$ catalyst.
- Pd/$NbOPO_4$ catalysts with various size were synthesized and simulated. The reductive etherification rates of 1-butanol and 4-heptanone increasing with Pd particle size (~5 nm optimum) over Pd/$NbOPO_4$

- CCPC Toolset Applied:
  - Atomistic modeling and catalyst synthesis and testing (CCB)
- Impact and Relevance:
  - Catalyst optimization for SAF production via CUBI







✓ C. Li, J. H. Miller, ,[3] N. J. LiBretto, A. L. Rein, H. A. Doan, M. Zhou, D. R. Vardon, S. Habas, and R. S. Assary, In preparation (2023)

Spillover at Metal-Support Interfaces Affect Susceptibility to Coking

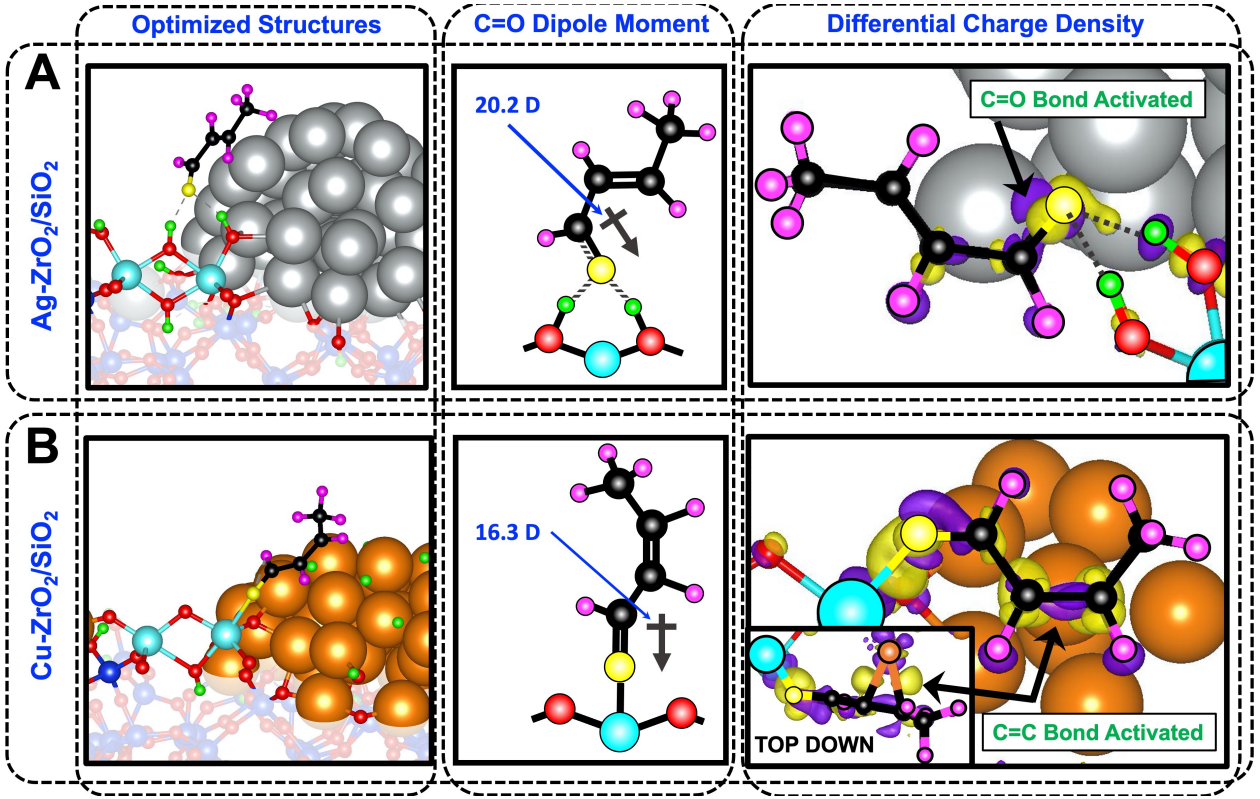
ChemCatBio
Chemical Catalysis for Bioenergy

C2+ Upgrading (Biochem-EtOH) | **CCPC** Atomic

- Using Cu instead of Ag, PNNL C2 upgrading team has improved the stability and selectivity of their Ag-based ethanol upgrading catalyst.
- Experiments: The Cu-based catalyst avoids reaction channels leading to coking. ***But why?***

- CCPC Toolset Applied:
  - DFT calculations, grand canonical free energy minimization, and chemical bonding analysis performed to investigate structural and chemical changes during reaction over both catalysts.

- Impact and Relevance:
  - Speciation and spillover of H_2 control the types of bonds activated. Metal-promoter interfaces are key to avoiding early dehydration and subsequent coking.



V. L. Dagle, G. Collinge, M. Rahman, A. Winkelman, D. Ray, W. hu, J. Z. Hu, L. Kovarik, M. Engelhard, J. Jocz, Y. Wang, M-.S. Lee, V-.A. Glezakou, R. Rousseau, R. Dagle ***Single-Step Conversion of Ethanol into n-Butene-Rich Olefins over Metal Catalysts Supported on ZrO_2-SiO_2 Mixed Oxides****. Applied. Catalysis B. (2023). Submitted*

Gregory Collinge (PNNL), Debmalya Ray (PNNL), Mal-Soon Lee (PNNL), Vassiliki-Alexandra Glezakou (ORNL), Roger Rousseau (ORNL)

Deactivation of Zeolite-Supported Cu-Y-Zn Ethanol Upgrading Catalyst is Thermodynamically Driven and Controlled by Zeolite pH

ChemCatBio
Chemical Catalysis for Bioenergy

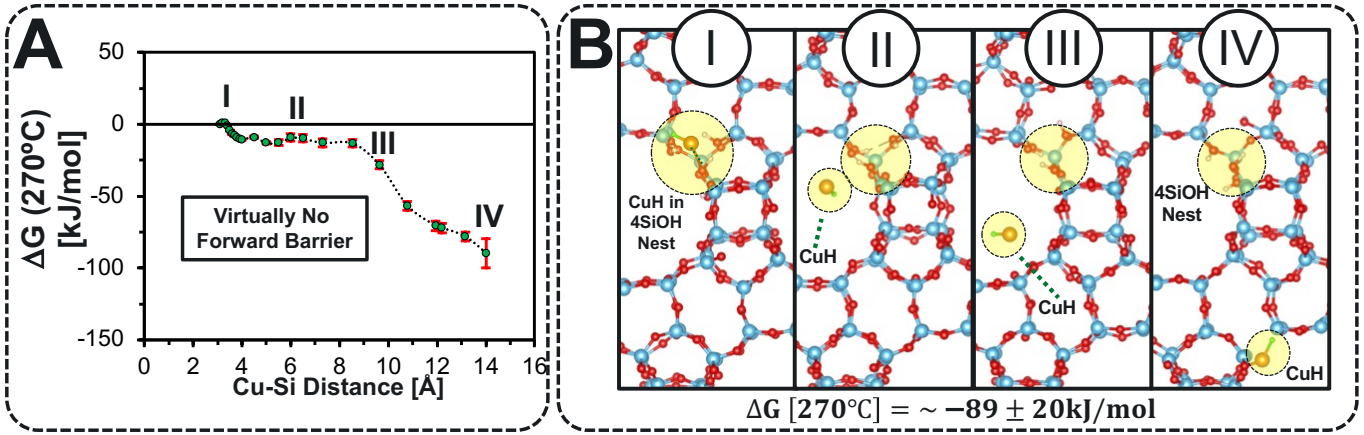
C2+ Upgrading (Biochem-EtOH) | **CCPC** Atomic

- Beta zeolite-supported Cu-Y-Zn catalyst for ethanol upgrading.
- Experiments: Deactivation by Cu sintering is observed over ~1-day time-on-stream, but high-temperature treatment in air, reverses sintering. ***Why? How?***

- CCPC Toolset Applied:
  - Ab initio molecular dynamics (AIMD) simulations plus enhanced free energy sampling to ascertain the mechanism and thermodynamics of deactivation.

- Impact and Relevance:
  - A full mechanism for deactivation and regeneration of ORNL's catalyst reveals strategies for preventing deactivation and/or accelerating regeneration.

Monomeric CuH (the identified active site) ejection from the zeolite defect. Enhanced free energy sampling reveals ejection to rapidly follow silanol nest protonation



S. Purdy, G. Collinge, J. Zhang, S. N. Borate, K. Unocic, Q. Wu, E. C. Wegener, N. Samad, S. Habas, T. R. Krause, J. W. Harris, M-.S. Lee, V-.A. Glezakou, R. Rousseau, K. Page, A. Sutton, Z. Li.

Improving the Regenerability of Copper Catalysis Through Atom Trapping in Zeolite Defects. *Paper Being Submitted*

Gregory Collinge (PNNL), Mal-Soon Lee (PNNL), Vassiliki-Alexandra Glezakou (ORNL), Roger Rousseau (ORNL)

Quantifying the Free Energy Reaction Profile for the Generation of Acetaldehyde from Ethanol

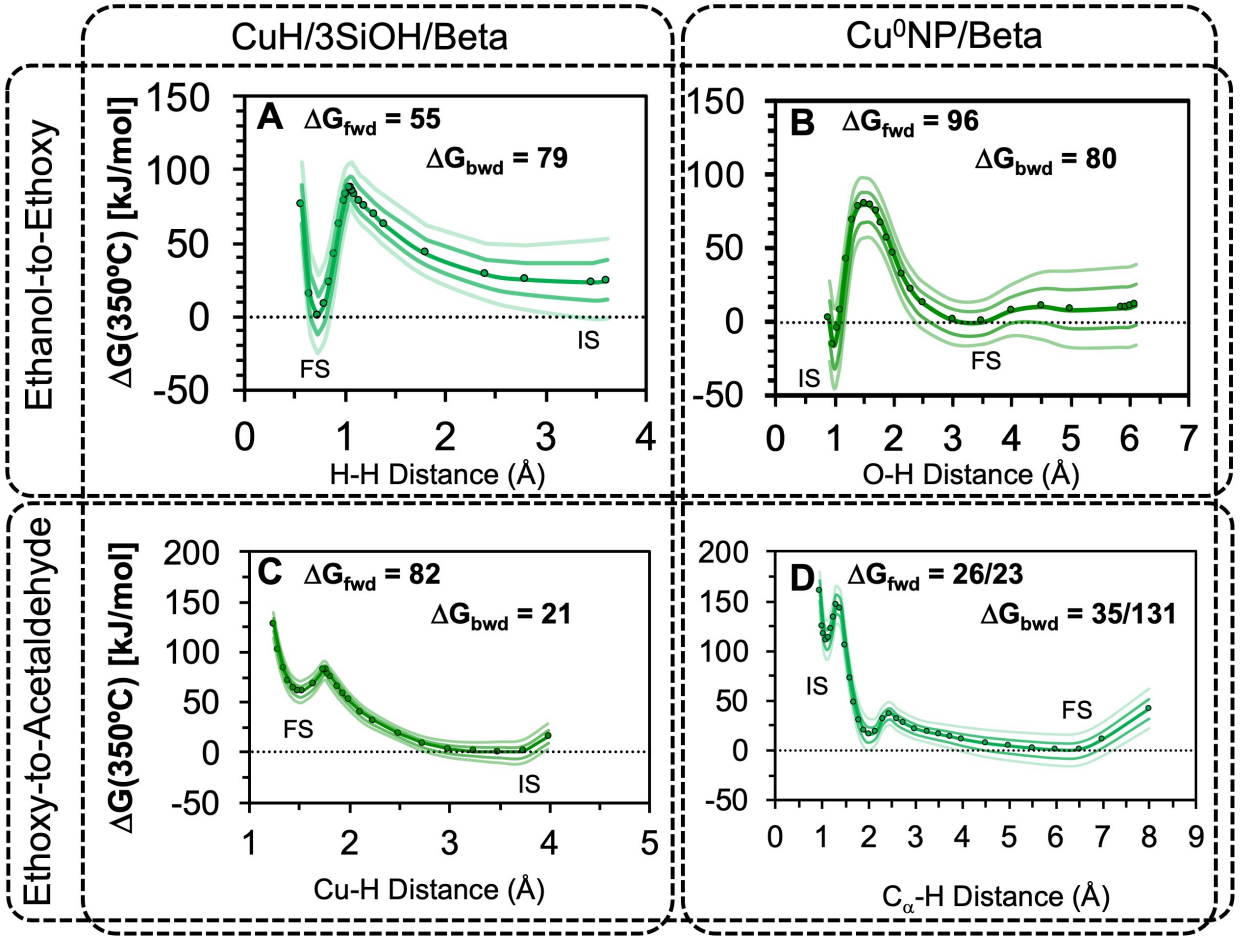
ChemCatBio
Chemical Catalysis for Bioenergy

C2+ Upgrading (Biochem-EtOH) | **CCPC** Atomic

- Beta zeolite-supported Cu-Y-Zn catalyst for ethanol upgrading.
- Experiments: Dehydrogenation activity of the catalyst is heavily impacted by the state of the Cu during reaction.

