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ChemCatBio
Chemical Catalysis for Bioenergy

CCPC
Consortium for Computational Physics and Chemistry

U.S. DEPARTMENT OF ENERGY
BIOENERGY TECHNOLOGIES OFFICE

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

DOE Bioenergy Technologies Office (BETO)
2021 Project Peer Review
March 8-26, 2021 (held virtually)

PI: Jim Parks (ORNL); **Task Leads and Liaisons:** Rajeev Assary (ANL), Yidong Xia (INL), Bill Rogers (NETL), Carrie Farberow (NREL), Peter Ciesielski (NREL), Bruce Adkins (ORNL), Charles Finney (ORNL), Roger Rousseau (PNNL), Vanda Glezakou (PNNL), Asanga Padmaperuma (PNNL)
[full list of CCPC team on last slide]

WBS: 2.5.1.301-307

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY
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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 by ChemCatBio to higher technical readiness levels, and
3. cost-effective scale-up of bioenergy catalytic conversion technologies relevant to industry.

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A multi-scale problem … A multi-lab solution

Heilmeier's Catechism:

- *What are you trying to do?*
  Accurately model bioenergy conversion processes with fundamental science theory.
- *How is it done today?*
  With a **multi-scale approach** that enables translation of science phenomena to process performance.
- *Why is it important?*
  Modeling enables cost-effective and time-effective R&D which bioenergy needs for commercialization.
- *What are the risks?*
  The largest risk is a disconnect of theory/modeling and experiment since combined they provide the greatest understanding of the science of bioenergy conversion.

Management

ChemCatBio
Chemical Catalysis for Bioenergy

Bioenergy Technologies Office (BETO) Consortia

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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Pacific Northwest NATIONAL LABORATORY

OAK RIDGE National Laboratory

NATIONAL ENERGY TECHNOLOGY LABORATORY

A multi-scale problem
… A multi-lab solution

Argonne NATIONAL LABORATORY

INL Idaho National Laboratory

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Agile BioFoundry

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

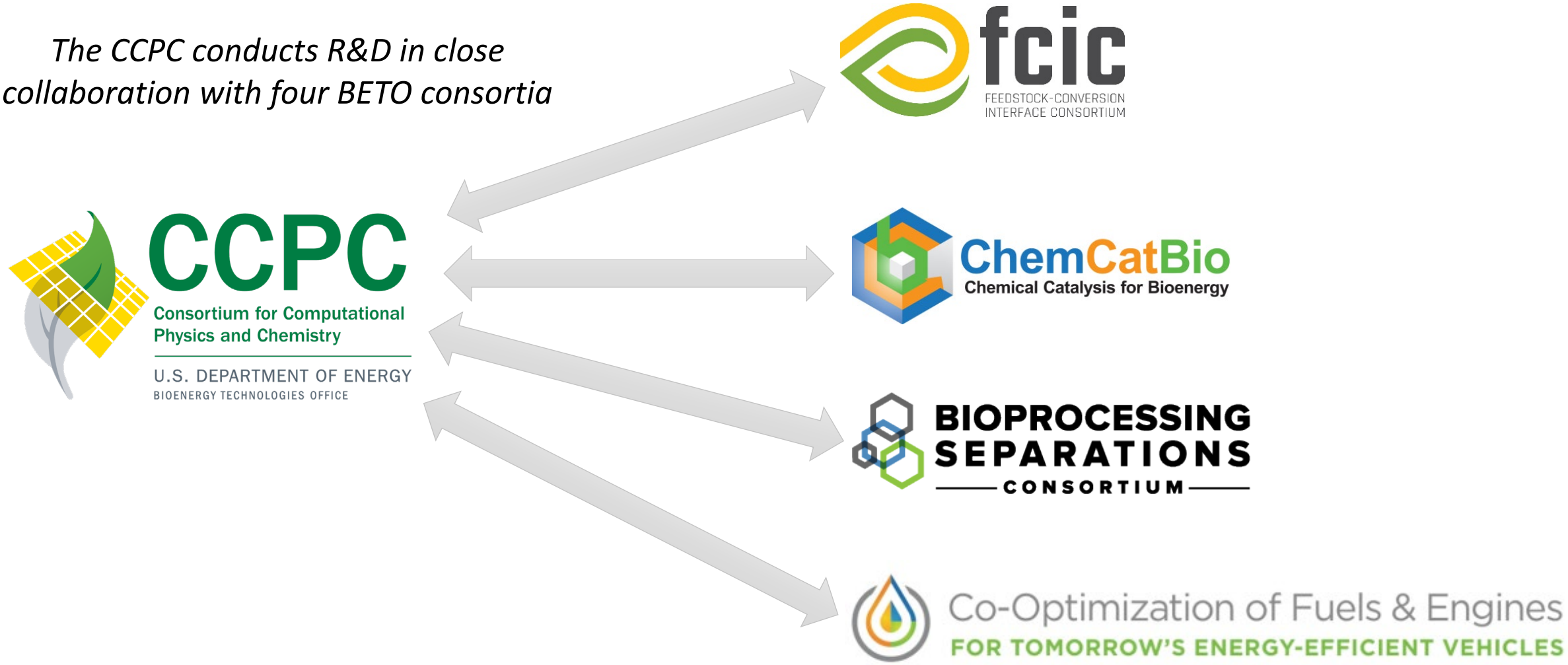
ChemCatBio Chemical Catalysis for Bioenergy

BIOPROCESSING SEPARATIONS CONSORTIUM

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

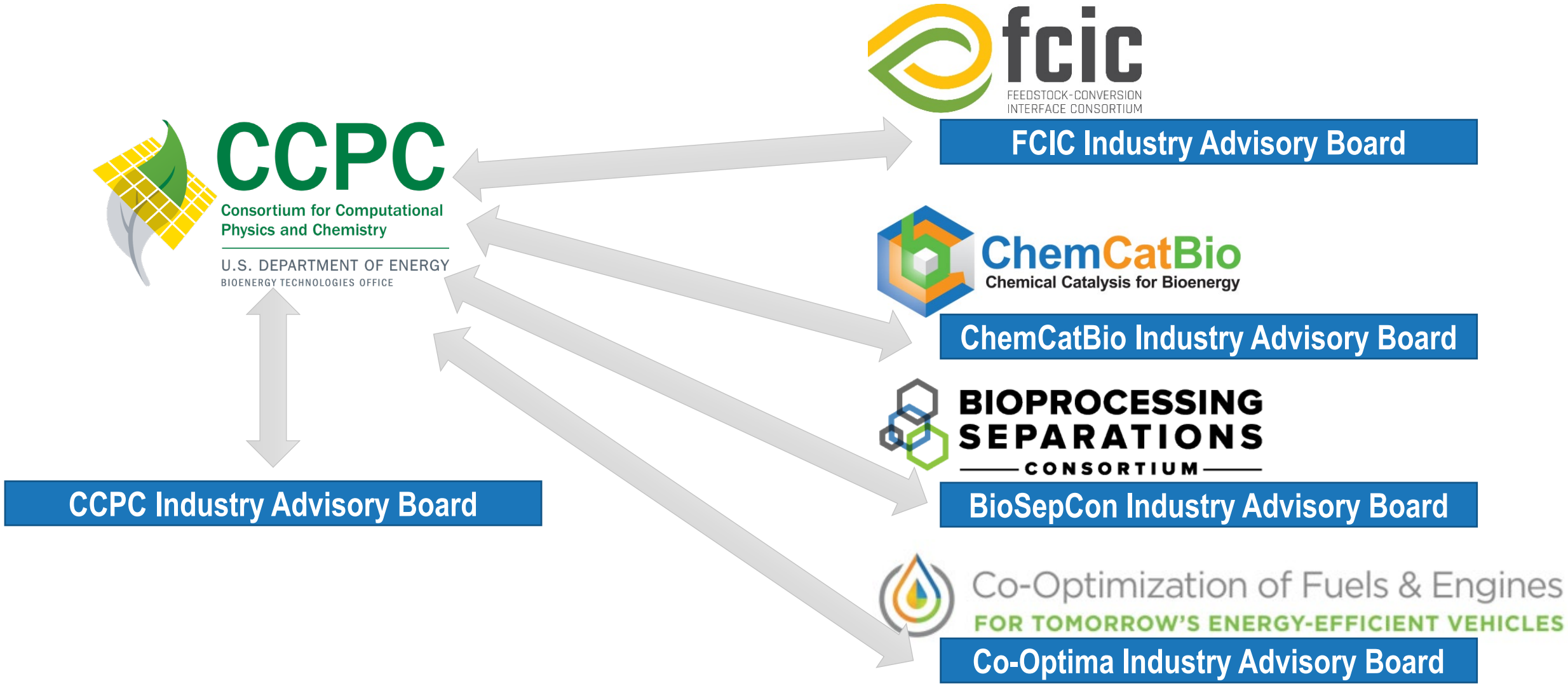
Bioenergy Technologies Office (BETO) Consortia

