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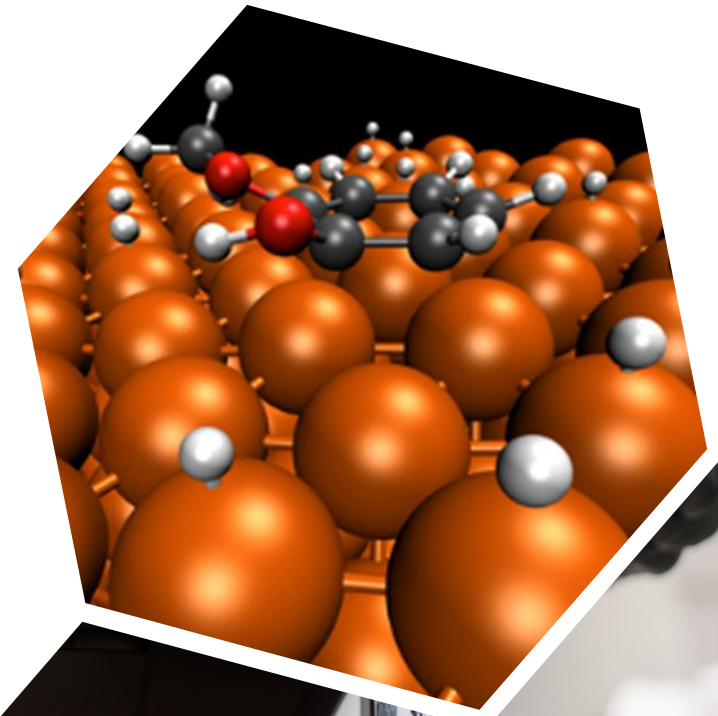
ChemCatBio
Chemical Catalysis for Bioenergy

CCPC
www.cpcbiomass.org

Consortium for Computational Physics and Chemistry (CCPC)



OAK RIDGE National Laboratory | Argonne NATIONAL LABORATORY | NETL NATIONAL ENERGY TECHNOLOGY LABORATORY | NREL NATIONAL RENEWABLE ENERGY LABORATORY | Pacific Northwest NATIONAL LABORATORY

PI: Jim Parks (ORNL); Task Leads: Rajeev Assary (ANL), Larry Curtiss (ANL), Bill Rogers (NETL), Syam Madhava (NETL), David Robichaud (NREL), Peter Ciesielski (NREL), Roger Rousseau (PNNL), Asanga Padmaperuma (PNNL)
[full list of CCPC team on last slide]

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
BIOENERGY TECHNOLOGIES OFFICE

ChemCatBio Foundation

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies

- **Catalytic Upgrading of Biochemical Intermediates** (NREL, PNNL, ORNL, LANL, NREL*)
- **Catalytic Upgrading of Indirect Liquefaction Intermediates** (NREL, PNNL, ORNL)
- **Catalytic Fast Pyrolysis** (NREL, PNNL)
- **Electrocatalytic and Thermocatalytic CO_2 Utilization** (NREL, ORNL*)

*FY19 Seed Project

Enabling Capabilities

- **Advanced Catalyst Synthesis and Characterization** (NREL, ANL, ORNL, SNL)
- **Catalyst Cost Model Development** (NREL, PNNL)
- **Consortium for Computational Physics and Chemistry** (ORNL, NREL, PNNL, ANL, NETL)
- **Catalyst Deactivation Mitigation for Biomass Conversion** (PNNL)

Industry Partnerships (Directed Funding)

- **Gevo** (NREL)
- **ALD Nano/JM** (NREL)
- **Vertimass** (ORNL)
- **Opus12**(NREL)
- **Visolis** (PNNL)
- **Lanzatech** (PNNL) - Fuel
- **Gevo** (LANL)
- **Lanzatech** (PNNL) - TPA
- **Sironix** (LANL)

Cross-Cutting Support

- **ChemCatBio Lead Team Support** (NREL)
- **ChemCatBio DataHUB** (NREL)

Approach: Goal Statement

Our Mission: To utilize core computational capabilities across the US DOE national laboratory system ***to enable and accelerate …***

(1) the development of new materials and

(2) optimize process scale-up

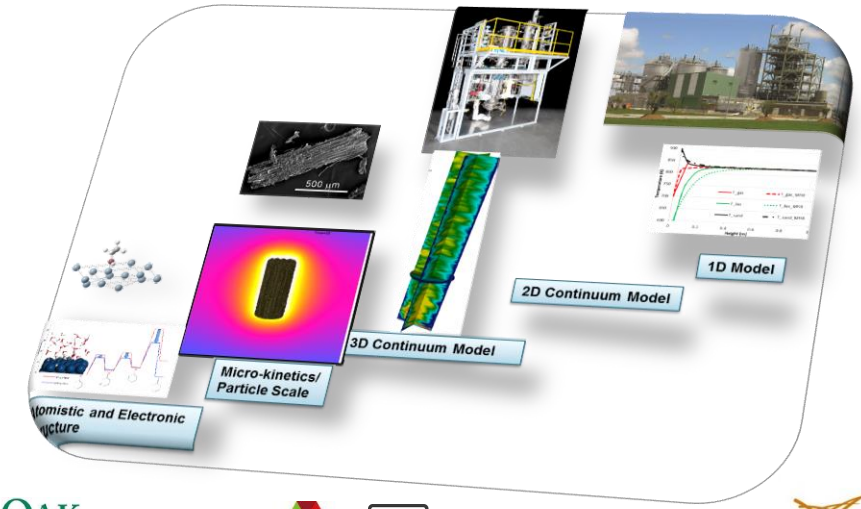
to advance the bioenergy economy.

Our Vision: The computational toolset developed by CCPC facilitates the modeling of biomass industrial technologies from atomic to process scales, thereby reducing the cost, time, and risk in commercializing bioenergy technologies.

CCPC

www.cpcbiomass.org

A multi-scale problem
… A multi-lab solution



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Approach: Quad Chart Overview CCPC-ChemCatBio

Timeline

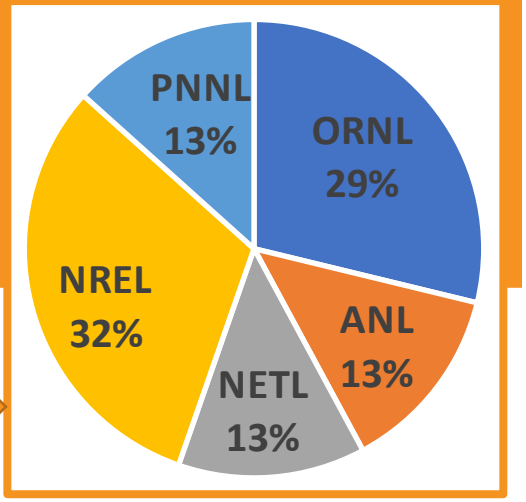
- Consortium Began in FY2013
- New AOP Began Oct. 1, 2018 (FY2019)
- Project end date: Sept. 30, 2021 (14% complete)

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	$11.8M	$3.15M	$3.28M	$3.28M/yr, $9.8M total

Partners:

ORNL: $945k (28.8%)
NREL: $1028k (31.3%)
PNNL: $437k (13.3%)
ANL: $437k (13.3%)
NETL: $433k (13.2%)

FY19 Budget by Lab



Barriers addressed

Ct-N. Multiscale Computational Framework toward Accelerating Technology Development

Ct-F. Increasing the Yield from Catalytic Processes

Ct-G. Decreasing the Time and Cost to Develop Novel Industrially Relevant Catalysts

Ct-D. Advanced Bioprocess Development

Objectives

(1) Accelerate discovery and optimization of cost-effective catalyst materials

(2) Translate catalyst discoveries to higher technical readiness levels by optimizing catalyst particle properties and designs, and

(3) Enable scale-up of bioenergy catalytic conversion technologies to process scales relevant to industry.

End of Project Goals

(1) Enable ChemCatBio to develop catalysts for verification of core BETO pathways and

(2) Complete a scaling transfer function for at least one conversion technology

Approach: Project Overview - Historic Timeline

FY13

Computational Pyroylsis 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
Ability to predict feedstock size-dependent pyrolysis yield demonstrated

FY17

ChemCatBio Launched
with CCPC, ACSC, and CCM enabling projects

ChemCatBio
Chemical Catalysis for Bioenergy

Accomplishment
Surface Phase Explorer tool released to public

FY18

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

fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

FY19

FY20

FY21

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

New Task Structure
implemented to align with BETO Verification Pathways

Peer Review Guidance
Interactions with Bioprocessing Separations Consortium initiated

BIOPROCESSING SEPARATIONS CONSORTIUM

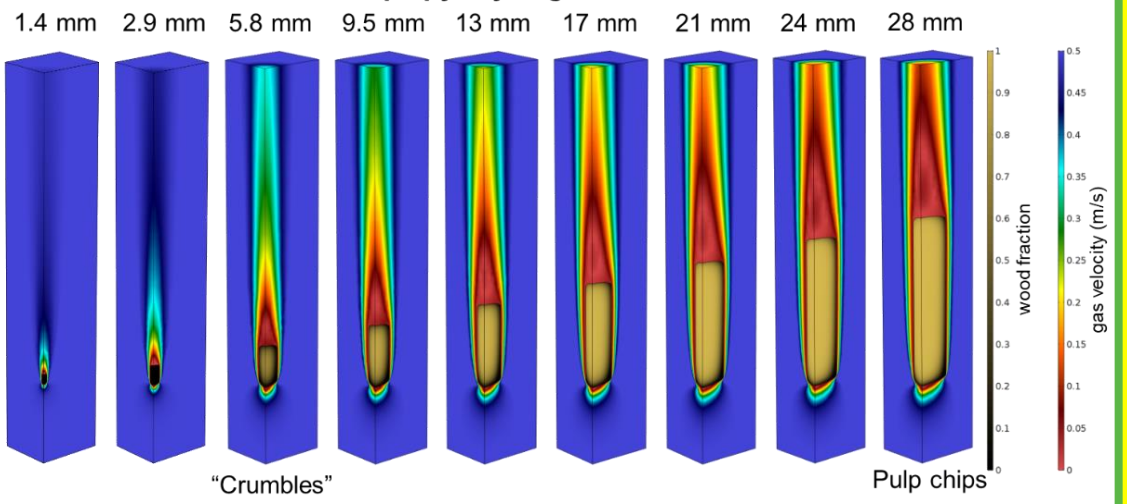
Redefined as **Consortium for Computational Physics and Chemistry (CCPC)** with focus on catalysis

Approach: Pyrolysis Model Results Aid Industry

Accomplishment

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

Pine chips pyrolyzing at 500°C, 30s mark

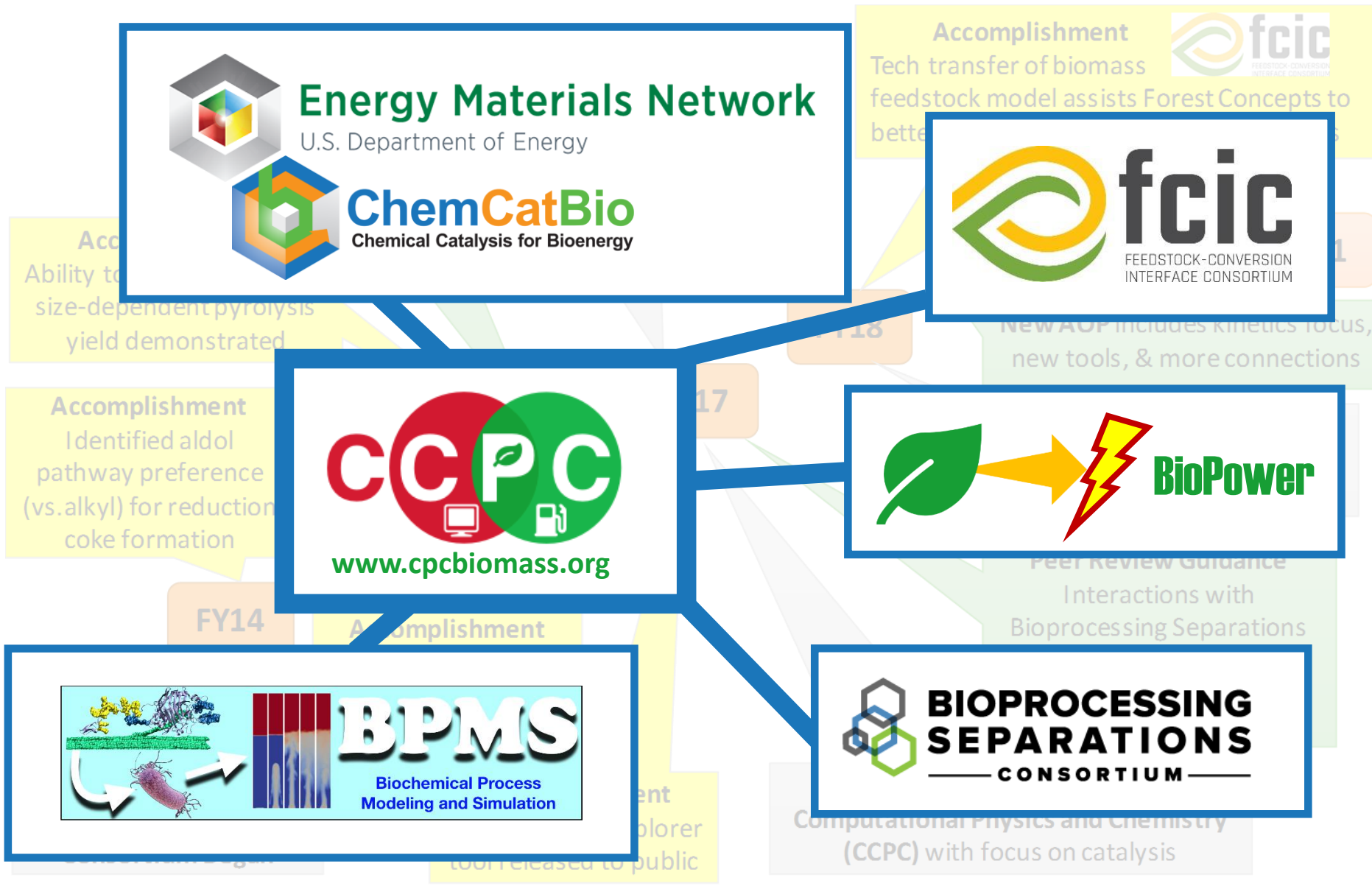


Relevance: *"The modeling data developed by NREL gave our company an understanding of how our production engineers can co-optimize reactors and feedstock properties to improve functional performance. This conversion data will also help our customers select the optimal feedstock for their specific conversion process."*

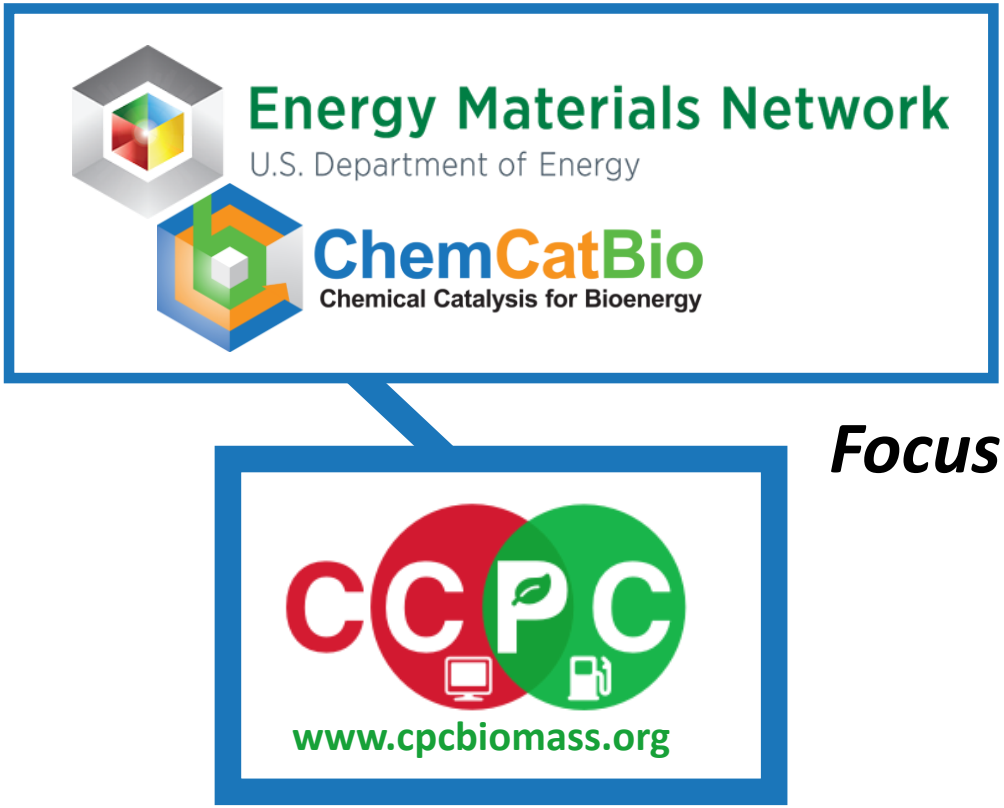
- **James H. Dooley**
  CTO, Forest Concepts

For more information, see ***Additional Slides*** *or* www.nrel.gov/news/program/2018/bioenergy-scientists-collaborate-with-industry-to-convey-feedstock-value-improve-biomass-conversion-processes.html

Approach: CCPC Connects Across BETO Program



Approach: CCPC-ChemCatBio Focus of Project



Focus of this presentation

Approach: Objectives, Challenges, and Success Factors

Objectives (from Annual Operating Plan):

(1) ***Accelerate discovery and optimization of cost-effective catalyst materials*** (compositional and structural) for bioenergy applications that result in experimentally observed improvements in metrics yield, selectivity, durability, lifetime, and cost,

(2) ***Translate catalyst discoveries*** by ChemCatBio to higher technical readiness levels by ***optimizing catalyst particle properties and designs*** to achieve maximum conversion efficiency and selectivity for specific catalytic conversion pathways, and

(3) ***Enable scale-up*** of bioenergy catalytic conversion technologies ***to process scales relevant to industry***, predict and optimize yield, and support BETO pathway verification and full plant techno-economic analyses.