- CCPC Toolset Applied:
  - Ab initio molecular dynamics (AIMD) simulations combined with enhanced free energy sampling to quantify the free energy profile of ethanol dehydrogenation over the Cu active site compared to sintered Cu^0.

- Impact and Relevance:
  - The Cu active site was computed to facilitate rapid dehydrogenation. Kinetic barriers are similar for the sintered Cu^0 nanoparticles.



Gregory Collinge (PNNL), Mal-Soon Lee (PNNL), Vassiliki-Alexandra Glezakou (ORNL), Roger Rousseau (ORNL)

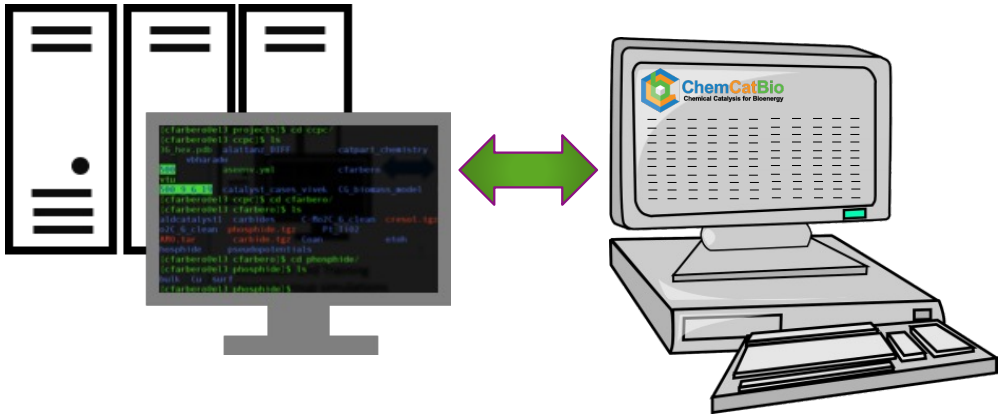
High-Throughput Calculations Enabling Population of DataHub

ChemCatBio
Chemical Catalysis for Bioenergy

DataHub	CCPC Atomic

- ChemCatBio DataHub *Catalyst Property Database* expanded to include 1000+ data values describing catalyst binding of **poisons common to biomass/waste conversion processes** and gas phase energies to enable data reuse

- CCPC Toolset Applied:
  - High-throughput quantum chemical calculations executed on NREL's DOE-EERE funded HPC resources
  - Develop scripts and APIs for automated data extraction and database upload
- Impact and Relevance:
  - First-of-kind set of contaminants/poisons database for bioenergy applications



cpd.chemcatbio.org

CCPC Contributors: Carrie Farberow (NREL), Sean Tacey (NREL)

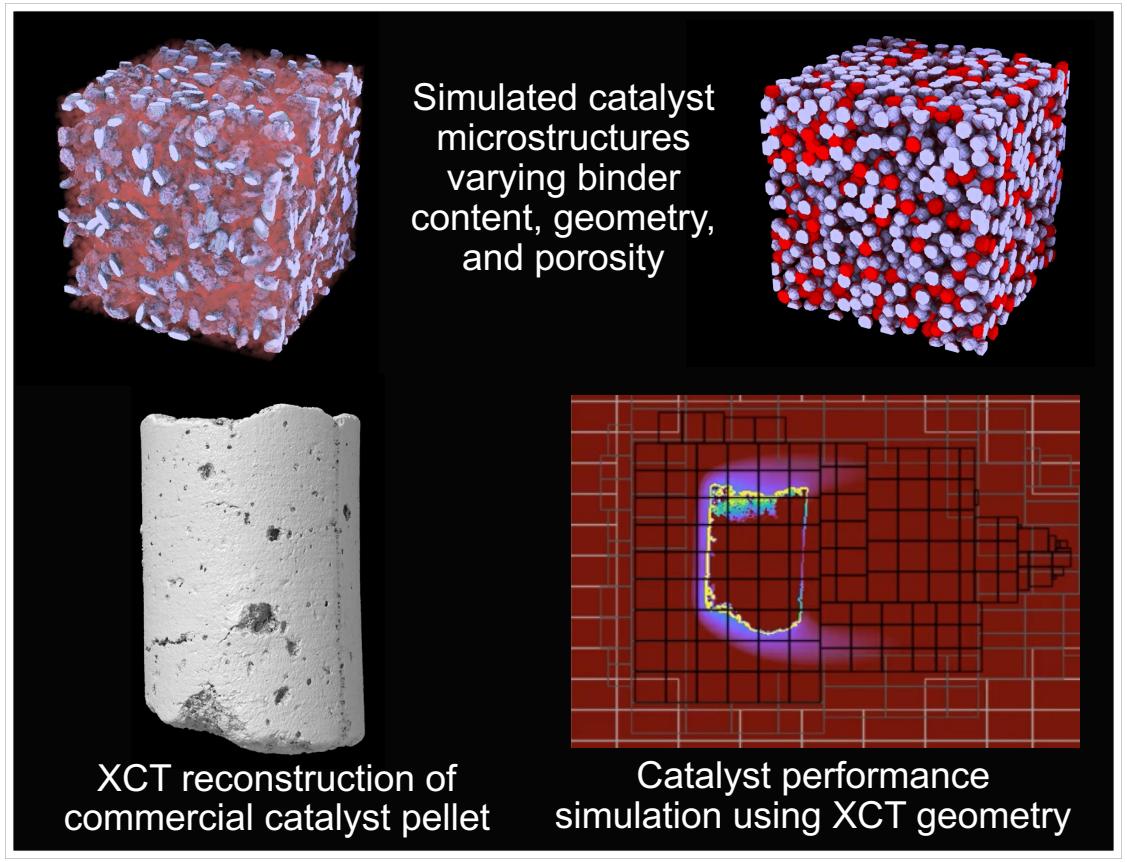
Modeling tools for catalyst particle size, shape, and porosity enable design and analysis of engineered catalysts for process scale-up

ChemCatBio
Chemical Catalysis for Bioenergy

C1 Upgrading (Gasification)	**CCPC** Meso
Catalytic Fast Pyrolysis (CFP)	**ACSC**

With Industry Partner JohnsonMatthey

  - Scale-up of catalytic processes usually requires transitioning from powdered catalyst to engineered particles (e.g., spheres, extrudates)
- CCPC Toolset Applied:
  - Modeling tools were developed to screen potential catalyst architectures prior to synthesis.
  - 3D X-ray reconstructions of commercial catalysts can also be directly imported for detailed performance simulations.
- Impact and Relevance:
  - New open-source code enables high-fidelity mesoscale simulations to optimize catalyst architecture for reactor configuration commercial performance targets



Sitaraman, H., Ciesielski, P. N., Crowley, M., Pecha, B., & Thornburg, N. (2022). Mesoflow: An Open-Source Reacting Flow Solver for Catalysis at Mesoscale (No. NREL/PR-2C00-83698). https://github.com/NREL/mesoflow

Jacob Miller (NREL), Meagan Crowley (NREL), Hari Sitaraman (NREL), Peter Ciesielski (NREL)

Biogenic Coke Oxidation Kinetics for Catalyst Regeneration

ChemCatBio
Chemical Catalysis for Bioenergy

Catalytic Fast Pyrolysis (CFP)	CCPC Reactor	CDM

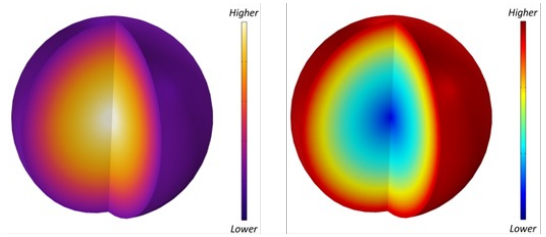
- Zeolite based catalyst regeneration and BFCC optimization
- Biogenic FCC coke is very different than petroleum FCC coke
- Combined particle scale (simplified) and reactor scale
- Two spent catalysts: (a) Geldart B (~700 mm) from 2FBR for method development, and (b) FCC (80 mm) catalyst from DCR

- CCPC Toolset Applied:
  - COMSOL bed models for deconvolution of combustion kinetics and mass/heat transport effects from TPO data (temperature programmed oxidation) complimented by spent and partially regenerated particle/coke characterization
  - MFiX models for pilot- and commercial-scale regenerators, with afterburn (freeboard combustion), catalyst cooler, etc
- Impact and Relevance:
  - First R&D program specifically aimed to understand nature of biogenic coke and consequences for BFCC design

TPO of Coked Catalysts

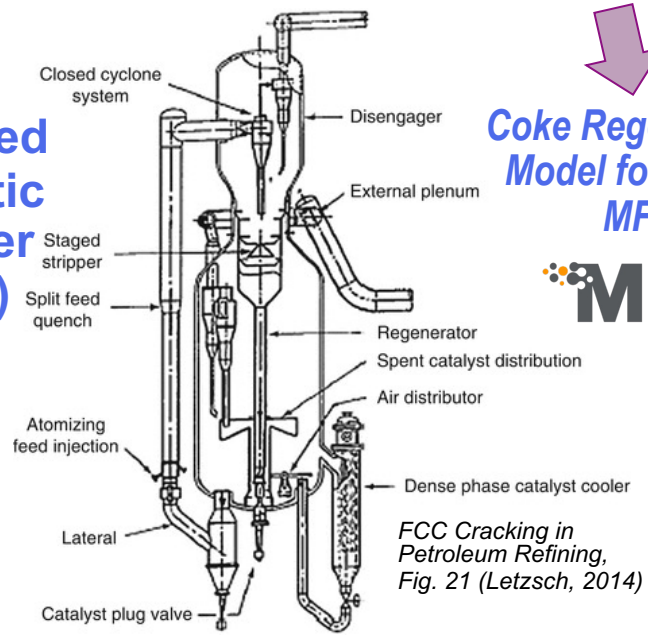
Kinetics Extraction via COMSOL

COMSOL



Temperature *O2 Concentration*

Fluidized Catalytic Cracker (FCC)



FCC Cracking in Petroleum Refining, Fig. 21 (Letzsch, 2014)

Coke Regeneration Model for FCC in MFiX

MFiX

Bruce Adkins (ORNL), Mehrdad Shahnam (NETL)

Scale Up of ChemCatBio Catalysts for Ethanol Conversion to SAF

ChemCatBio
Chemical Catalysis for Bioenergy

C2+ Upgrading (Biochem-EtOH) | **CCPC** Reactor

- Conversion of EtOH to C4 higher olefin SAF precursors
- Routes avoid endothermic dehydration of EtOH to ethylene, resulting in considerable process simplification
- PNNL route: Cu-Zr/SiO_2 and Ag-Zr/SiO_2
- ORNL route: Cu-Zn-Y/BEA