The CCPC conducts R&D in close collaboration with four BETO consortia



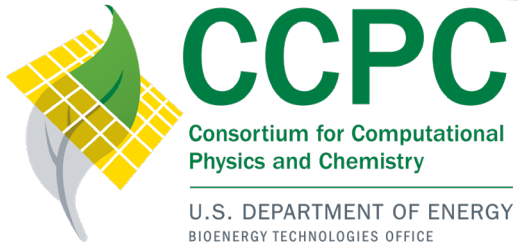
CCPC Industry Engagement via Advisory Boards

The CCPC engages with industry via consortia-specific Industry Advisory Boards as well as a CCPC Industry Advisory Board (renewed in early 2021 with focus on computational application knowledge in industry)



CCPC Management Approach Utilizes Technical Liaisons

CCPC designated Technical Liaisons and additional leadership roles in multiple consortia enable covering wide expanse of bioenergy R&D across BETO



CCPC Coordination
PI: Jim Parks
BETO TM: Trevor Smith

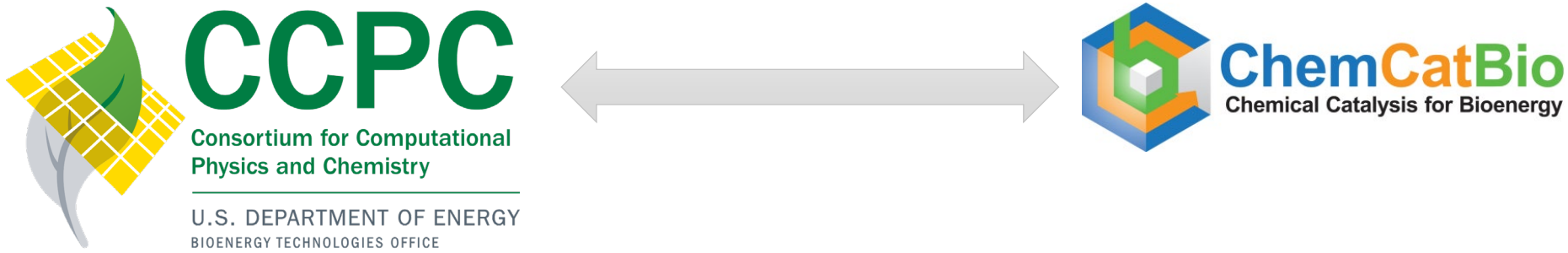
Technical Liaison: Peter Ciesielski
FCIC Task 3 Lead: Yidong Xia
FCIC Task 6 Co-Lead: Jim Parks

Technical Liaison: Rajeev Assary
Six CCPC members on Steering Committee

Technical Liaison: Vanda Glezakou

Technical Liaison: Seonah Kim

CCPC Management Approach Utilizes Technical Liaisons



The technical portion of this presentation is focused on ChemCatBio research.

CCPC research for other consortia is being covered
in their respective Peer Review sessions.

Management: ChemCatBio Foundation – FY21

Integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Catalytic Technologies

Catalytic Upgrading of Biochemical Intermediates
(NREL, PNNL, ORNL, LANL)

Upgrading of C1 Building Blocks
(NREL)

Upgrading of C2 Intermediates
(PNNL, ORNL)

Catalytic Fast Pyrolysis
(NREL, PNNL)

Electrocatalytic CO_2 Utilization
(NREL)

Enabling Capabilities

Advanced Catalyst Synthesis and Characterization
(NREL, ANL, ORNL)

Consortium for Computational Physics and Chemistry
(ORNL, NREL, PNNL, ANL, NETL)

Catalyst Deactivation Mitigation for Biomass Conversion
(PNNL)

Industry Partnerships (Phase II Directed Funding)

Opus12 (NREL)

Visolis (PNNL)

Sironix (LANL)

Cross-Cutting Support

ChemCatBio Lead Team Support (NREL)

ChemCatBio DataHUB (NREL)

CCPC Coordination, Integration, and Outreach

In addition to the consortia collaborations, the CCPC also manages and operates important computational R&D programs with BETO and manages outreach and tech transfer for CCPC outcomes

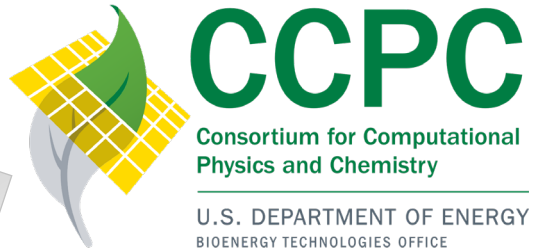
New!

Direct Funding Assistance Program (Launched in FY2020):
3 Industry-led collaborative projects with CCPC start in FY2021

forestconcepts

Catalyxx

Pyran



New!

BETO-HPC Program in High Performance Computing (Launched in FY2020):
Dedicated computational resources allocated via user facility mechanism to BETO researchers

Summit

Ridge

Outputs, Outreach, & Tech Transfer

- Peer-Reviewed Publications
- Conference Presentations
- Public Webinars
- Industry Visits/Webinars
- Website for Public Outreach www.cpcbiomass.org
- Public Open-Source Code github.com/ccpcode

python™ MFiX

End Goal is Impact to Support the Bioenergy Industry with Unique Computational Science Toolsets

Supporting Development of ChemCatBio DataHub: Catalyst Property Database

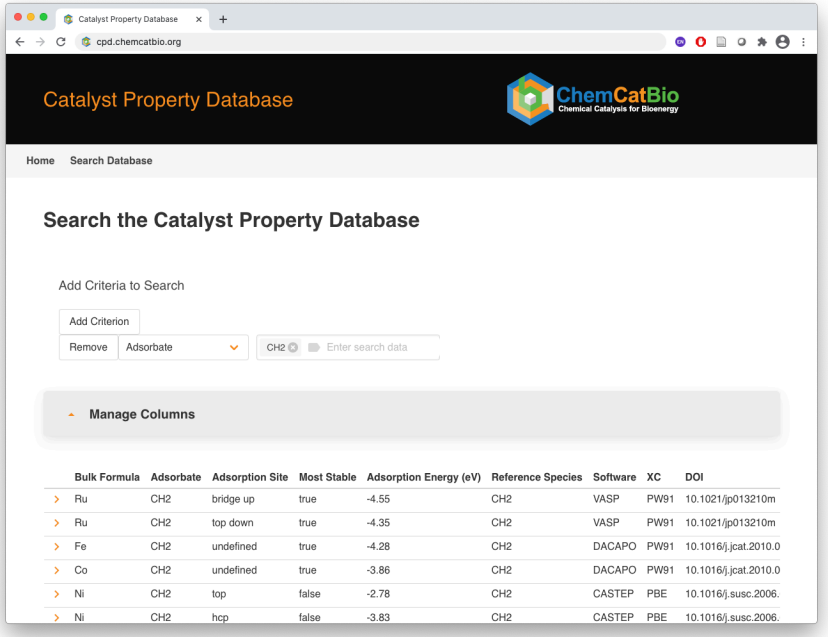
The Catalyst Property Database (CPD)

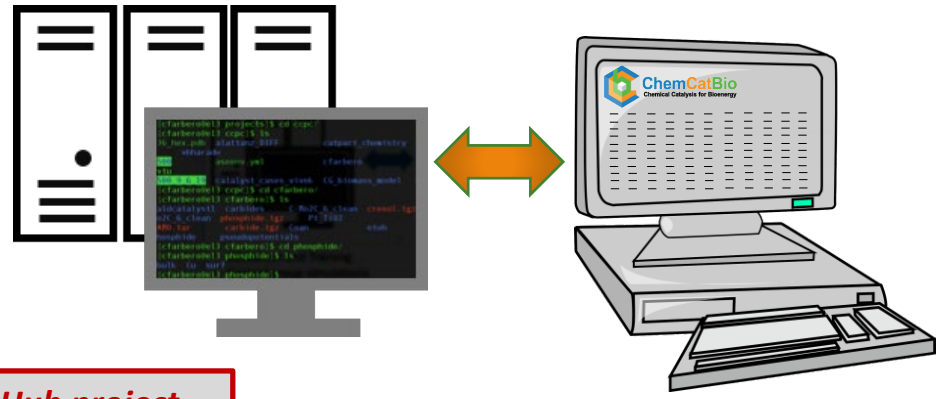
- A centralized, searchable repository of catalyst properties
- Initial release: DFT-computed adsorption energies for intermediates on catalyst surfaces
- Publicly accessible
- Data subject to quality control

CCPC Key Contributions and Impact:

- Contribute critical quantum chemistry expertise to inform database and user interface development
- Provide and curate data through (1) literature mining and (2) executing simulations

cpd.chemcatbio.org





Energy Materials Network
U.S. Department of Energy

ChemCatBio
Chemical Catalysis for Bioenergy

In collaboration with the ChemCatBio Data Hub project

Approach

ChemCatBio
Chemical Catalysis for Bioenergy

CCPC Timeline: Continued Evolution to Meet Needs

New logo in 2021

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DFO Projects Launch
DOE supported industry assistance from CCPC
forestconcepts
Catalyxx
Pyran

ChemCatBio Launched
with CCPC, ACSC, and CCM enabling projects
ChemCatBio
Chemical Catalysis for Bioenergy