Challenges:

- Vast array of material possibilities and combinations (zeolite, metal oxide, metal carbide, crystalline vs. defect sites, etc.)
- Complex surface science, biomass-specific chemistry, and chemisorption/diffusion phenomena

Approach: *Tackle Challenges that Need Computation*

- Density Functional Theory (DFT) simulation of catalyst surface chemistry and Molecular Dynamic (MD) simulation of diffusion in nanoscale pores
- ***New!*** Artificial Intelligence techniques for material screening to guide research being investigated

Success Factors:

- Science-based understanding of catalysis
- Success of ChemCatBio projects discovering catalysts of industry interest

Need experimental data including from Advanced Catalyst Synthesis and Characterization

Approach: Objectives, Challenges, and Success Factors

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Challenges:

- A complex mixture of chemical and physical processes occur in catalyst particle ***and*** the particle is changing (coking) over time (in stream)

Approach: *Tackle Challenges that Need Computation*

- Generate comprehensive particle model capturing all chemistry and physics in process conditions (using Finite Element modeling)
- Develop reduced-order particle models for translation into process scale models

Success Factors:

- Catalysts that are practical for industry applications (optimal conversion with longevity)
- Sub-models and parameters to enable process scale simulations

Need experimental data including from Advanced Catalyst Synthesis and Characterization

Approach: Objectives, Challenges, and Success Factors

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Challenges:

- Multiphase flow and inherent chemistry and physics is highly complex
- Vast array of reactor designs & operational space
- Critical parameters like residence time are extremely difficult to measure experimentally

Approach: *Tackle Challenges that Need Computation*

- Utilize MFiX & other open source codes to develop comprehensive multi-phase flow reactor models
- ***New!*** Determine kinetic rates with dedicated effort in collaboration with experimentalists

Success Factors:

- Science-based prediction of conversion (demonstrates fundamental understanding)
- Successful scale up of industrial relevant catalysis and BETO Verification of pathways

Need experimental data including from Advanced Development and Optimization teams

Approach: Objectives, Challenges, and Success Factors

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The CCPC leverages **DOE Basic Energy Sciences** program including **Catalysis Science** and **Advanced Scientific Computer Research (ASCR)** programs

U.S. DEPARTMENT OF ENERGY | Office of Science

A ***common shared risk*** is the potential to be limited by computing resources. ***New!*** This risk is being mitigated by an emerging strategy to share resources across the national labs

Approach: Objectives, Challenges, and Success Factors

Objectives (from Annual Operating Plan):

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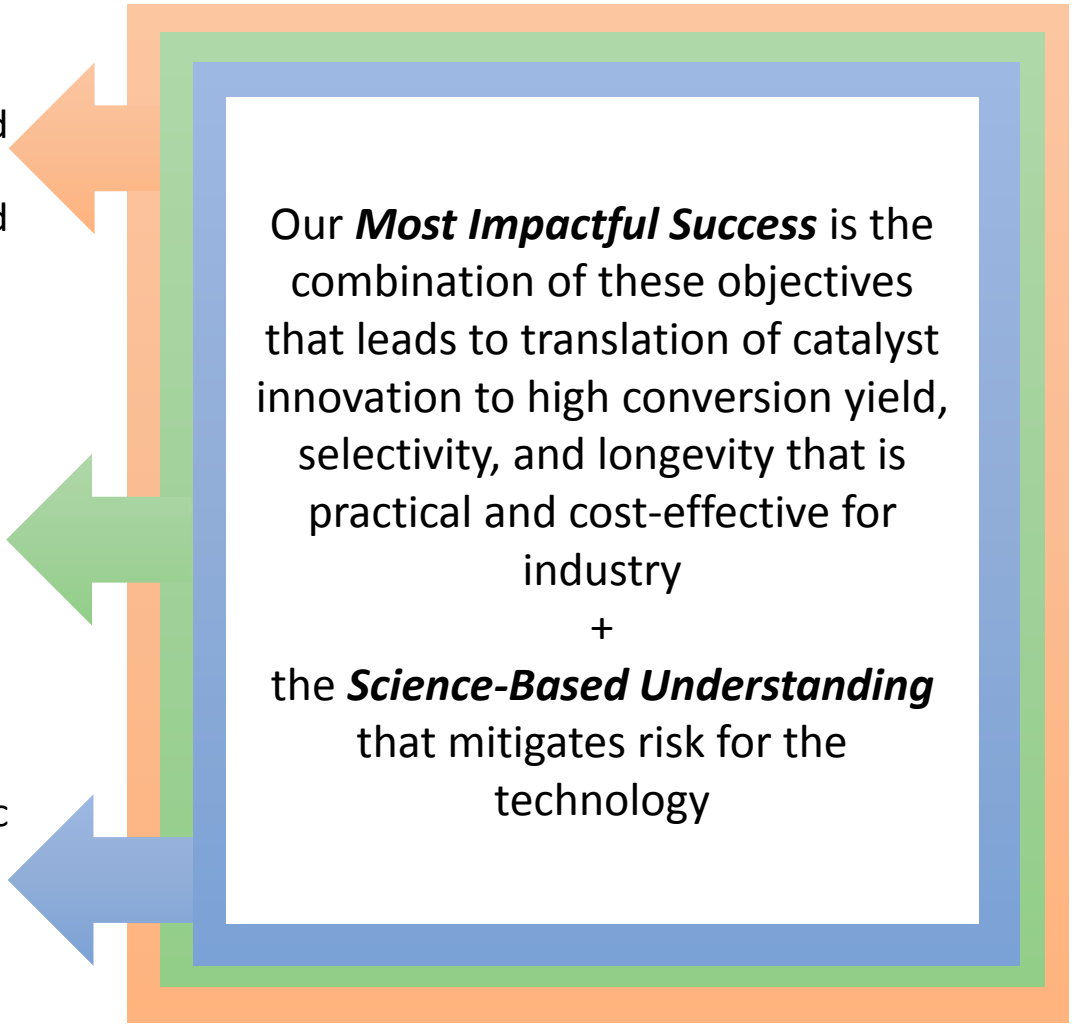


Approach: Task Structure (Adopted in FY2018)

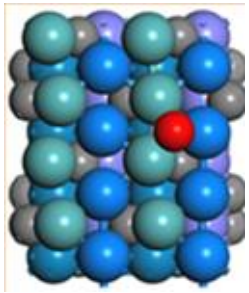
Task

Catalysis Modeling at Atomic Scales

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Argonne NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

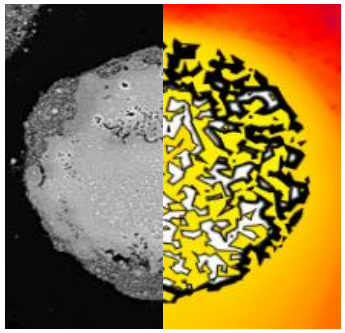


Investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists

Task

Catalyst Particle Modeling at Meso Scales

NREL NATIONAL RENEWABLE ENERGY LABORATORY



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

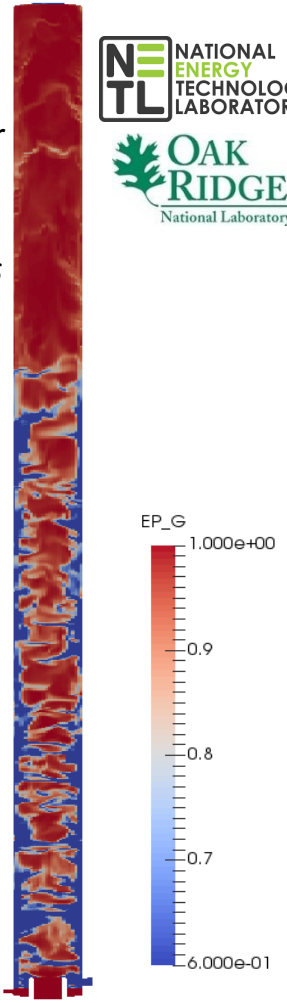
Task

Conversion Modeling at Process Scales

Determining optimal process conditions for maximum yield and enable scale-up of ChemCatBio catalysts

NATIONAL ENERGY TECHNOLOGY LABORATORY

OAK RIDGE National Laboratory



Task

Coordination, Integration, and Industry Outreach

OAK RIDGE National Laboratory

Coordinate R&D, outreach, & industry engagement

CCPC Industry Advisory Panel

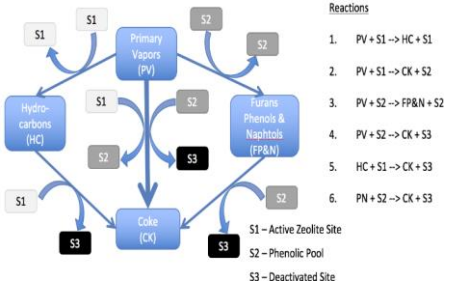
David Dayton (RTI), George Huff (MIT, retired BP), Jack Halow (Separation Design Group), Steve Schmidt (WR Grace), Tom Flynn (Babcock & Wilcox)

Task

New!

Kinetics: Fundamental Reaction Rates for Modeling

Guide efficient technology scale-up, enabling performance gains achieved by ChemCatBio to be maintained at pilot scale



Approach: CCPC Connects Across ChemCatBio and BETO

Techno-Economic Analysis (TEA)

TEA provides BETO-wide guidance

ChemCatBio
Chemical Catalysis for Bioenergy

ChemCatBio Industry Advisory Board

Catalytic Fast Pyrolysis

Catalytic Upgrading of Biochemical Intermediates

Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates

New! Electrocatalytic and Thermocatalytic CO_2 Utilization

Advanced Catalyst Synthesis and Characterization

New! Catalyst Deactivation Mitigation for Biomass Conversion

Catalyst Cost Model Development

CCPC
www.cpcbiomass.org

Advanced Development and Optimization (ADO)

ADO Process Scale Up for Production Environments

ADO Engineering of Catalyst Scale Up

Pilot-Scale Ex-situ CFP with DCR System

Industry Stakeholders
CCPC Industry Advisory Panel

Catalyst Innovation and Catalyst-Process Development

Accelerate and Enable

Verified Proof of Performance on Engineering-Scale Systems

Approach: Coordination, Integration, & Outreach

Inputs

BETO Multi-Year Program Plan

CCPC Industry Advisory Panel

David Dayton (RTI), George Huff (MIT, retired BP), Jack Halow (Separation Design Group), Steve Schmidt (WR Grace), Tom Flynn (Babcock & Wilcox)

ChemCatBio Industry Advisory Board

BETO Peer Review

Literature Reviews

Invited Webinars

CCPC

Quarterly Face-to-Face Meetings

Frequent sub-team conf calls

Participation in ChemCatBio events

New! Designated Liaisons for interfacing across BETO

Outputs, Outreach, Tech Transfer

Peer-Reviewed Publications

Conference Presentations

Public Webinars

Industry Site Visits/Webinars

Website
www.cpcbiomass.org

Public Open-Source Code
github.com/ccpcode

python™ MFiX

Strategic Tech Transfer

End Goal is Impact to Support the Bioenergy Industry

Progress: Atomic Catalyst Models Accelerate the Discovery and Optimization of Cost-effective Materials across ChemCatBio

New metal-doped zeolites

- Catalytic upgrading of pyrolysis products
- Design new Ga-doped zeolites for dehydration reaction in CFP

Bimetallic catalysts for selective carboxylic acid reduction

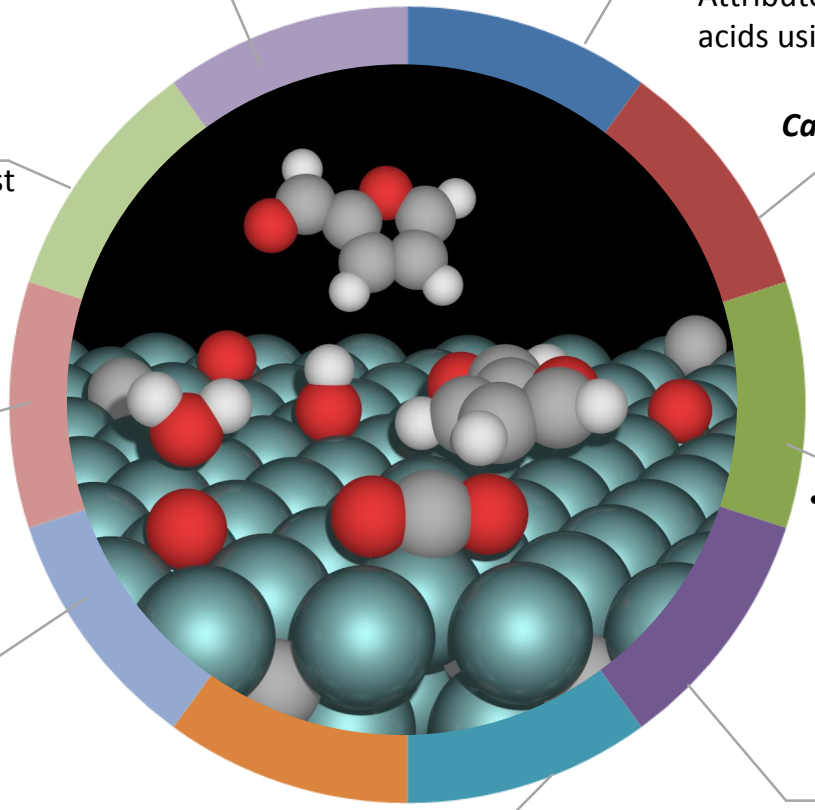
- Catalytic Upgrading of Sugars
- Attribute selective reduction of carboxylic acids using RuSn

Selectivity of metal catalyst

- Selectivity of $Ag/SiO_2/ZrO_2$ catalyst towards Ethanol Upgrading

Catalyst screening for dehydrogenation

- Develop predictive alkyl zeolite model for dehydrogenation using metal-doped BEA zeolites