- CCPC Toolset Applied:
  - Leveraging numerical "know-how" from modeling Guerbet EtOH upgrading with 26 species and 22 reactions demonstrated feasible in Catalyxx DFO for up to 5-ton bed reactor
  - Rate expressions specific to this chemistry under development
- Impact and Relevance:
  - Commercialization of thermocatalytic C2-to-SAF technologies being developed at PNNL and ORNL

$$C_2H_6O(ethanol) \xrightarrow{k_1} C_2H_4O(acetaldehyde) + H_2$$

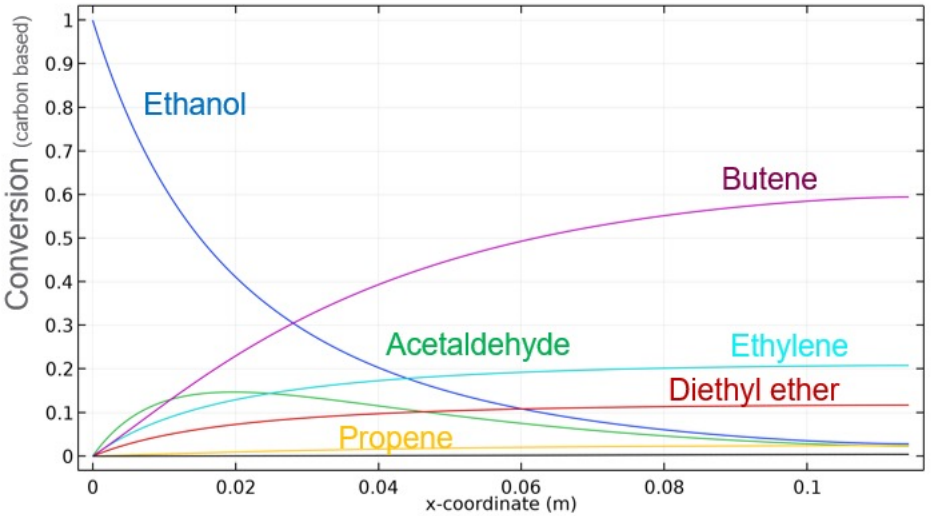
$$2C_2H_6O(ethanol) \xrightarrow{k_8} C_4H_{10}O(\text{di-ethyl-ether}) + H_2O$$

$$C_2H_6O(ethanol) \xrightarrow{k_9} C_2H_4(ethylene) + H_2O$$

$$2C_2H_4O(acetaldehyde) + 2H_2 \xrightarrow{k^*} C_4H_8(butene) + 2H_2O$$

$$2C_2H_4O(acetaldehyde) + \frac{1}{2}O_2 \xrightarrow{k_p} C_3H_6(propene) + CO_2 + H_2O$$

$$C_4H_8(butene) + H_2 \xrightarrow{k_{10}} C_4H_{10}(butane)$$



Paul Humble (PNNL)
Bruce Adkins and Canan Karakaya (ORNL)

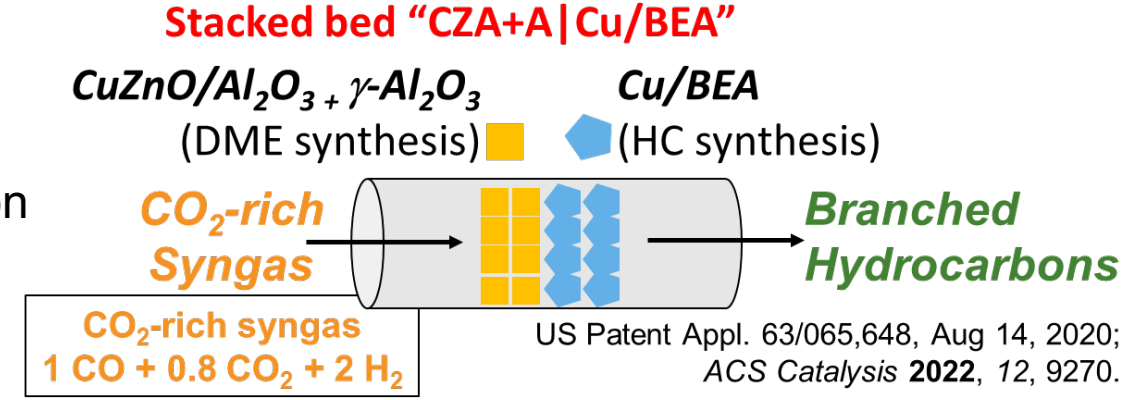
Stacked- and Mixed-Bed Modeling to Optimize CO_2–Rich Syngas Upgrading

ChemCatBio
Chemical Catalysis for Bioenergy

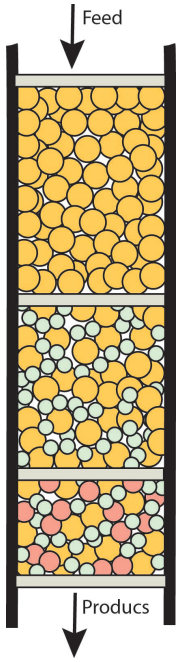
C1 Upgrading (Gasification)	CCPC Reactor

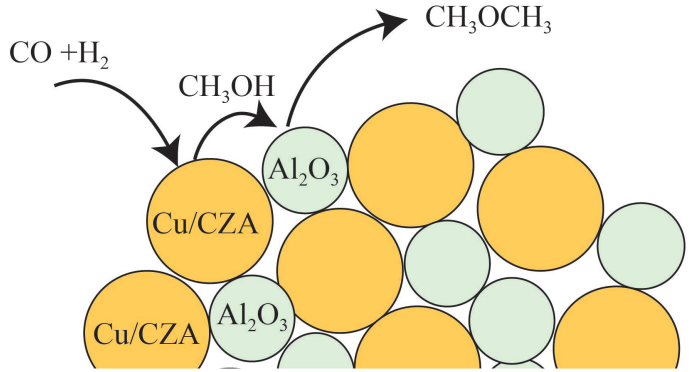
- Multiple catalysts (Cu/BEA+CZA+Al_2O_3) for hydrocarbon production via methanol and dimethyl ether (DME)
- What is the optimal catalyst bed geometry?

- CCPC Toolset Applied:
  - A packed reactor model to describe the process in a mixed catalyst, multi-bed system
  - Represents complex chemistry (23 reactions) over multiple catalyst
  - Captures the complex nature of process, heat mass transfer catalytic chemistry
  - Incorporates intraparticle scale heat and mass transfer
  - Validated heat and mass transfer features
- Impact and Relevance:
  - Scalable reactor models (lab scale to pilot+) for process design and optimization
  - Validated reaction chemistry (enables risk mitigation for scale up



US Patent Appl. 63/065,648, Aug 14, 2020;
ACS Catalysis **2022**, *12*, 9270.





Canan Karakaya (ORNL), Bruce Adkins (ORNL), Peter Ciesielski (NREL)

Progress & Outcomes: BETO-HPC

The BETO-High Performance Computing Program (BETO-HPC)

The Bioenergy Technologies Office (BETO) partnered with the Advanced Manufacturing Office and the Oak Ridge Leadership Computing Facility (OLCF) to acquire and host access to High Performance Computing (HPC) resources.

Launched in FY2020, BETO-HPC is a BETO-specific user program operated by the CCPC and OLCF providing ~100M core-hrs per year access to:

18 nodes (16,200 core equivalent)
Hybrid CPU-GPU

40 CPU nodes (5120 core equivalent)
5 CPU+GPU (1750 core equivalent)

Summit (right) and Frontier (below) supercomputers at the Oak Ridge Leadership Computing Facility

Summit (200 PetaFlops max): #1 fastest computer in 2018* (now #5)

Frontier (1.6 ExaFlops max): #1 fastest computer in 2022*

Over the next year the OLCF User Facility will transition from Summit to Frontier

*based Top500 List at top500.org

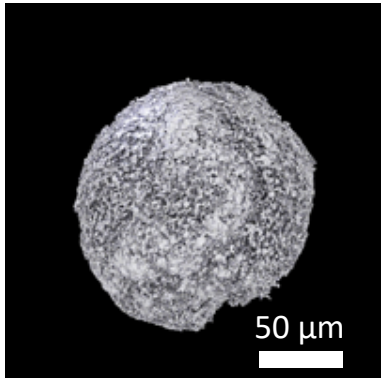
BETO-HPC User Facility Projects Span BETO Program Areas

BETO Area	NL	PI(s)	Summary	Industry Partner
Feedstock Technologies	ORNL	Lianshan Lin	Large-scale digital twins of a real rotary shear machine can be used to study feedstock comminution and to help optimize the cutters design to improve the tool lifetime and processing efficiency.	Forest Concepts forestconcepts
Conversion Technologies	NREL	Carrie Farberow	Atomic-scale simulations have advanced the development of Pt/TiO2 catalysts for CFP upgrading by providing insight into observed carbon efficiency and the effect of alkali impurities on product yields.	
Data, Modeling, & Analysis (DMA)	ORNL	Yan Liu	Models how farmers can adapt to a wetter eastern US under climate-change projections by planting deep-rooted perennial crops that can withstand flooding, increase infiltration rates, and protect water quality of rivers as floods become more frequent.	
Systems Development & Integration (SDI)	NREL	Hariswaran Sitaraman	Computational tools help conversion plants handle highly variable solid feedstocks to avoid upstream process upsets such as hopper arching and screw-feeder plugging.	
Systems Development & Integration (SDI)	NREL	Hariswaran Sitaraman	Prediction of catalyst reactivity and deactivation for biomass pyrolysis vapor upgrading to tune catalyst residence time in large-scale catalytic pyrolysis reactors for production of renewable fuels and chemicals from biomass/plastics.	
Systems Development & Integration (SDI)	ORNL	Flavio Dal Forno Chuahy	Optimizing the engine piston geometry, injection strategies, and fuel physical properties simultaneously can find synergistic effects between decarbonized fuels and engine designs.	Cummins
DMA & SDI	LBNL	Vi Rapp & Ana Comesana	The 'Feedstock to Function' tool encourages innovation and accelerates early R&D of sustainable aviation fuels (SAFs) by enabling users to rapidly and seamlessly screen properties, cost, and emissions of viable SAF molecules.	
Feedstocks & Conversion	ORNL	Oluwafemi Oyedeji	Couples single-particle and reactor models developed under the CCPC to capture the critical particle-scale effects that occur under oxidative pyrolysis for more accurate yield predictions.	