Accomplishment
Tech transfer of biomass feedstock model assists Forest Concepts to convey product value to customers
fcic
FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM

Accomplishment
Modeling outcomes provided critical input into Catalytic Fast Pyrolysis decisions

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

Go/No-Go Passed
Kinetics application

BETO-HPC Launched
Dedicated BETO High-Performance Computing
summit

FY21
FY20
FY19
FY18
FY17
FY16
FY15
FY14
FY13

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

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

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

Accomplishment
Surface Phase Explorer tool released to public

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 expanded focus on catalysis

Original logo in 2013

Computational Pyrolysis Consortium Began

Consortium for Computational Physics and Chemistry (CCPC)

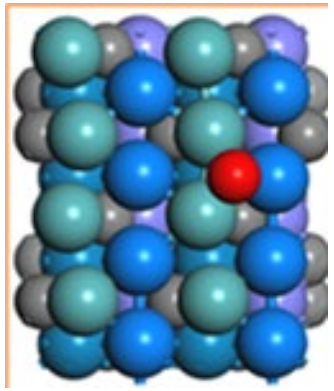
Task

Catalysis Modeling at Atomic Scales

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Argonne NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

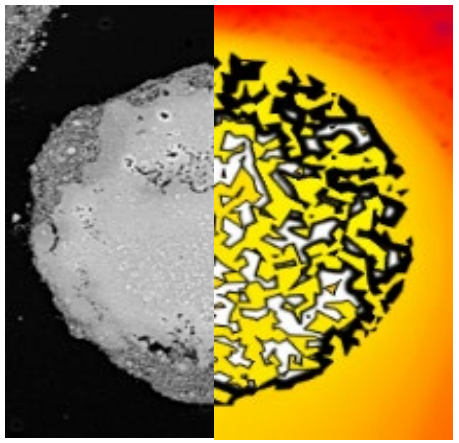


Investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists

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

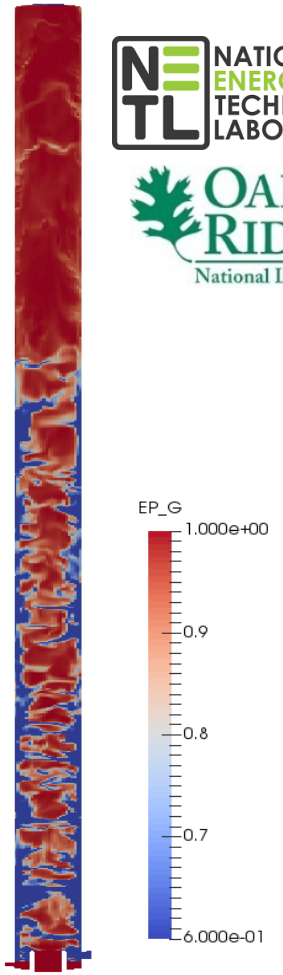
Task

Conversion Modeling at Reactor 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

Task

CO_2 Conversion

New!

Multi-scale modeling and simulation to enable efficient CO_2 conversion

Risks and Mitigation Strategies

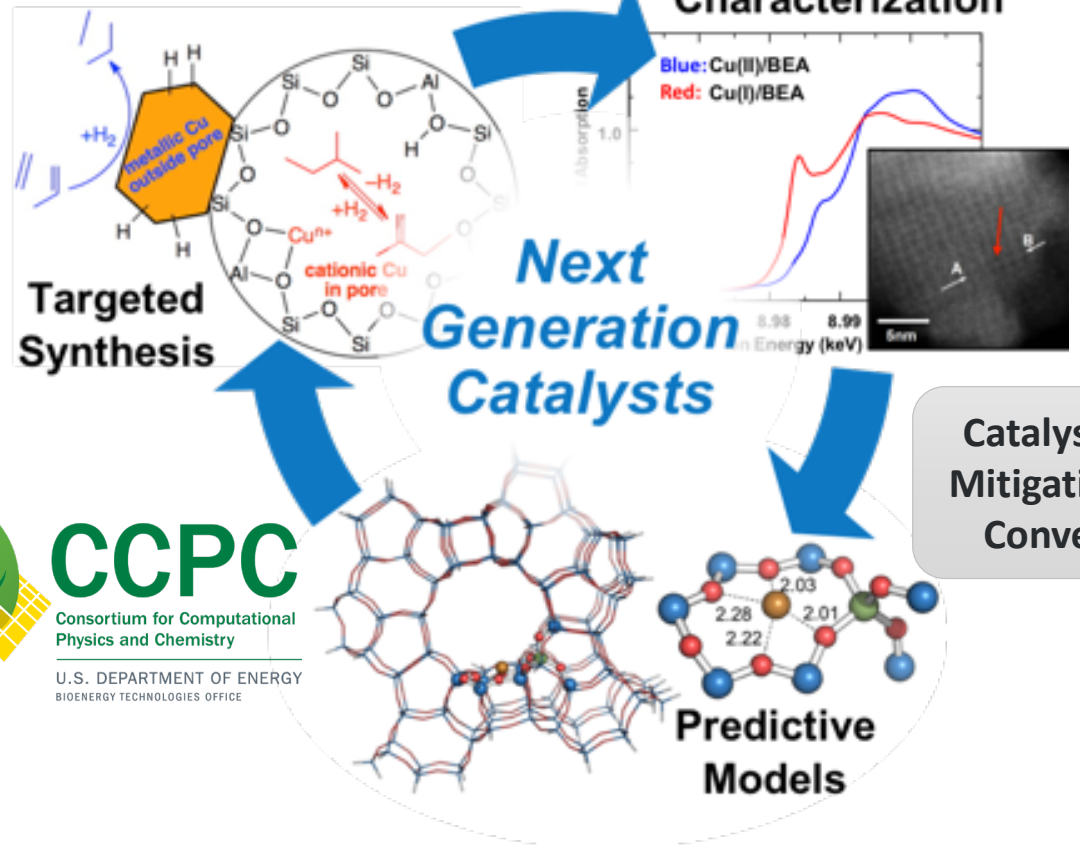
Risk
Model vs. Real Catalyst Surface Structure
High Degree of Process Complexity
High Performance Computing Availability

Mitigation

ChemCatBio
Chemical Catalysis for Bioenergy

Accelerated catalyst and process development cycle

Advanced Catalyst Synthesis and Characterization Project



Catalyst Deactivation Mitigation for Biomass Conversion Project

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BIOENERGY TECHNOLOGIES OFFICE

Risks and Mitigation Strategies

Risk
Model vs. Real Catalyst Surface Structure
High Degree of Process Complexity
High Performance Computing Availability

Mitigation

(1) Multiscale modeling approach
(2) Close collaboration with experimental pathway projects for validation of models
(3) Utilization of reduced-order models and lumped kinetics when appropriate

Risks and Mitigation Strategies

Risk
Model vs. Real Catalyst Surface Structure
High Degree of Process Complexity
High Performance Computing Availability

Mitigation

The BETO-HPC Program

…more info in upcoming slides

Responses to Previous Reviewers' Comments (FY2019 Peer Review)

- **Positive Feedback:**
  - *"…a **very impressive effort that covers many scales** of catalyst/reactor performance."*
  - *"A well organized, expansive center level effort which did an excellent job of demonstrating its **pervasive value throughout CCB [ChemCatBio]**."*
  - *"The approaches taken by computational physics and chemistry team are the **scientifically sound application of mathematical models** to problems arise from biomass conversion technologies."*
  - *"The operation of the CCPC is to what all the Enabling Capability projects might aspire. What a **solid, helpful, impactful consortium.**"*
- **Advice and Constructive Criticism:**
  - *"**Experimental validation will always continue to be the key** to computational programs building both the researchers and process deign engineer's confidence as reasonable agreement is reached at all scales."*
    - ***Response:** We agree and continue to observe the critical need for high quality experimental validation. We continue to improve in our interactions with experimentalists toward this key.*
  - *"Atomic scale activities should continue to show clearly how the computer experimental results will be incorporated in reaction engineering models for MFiX and the anticipated implications of these new simulations." & "CCPC has an opportunity to demonstrate how all of these efforts mathematically fit together at least at a simple first approach **to establish the "knowledge train" for a commercial design basis**."*
    - ***Response:** Yes, we like the "knowledge train" objective to bridge our multi-scale models. We have made progress in linking kinetics and meso-scale models to fixed bed reactor models. We have more progress to complete our "train" from atomic to reactor.*
  - *"…the group is encouraged to **pursue leverage with the existing basic science programs**."*
    - ***Response:** We agree. We have leveraged basic energy sciences programs specifically related to atomic-scale catalysis modeling techniques.*
  - *"…**machine learning algorithms might be a great fit** for these multiscale reactor models…."*
    - ***Response:** We agree. We have leveraged machine learning tools and continue to pursue this approach along with high-performance computing.*

Note: select reviewer comments shown. For full reviewer assessment, see 2019 BETO Peer Review Report at www.energy.gov/eere/bioenergy/2019-project-peer-review-report

New Directions for the CCPC in High Performance Computing

The BETO-HPC Program

The Bioenergy Technologies Office (BETO) has 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 dedicated HPC resource operated as a user program by the CCPC and OLCF providing ~100M core-hrs per year access to:

Ridge

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

summit

18 nodes (16,200 core equivalent)
Hybrid CPU-GPU
#2 most powerful computer in world*

Summit supercomputer at Oak Ridge Leadership Computing Facility

*based on Nov. 2020 Top500 List at top500.org (Fugaku in Japan is current #1)

A New Approach for the CCPC Being Pursued on Summit

- The BETO-HPC computing resources open a new paradigm for computational science, and the CCPC is investigating approaches for utilizing high performance computing to advance bioenergy
- Six (6) BETO-HPC projects approved to-date
  - CCPC scientists leading three (3) BETO-HPC projects

BETO-HPC Project: Massive-GPUs Simulation of High-Solids Biomass Slurry Flow (Yidong Xia, INL)

BETO-HPC Project: Atomic-scale Modeling for Heterogeneous Catalyst Development for Catalytic Fast Pyrolysis (Carrie Farberow, NREL)

BETO-HPC Project: Atomistic Computational Catalysis (Rajeev Assary, ANL)

Challenges include: software/code readiness, approach, validation challenges, etc.