Ethanol conversion in zeolites

- Identify entropy contribution in ethanol conversion over zeolites

Optimize catalytic activity of Metal carbides

- Design metal carbides catalysts with enhanced deoxygenation and stability via QM and screening descriptors

Diffusivity during CFP

- Studied the diffusion in both micro/mesoporous zeolites to provide guidance that results in substrate access to catalyst active sites and remove coke precursors

Co-adsorption of ketones and water on MgO surfaces

- Explain H_2O effect on ketone self-condensation on MgO(111) and MgO(100)
- Develop new SPE (Surface Phase diagrams) tool for metal catalyst

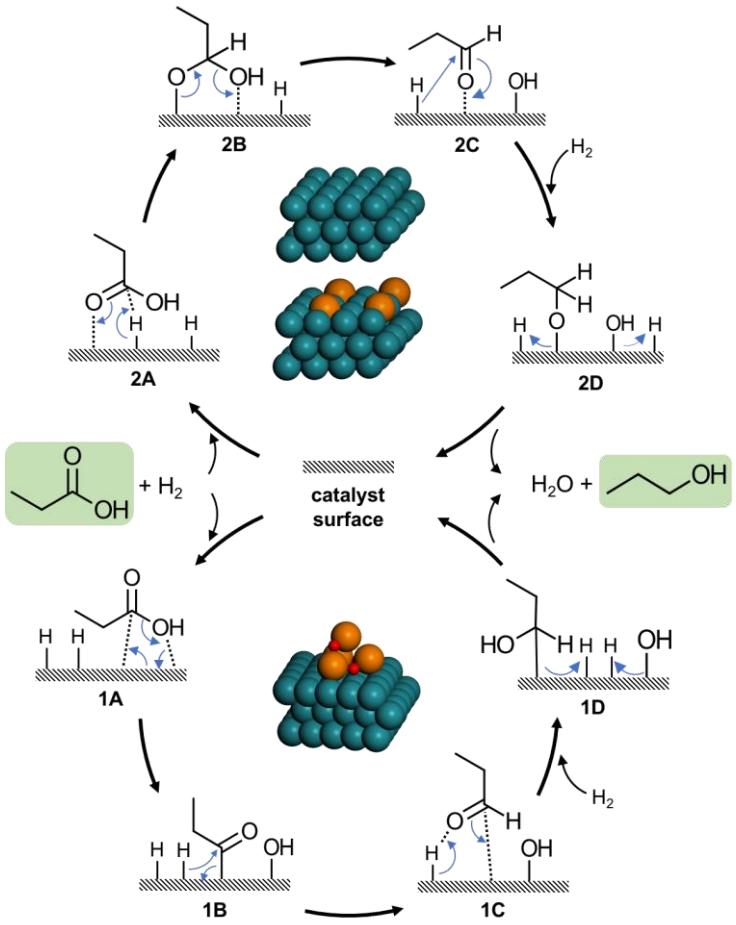
Data Science

- Started new machine learning capability for catalyst discovery applications

Progress: Developing a Holistic View of Inverse Bimetallic Catalysts for Selective Carboxylic Acid Reduction

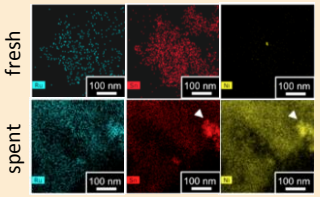
- Used density functional theory (DFT) to identify RuSn structure and function
- Determined driving forces in RuSn reconstruction, proposed alternative Ni-resistant formulations
- Revealed structure-selectivity relationships for the design of new catalyst motifs: *inverse bimetallic catalysts*

Relevance: model predicts performance of catalytic sites by understanding structure-function relations.



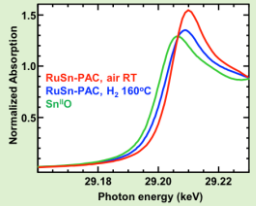
ORNL

SEM-EDS Spectroscopy



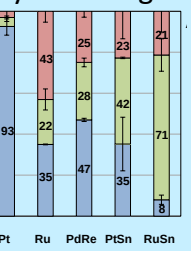
ANL

XAS/EXAFS/XANES



NREL

Catalytic testing



CCPC-Atomic [NREL] ⟷ **ChemCatBio CUBI** ⟷ **ACSC** [NREL, ORNL, ANL]

Vardon et al., ***ACS Catalysis***, 2017, 7 (9), 6207-6219.

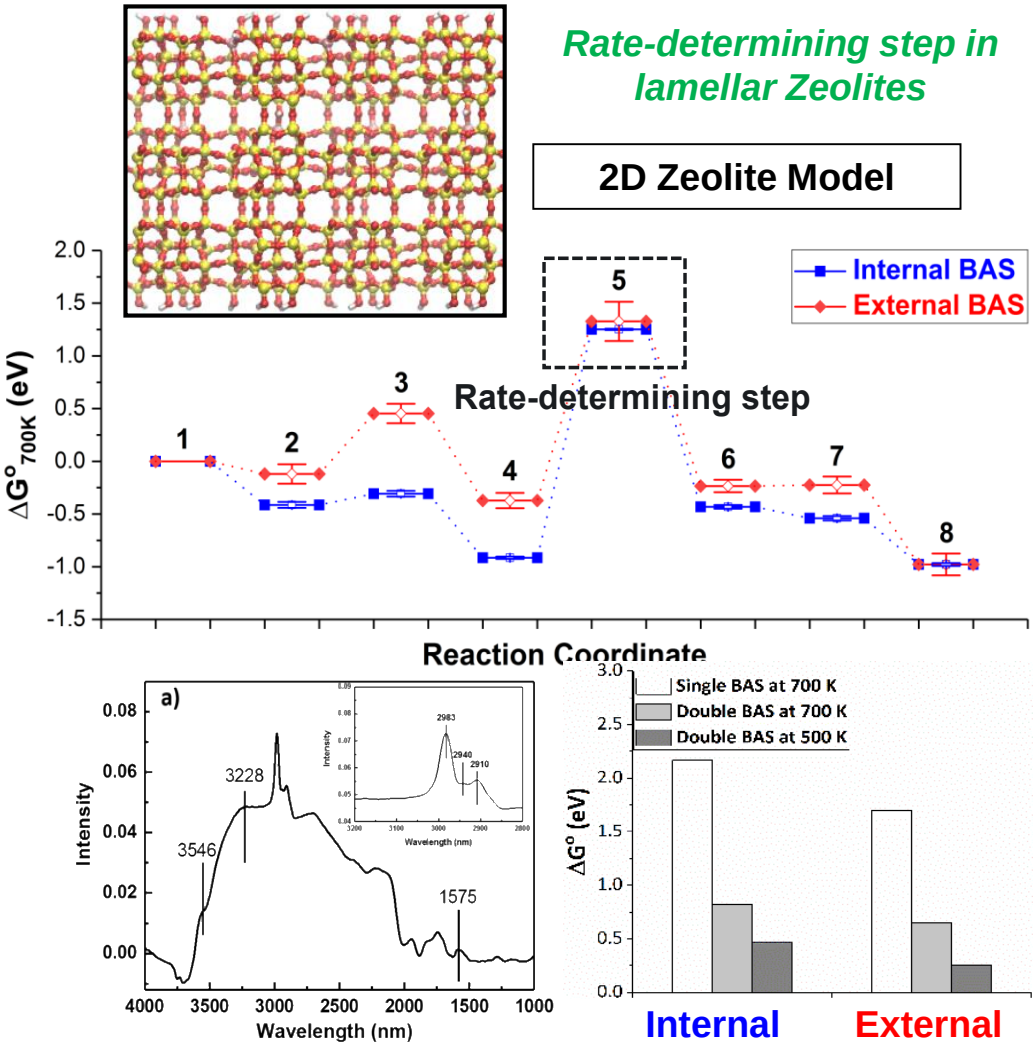
Vorotnikov et al., *submitted* (target: Nature Catalysis)

Progress: Ethanol Conversion Under Pore Confinement

- Design of 2D-pillared MFI zeolite model
- Ethoxy-mediated conversion is energetically preferable at interior BAS at low T
- Double occupied cages predicted to be superior than single mitigating entropic bottlenecks
- Experimental validation of mechanism by DRIFTS/DSC in collaboration with Z. Li (IDL/ORNL)
- In progress: models of Y/Cu/Zn Zeolites for ethanol upgrading

Relevance: CCPC identified that catalysis was limited by entropic penalties and suggested building double BAS catalysts to enhance conversion.

CCPC-Atomic [PNNL] ⟷ **ChemCatBio CUBI/IDL**



"Conversion of EtOH over 2D Zeolites" in preparation, 2019, Simuk, Lee, Li, Zhang, Akhade, Padmaperuma, Glezakou, Rousseau

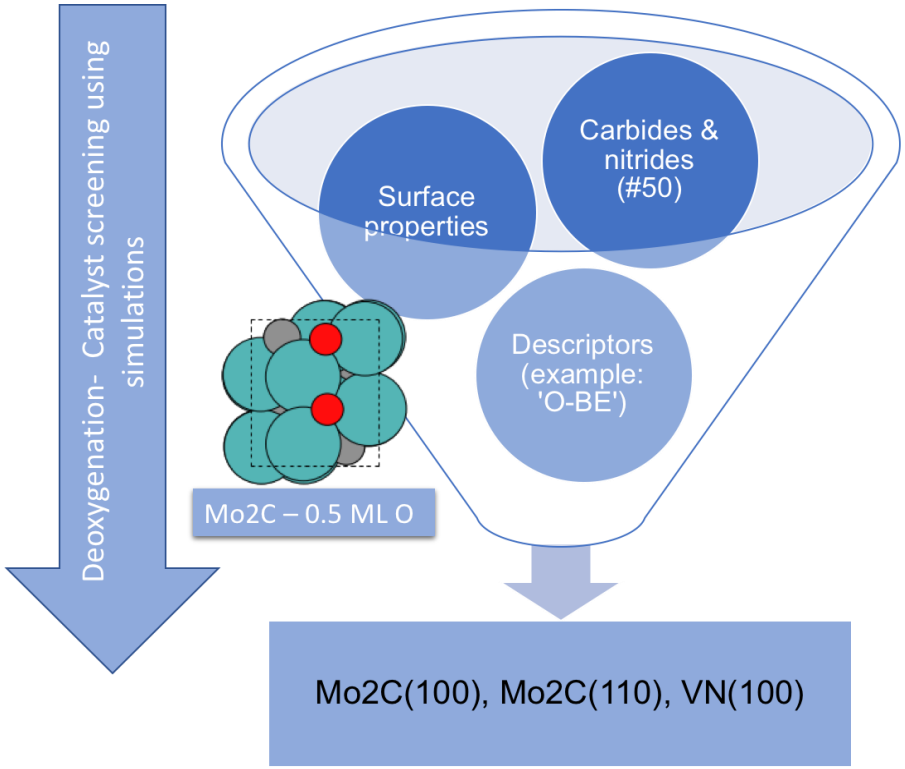
Progress: Design Catalysts with Enhanced Activity & Stability

- Using quantum simulations, performed catalyst screening of 50 transition metal carbides/nitride surface catalysts and **two** best candidates were proposed (Mo_2C(110) & VN(100)).
- At higher catalyst surface coverage, the carbon binding is exothermic due to the graphitic carbon formation, which is a significant cause of catalytic deactivation.

Relevance: *A priori* identification of most active and selective catalysts for crucial deoxygenation reactions via reliable predictive modeling reduces the cost of the catalyst discovery

CCPC-Atomic [ANL, NREL] ⟷ **ChemCatBio CFP**

Quantum chemical screening for catalyst discovery for deoxygenation



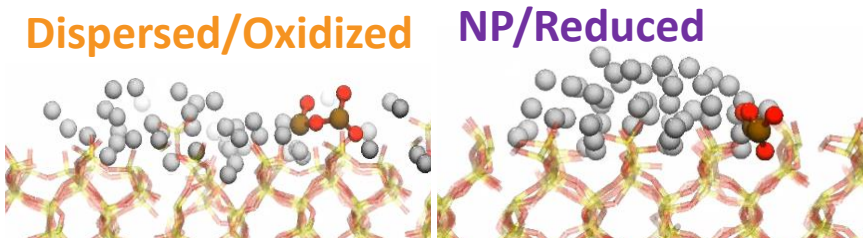
Assary et al. in preparation
Assary et al, 255th ACS Meeting, New Orleans, LA, US

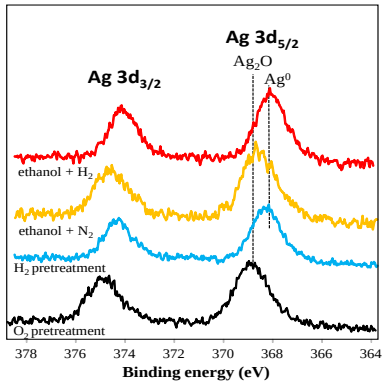
Progress: Selective Ethanol Upgrading Using $Ag/SiO_2/ZrO_2$

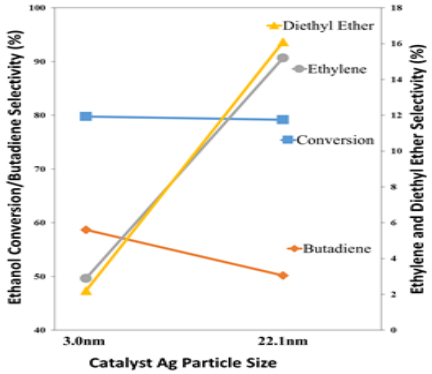
- Understand how the size/shape of metal particles affects on butane/butene/butadiene production
- Oxidized Ag promotes selectivity of EtOH to butadiene, while reduced Ag (NP) favors the selectivity towards **butene** formation
- Validation of catalyst state/selectivity in collaboration with Dagle (IDL/PNNL)

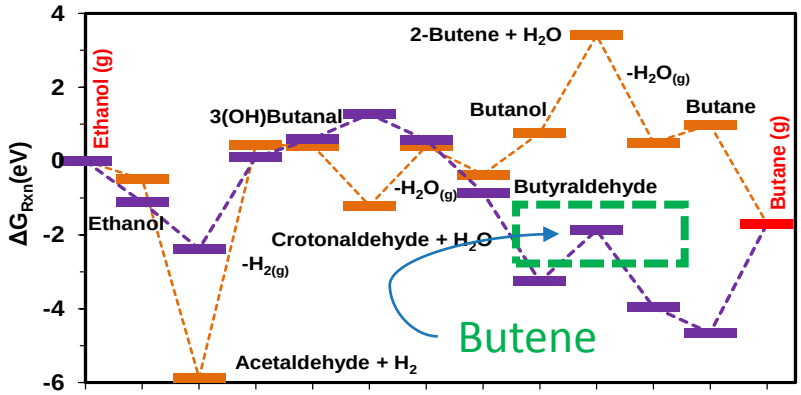
Relevance: CCPC determine correlations between the catalyst composition, reactivity and product selectivity to validate, guide and improve catalyst design targeted to enhance control towards butadiene and/or butenes

CCPC-Atomic [PNNL] ⟷ **ChemCatBio IDL**









"Conversion of Ethanol to Butene/Butadiene over $Ag/ZrO_2/SiO_2$ Catalysts" in preparation, 2019, Wilkelman, Akhade, Kovarik, Glezakou, Rousseau, Dagle, Dagle

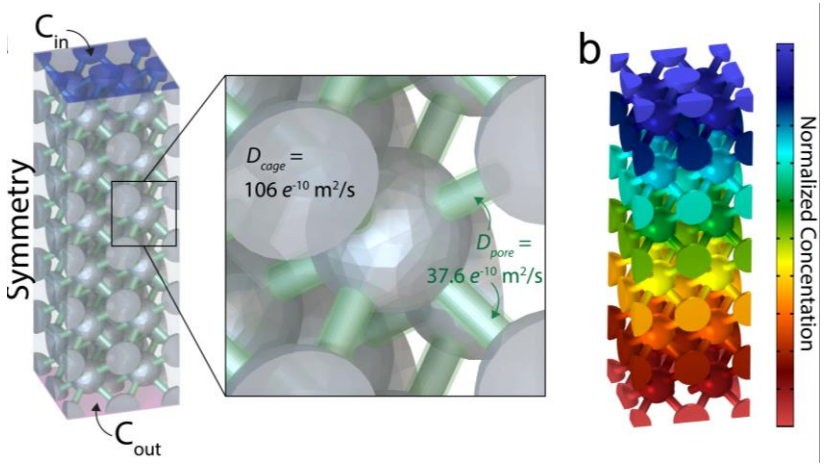
Progress: $Ag/SiO_2/ZrO_2$ Performance Further Optimized with Meso Scale Model of SBA-16 Support