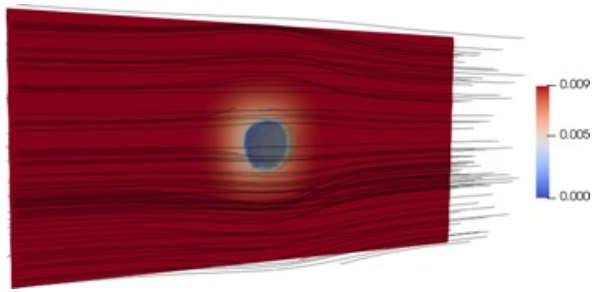
A Wide Range of Bioenergy Applications Studied on BETO-HPC

Catalyst Particle Reactivity and Deactivation (Hariswaran Sitaraman)

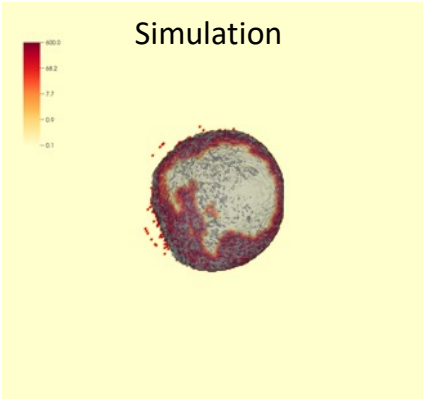
Zeolite catalyst particle

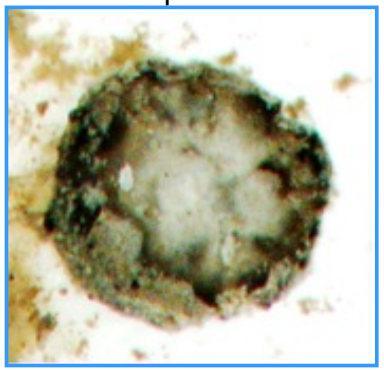


Reactant flow



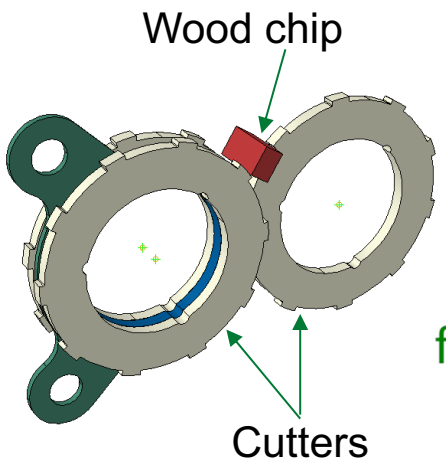
Catalyst deactivation



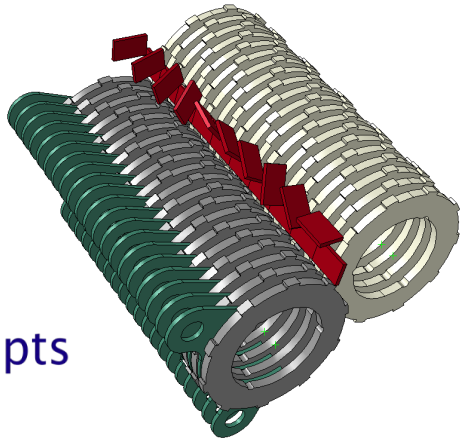


Feedstock Pre-Processing (Lianshan Lin)

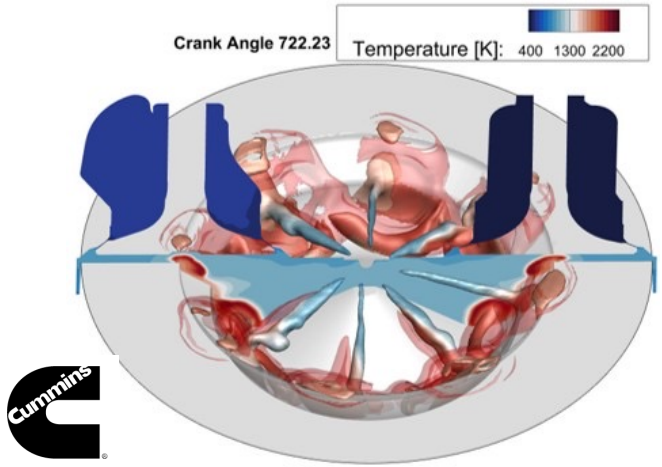
Simple model (PC-scale)



Digital twin (HPC-scale)



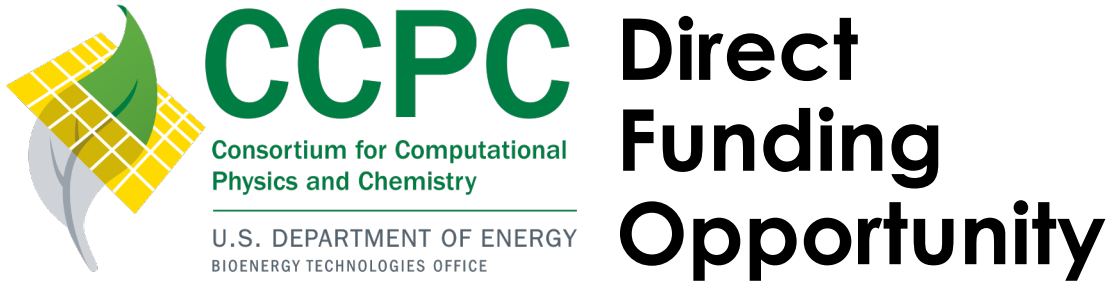
Biofuel Combustion (Flavio Dal Forno Chuahy)



Moving Forward with BETO-HPC

- Summit will phase out (and be recycled) as Frontier comes on-line
- Ridge will remain available for use
- Lessons Learned:
  - BETO-HPC has provided an excellent trial platform for BETO researchers (particularly for trying code on GPU-based computers)
  - Projects with original code worked well (with support from OLCF)
  - Using licensed software was problematic
- Recommendations Moving Forward:
  - Focus BETO resources on software readiness and user support
  - CCPC and OLCF continue to assist BETO researchers on HPC access
  - Work with Office of Science programs addressing similar challenges

Progress & Outcomes:
CCPC Direct Funding Opportunity



CCPC Models Enabling Industry Partners

BETO Webinar Presented in Oct. 2022*

CCPC
Consortium for Computational Physics and Chemistry
U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE


Yidong Xia (INL)


Peter Ciesielski (NREL)


Canan Karakaya (ORNL)


Bruce Adkins (ORNL)

Three projects supported by the Bioenergy Technologies Office in the CCPC Direct Funded Opportunity program.

forestconcepts™

Dr. Jim Dooley
Chief Technology Officer
Forest Concepts, LLC

PYRAN
The 5-Carbon Company


Dr. Kevin Barnett
Chief Technology Officer
Pyran

Catalyxx


Joaquín Alarcón
President and Chief Executive Officer
Catalyxx, Inc.

Budget (over 18-24 month period)

$432k ($540k with cost share)

$300k ($400k with cost share)

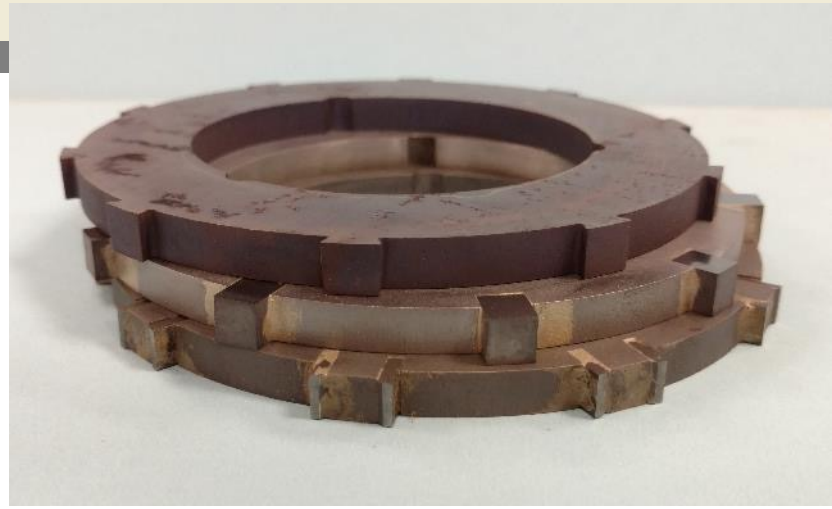
$300k ($400k with cost share)

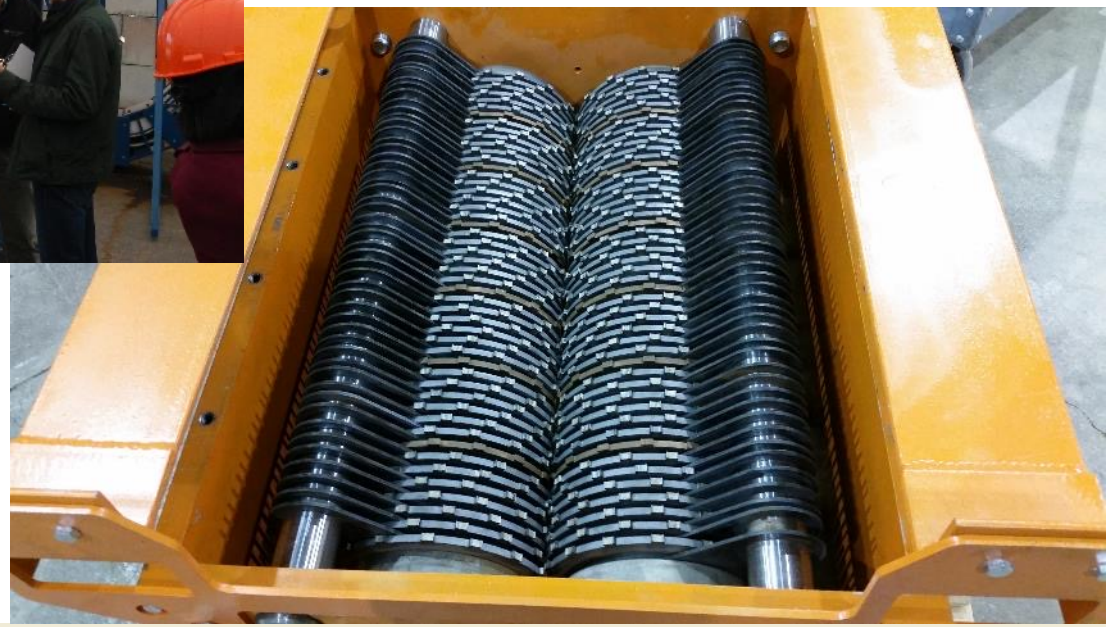
*www.youtube.com/watch?v=6IpMGfcAi8U

The "Forest Concepts' Crumbler® Rotary Shear"

"Sort of like a paper shredder"

- Cutter thickness controls particle size
- Processes any moisture content from dry to wet
- Specific energy fairly independent of moisture
- Quiet
- Dust control not needed for most materials