This project uses high performance computing resources located at Oak Ridge National Laboratory and provided by the Bioenergy Technologies Office.

The end goal is to utilize BETO-HPC Summit nodes to evaluate algorithms that can enable advanced approaches in computational science for bioenergy. If successful, larger user allocations on Summit can be acquired via the OLCF User Facility program (operated by DOE Office of Science).

FY2020 Go/No-Go Passed: Kinetics Approach Assessment

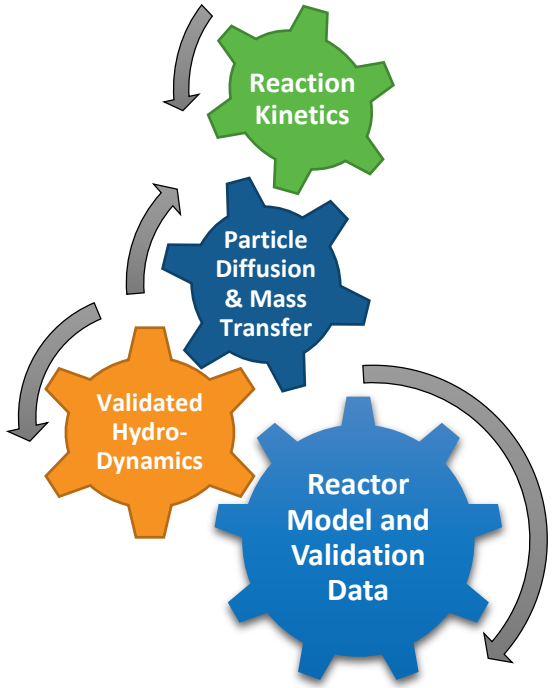
Go/No-Go Criteria:

- 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.

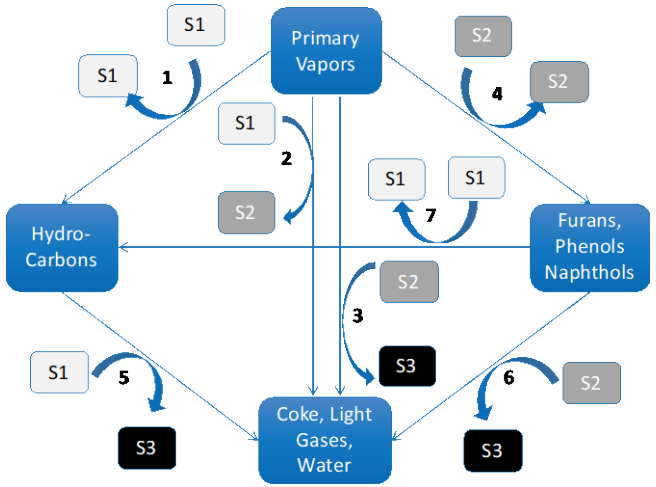
Outcome: Go *(Milestone Achieved*)*

- Kinetics implemented in multiple models
- Experimental validation on 2 reactors (2FBR, TCPDU)
- 5 publications to-date

Critical elements to reactor & process model include reaction kinetics

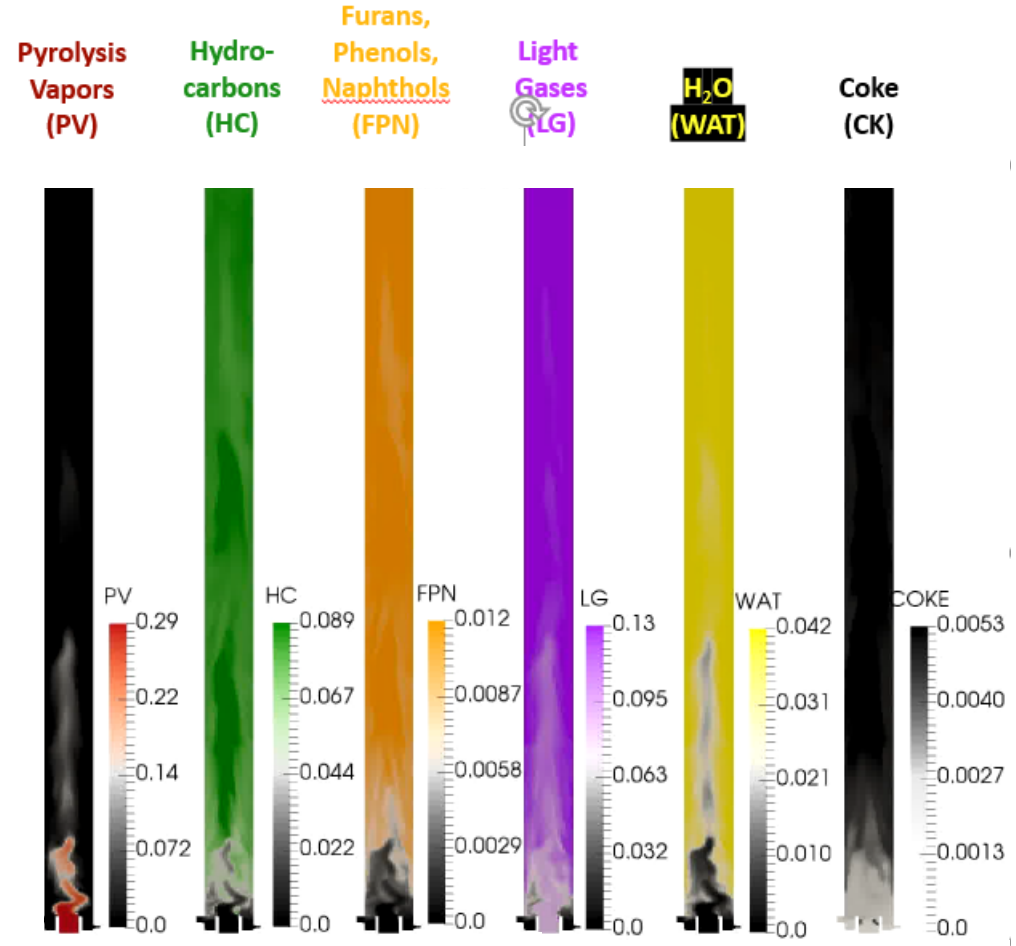


Kinetic reaction pathway developed and applied by CCPC team for Catalytic Fast Pyrolysis



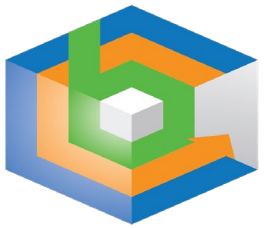
Dedicated kinetics R&D launched in FY18 successful with method being applied in ongoing CCPC R&D

Kinetics implemented in full CFD (MFiX) reactor simulation of Catalytic Fast Pyrolysis vapor upgrading in TCPDU reactor



*Achieved in close collaboration with ChemCatBio and NREL 2FBR & TCPDU Experimental Teams