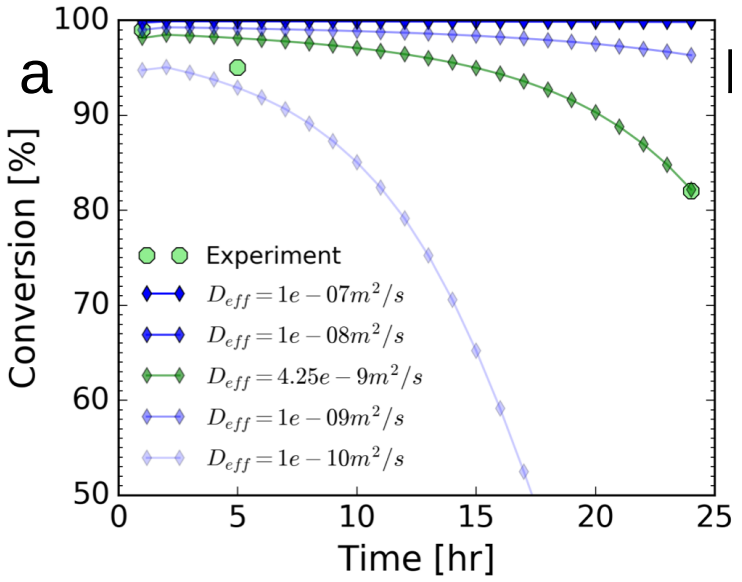
Objective: Develop a multi-scale modelling approach to study deactivation in the ethanol to butadiene process and guide catalyst design by exploring catalyst architecture activity lifetimes

Approach:

- Domain-specific diffusion coefficients for reactants and products are determined using Molecular Dynamics simulations and enable the calculation of effective diffusivities through the SBA-16 microstructure.
- Transport independent kinetic parameters for a simplified reaction scheme are estimated by fitting multiscale ethanol conversion simulations to experimental data.

Relevance: Model predicts methods for increasing conversion and lifetime via reducing pore size and catalyst particle diameter (optimize architecture). IDL team pursuing experimental validation.



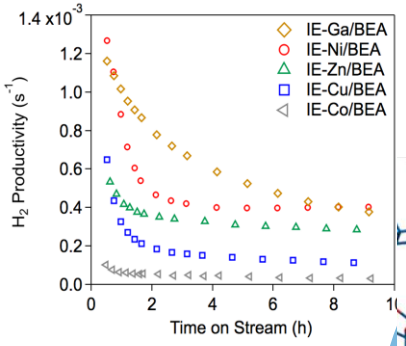


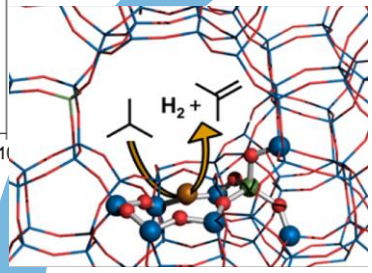
CCPC-Atomic [PNNL] ⟷ **CCPC-Meso** [NREL] ⟷ **ChemCatBio IDL**

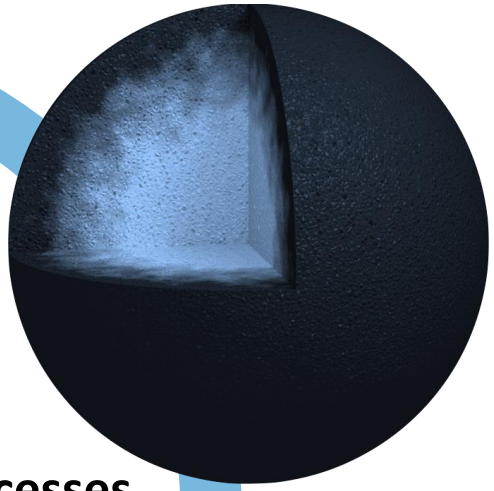
Relevance: CCPC Atomic-Level Fundamental Calculations Support *A Priori* Catalyst Design Process

Provide guidance for next generation catalyst design

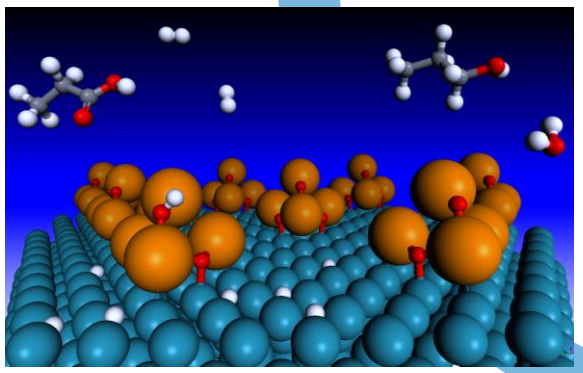
- Support architectures to enhance **selectivity** & **longevity**
- Identify key atomic-level descriptors that control catalytic **activity** & **selectivity**

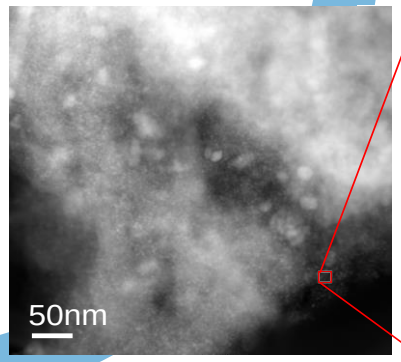


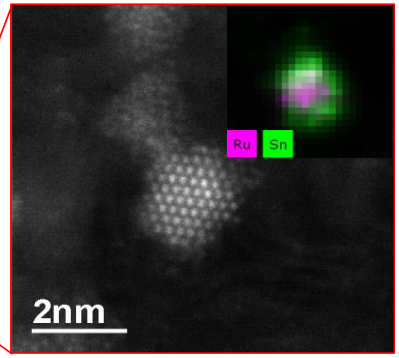




***A Priori* Design of Catalytic Processes**

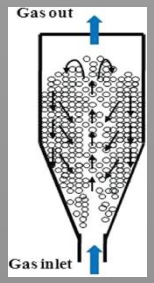


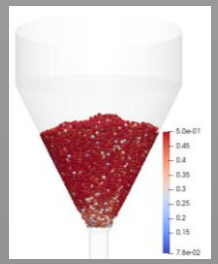




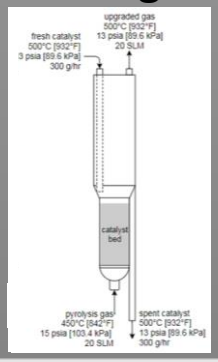
Progress: Reactor Models Cover Wide Range of Scale and Type

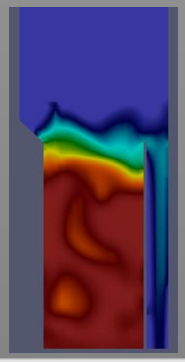
Spouted Bed (Kinetics)





2” Fluidized Bed Reactor Vapor Phase Upgrader (Bubbling Fluidized Bed)



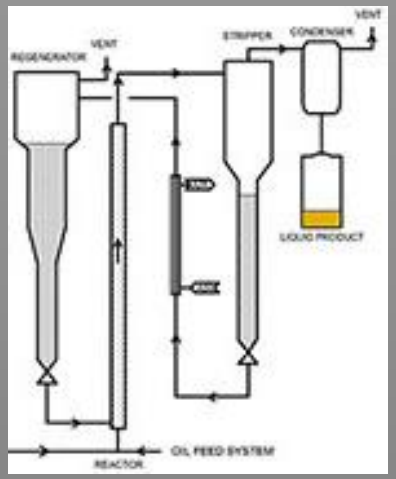


~883 sec Residence Time

500-900 micron particles

0.5 kg/hr flow rate

Davison Circulating Riser (DCR)

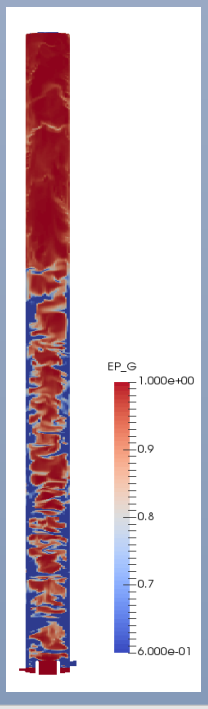


~3 sec Residence Time

80-100 micron particles

2 kg/hr flow rate

R-Cubed Reactor (TCPDU)



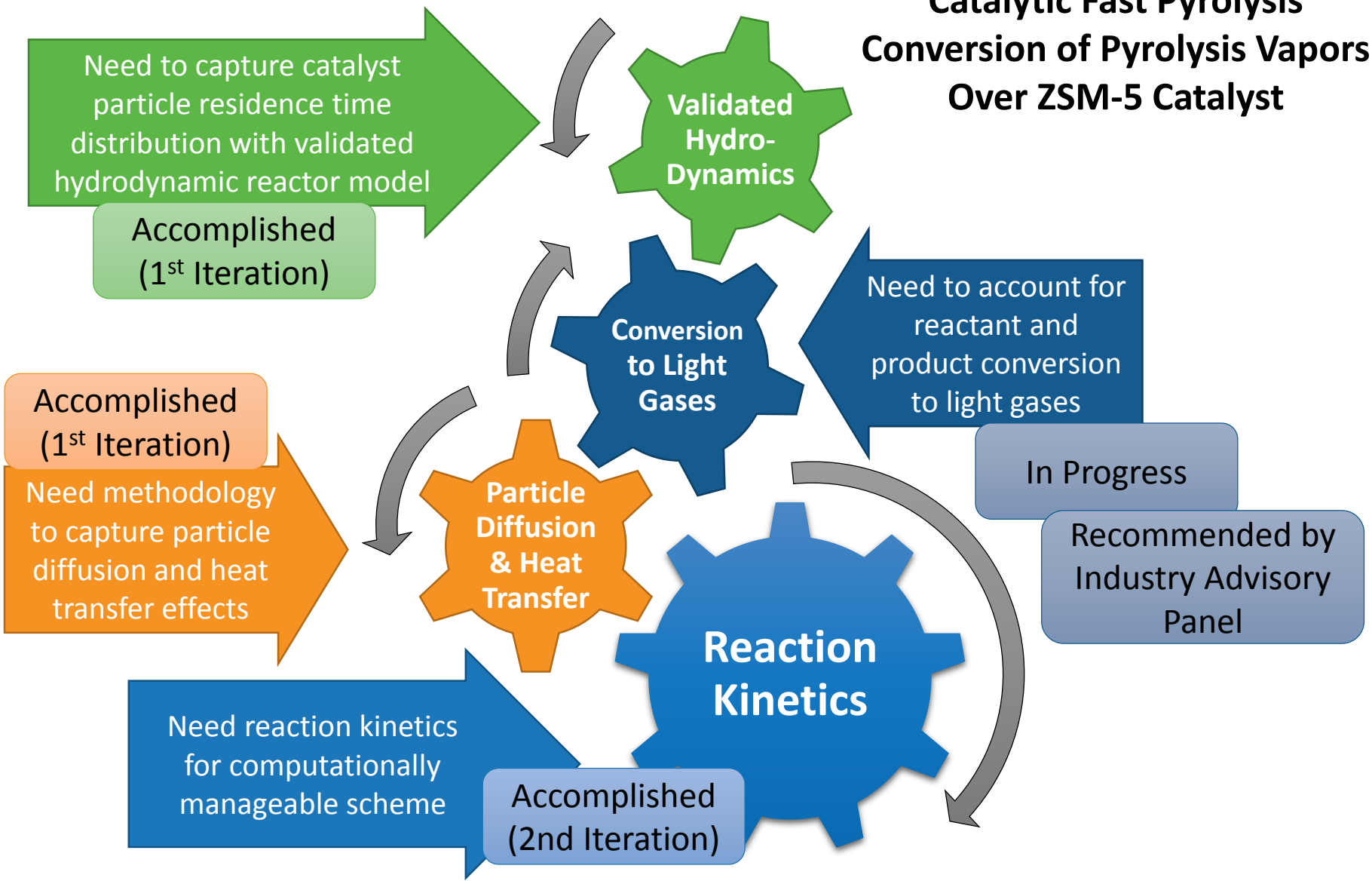
~10 sec Residence Time

80-100 micron particles

15 kg/hr flow rate

Progress: Grand Challenge of Predicting Yield Requires Many Elements to Capture Physics & Chemistry

Catalytic Fast Pyrolysis Conversion of Pyrolysis Vapors Over ZSM-5 Catalyst

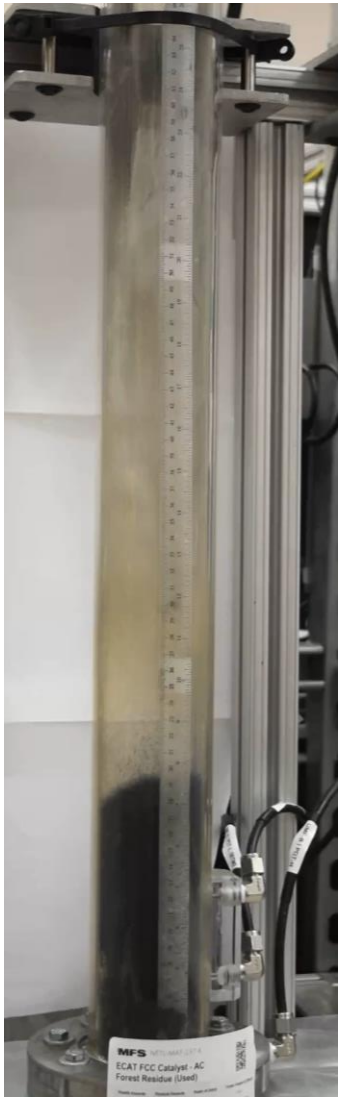


Progress: Validation of R-Cubed Model Hydrodynamics

- MFiX Computational Fluid Dynamic models of upgrading reactors capture residence time of catalyst particles
- R-Cubed reactor team provided validation data over designed experimental matrix
- NETL cold flow reactor enables further validation of catalyst particle drag models

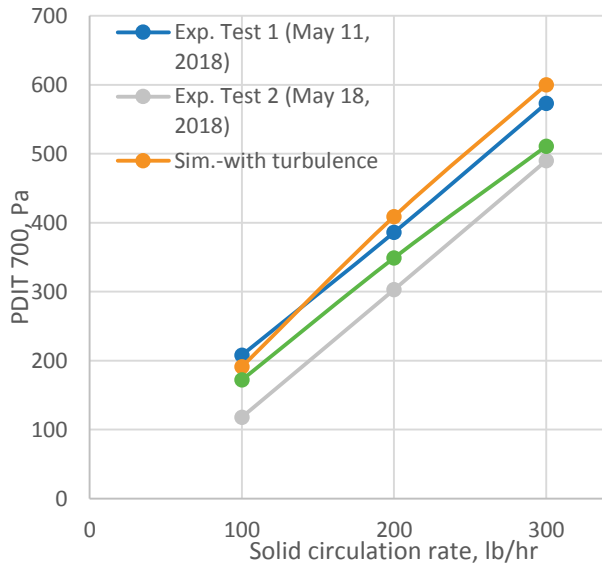
Relevance: Model enables accurate capture of critical residence times of catalyst particles (experimentally very difficult to measure)