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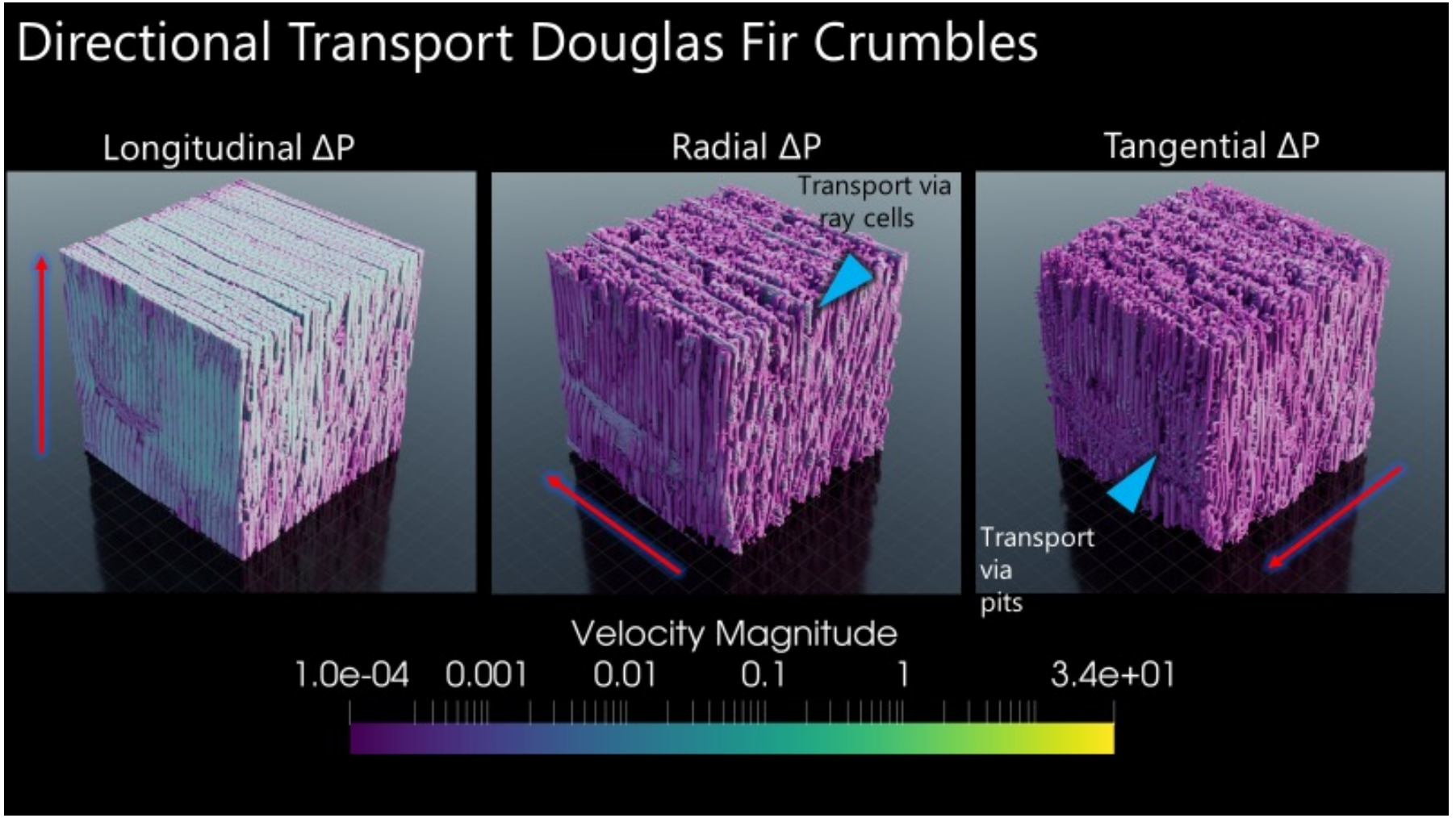
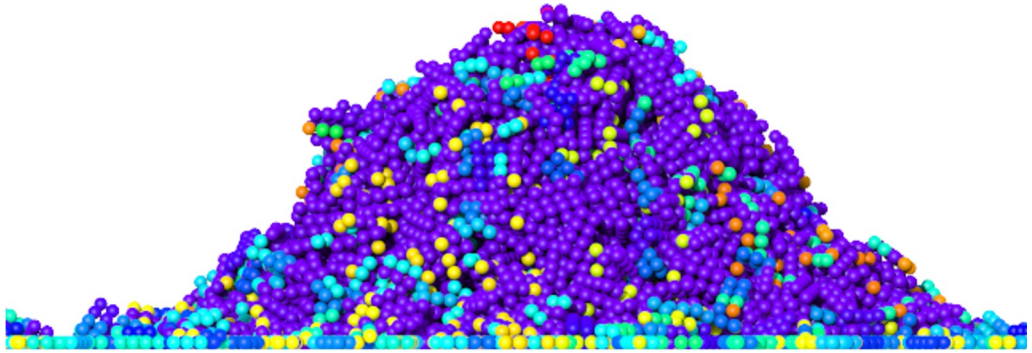
CCPC Modeling Role(s):
(1) Determine transport
(2) Determine flowability

Directional Transport in Biomass Particles

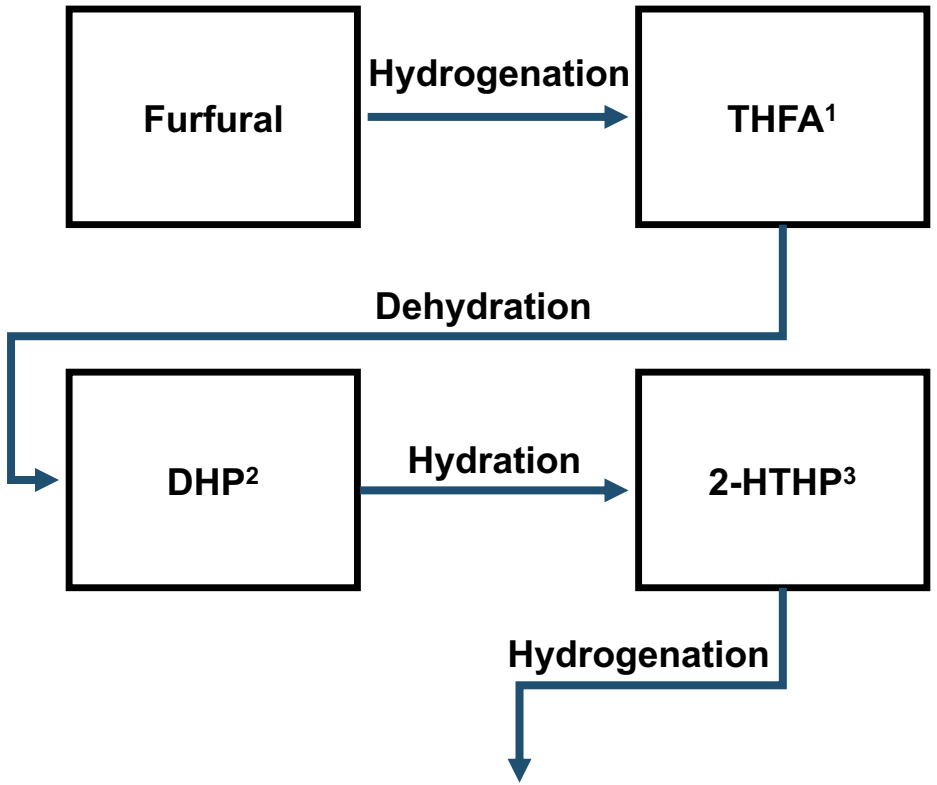


Flowability Modeling – Angle of Repose



Application of Discrete Element Modeling to predict angle of repose for bulk biomass.

Pyran's Process for Sustainable 1,5-Pentanediol (PDO)



Pyran's PDO could lead to a cumulative reduction in GHG of 6 Gt by 2050 relative to traditional alternatives.

- Adipic acid,[1] the standard building block for HDO, is produced primarily through oil refining – generating ~23 kg CO_2/kg.
- In contrast, Pyran PDO generates ~1 kg CO_2/kg.

~95% CO_2 Reduction!!! & 20-40% Lower Cost

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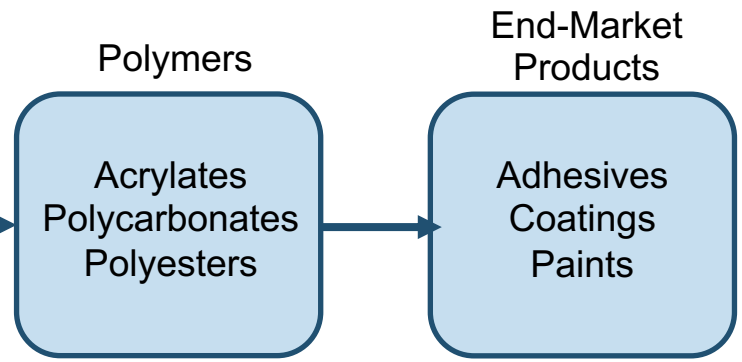
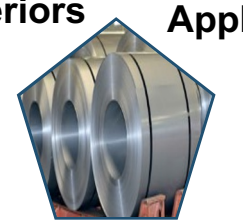
CCPC Modeling Role:
(1) Enable Scale Up
(bench scale to pilot scale)




Car Interiors


Appliances

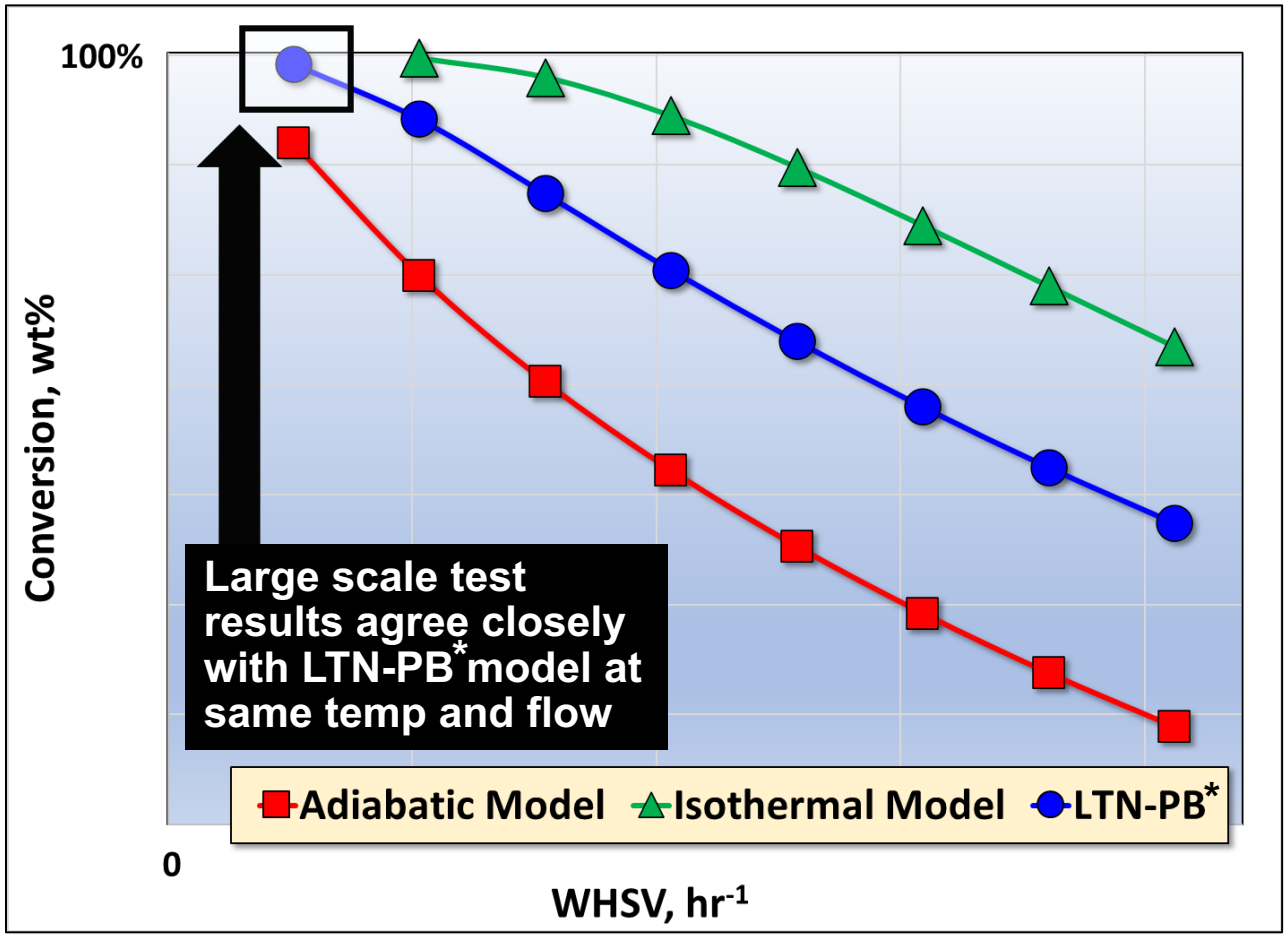

Metal Coil Coatings


Inks

1. Tetrahydrofurfuryl Alcohol.
2. Dihydropyran.
3. 2-Hydroxytetrahydropyran.

CCPC Model Supports Pyran Scaleup Step of ~1,000X!!