Impact:
Atomic-Scale Modeling



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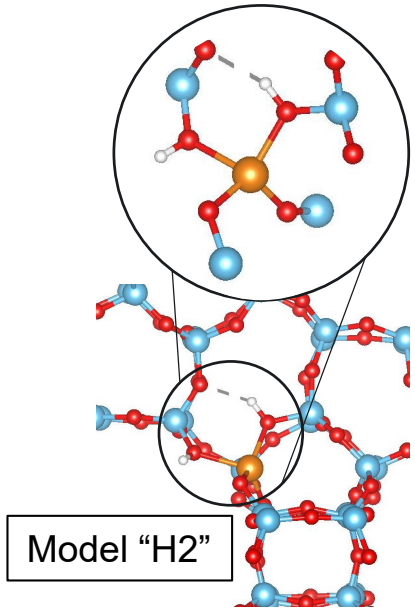
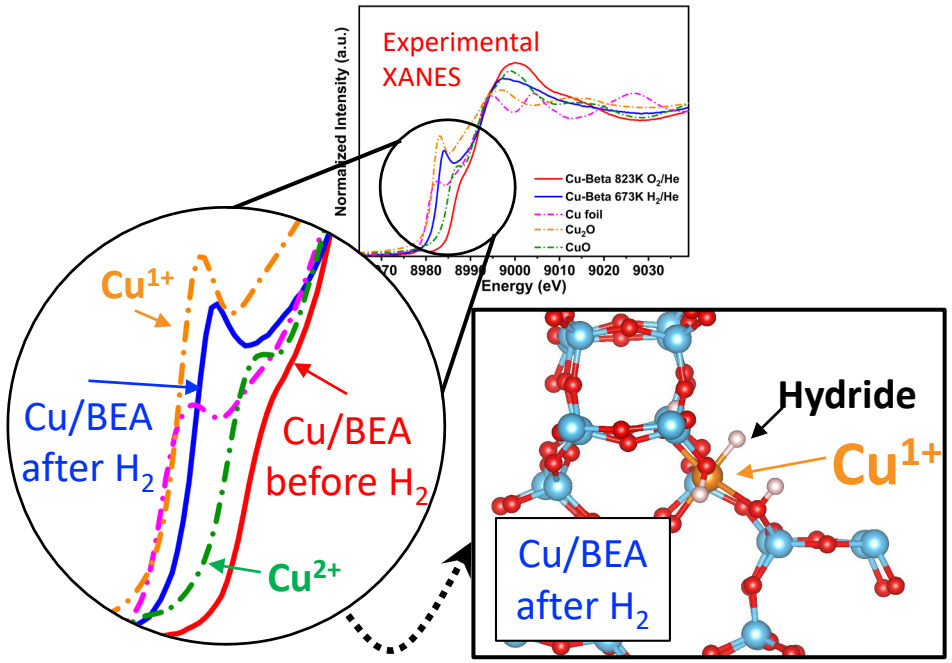
Role of H_2 on Cu oxidation state in Cu-Zn-Y/BEA (Beta) zeolite for upgrading of ethanol explains experimental results of varying selectivity with H_2 partial pressure

Model identifies location of Cu active site in zeolite → ***XANES experimental results validate model Cu site oxidative state predictions*** → ***Results relevant to product selectivity dependence on H_2 partial pressure***





H_2 Partial Pressure (kPa)	Conversion (%)	Product Selectivity			
		$C_{3+}^{=}$	Butadiene	Oxygenates	Paraffins
101	96.4	72.6	0.3	9.4	0.6
75	95.8	72.9	0.5	9.0	0.5
50	94.5	70.6	1.7	10.5	0.3
25	93.0	65.2	8.3	10.3	0.2
0	90.6	24.8	47.5	10.7	0.1

Not all products shown in table (for full table, see C2+ Upgrading talk)

- Model investigates the structure of Cu-Zn-Y/BEA zeolite and the reaction pathways in operation during ethanol upgrading
- Capabilities developed in **Basic Energy Sciences** catalysis program applied: (1) Simulate spectroscopies to ensure model. (2) Utilize AIMD and statistical mechanics to determine thermodynamics. (3) Use CINEB and/or Constrained MD to determine kinetics.
- Y also has a role due to Lewis acidity; ongoing research to understand relative role of Y to Cu effect shown will further correlate atomic scale theory with experimental findings

In collaboration with the C2+ Upgrading and Advanced Catalyst Synthesis and Characterization (ACSC) projects

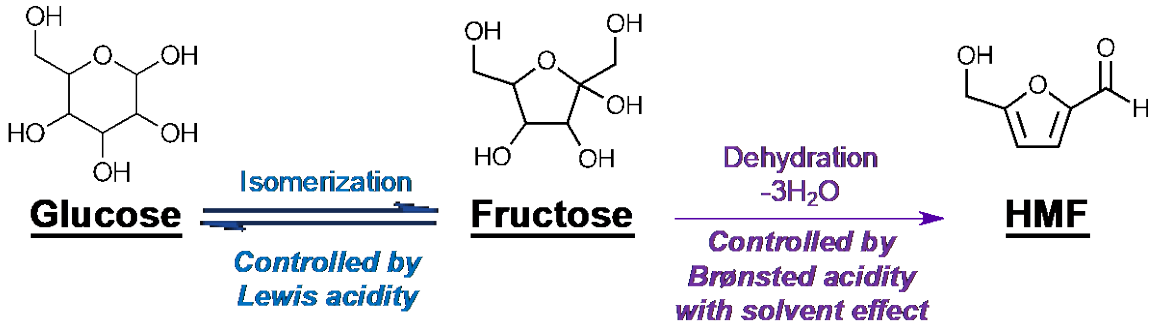
Impact:

(1) Experimental and model results validate role of H_2 on Cu site and resulting effect on product selectivity

(2) H_2 partial pressure can be adjusted to produce middle distillate and butadiene simultaneously

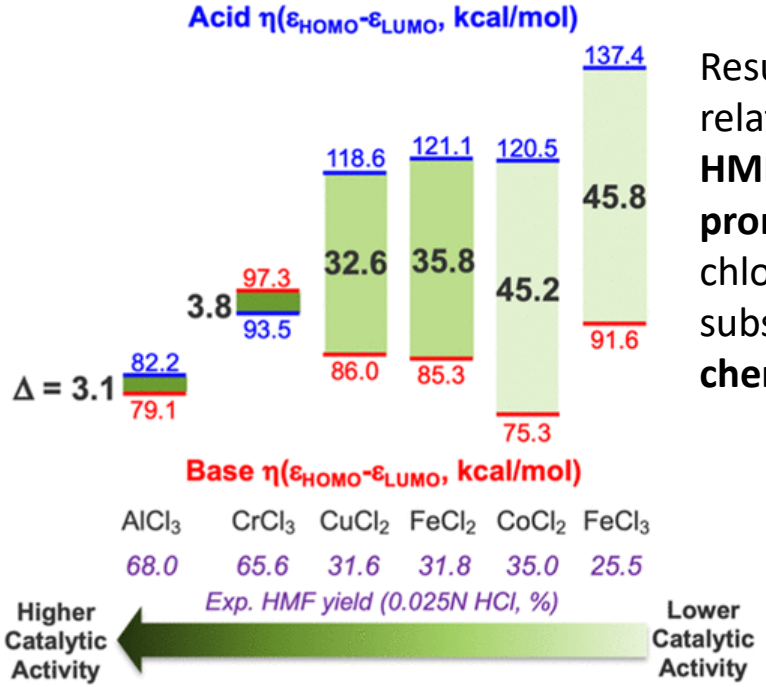
(3) Preliminary TEA indicates coproduction of butadiene can significantly reduce MFSP

Lewis acid and solvent effect on glucose conversion to hydroxymethylfurfural (HMF)



- HMF is an important renewable platform compound that can be obtained from biomass feedstocks through glucose conversion. A **key challenge** is **maximizing** the **HMF yield**
- Approach: combine experimental (CUBI project) and computational (CCPC atomic-scale) tools to identify key catalyst and organic solvent descriptors determining the HMF yield

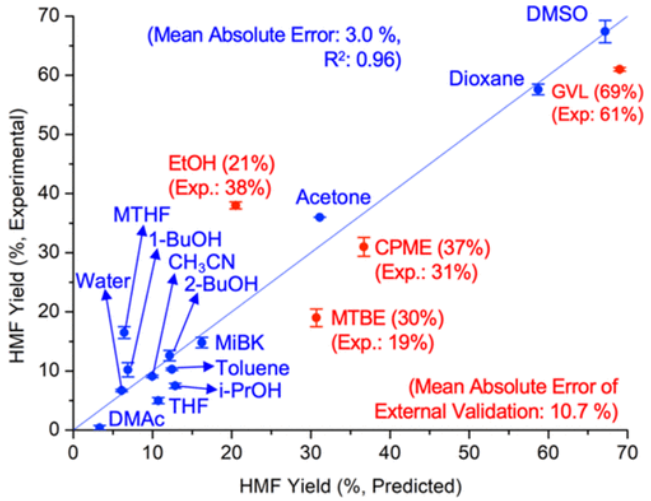
Lewis Acid Catalyst



Result: Established relationship revealing that **HMF production** is **promoted** when the metal chloride catalyst and substrate had a **similar chemical hardness**.