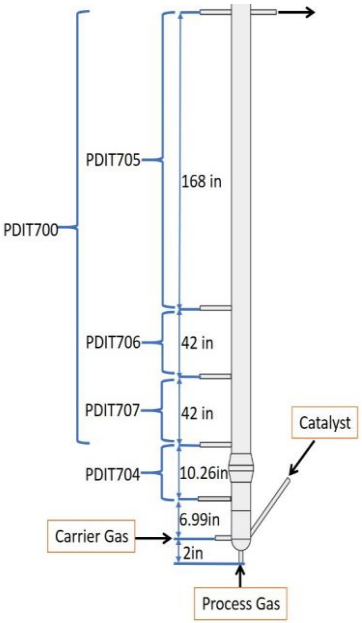
Cold Flow Reactor (NETL)



Validated Hydro-Dynamics

	Experimental matrix					
No.	Process N2, SLM	Carrier N2, SLM	Heater temps, °C	Process gas temp, °C	Catal kg/	a)
0	400	130	500	500		50
1	400	130	500	500		50
2	400	130	500	500	136 (	
3	300	130	500	500	91 (2	50
4	500	130	500	500	91 (2	50
5	400	130	500	400	91 (200)	50
6	400	130	500	600	91 (200)	50
7	400	230	500	500	91 (200)	50
8	400	330	500	500	91 (200)	50
9	400	130	500	500	91 (200)	25
10	400	130	500	500	91 (200)	75





CCPC-Process [NETL, ORNL] ↔ **ChemCatBio CFP** ↔ **ADO-TCPDU** [NREL]

Progress: Mesoscale Models of Reaction, Diffusion, and Deactivation in ZSM-5 Catalyst Particles

Particle Diffusion & Heat Transfer

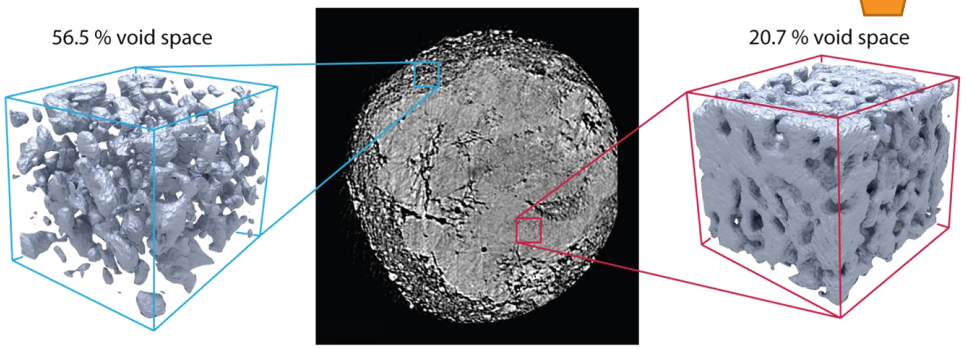
Objective: Develop a mesoscale simulation that decouples transport effects from kinetics of reaction and deactivation.

Approach:

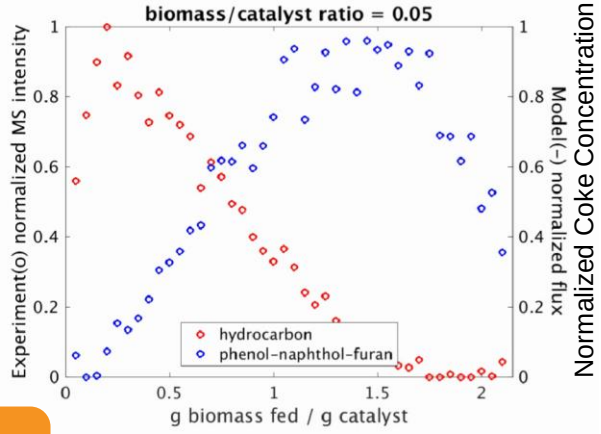
- Atomic modeling results (MD) simulations to determine molecular diffusion coefficients.
- Quantitative analysis of 3D image data (XCT) used to develop model for bulk transport in heterogenous porous media.

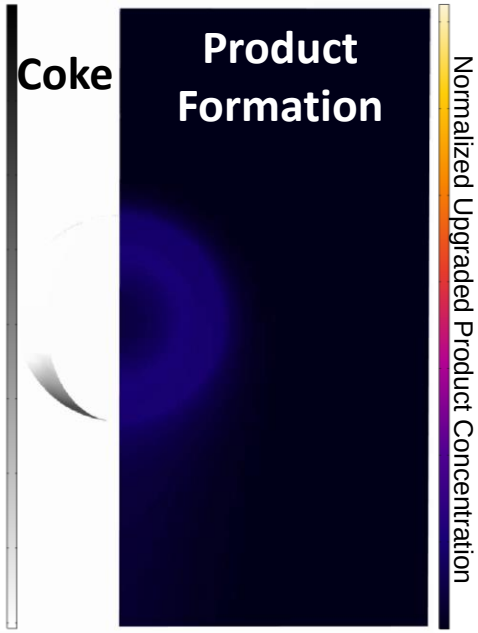
Relevance: simulation tool enables computational investigation of catalyst architectural features such as porosity and particle size

Experimental Characterization via X-Ray Computational Tomography



Reaction/Diffusion/Deactivation Model Compared to Experimental Results





CCPC [NREL] ↔ ChemCatBio CFP ↔ ChemCatBio ACSC

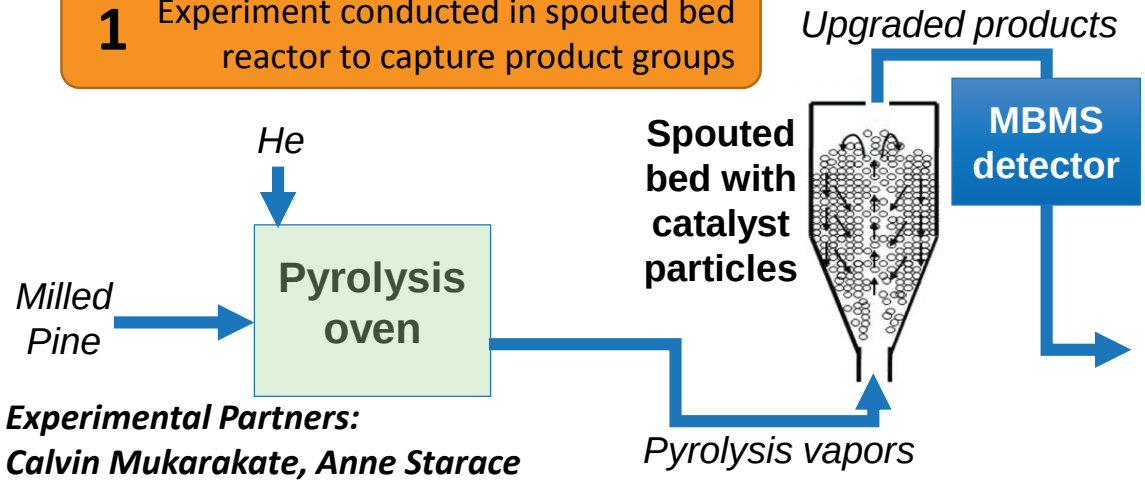
Progress: Close Collaboration Between Experimentalists and Modelers Enables Kinetic Rate Parameters to be Determined

Reaction Kinetics

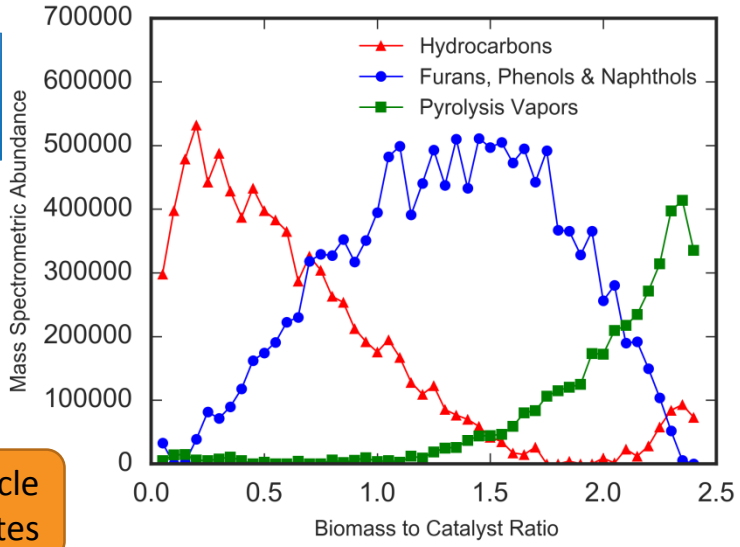
Relevance: kinetics specific to biomass pyrolysis vapors and catalysts of interest are critical and fill void in technical literature

Adjaye, Broadbelt, Klein, & others part of our search*

1 Experiment conducted in spouted bed reactor to capture product groups



Experimental Partners:
Calvin Mukarakate, Anne Starace



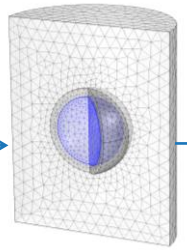
2 Kinetic rates extracted by using particle scale model to analyze data & extract rates

- Species
- Experimental Yields

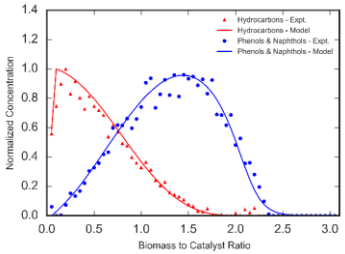
- Porosities
- Diffusivities
- Architecture
- Reaction Scheme

Initial Guess

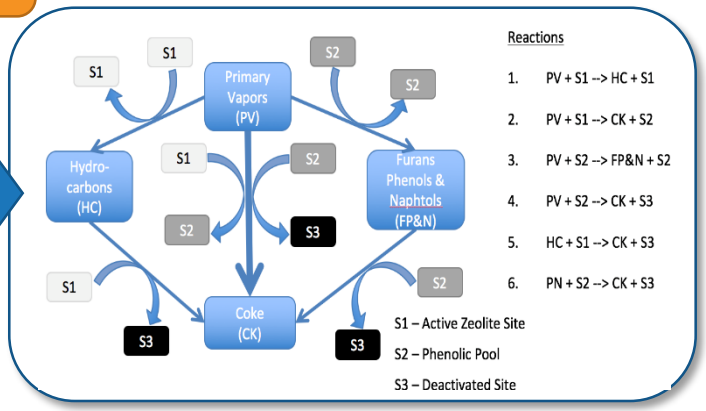
- Kinetic Rate Parameters



FEM simulation



External optimization routine

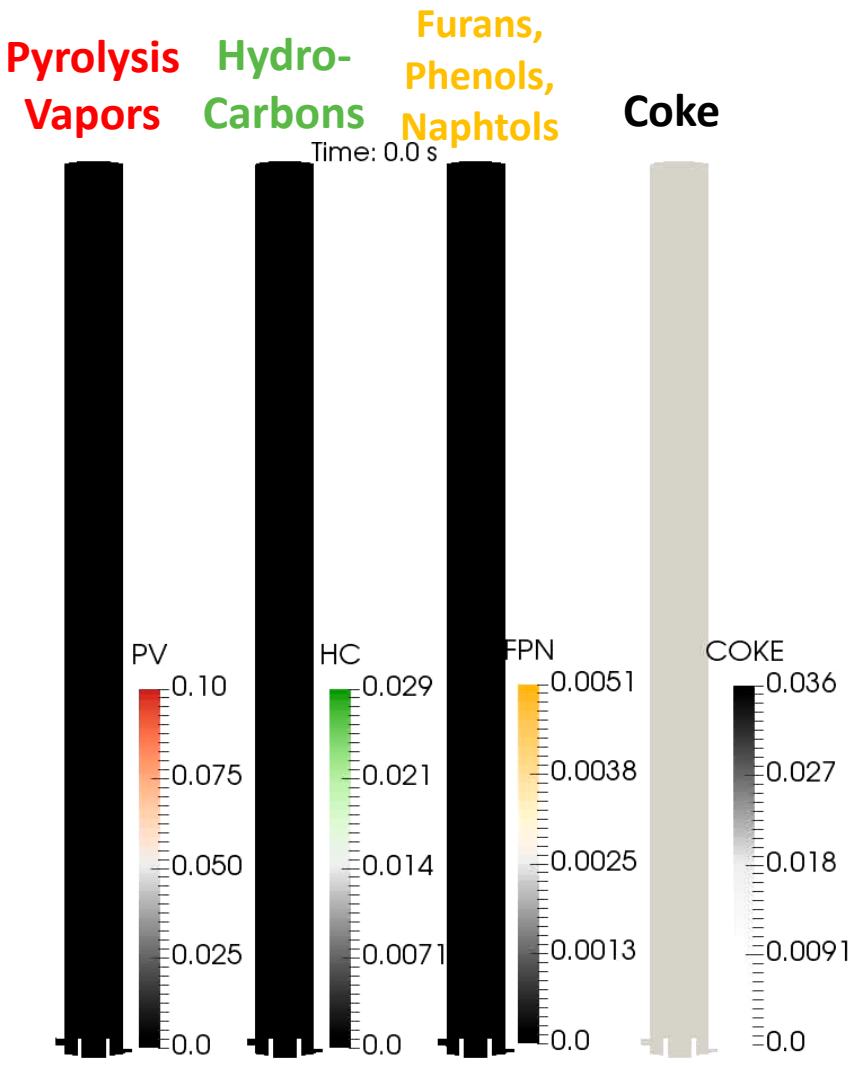


Reaction Pathway with Kinetic Rates

Progress: Application of Kinetics to R-Cubed Riser

- Kinetics generated from spouted bed reactor experiments ***and*** particle scale diffusion and heat transfer effects ***have been applied*** to R-Cubed Riser MFiX model to predict product yield
- Our methodology has been implemented. Initial results are encouraging but await experimental validation

Relevance: A validated model can enable translation of ChemCatBio catalyst technologies to industry-relevant scale



CCPC [NETL, NREL, ORNL] ↔ **ChemCatBio CFP** ↔ **ADO-TCPDU** [NREL]

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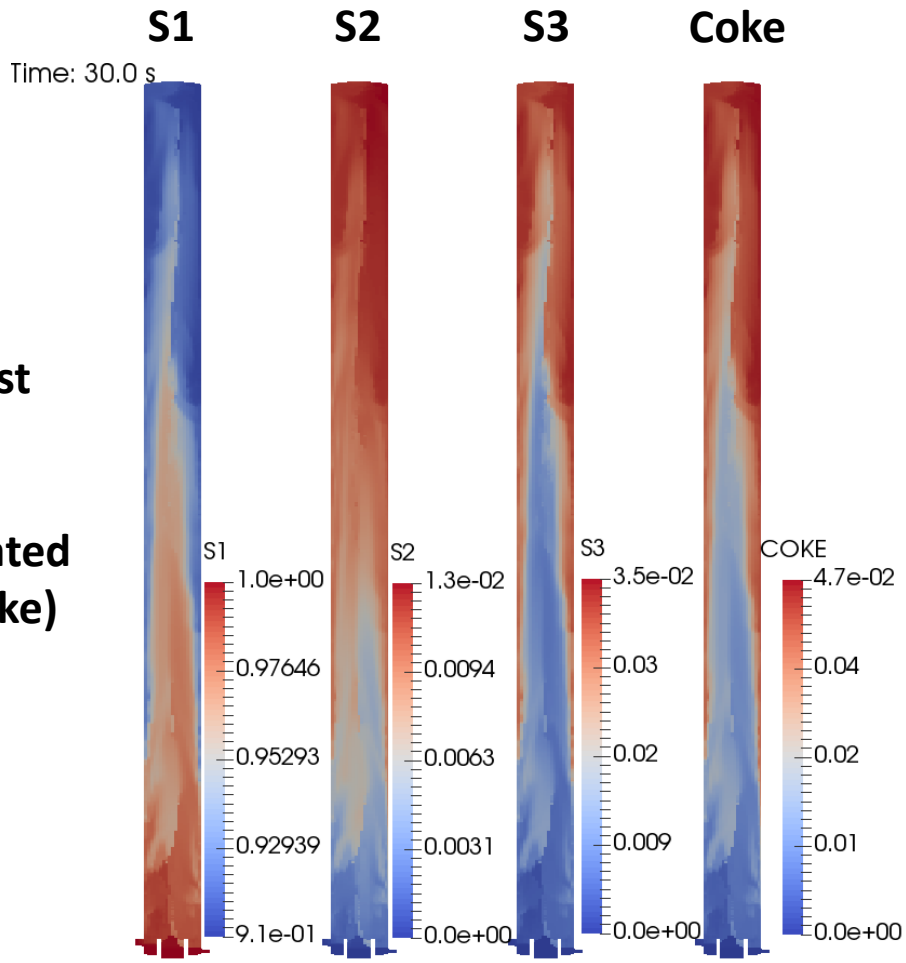
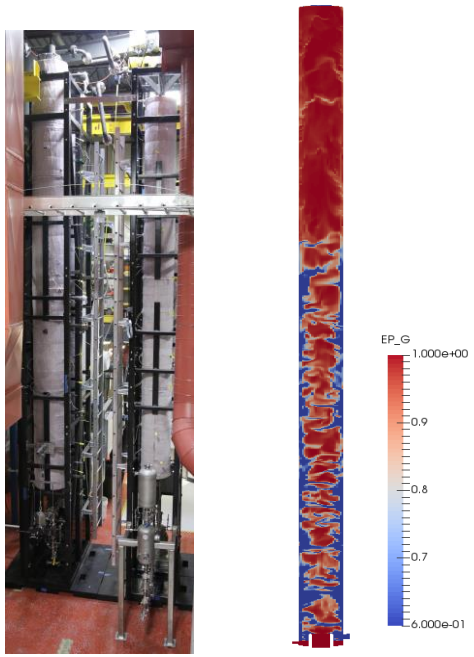
Catalyst Sites and **Deactivated Site (Coke)**