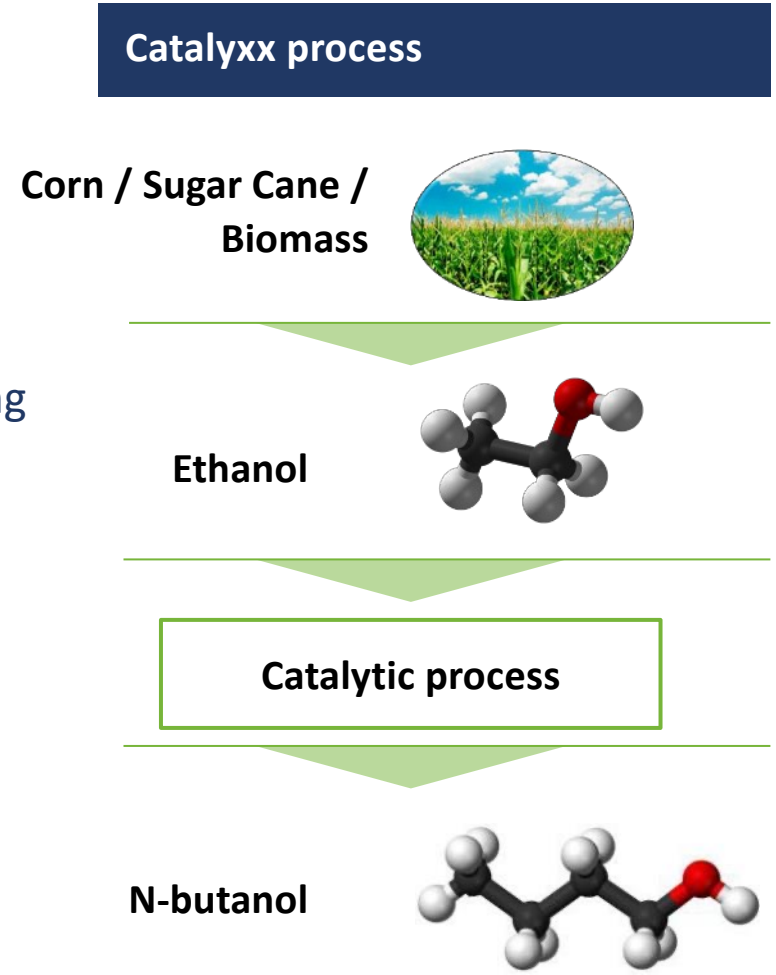
Multiple reactor system holds 100's of kgs of catalyst



*LTN-PB=Local Thermal Non-equilibrium-Packed Bed

Catalyxx produces renewable chemicals and fuels via Guerbet's reaction

- Catalyxx, incorporated in 2017, is a **renewable** chemical and fuel technology company that has fully **developed and successfully tested** a new and disruptive technology to produce n-biobutanol and other longer-chain linear alcohols.
- Butanol is produced by condensing ethanol using Catalyxx's patented catalyst and its thermochemical catalytic process, following the mechanisms of Guerbet's reaction.
- Economic and environmental **value**:
  - Lower cost of production of butanol: **60% lower cost** than the existing petrochemical route.
  - **Up to 85% lower CO_2 emissions**.
- The N-butanol is a widely used chemical commodity and has a **market size** of $5bn and is expected to steadily grow in the coming years.
- The technology is **fully protected** by five international families of patents.



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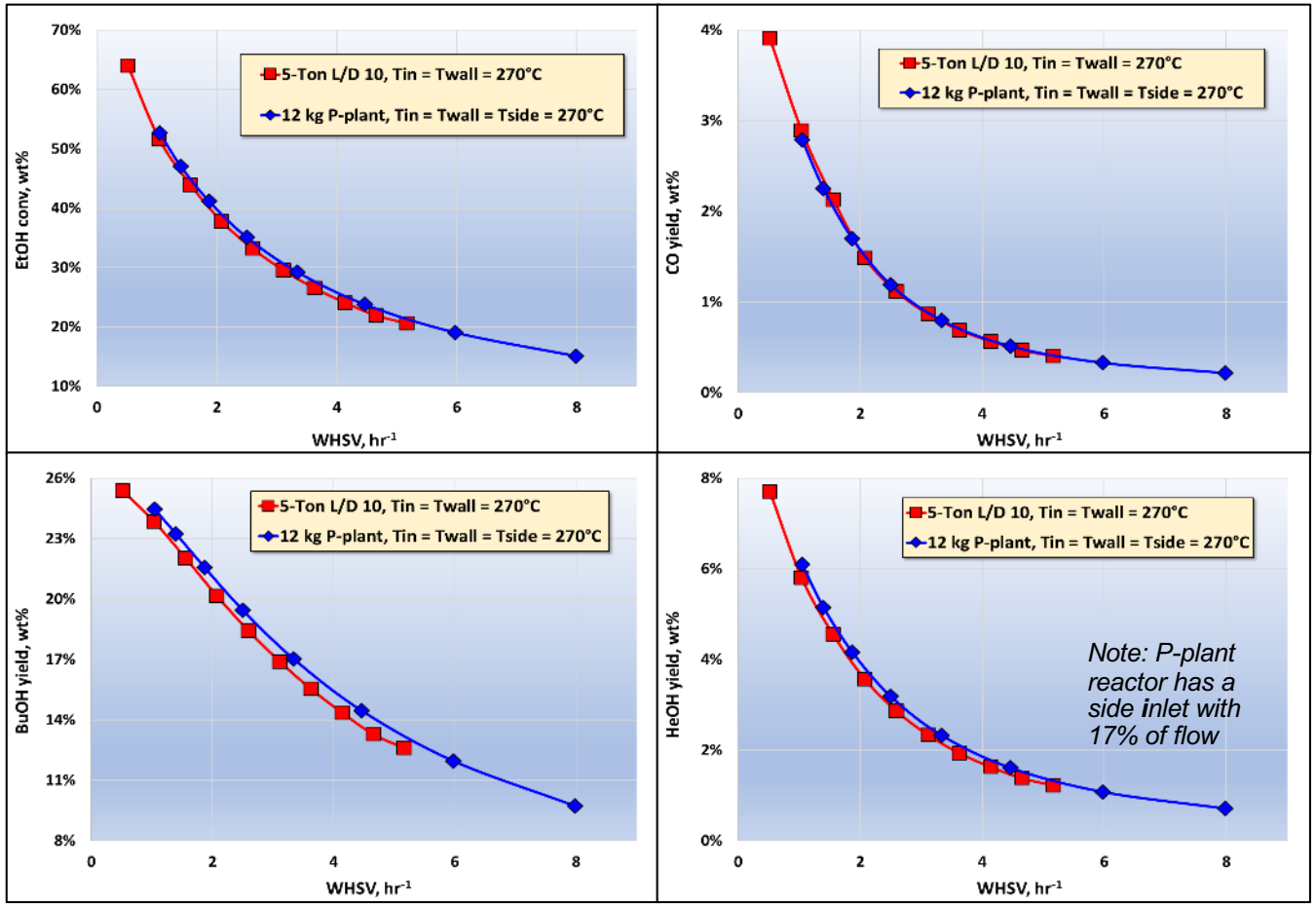
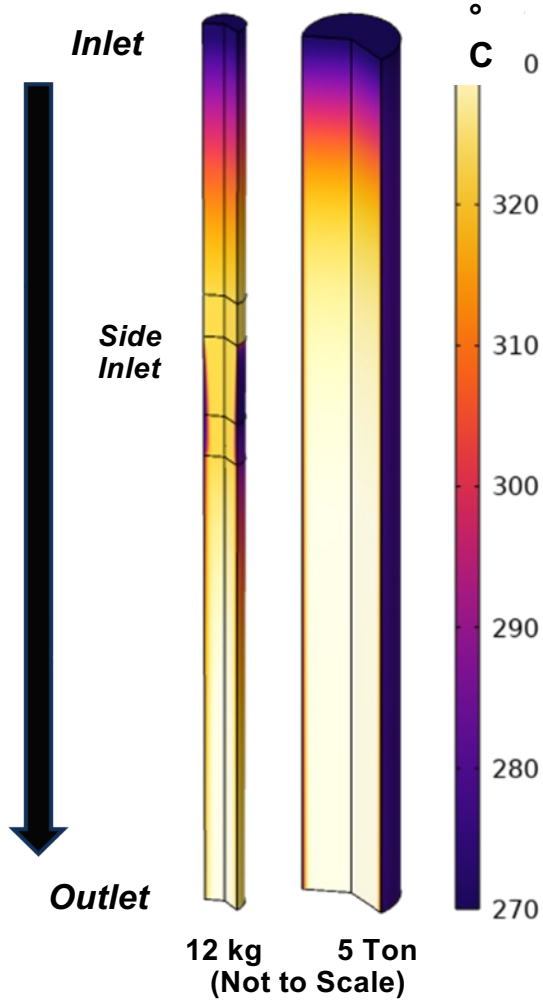
CCPC Modeling Role:
(1) Enable predictive simulation of scaled up reactors

CCPC modeling demonstrated 5-ton reactor scale was feasible, with yields similar to pilot-scale beds





The simulation provided Catalyxx with a tool to optimize the 5-ton reactor and reduces scale-up risks, knowing that the model shows similar behaviors independently of scale.

Statements from Our Valued Industry Partners

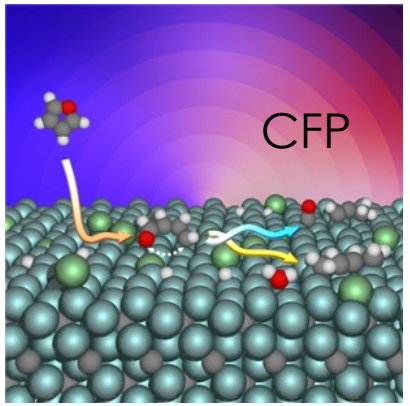
- From Dr. Jim Dooley, Chief Technology Officer, Forest Concepts, LLC:
  - *Forest Concepts is now in a position to help our clients and customers specify feedstocks and processing equipment systems based on a much better understanding of the effects of particle properties.*

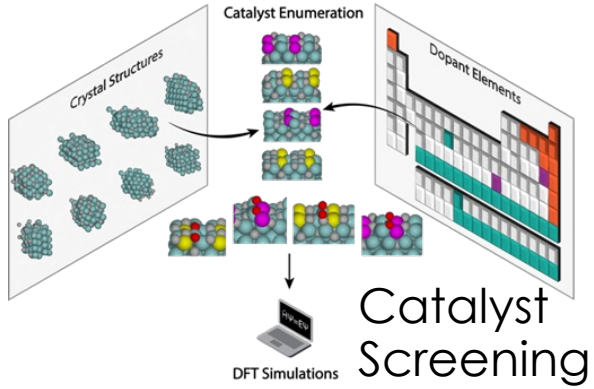
    We are using the new knowledge to refine our equipment designs and toll processing operations.
- From Dr. Kevin Barnett, Chief Technology Officer, Pyran:
  - *This DFO project allowed us to access invaluable CCPC modeling expertise that was instrumental in accelerating the scale up of our technology to produce renewable 1,5-pentanediol. The modeling groundwork developed for this project can serve as a foundation to further scale up our reactions and design commercial scale processes to bring bio-based products to market.*
- From Joaquín Alarcón, President & CEO Catalyxx Inc.:
  - *Well, I think the people that work with us are very smart; they deploy the wealth of knowledge and very good ideas. And you know, working with the BETO office is fantastic because it also provides capability to our solutions, having people that trust what we do and that have an excellent profile and excellent background is very encouraging for us. So we can just at least for myself, yes, can say thank you, thank you, thank you."*