In collaboration with Catalytic Upgrading of Biochemical Intermediates (CUBI) project

Solvent Effect

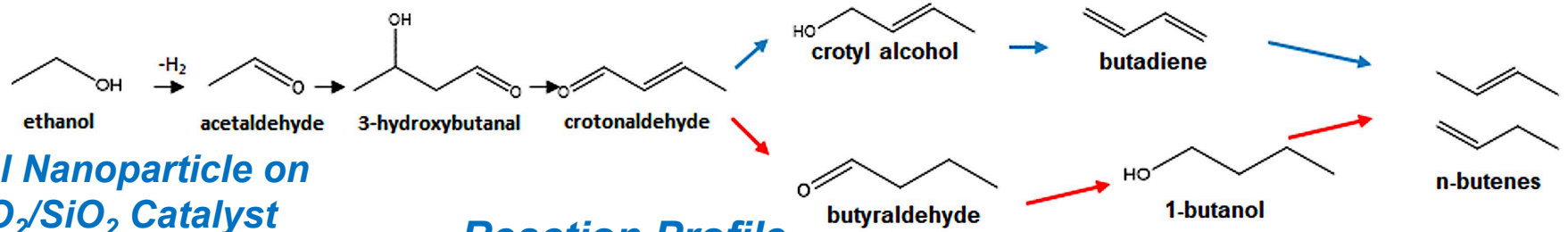


Result: Developed **multivariate model to predict experimental HMF yields** in water-organic cosolvent systems

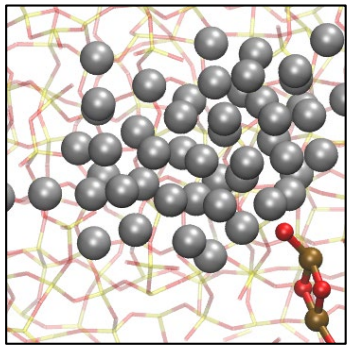
Impact: Established **criteria for choosing Lewis Acid catalyst and organic solvent** to **maximize HMF production** in glucose conversion

Y. Kim, A. Mittal, D. J. Robichaud, H. M. Pilath, B. D. Etz, P. C. St. John, D. K. Johnson, S. Kim, "Prediction of Hydroxymethylfurfural Yield in Glucose Conversion through Investigation of Lewis Acid and Organic Solvent Effects" *ACS Catalysis* (2020) 10, 14707

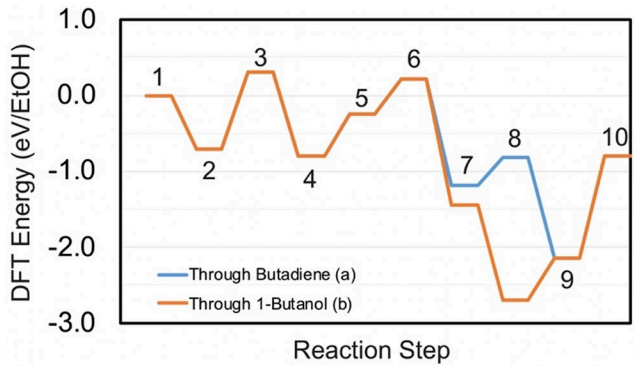
Reaction pathway to minimize coke formation for increased time on stream shown via model of reaction thermodynamics for metal nanoparticles on ZrO_2/SiO_2



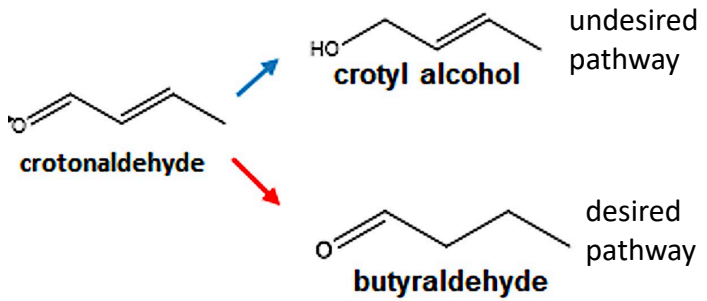
Metal Nanoparticle on ZrO_2/SiO_2 Catalyst



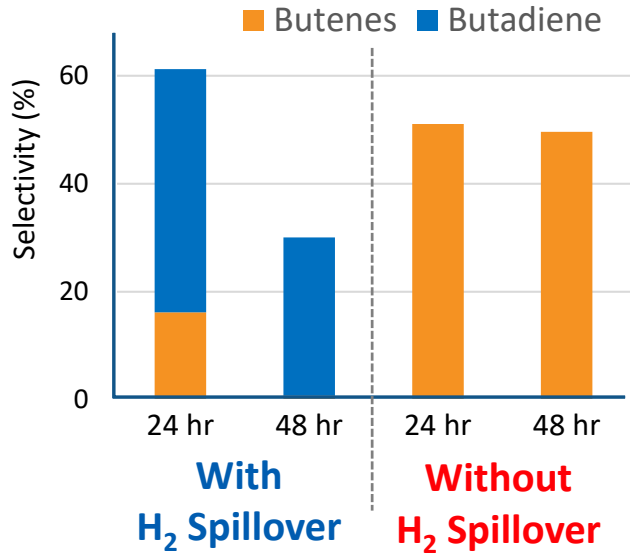
Reaction Profile



Critical Branch Point



Improved Durability & Butene/Butadiene Selectivity



Approach:

- Employ ab initio molecular dynamics (AIMD), statistical mechanics, and reaction coordinate constrained optimizations to determine reaction thermodynamics and kinetics of competing pathways on metal nanoparticle catalyst supported on ZrO_2/SiO_2.

Impact:

(1) Model enables understanding the role of catalyst in each step of the cascading sequence of reactions.

(2) Different metal formulations have been computationally screened to find catalyst that avoids selectivity to butadiene which is a coke precursor.

(3) Improved durability and selectivity to butene result.

In collaboration with the C2+ Upgrading project

Akhade, ,et al. (2020). Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts. *Journal of Catalysis*, *386*, 30-38.

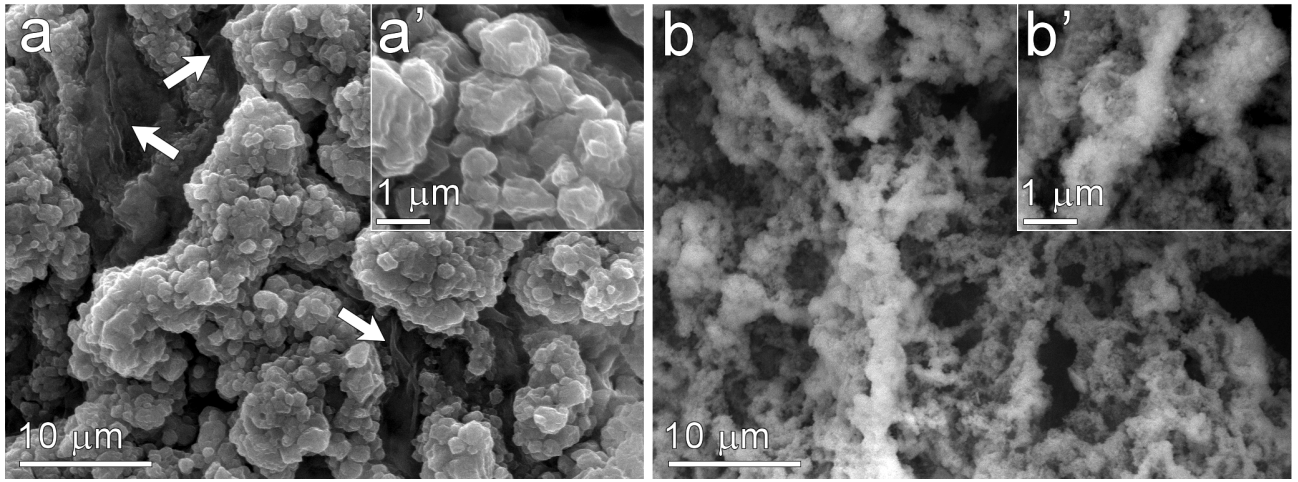
Dagle, V. L., et al. (2020). Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO2/SiO2 Catalysts. *ACS Catalysis*, *10*(18), 10602-10613.

Impact:
Meso-Scale Modeling

ChemCatBio
Chemical Catalysis for Bioenergy

Mesoscale modeling predicts synthesis targets for optimal catalyst particle porosity for improved performance

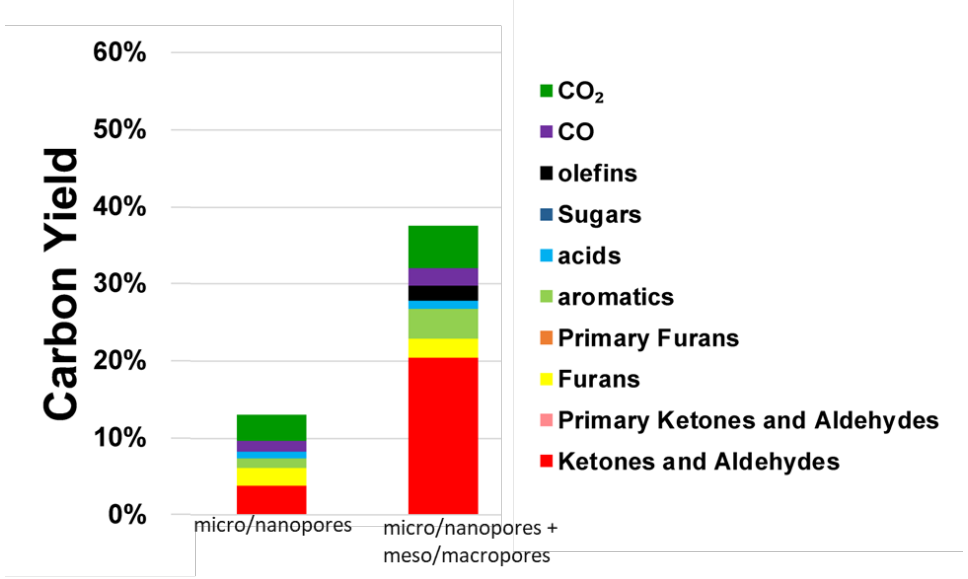
- Mesoscale simulations performed in 2018/2019 investigating catalyst pore size predicts *introducing additional meso- and macro pores will improve catalyst activity lifetime*
- Based on these predictions, a nanocellulose catalyst templating method was developed to increase meso/macro porosity
- As predicted, templated catalysts with larger pores were shown to out-perform catalysts with micro/nanopores in CFP experiments, *even though the total surface area was lower*
- This templating method is being extended to the Pt/TiO_2 system in FY21 in collaboration with the Engineering of Catalyst Scale Up project in the Systems Development and Integration Program