CCPC [NETL, NREL, ORNL] ↔ **ChemCatBio CFP** ↔ **ADO-TCPDU** [NREL]

Relevance: Translation of ChemCatBio Innovations to Industry and BETO Program Verification Success

- **Goal:**
  provide state-of-the-art methodology for translating ChemCatBio bioenergy catalytic upgrading to industry-relevant scales
- **Approach:**
  CCPC modeling approach combines science-based tools to capture key phenomena across all scales
- **Relevance:**
  - CCPC-developed kinetics fill void in bioenergy community
  - Prediction of catalytic performance at industry-relevant scales
  - Bridging function between BETO programs (ChemCatBio to Advanced Development and Optimization)
  - Capability to design and optimize reactors to enable success for BETO Verification (Catalytic Fast Pyrolysis, 2022)



Translate ChemCatBio catalysis innovations to industry-relevant scales

ChemCatBio
Chemical Catalysis for Bioenergy

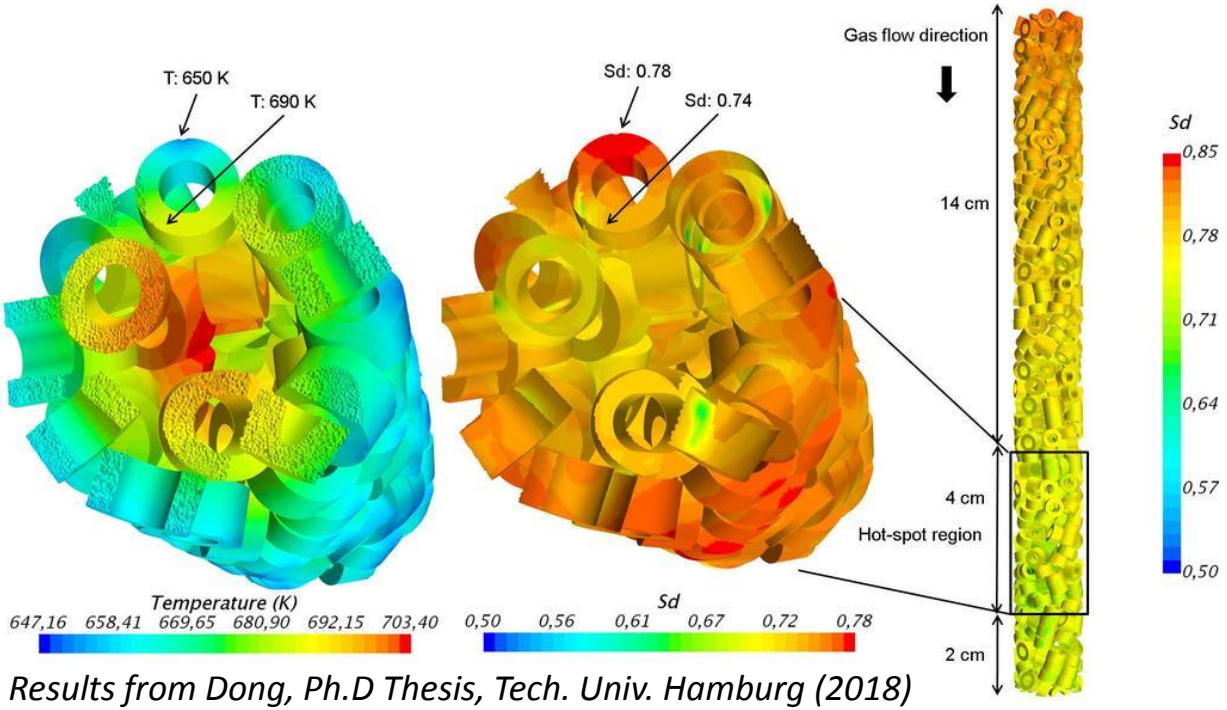
Future Work: Enabling Catalytic Fast Pyrolysis (CFP) Verification

Objective 1: aid CFP team in design, operation, and optimization of fixed bed reactor

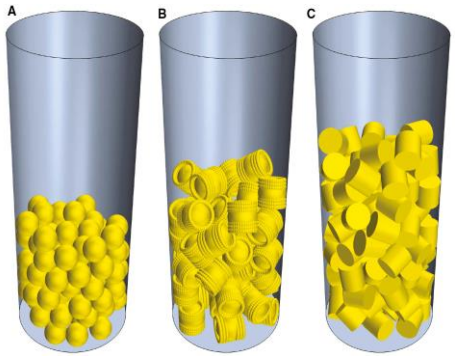
Heat Transfer Effects

Regeneration: strongly exothermic. Models must be able to predict hot spots to avoid loss of catalyst activity

Pyrolysis vapor deoxygenation: information on heat of reaction is sparse but essential to successful modeling



Results from Dong, Ph.D Thesis, Tech. Univ. Hamburg (2018)



Jurtz doi.org/10.1515/revce-2017-0059

Spatial Effects

Complex void space topology

Porosity and intraparticle diffusion

Flow uniformity & packing design

Relevance: Comprehensive understanding of design and operational spaces is critical for Catalytic Fast Pyrolysis (CFP) Verification

Note: model results shown from literature search (not CCPC)

Future Work: Enabling Catalytic Fast Pyrolysis (CFP) Verification

Objective 2: develop kinetics to support fixed bed reactor modeling (Objective 1)

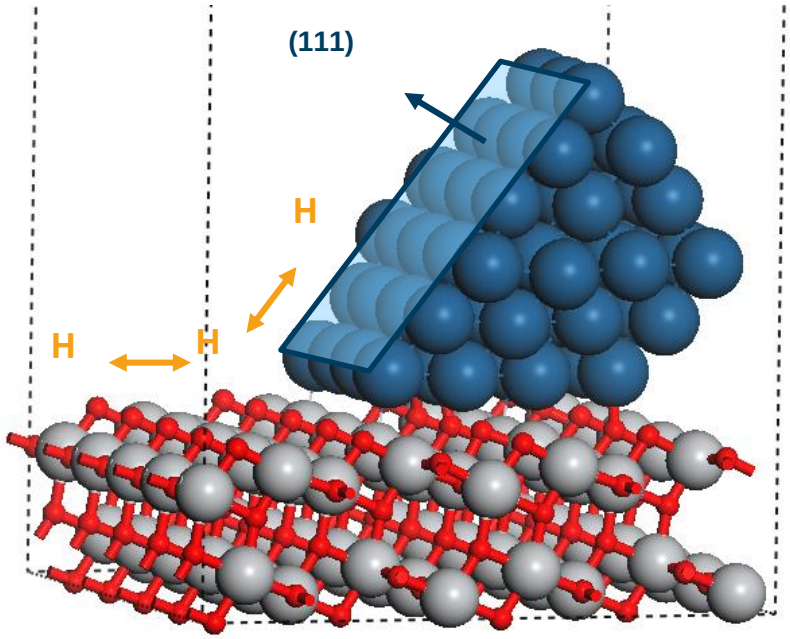
- Determine **kinetic rates** for Pt/TiO_2 catalysis to support fixed bed reactor models

Relevance: kinetics are needed to enable scale-up and predict performance at reactor scale for CFP Verification

Objective 3: understand strong metal surface interactions of Pt on TiO_2

- **Atomic scale** modeling of Pt/TiO_2 catalyst to understand H spillover and strong metal surface interactions that affect performance

Relevance: fundamental understanding of complex interface between Pt and support enables mitigation of risks for CFP Verification

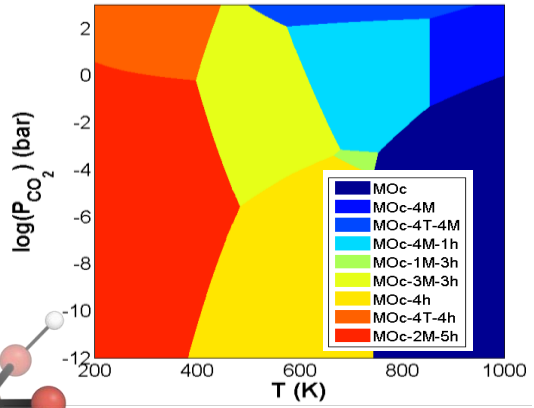


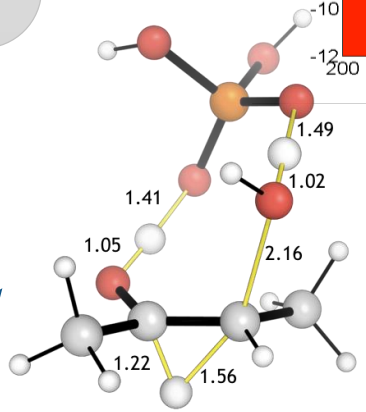
Pt/TiO_2 catalyst model in progress (NREL)

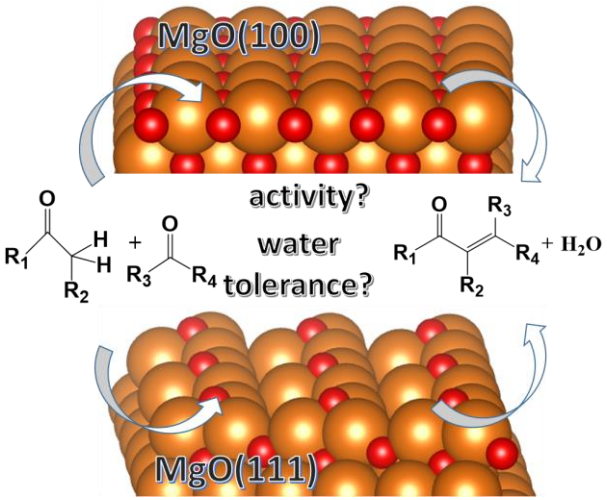
Future Work: Design Catalytic Reactions for Catalytic Upgrading of Biochemical Intermediates (CUBI)

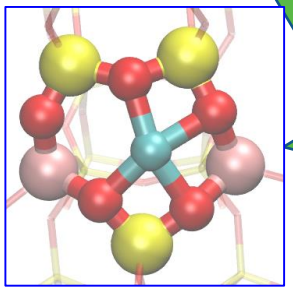
Objectives:

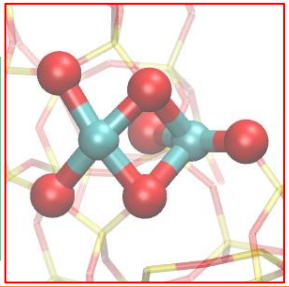
1. Establish design principles for efficient catalysts
2. Assist experimental efforts to identify optimum conditions for reactions
3. Using verified descriptors, screen catalysts for experimental studies











Relevance: simulations of wide range of materials accelerates catalyst R&D

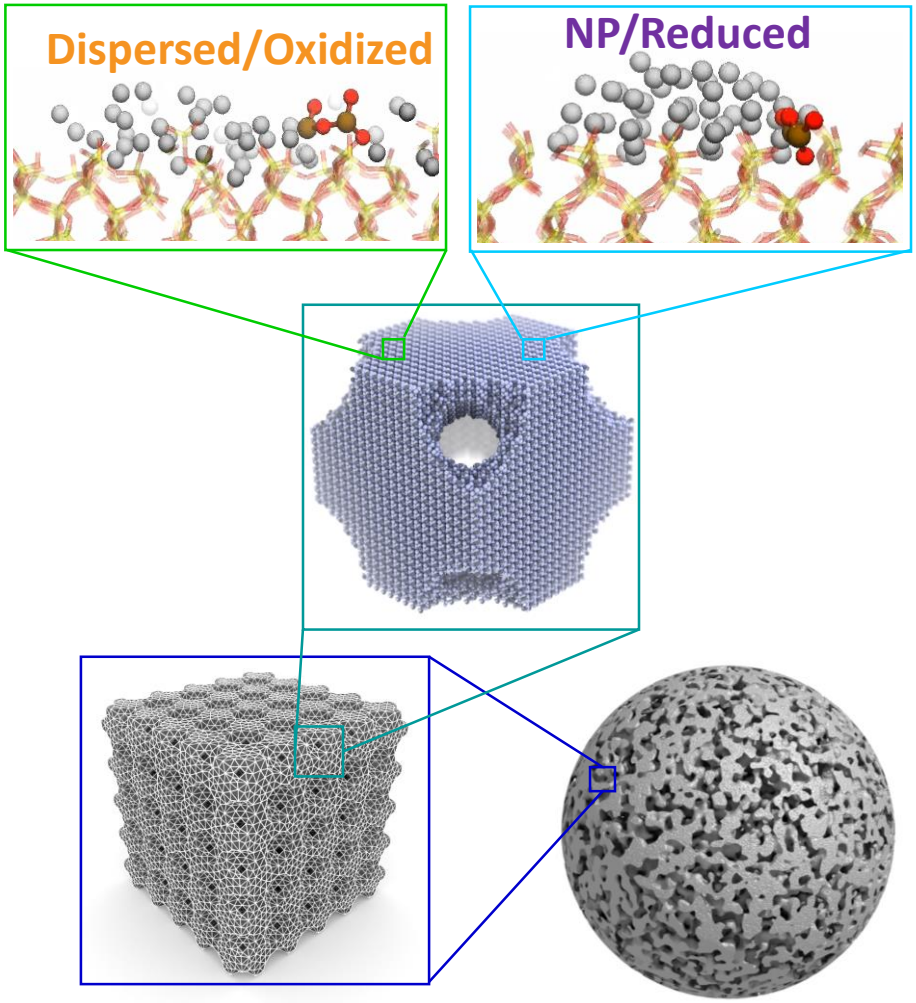
Selected systems

- Lewis acid -Furfural upgrading
- Metal phosphate BDO upgrading
- Metal oxide Ketone condensation
- HZSM-5 Dehydration

Future Work: Couple Atomic and Meso Scale Phenomena to Optimize $Ag/SiO_2/ZrO_2$ for Indirect Liquefaction (IDL)

Objective:
improve $Ag/SiO_2/ZrO_2$ catalyst yield and selectivity via optimization with atomic and meso scale simulations

- Leverage previous work from atomic scale and mesoscale simulations to develop multiscale simulation framework
- Elucidate the interplay of intraparticle transport phenomena and active site distribution in the bi-functional catalyst
- Use simulations to guide co-optimization of site density and support architecture to enhance yield and selectivity



Relevance: control of coupling of atomic and meso scale effects can enable optimization of catalyst