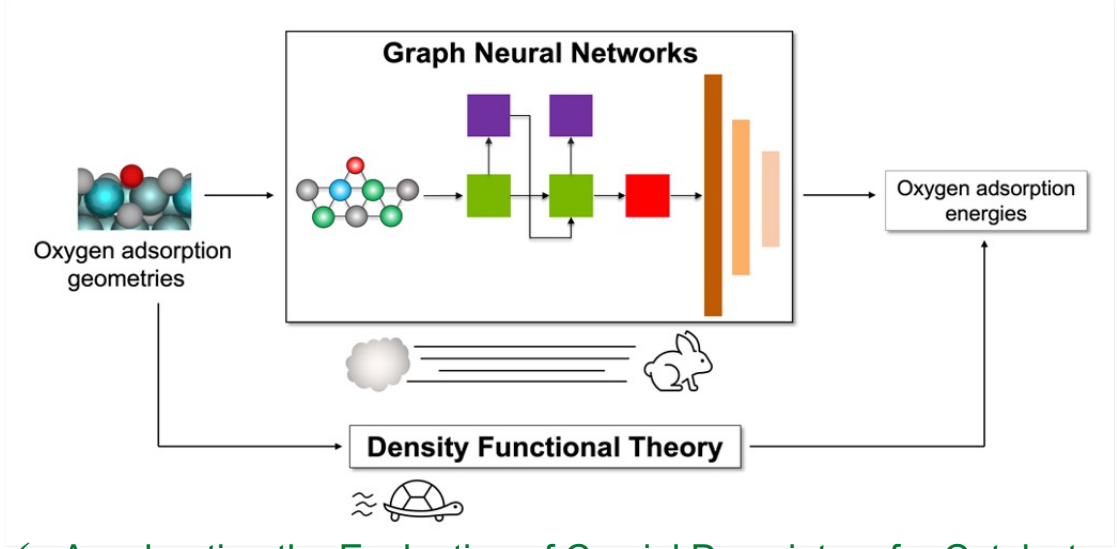
Impact

Catalyst Discovery Capabilities Utilize Artificial Intelligence (AI)

- Catalyst Innovation via AI
  - Developed new AI capabilities to CCPC relevant to early TRL-catalyst developments
  - Catalyst-substrate binding strength prediction is time consuming. We have developed a deep learning model that can predict fast (milli seconds) oxygen adsorption energy for Mo_2C –based CFP catalysts
  - Developed an intelligent workflow for developing accelerated DFT-based catalyst models in HPC machines (performed 20K DFT calculations in Theta Argonne)
- Tool and data development
  - https://github.com/MolecularMaterials/nfp
  - https://acdc.alcf.anl.gov/mdf/detail/doan_datasets_accelerating_representations_v1.1/



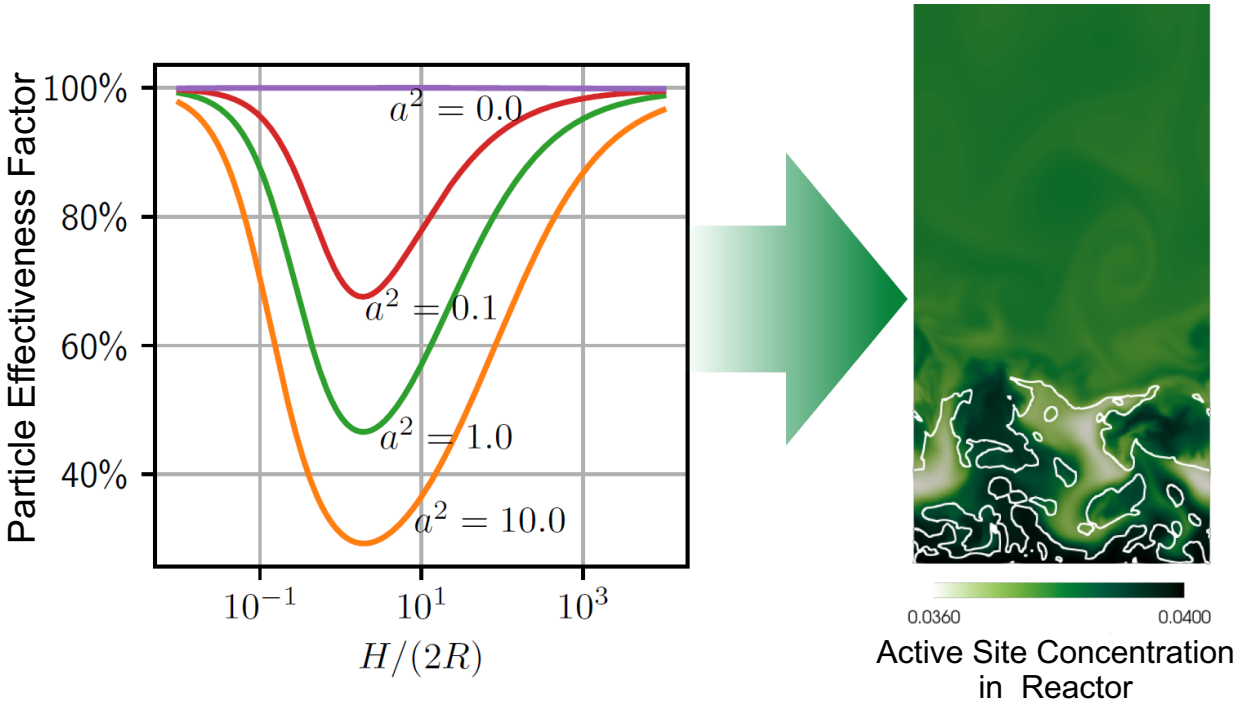




✓ Accelerating the Evaluation of Crucial Descriptors for Catalyst Screening via Message Passing Neural Network, H. A Doan, C. Li, L. Ward, M. Zhou, L. A. Curtiss, R. Assary, **Digital Discovery**, **2023**, DOI: 10.1039/D2DD00088A

New Reduced Order Models for Cascading Reactions in Engineered Catalysts Enable Rapid Particle/Reactor Scale Multiscale Coupling

- Computationally Efficient Particle Effects
  - Detailed simulations of particle-scale catalyst behavior are too computationally expensive for direct integration with reactor-scale simulations.
  - New theory and fast-solving mathematical algorithms were developed to account for transport limitations in arbitrarily shaped catalyst particles.
- Impact and Relevance:
  - De-risk of scale up via fast integration between particle and reactor scales, which greatly accelerates predictions of engineered catalyst performance at industrially relevant scales

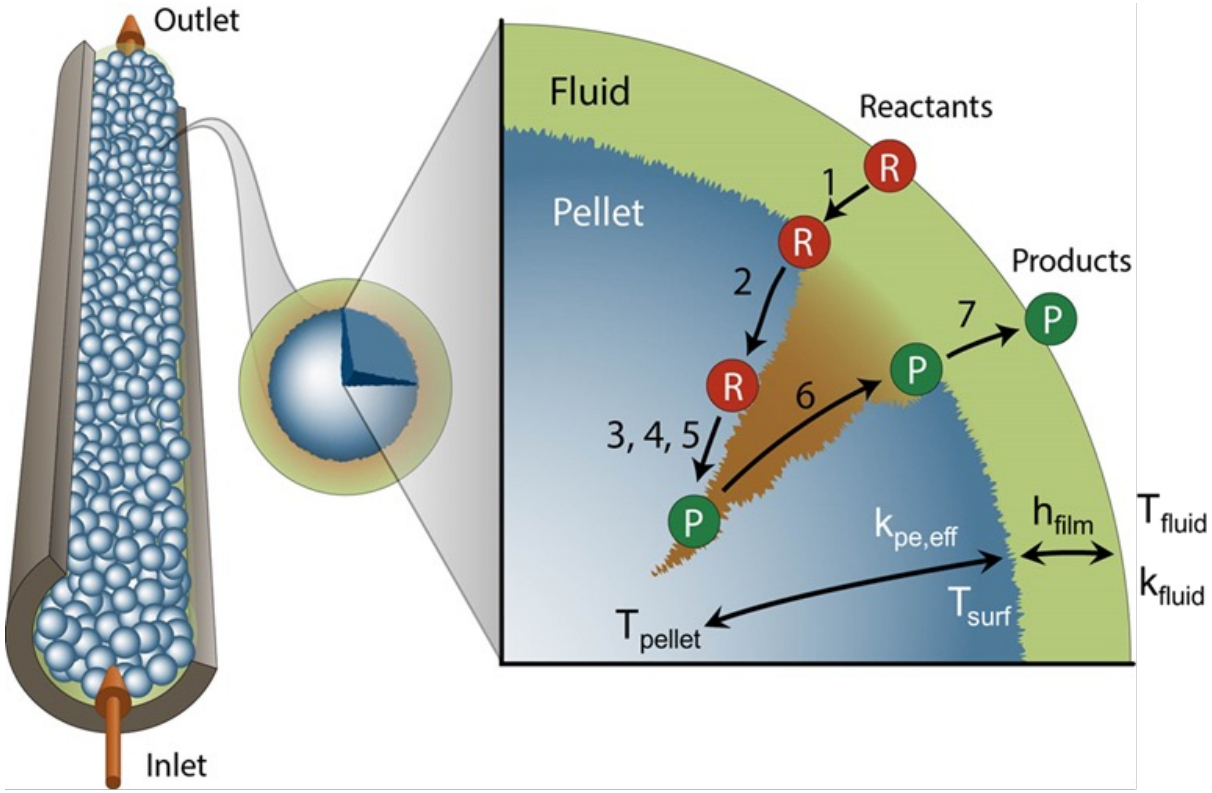


Wakefield, J. P., Lattanzi, A. M., Pecha, M. B., Ciesielski, P. N., & Capecelatro, J. (2023). Fast estimation of reaction rates in spherical and non-spherical porous catalysts. Chemical Engineering Journal, 454, 139637.

Brennan Pecha (NREL) and Peter Ciesielski (NREL) in collaboration with University of Michigan (CCPC Alumni Aaron Lattanzi, now at LBNL)

State of the art packed-bed models enable design and optimization of packed-bed reactors in micro-macro scale: De-risks scale-up

- State-of-the-Art Packed-Bed Models
  - Heat transfer in axial and radial directions
  - Incorporates reactor scale and particle scale
  - Heat/mass transfer, external and intra-particle
  - No assumption on rate limiting step/species
  - Lab-scale to commercial scale applications
- Impact and Relevance:
  - Enables de-risking scale-up
  - Optimization of operating conditions for max yield
  - Prediction of hot spot formation, T, p, C profiles
  - Optimization of pellet properties (porosity, pore size, pellet size)



1. Diffusion of R through boundary film, 2. Diffusion of R into pores, 3. Adsorption of R on catalyst surface, 4. Reaction R → P, 5. Desorption of P from catalyst surface, 6. Diffusion of P out of pore, 7. Diffusion of P through boundary film

Summary

- Objective:
  - Develop and apply fundamental science-based computational toolsets that enable and accelerate bioenergy technologies
- Approach:
  - A multi-scale problem…a multi-lab solution
- Progress and Outcomes:
  - ChemCatBio catalysis innovation enabled by atomic-scale modeling
  - Meso-scale modeling enabling ChemCatBio focus on transition to engineered catalysts
  - Reactor-scale modeling de-risking scale up of complex bioenergy technologies
  - BETO-HPC program successful with lessons learned to focus on software readiness
- Impact:
  - CCPC models enabling industry partners to advance bioenergy via CCPC DFO program

Quad Chart: CCPC-ChemCatBio AOP

Timeline [new 3-yr AOP cycle]

- *Project start date: October 1, 2022*
- *Project end date: September 30, 2025*

	FY22 Costed	Total Award
DOE Funding	*FY22 Costs (previous AOP cycle): $2M over 5 national labs*	*$2M over 5 NLs* *ORNL: $700k* *ANL: $250k* *NREL: $600k* *NETL: $250k* *PNNL: $200k*
Project Cost Share *		

TRL at Project Start: 1

TRL at Project End: 5

Note: Range of TRLs in project due to range of modeling tasks

Project Goal

Develop & apply a fundamental science-based computational toolset that enables & accelerates …

1. *discovery and optimization of cost-effective catalyst materials for bioenergy applications,*
2. *translation of catalyst discoveries to higher technical readiness levels, and*
3. *cost-effective scale-up of bioenergy technologies relevant to industry.*

End of Project Milestone

Develop a predictive model for engineered catalyst properties. This milestone is joint between the C1, CCPC, CDM, and ACSC projects.