Nanocellulose templated catalyst before (left) and after (right) burnout

Impact:
(1) Mesoscale model predicted performance improvement from catalyst porosity design which was experimentally validated
(2) Results gave increased yield of C products from fast pyrolysis vapor upgrading due to addition of larger pores with nanocellulose template technique

In collaboration with the Catalytic Fast Pyrolysis, Advanced Catalyst Synthesis and Characterization (ACSC), and Engineering of Catalyst Scale Up (in SDI Program) projects



Moyer, K., Conklin, D. R., Mukarakate, C., Vardon, D. R., Nimlos, M. R., & Ciesielski, P. N. *Frontiers in chemistry, 2019*

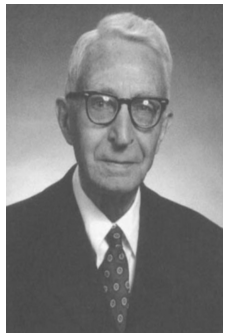
Extending classic fundamentals to solve new catalysis problems – cascading reactions with diffusion limitations

- **The State of the art** for accounting for diffusion limitations in porous catalysts was developed by Thiele (1930s) and Aris (1970s)
- **Problem:** The classic mathematical framework described by the Thiele Modulus and Effectiveness Factor does not allow for complex, multi-step reactions
- **Solution:** The CCPC team extended this classic theory using matrix-vector form to account for sequential, diffusion-limited reactions with deactivation
- **The Multicomponent Effectiveness Vector** is a new mathematical tool for analyzing diffusion limitations for cascading reaction mechanisms in catalyst pellets:

$$\eta = \bar{\mathbf{P}}\bar{\mathbf{D}}\left(\frac{3C_{Bi}}{\lambda}\left(\sqrt{\lambda}\coth(\sqrt{\lambda})-1\right)\right)\bar{\mathbf{P}}^{-1}\hat{\mathbf{C}}_{\mathrm{Rat},\infty}$$

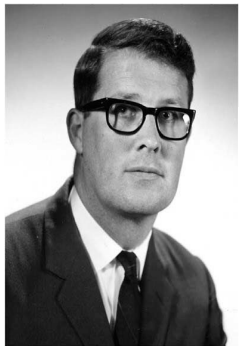
Impact:
New Multicomponent Effectiveness Vector approach to diffusion in/out of catalyst particles enables multiscale models to rapidly and simultaneously couple intra-particle and bulk transport phenomena to complex reaction mechanisms.

In collaboration with the Catalytic Fast Pyrolysis and Advanced Catalyst Synthesis and Characterization (ACSC) projects



Earnest Thiele:
Thiele Modulus

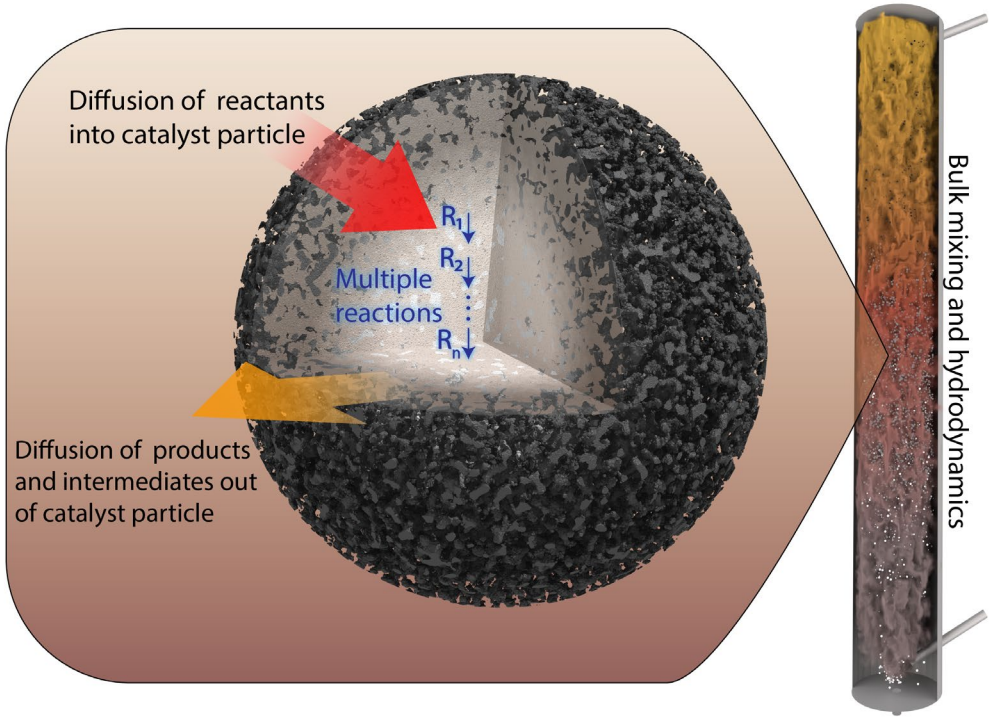
$$\phi = \sqrt{\frac{ka^2}{D_{\mathrm{eff}}}}$$



Rutherford Aris:
Effectiveness Factor

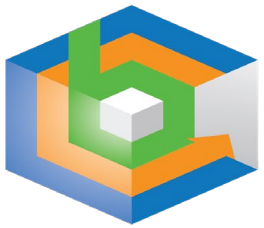
$$\eta = \frac{3C_{Bi}}{\phi^2}\left(\phi\coth(\phi)-1\right)$$

$$C_{Bi} = \frac{Bi}{\left(\phi\coth(\phi)-1+Bi\right)}$$



Lattanzi, A. M., Pecha, M. B., Bharadwaj, V. S., & Ciesielski, P. N. **2019**. *Chemical Engineering Journal*

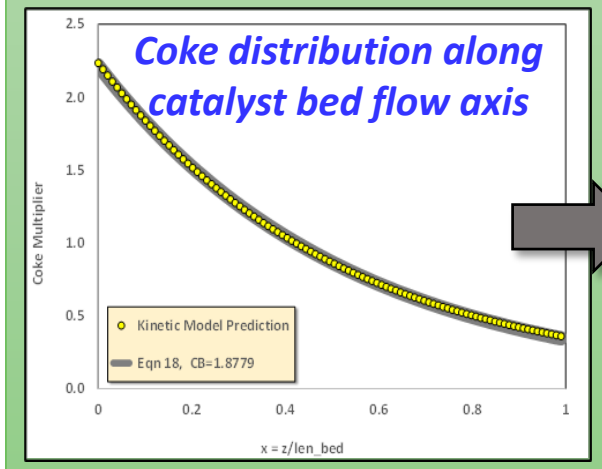
Impact:
Reactor-Scale Modeling



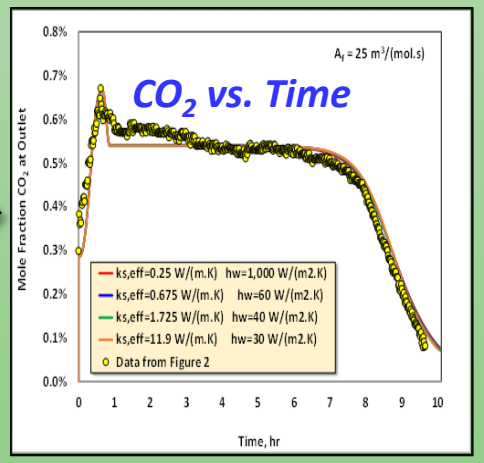
ChemCatBio
Chemical Catalysis for Bioenergy

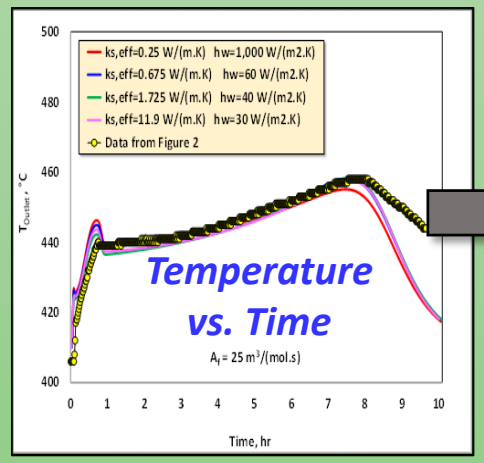
Coke oxidation in catalytic packed bed reactor captured by model

Step 1: Apply coke profile from Pt/TiO_2 upgrading kinetic model

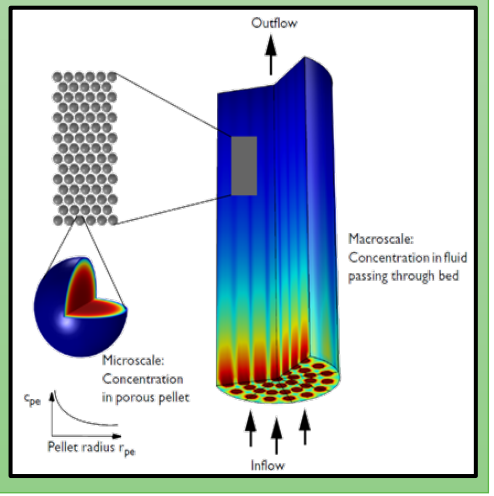


Step 2: Use 2D axisymmetric model to extract parameters from 2FBR data. Validate accuracy with CO_2 and temperature data.