Future Work: Go/No-Go Review in FY2020

Kinetics Approach Assessment
demonstrate ability of process models to predict catalytic upgrading conversion efficiency and coking degradation rates

"Go" Next Steps:
- Transfer toolsets to industry including providing open-source code to public
- Apply toolset to optimize catalyst architecture, process controls, and reactor designs

"No-Go" Next Steps:
- Reassess approach

FY2019	FY2020	FY2021

Catalysis Innovation
show acceleration of the catalyst innovation cycle with a net reduction in R&D cost and time

"Go" Next Steps:
- Identify best approaches and keep using
- Consider new toolsets to further accelerate catalyst innovation (AI, machine learning)

"No-Go" Next Steps:
- Reassess approach

Summary: Consortium for Computational Physics and Chemistry (CCPC) for ChemCatBio

Approach: Utilize core computational capabilities ***to enable and accelerate …***
(1) the development of new materials and
(2) optimize process scale-up ***… to advance the bioenergy economy.***

Progress

Atomic Scale calculations of numerous catalyst material combinations have aided experimental pathway projects

Meso Scale catalyst particle models capture heat transfer and diffusion effects for wide range of architectures

Process Scale reactor models capture critical hydrodynamics and calculate conversion with bioenergy kinetics

Relevance

Enables ChemCatBio teams to **accelerate** progress & provides **fundamental understanding** of catalyst surface science phenomena

Provides means to **optimize catalyst particle architecture** and enables determination of **kinetics** and other critical parameters

Methodology progressing for process **optimization and scale-up** to industry relevant scales and BETO Verification

Future Work:
- Design/optimize fixed bed reactor system for Catalytic Fast Pyrolysis Verification
- Complete & validate reactor models with kinetics for pyrolysis vapor upgrading (ZSM-5)
- Optimize $Ag/SiO_2/ZrO_2$ on SBA-16 support for ethanol conversion to butadiene/butene

Acknowledgements*

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Stuart Daw
Emilio Ramirez
Zach Mills
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Peter Ciesielski
Seonah Kim
Lintao Bu
Tom Foust
Vassili Vorotnikov
Carrie Farberow
Mark Nimlos
Brandon Knott
Brennan Pecha
Vivek Bharadwaj
Aaron Lattanzi

Pacific Northwest NATIONAL LABORATORY

Roger Rousseau
Vanda Glezakou
Asanga Padmaperuma
Simuck Yuk
Bob Weber*
Sneha Akhade*
David Cantu*

NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

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Tingwen Li*
Dirk VanEssendelft*
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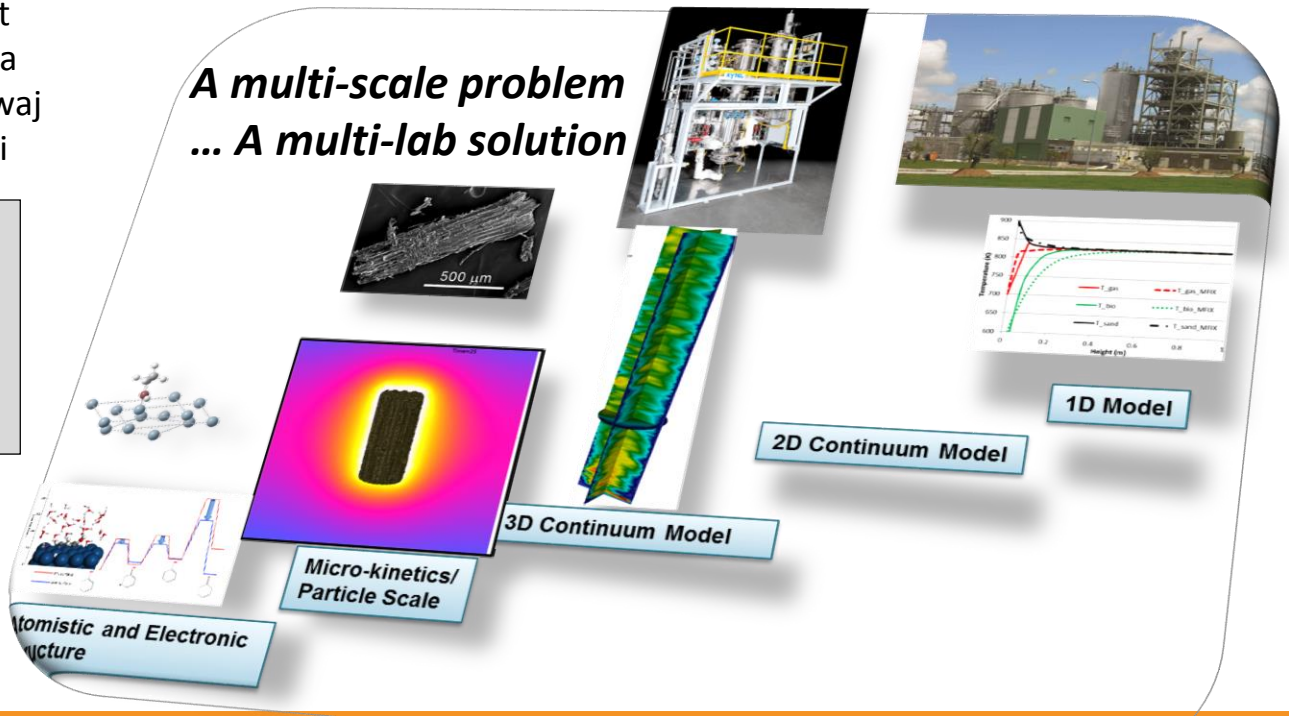
Rajeev Assary
Mingxia Zhou
Hieu Doan
Lei Cheng
Cong Liu
Dale Pahls*

Industry Advisory Panel

David Dayton (RTI), George Huff (MIT, retired BP),
Jack Halow (Separation Design Group), Steve Schmidt (WR Grace),
Tom Flynn (Babcock & Wilcox)



CCPC

www.cpcbiomass.org

*includes current and former CCPC contributors

ChemCatBio
Chemical Catalysis for Bioenergy

Additional Slides

Consortium for Computational Physics and Chemistry - ChemCatBio

Additional Slides: 2017 Peer Review - Reviewer Comments

Overall Impressions:

- There is an impressive amount of work for programs. The budget is quite high but necessary for all teams to succeed and accelerate programs. Continue what the team is doing as they are doing well. Do not change anything. There is an impressive amount of publications as well since the last review. I applaud the team and their ability to influence and impact programs in such a complex set of programs. I give this team my highest ratings.
- There is a very high impact for the cost of the project. One wonders where the resources are coming from to accomplish all that was reported and if this can be continued in the future. Predicting the performance of process from small-scale experiments requires a strong modeling effort that can identify potential problems. The phase behavior in the converter and the effect of particle and reactor hold up as the scale increases are critical factors that can be predicted using the models developed by this group. It will be particularly important to access the effects of the reactor configuration, including the shape, size inlet design, etc.
- This is a great project with lots of valuable information available for other bioenergy projects. The industry advisory panel helps focus the work on areas that will accelerate the commercialization of bioenergy technologies. The project leverages several experts from multiple laboratories and organizations. This is exciting work.
- Overall, this is a solid program with a number of significant historical contributions, as well as quite a few potentially promising contributions in the future. Models are a critical component for both communication and commercialization. CCPC's high level of competency and expertise in this area is priceless for both BETO and the public. Focus on scalability, bio-complexity , and basic catalysis science is spot on and reflects good understanding of most of the major variables that drive commercialization in the bioenergy/biofuels industry.
- These are impressive project accomplishments to date. Congratulations! If the modeling tools can be successfully applied to the benefit of the catalytic project teams, this will have been a very valuable program.

The text on this slide is a direct quote from the 2017 Project Peer Review of the U.S. Department of Energy Bioenergy Technologies Office final report available at www.energy.gov/eere/bioenergy/downloads/2017-project-peer-review-report (pp. 291-3)

Additional Slides: Responses to Previous Reviewers' Comments

Reviewer Comments	CCPC Responses
General positive impressions & comments	***The positive feedback is appreciated. We have continued practicing the highlighted approaches*** including: (1) use of the industry advisory panel, (2) alignment/collaboration with biomass conversion projects, (3) open-source code and tech transfer mechanisms, (4) emphasis on capturing biomass complexity in scalable models, and (5) study of zeolite catalysis transport and deactivation mechanisms.
Tech transfer of methodologies and models to commercial partners	By design, we utilize open-source code and publish codes on GitHub (with a link accessible from our CCPC website) as well as results in peer-reviewed journals. This enables the potential for tech transfer of our models; however, the reviewer comments were quite useful as we have re-examined our approach for tech transfer and ways in which we can be more proactive. As a result, in FY2018, we added a specific milestone to transfer our biomass particle model (a mature model). We approached numerous entities with the intent to transfer the model. ***Ultimately, we succeeded in transferring the model to Forest Concepts, and the results were a major highlight for our program*** (see next slide and press release at www.nrel.gov/news/program/2018/bioenergy-scientists-collaborate-with-industry-to-convey-feedstock-value-improve-biomass-conversion-processes.html). We learned lessons in this process too. In this case, the industry partner was only interested in the model results (and not in being able to operate the model themselves). So, we ran the model for their case and needs.
Expanding scope to include separations	***This recommendation from the review panel was extremely beneficial and insightful.*** We responded by scheduling a series of web conferences with the Bioprocessing Separations Consortium (SepCon) in which we discussed CCPC modeling capabilities and SepCon modeling needs. The result was a vast array of opportunities where existing CCPC modeling toolsets and capabilities could be adapted to meet SepCon modeling needs. We initiated starter projects in FY2018 to begin progress in this area. We faced limitations early on due to the fact that no resources were identified in the BETO Separations program for modeling, and our CCPC-ChemCatBio resources are designated for supporting the ChemCatBio objectives. As a result, we have formed a more holistic strategy for the CCPC to serve and coordinate modeling needs across BETO. We are working closely with SepCon and BETO Technology Managers to specifically identify resources to support modeling for separations in the next AOP cycle for SepCon which begins in FY2020. And, we have designated a liaison to SepCon to foster the efforts.

Three comment areas and associated responses on highlighted on this slide. Other comments and our responses can be found in the 2017 Project Peer Review of the U.S. Department of Energy Bioenergy Technologies Office final report available at www.energy.gov/eere/bioenergy/downloads/2017-project-peer-review-report (pp. 291-3)

Additional Slides: Pyrolysis Model Results Aid Industry

Objective: Leverage validated pyrolysis models to support industry partners

Approach:

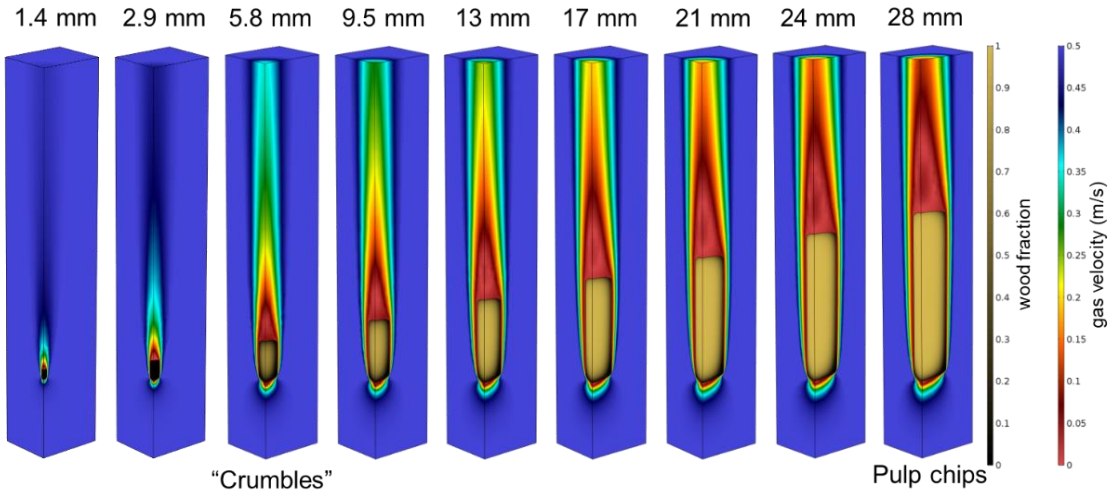
- Models were parameterized to represent a range of Forest Concepts' feedstock products
- FC used results to communicate value of precision feedstocks to customers

Relevance: *"The modeling data developed by NREL gave our company an understanding of how our production engineers can co-optimize reactors and feedstock properties to improve functional performance. This conversion data will also help our customers select the optimal feedstock for their specific conversion process."*

- James H. Dooley
  CTO, Forest Concepts

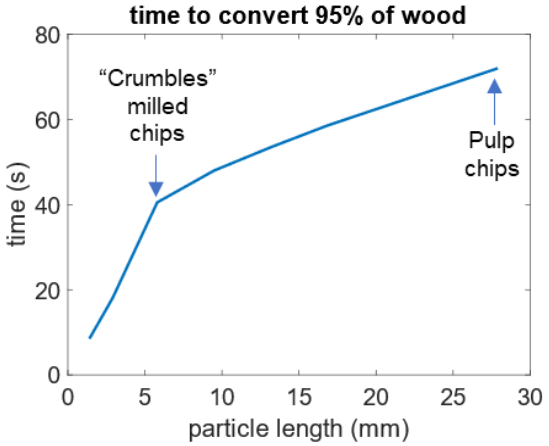
Industry Partner: Forest Concepts

Pine chips pyrolyzing at 500°C, 30s mark



NREL scientists visualizing data

Conversion times, particle size



Additional Slides: Go/No-Go Reviews

- The last Go/No-Go Review for this project was in FY2016. The stage was passed (Go), and technical results were shared at the 2017 Peer Review.
- The next Go/No-Go Review for the project is scheduled for FY2020 and is summarized in the table below (verbatim from Annual Operating Plan).

Name	Description	Criteria	Date
Kinetics Approach Assessment	Based on modeling at atomic, meso, and process scales, demonstrate a technique for predicting conversion at commercially-relevant scales for ChemCatBio catalytic upgrading processes. The outcome of this go/no-go decision will determine: (1) is the CCPC-CCB approach toward kinetics definition in highly complex bioenergy applications valid and feasible; should more extensive approaches be pursued such as micro-kinetics-based approaches.	Using kinetics data extracted from data from designed experiments with ChemCatBio colleagues, demonstrate ability of process models to predict catalytic upgrading conversion efficiency and coking degradation rates.	4/30/2020
Catalysis Innovation	In close collaboration with ChemCatBio experimentalists, modeling will be utilized to accelerate catalyst innovation.	Using an experiment-only base case as reference, show acceleration of the catalyst innovation cycle (design to experimental results) with a net reduction in R&D cost and time to results.	4/30/2020

Additional Slides: Publications, Patents, Presentations, Awards, and Commercialization - Slide 1 of 7

Patents, Commercialization, Tech Transfer, and Open-Source Code

Note: The CCPC by design produces open-source code models that are publicly available on GitHub (github.com/ccpcode) with a link to the site on the CCPC website (www.cpcbiomass.org). Therefore, our tech transfer output is primarily in the form of the open-source code, and we cite here the resulting commercial impacts and open source codes made publicly available.

Tech Transfer/Commercial Impact (since 2017 Peer Review):

- Tech transfer of biomass feedstock pyrolysis model to aid Forest Concepts in product characterization
  - The CCPC performed detailed thermochemical conversion simulations with our biomass feedstock particle model to characterize the fast pyrolysis yield of select Forest Concepts products. The results provided new information for performance and valuation of products for Forest Concepts and their customers in bioenergy applications. The commercial impact was acknowledged by Forest Concepts Chief Technology Officer James Dooley and was featured in a press release (www.nrel.gov/news/program/2018/bioenergy-scientists-collaborate-with-industry-to-convey-feedstock-value-improve-biomass-conversion-processes.html). [Peter Ciesielski et al.]