Funding Mechanism

Lab Call (Annual Operating Plan or "AOP")

Project Partners

- ChemCatBio NLs and Industry Advisory Board
- Advanced Catalyst Synthesis and Characterization (ACSC) Project
- Catalyst Deactivation Mitigation (CDM) Project

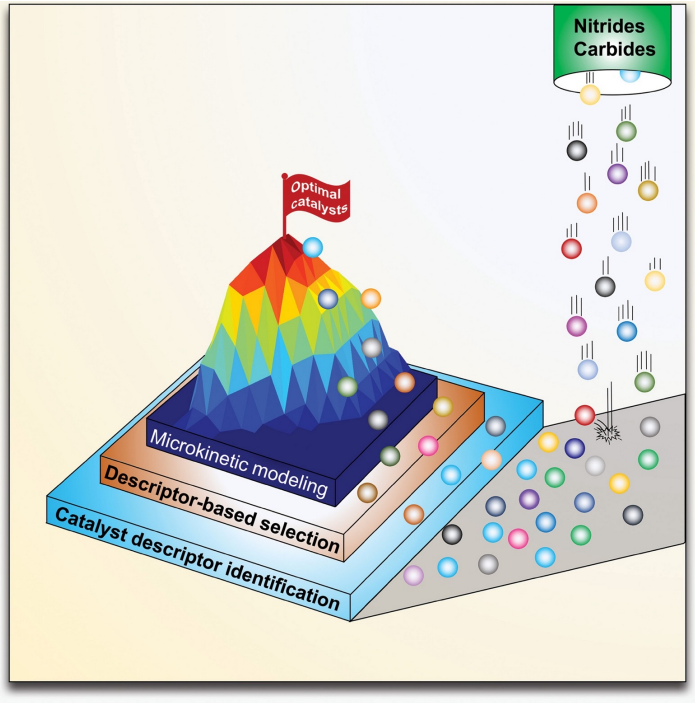
Additional Slides [for Review Panel]

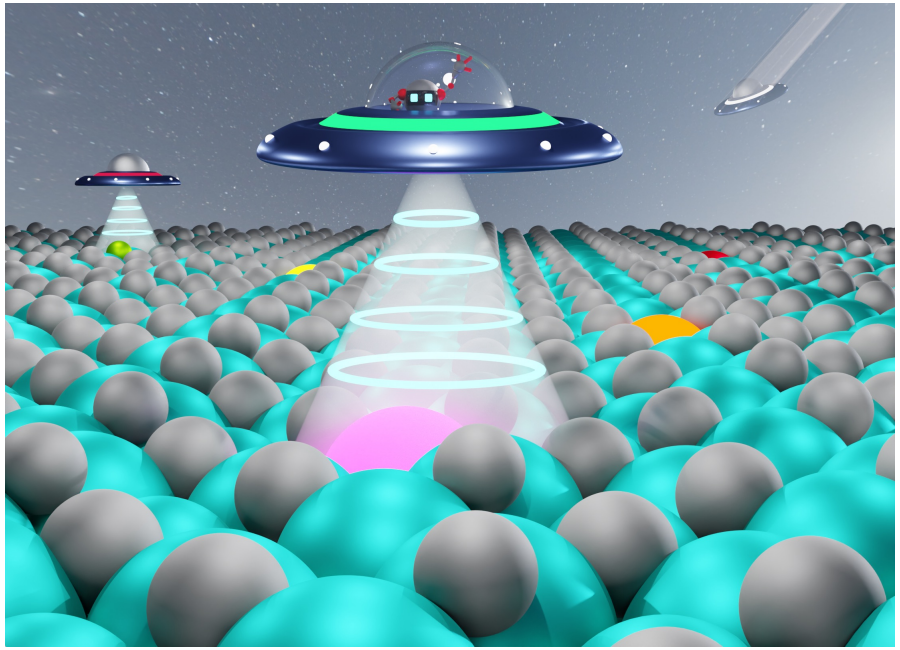
Responses to Previous Reviewers' Comments

- **Generally positive feedback; compliments were given to modeling at all scales (atomic, meso, reactor):**
  - *"The CCPC has demonstrated how the impact of the consortium will impact the catalysis and reaction engineering community at all scales of modeling."*
  - *"The computational screening work for HDO activity on transitional metal nitrides and carbides was fascinating and appears to be very promising. This is an example of an acceleration tool."*
  - *"The multi-component effectiveness factor vector concept is a good approach for the reaction engineering community and will be important for condensed phase analysis at the meso-scale."*
  - *"At the reactor scale, the team realizes their impact on predicting hot spots and other commercial scale operational impacts on the CFP upgrading reactor."*
  - *"This project, dedicated to computational support for catalytic and other projects, is the kind of cross-cutting project that seems to be the type of fundamental enabling work that is the core purpose of BETO/ EERE."*
- **Comments citing concern or question:**
  - *"The extent at which this acceleration and enabling effort is measured was not mentioned."*
    - **This is an important comment, and it is difficult to quantify our "acceleration". Need to identify a methodology.**
  - *"The communication frequency at which the CCPC interacts with the liaisons was not explicitly addressed."*
    - **Overall, about monthly interaction amongst task leads and liaisons in CCPC occurred as virtual (Teams) meetings during COVID. We have restarted our CCPC Face-to-Face meetings again; however, there is some turnover in liaison roles due to decreasing budgets and personnel changes.**
- **No major "Red Flag" negative comments**
- **Other notable commentary:**
  - *"The reactor scale work is ready for hand-off to any established EPC ready to do FEL work on this process."*
    - **This is a very positive comment, but maybe a little too strong? Certainly, this points toward looking into tech transfer. Thinking an internal review of our toolkit might be best place to start.**
  - *"It would be beneficial if these data and tools would be managed and distributed in a way to the benefit the funding agencies and the public."*
    - **We are doing this, but perhaps the comment means we need to do better?**
  - *"The atomic scale analysis of Pt/TiO2 materials must lead to the development of a fast synthesis strategy preferably a high-throughput method."*
    - **This comment not exactly clear, but probably the take away is that we should collectively think about where our high-throughput methods are going.**

Publications Selected for Cover Images (since Jan. 2021)

1. Accelerating the Evaluation of Crucial Descriptors for Catalyst Screening via Message Passing Neural Network, Hieu A Doan, Chenyang Li, Logan Ward, Mingxia Zhou, Larry A. Curtiss, Rajeev Assary, **Digital Discovery**, **2023**, Inside Cover, Feb 2023
2. *Identification of Active Metal Carbides and Nitrides Catalytic Facets for Hydrodeoxygenation Reactions*, Mingxia Zhou, Hieu A. Doan, Larry A. Curtiss, Rajeev Assary†, ***Journal of Physical Chemistry C***, **2021**, 125, 16, 8630-8637 (**Cover image**)





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1. "Assessing the Role of Surface Carbon on the Surface Stability and Reactivity of β-Mo_2C Catalysts," Carrie Farberow, Sean Tacey, and Matt Jankousky. ACS Colloid & Surface Science Symposium, Golden, CO July 2022 (Invited)
2. "Assessing the Role of Surface Carbon on the Surface Stability and Reactivity of β-Mo_2C Catalysts" Carrie Farberow, Sean Tacey, and Matt Jankousky. North American Catalysis Society NAM27, New York, NY. May 2022
3. "Assessing the role of interfacial and metal sites in Pt/TiO_2-catalyzed acetic acid hydrodeoxygenation" Sean Tacey, Carrie Farberow. North American Catalysis Society NAM27, New York, NY. May 2022
4. "Accelerating research with the catalyst property database" Sean A. Tacey, Qiyuan Wu, Carrie A. Farberow, Kurt M. Van Allsburg. North American Catalysis Society NAM27 Poster Presentation, New York, NY. May 2022
5. "Catalytic Descriptors for CO_2 Methanation on Transition-Metal Catalysts" Michelle Nolen, Sean Tacey, Stephanie Kwon, Carrie Farberow. North American Catalysis Society NAM27 Poster Presentation, New York, NY. May 2022
6. "Assessing the role of interfacial and metal sites in Pt/TiO_2-catalyzed acetic acid hydrodeoxygenation" Sean Tacey, Carrie Farberow. Rocky Mountain Catalysis Society Poster Presentation, Golden, CO. April 2022
7. "Catalytic Descriptors for CO_2 Methanation on Transition-Metal Catalysts" Michelle Nolen, Sean Tacey, Stephanie Kwon, Carrie Farberow. Rocky Mountain Catalysis Society Poster Presentation, Golden, CO. April 2022.
8. "First-principles modeling of the effect of surface modification strategies on hydrogenation catalysis," Carrie Farberow. AIChE Annual Meeting, *Pioneers in Catalysis and Reaction Engineering,* Boston, MA and Virtual, November 2021 (Invited)
9. "Assessing the role of the support in acetic acid hydrodeoxygenation selectivity on Pt/TiO2," Sean Tacey. ACS Fall Meeting, Atlanta, GA and Virtual, August 2021.
10. "Determining the role of synthesis and reaction conditions on the exposed surface and shape of β-Mo2C catalysts," Sean Tacey. ACS Fall Meeting, Atlanta, GA and Virtual, August 2021.

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11. Rajeev S. Assary, Atomistic Modeling and AI for Energy Storage and Conversion Chemistry, HPC4Energy Innovation, LLNL, April 8, 2022 (Keynote Lecture, invited)
12. Rajeev S. Assary, Insights into the Molecular Materials for Energy: Lets start from Computations, Directors Special Colloquium, Feb 10, Beckman Institute, University of Illinois, Urbana Champaign, 2023 (*Invited)
13. Rajeev S. Assary, Predictive Simulations for Energy Storage and Chemical Catalysis, Physical and Computational Sciences Directorate, PNNL, WA, June 28, 2022 (Invited)
14. Rajeev S. Assary, Predictive Simulations for Energy Storage and Chemical Catalysis, Center of Nano Scale Materials, November 2022. (Invited)
15. Chenyang Li, Rajeev S. Assary, Ketonization and Etherification Reactions for Sustainable Biomass Conversion, AiChE annual meeting, Phoenix, AZ, Nov 2022 (Contributed)
16. Michael Cordon, Junyan Zhang, Stephen Purdy, Evan C Wegener, Kinga A Unocic, Lawrence Allard, Mingxia Zhou, Rajeev Assary, Jeffrey T Miller, Theodore Krause, Dongxia Liu, Zhenglong Li, Selective Butene Formation in Direct Ethanol to C3+ Olefin Valorization over Zn-Y/Beta and Single-Atom Alloy Pt-Cu Composite Catalysts Using in Situ Generated Hydrogen, AIChE annual meeting, 2021 (Virtual, Contributed)
17. B. Adkins (presenting) and C. Karakaya, “Importance of Heat Transfer Model Selection in Scale-up and Optimization of Packed Bed Reactors for Reweable Fuels and Chemicals”, COMSOL Webinar, March 2023
18. B. Adkins (presenting) and C. Karakaya, “A Model-Informed Approach for Fixed Bed Catalyst Testing and Process Development at Pre-Pilot Scale”, AIChE Annual Meeting, Houston Texas, March 2023
19. B. Adkins (presenting) and C. Karakaya, “Scaleup Modeling of Highly Nonisothermal Biofuel and Biochemical Production Processes”, ACS Spring Meeting, Indianapolis Indiana, March 2023
20. B. Adkins (presenting) and C. Karakaya, “Importance of Conjugate Heat Transfer in Modeling of Fixed Bed Reactors for Renewable Fuels and Chemicals”, NETL Multiphase Workshop, Morgantown West Virginia Aug 2022
21. B. Adkins (presenting) and C. Karakaya, “Computational Evaluations of Fixed Bed Catalytic Reactors for Renewable Fuels and Chemicals”, ACS Spring Meeting, San Diego California, March 2022

Awards (since Jan. 2021)

- Michelle Nolen, North American Catalysis Society NAM27 *Kokes Student Travel Award*, New York, NY 2022.
- Michelle Nolen, ACS Colloids *Langmuir Graduate Student Oral Presentation Award*, Golden, CO 2022