Tech Transfer/Commercial Impact (since project inception):

- Surface Phase Explorer Website-Based Tool (spe.nrel.gov)
  - The CCPC made a publicly available web-based tool called “Surface Phase Explorer” which enables: (1) construction of surface ab initio phase diagrams for single species adsorbing to a surface as well as coadsorption of two species to a surface and (2) visualization of the Wulff Construction of the surface at any temperature and pressure. [Vassili Vorotnikov et al.]
- Commercial Software Impact: CSFMB©/CeSFaMB™
  - The CCPC assisted Prof. de Souza-Santos (Brazil) in including biomass pyrolysis chemistry into new version of CSFMB© commercial software (see www.csfmb.com) [C. Stuart Daw et al.]

Additional Slides: Publications, Patents, Presentations, Awards, and Commercialization - Slide 2 of 7

GitHub Open-Source Code and Supporting Documentation (since 2017 Peer Review):

- github.com/ccpcode/chemics-reactors
  - A Python-based program for implementing network models of multiphase reactors (beta version) [Jonathan Sutton et al.]
- github.com/ccpcode/kinetic-schemes
  - A repository of various kinetic reaction schemes for biomass pyrolysis based on the literature. The kinetics are presented in Python-based code and include the CCPC kinetics which are a combination of the Di Blasi (1993), Chan (1985), and Liden (1988) kinetic schemes. [Gavin Wiggins et al.]
- github.com/ccpcode/docs-tcpdu
  - Supporting documentation for the NREL ThermoChemical Process Development Unit (TCPDU) [Gavin Wiggins, Katie Gaston et al.]
- github.com/ccpcode/docs-2fbr
  - Supporting documentation for the NREL 2" Fluidized Bench Reactor (2FBR) and associated Vapor Phase Upgrading reactor [Gavin Wiggins, Rick French et al.]
- github.com/ccpcode/nrel-2fbr-particles
  - Particle characterization data for catalyst particles used in experiments and models of the NREL 2" Fluidized Bench Reactor (2FBR) Vapor Phase Upgrading reactor [Gavin Wiggins, Rick French et al.]

GitHub Open-Source Code and Supporting Documentation (since project inception):

- github.com/ccpcode/low-order-reactor
  - A low-order reactor model that utilizes a CSTR (continuously stirred tank reactor) modeling approach to estimate fast pyrolysis yields from bubbling fluidized bed reactors based on a give particle size distribution and associated low-order particle sub-model. [Gavin Wiggins, C. Stuart Daw et al.]
- github.com/ccpcode/low-order-particle
  - Python-based low-order particle model for modeling heat transfer and pyrolysis as a function of particle size and shape. This sub-model was developed based on high-order models of particle pyrolysis with COMSOL and feeds the low-order reactor model above. [Gavin Wiggins, Peter Ciesielski et al.]

Awards

Awards (since 2017 Peer Review):

- Poster Presentation Award to Emilio Ramirez for Second Place in the Student Research Poster Presentation category at the *Thermal and Catalytic Sciences (TCS) Symposium for Biofuels and Bioproducts*, October 8-10, 2018.

  Note: Emilio is a Ph.D. graduate student at the University of Tennessee who is conducting his dissertation research in multiphase modeling of fast pyrolysis in bubbling fluidized beds (anticipated graduation in May 2019). His poster was entitled "Computational study on biomass fast pyrolysis: Hydrodynamic effects in a laboratory-scale fluidized bed".

Emilio Ramirez (second from left) with poster presentation award from TCS2018

Additional Slides: Publications, Patents, Presentations, Awards, and Commercialization - Slide 4 of 7

Publications [26 since January 1, 2017; 55 Total since Project Inception]

Publications (with publication date since January 1, 2017):

1. Bharadwaj VS, Pecha MB, Lebarbier Dagle V, Dagle RA, Ciesielski PN (2019). Multi-scale simulation of reaction, transport and deactivation in SBA-16 supported catalysts for the conversion of ethanol to butadiene. Submitted to *Catalysis Today*.
2. Zhou M, Cheng L, Lu B, Curtiss LA, Assary RS (2019). Role of Ga sites on furan decarbonylation over Ga/ZSM-5 – A first-principle investigation. Submitted to *Industrial Engineering Chemistry Research*.
3. Gao X, Li T, Rogers WA (2018). Assessment of mesoscale solid stress in coarse-grid TFM simulation of Geldart A particles in all fluidization regimes. *AIChE Journal* 64(10): 3565–3581. doi:10.1002/aic.16341
4. Ciesielski PN, Pecha MB, Bharadwaj VS, Mukarakate C, Leong GJ, Kappes B, Crowley MF, Kim S, Foust TD, Nimlos MR (2018). Advancing catalytic fast pyrolysis through integrated multiscale modeling and experimentation: Challenges, progress, and perspectives. *Wiley Interdisciplinary Reviews: Energy and Environment* 7(4). doi:10.1002/wene.297
5. Krishna SH, Assary RS, Rashke QA, Schmidt ZR, Curtiss LA, Dumesic JA, Huber GW (2018). Mechanistic insights into the hydrogenolysis of levoglucosanol over bifunctional platinum silica-alumina catalysts. *ACS Catalysis* 8(5): 3743–3753. doi:10.1021/acscatal.7b03764
6. Gao X, Li T, Sarkar A, Lu L, Rogers WA (2018). Development and validation of an enhanced filtered drag model for simulating gas-solid fluidization of Geldart A particles in all flow regimes. *Chemical Engineering Science* 184: 33–51. doi:10.1016/j.ces.2018.03.038
7. Bu L, Nimlos MR, Robichaud DJ, Kim S (2018). Diffusion of aromatic hydrocarbons in hierarchical mesoporous H-ZSM-5. *Catalysis Today* 312: 73–81. doi:10.1016/j.cattod.2018.02.012
8. Knott BC, Nimlos CT, Robichaud DJ, Nimlos MR, Kim S, Gounder R (2018). Consideration of the aluminum distribution in zeolites in theoretical and experimental catalysis research. *ACS Catalysis* 8(2): 770–784. doi:10.1021/acscatal.7b03676
9. Zhou M, Cheng L, Choi J-S, Lu B, Curtiss LA, Assary RS (2018). Ni-doping effects on oxygen removal from an orthorhombic Mo2C(001) surface: A density functional theory investigation. *Journal of Physical Chemistry C* 122(3): 1595–1603. doi:10.1021/acs.jpcc.7b09870
10. Pecha MB, Ramirez E, Wiggins GM, Carpenter D, Kappes B, Daw CS, Ciesielski PN (2018). Integrated particle- and reactor-scale simulation of pine pyrolysis in a fluidized bed. *Energy and Fuels* 32(10): 10683–10694. doi:10.1021/acs.energyfuels.8b02309.

Publications [26 since January 1, 2017; 55 Total since Project Inception]

Publications (with publication date since January 1, 2017*) [cont. from previous slide]*:

11. Sutton JE, Wiggins GM, Daw CS (2018). Chemics-Reactors: A preliminary Python program for implementing network models of multiphase reactors. *Oak Ridge National Laboratory Report* ORNL/TM-2017/748.

12. Likith SRJ, Farberow CA, Manna S, Abdulslam A, Stevanović V, Ruddy DA, Schaidle JA, Robichaud DJ, Ciobanu CV (2018). Thermodynamic stability of molybdenum oxycarbides formed from orthorhombic Mo_2C in oxygen-rich environments. *Journal of Physical Chemistry C* 122(2): 1223–1233. doi:10.1021/acs.jpcc.7b11110

13. Iisa K, Watson MJ, ten Dam J, Dutta A, Baldwin RM, Mukarakate C, Kim S, Robichaud DJ, Nimlos MR (2018). Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. *Green Chemistry* 20: 567–582. doi:10.1039/C7GC02947K

14. Vardon DR, Settle AE, Vorotnikov V, Menart MJ, Eaton TR, Unocic KA, Steirer KX, Wood KN, Cleveland NS, Moyer KE, Michener WE, Beckham GT (2017). Ru-Sn/AC for the aqueous-phase reduction of succinic acid to 1,4-butanediol under continuous process conditions. *ACS Catalysis* 7(9): 6207–6219. doi:10.1021/acscatal.7b02015

15. Ciesielski PN, Wiggins GM, Daw CS, Jakes JE (2017). Simulating Biomass Fast Pyrolysis at the Single Particle Scale, Chapter 11 in Fast Pyrolysis of Biomass: Advances in Science and Technology, pp. 231–253. doi:10.1039/9781788010245-00231

16. Farberow CA, Cheah S, Kim S, Miller JT, Gallagher JR, Hensley JE, Schaidle JA, Ruddy D (2017). Exploring low-temperature dehydrogenation at ionic Cu sites in beta zeolite to enable alkane recycle in dimethyl ether homologation. *ACS Catalysis* 7(5): 3662–3667. doi:10.1021/acscatal.6b03582.

17. Kunz L, McDonough R, Bu L, Cywar R, Yung MY, Chupk G, Liu C, Patalano R, Iisa K, Nimlos MR, Assary RS, Curtiss LA, Kim S, Robichaud DJ (2017). Kinetic determination of alcohol dehydration to olefins over zeolites. Submitted *to Journal of Physical Chemistry.*

18. Pecha MB, Garcia-Perez M, Foust TD, Ciesielski PN (2017). Estimation of heat transfer coefficients for biomass particles by direct numerical simulation using microstructured particle models in the laminar regime. *ACS Sustainable Chemistry & Engineering* 5(1): 1046–1053. doi:10.1021/acssuschemeng.6b02341.

19. Bu L, Nimlos MR, Robichaud DJ, Kim S (2017). Diffusion of biomass pyrolysis products in H-ZSM-5 by molecular dynamics simulations. *Journal of Physical Chemistry C* 121(1): 500–510. doi:10.1021/acs.jpcc.6b10871.

Publications [26 since January 1, 2017; 55 Total since Project Inception]

Publications (with publication date since January 1, 2017*) [cont. from previous slide]*:

20. Foust TD, Ziegler JL, Pannala S, Ciesielski PN, Nimlos MR, Robichaud DJ (2017). Predictive model for particle residence time distributions in riser reactors. Part 1: Model development and validation. *ACS Sustainable Chemistry & Engineering* 5(4): 2847–2856. doi:10.1021/acssuschemeng.6b02384.

21. Foust TD, Ziegler ZL, Pannala S, Ciesielski PN, Nimlos MR, Robichaud DJ (2017). Catalyst residence time distributions in riser reactors for catalytic fast pyrolysis. Part 2: Pilot-scale simulations and operational parameter study. *ACS Sustainable Chemistry and Engineering* 5(4): 2857–2866. DOI: 10.1021/acssuschemeng.6b02385

22. Ramirez E, Finney CEA, Pannala S, Daw CS, Halow JS, Xiong Q (2017). Computational study of the bubbling-to-slugging transition in a laboratory-scale fluidized bed. *Chemical Engineering Journal* 308: 544–556. doi:10.1016/j.cej.2016.08.113

23. Drouin BJ, Benner DC, Brown LR, Cich MJ, Crawford TJ, Devi VM, Guillaume A, Hodges JT, Mlawer EJ, Robichaud DJ, Oyafuso F, Payne VH, Sung K, Wishnow EH, Yu S (2017). Multispectrum analysis of the oxygen A-band. *Journal of Quantitative Spectroscopy and Radiative Transfer* 186: 118–138. doi:10.1016/j.jqsrt.2016.03.037.

24. Xiong, Q.; Robichaud, D. J. (2017). Computational Studies of Pyrolysis and Upgrading of Bio-oils: Virtual Special Issue, *ACS Sustainable Chemistry & Engineering* 5(4): 2782. doi: 10.1021/acssuschemeng.7b00805

25. Logan C. Thompson, Peter N. Ciesielski, Mark W. Jarvis, Calvin Mukarakate, Mark R. Nimlos, and Bryon S. Donohoe (2017). Estimating the Temperature Experienced by Biomass Particles during Fast Pyrolysis Using Microscopic Analysis of Biochars. *Energy Fuels* 31 (8): 8193–8201. DOI: 10.1021/acs.energyfuels.7b00791

26. L.D. Dellon, C.-Y. Sung, D.J. Robichaud, L.J. Broadbelt (2017). Group Additivity Determination for Oxygenates, Oxonium Ions, and Oxygen-Containing Carbenium Ions. *Industrial & Engineering Chemistry Research*, 56(37): 10259-10270. doi: 10.1021/acs.iecr.7b02605

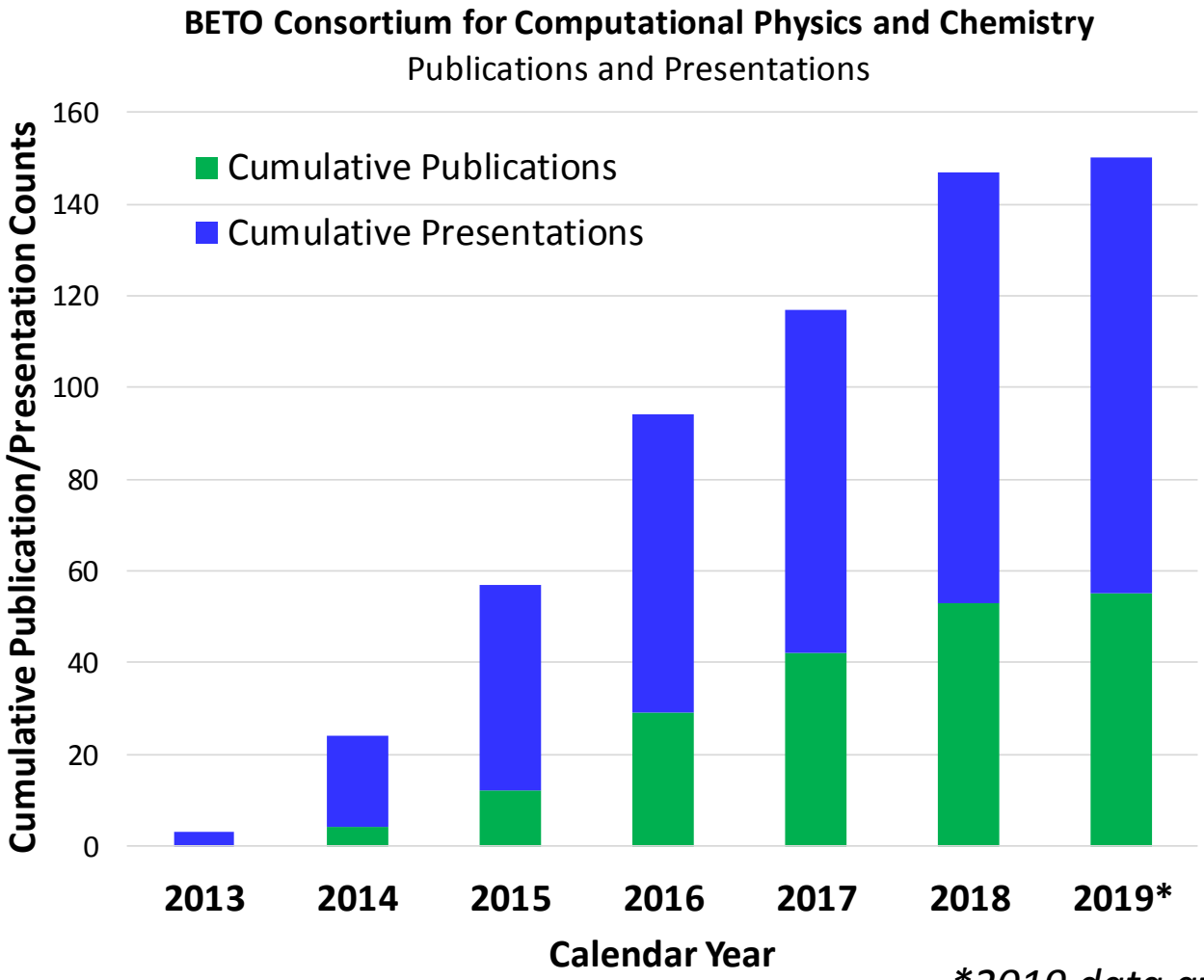
Presentations

Presentations since January 1, 2017: 30

Presentations since Inception of Project (2013): 95 Total

Publications and Presentations

Summary Graph of Publications and Presentations To-Date for Project



**2019 data at Feb. 14, 2019*