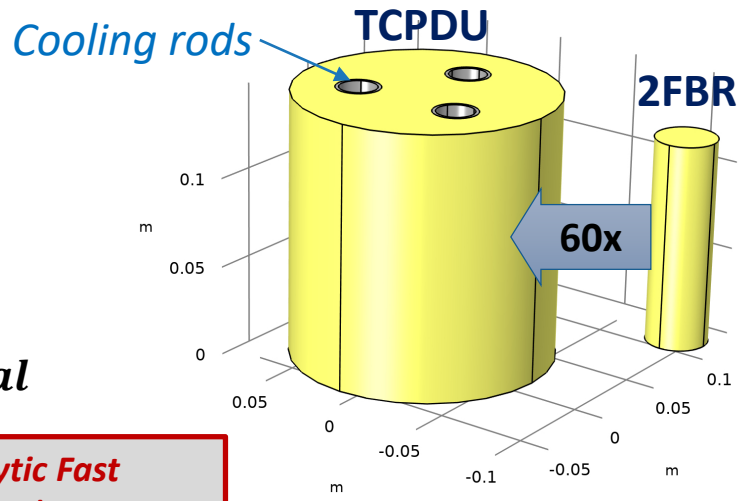


Step 3: Build 3D model using COMSOL Reactive Pellet Bed with particle resolution as low as 42 (real/virtual)



- **Challenge:** design catalytic packed bed reactor at 60x scale of 2FBR system
- **Need:** a computational model of the Pt/TiO_2 catalyst reactor that captures coke oxidation and associated thermal exotherms accurately

$$2FBR \xrightarrow{60\ X} TCPDU \xrightarrow{?} Commercial$$



2FBR=2" Fluidized Bed Reactor (2" diameter reactor)
TCPDU=ThermoChemical Process Development Unit (15 kg/hr biomass flow)

Impact:
Model of coke distribution along catalytic packed bed reactor and associated kinetics for coke oxidation enable predictive design of coke oxidation effects on reactor temperatures

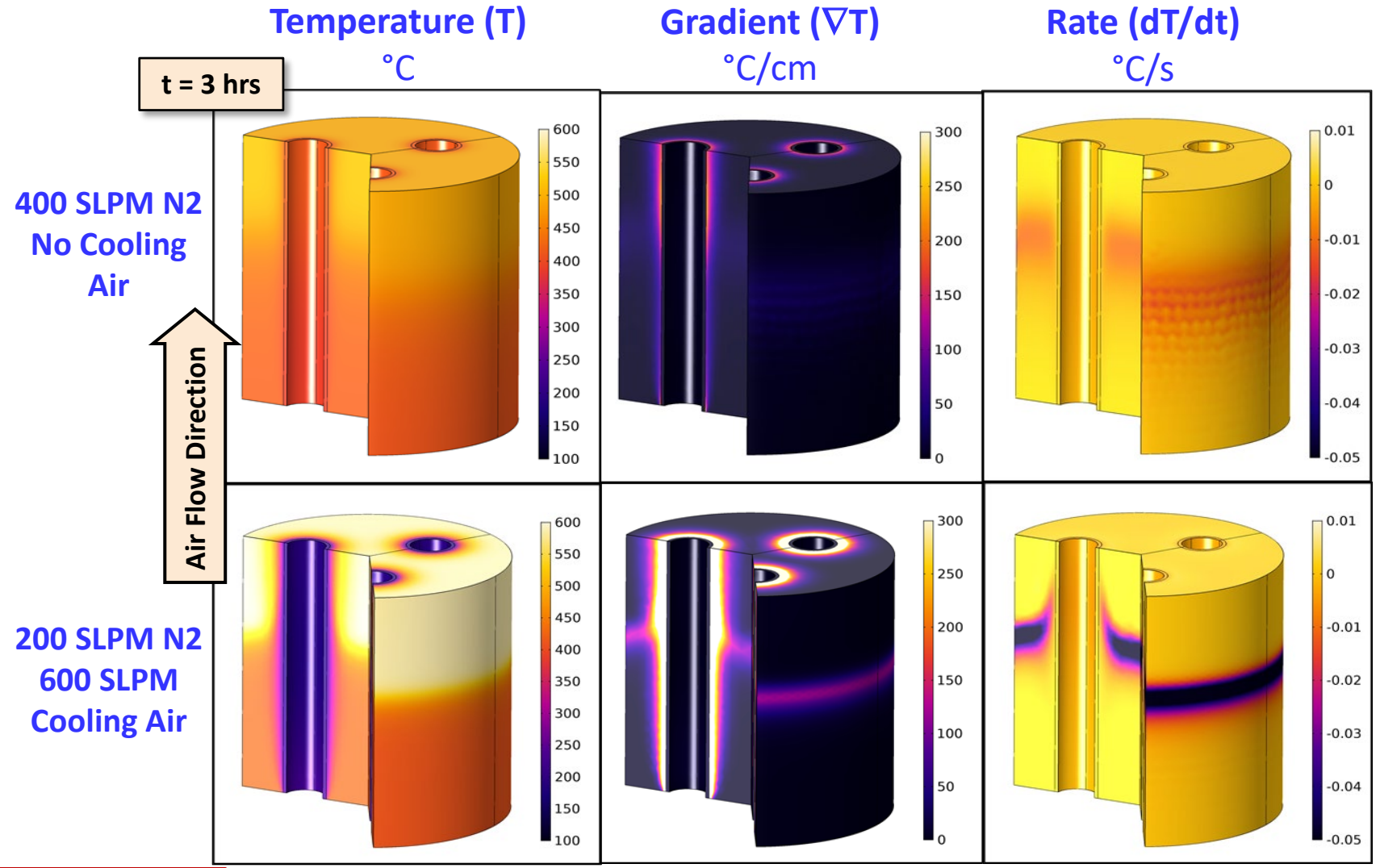
In collaboration with the ChemCatBio project on Catalytic Fast Pyrolysis, the Systems Development and Integration (SDI) program, and Thermochemical Process Development Unit (TCPDU) team

B.D. Adkins et.al, *Predicting thermal excursions during in-situ oxidative regeneration of packed bed catalytic fast pyrolysis catalyst,* submitted to *Reaction Chemistry and Engineering*

CCPC reactor models inform path forward for Catalytic Fast Pyrolysis

- Packed Bed Reactor for Pt/TiO_2 catalyst constructed *in silico* to understand thermal excursions and associated stresses during coke regeneration
- Kinetics for Pt/TiO_2 determined with CCPC developed techniques with data from Catalytic Fast Pyrolysis experimentalists
- Results identified peak temperatures that would damage Pt/TiO_2 structure and likely cause attrition from thermally-induced mechanical stresses

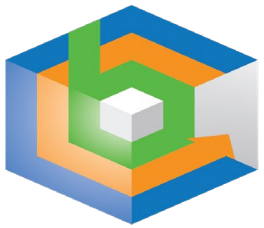
Impact:
Critical decisions on next steps for Catalytic Fast Pyrolysis project informed by model predictions of temperature spikes and gradients that predict catalyst damage in 60x scale up step



In collaboration with the ChemCatBio project on Catalytic Fast Pyrolysis, the Systems Development and Integration (SDI) program, and Thermochemical Process Development Unit (TCPDU) team

B.D. Adkins et.al, *Predicting thermal excursions during in-situ oxidative regeneration of packed bed catalytic fast pyrolysis catalyst,* submitted to *Reaction Chemistry and Engineering*

Progress and Accomplishments



ChemCatBio
Chemical Catalysis for Bioenergy

Atomic-scale Structure-function Relationships Inform R&D of Multifunctional HDO Catalysts

Bifunctional Pt/TiO_2 **catalysts** are **active** toward **hydrodeoxygenation (HDO)** reactions for CFP upgrading. Catalyst R&D is targeting improved selectivity to deoxygenation products and mitigating deactivation.

Computational Approach: Develop **atomic-scale models** of **Pt metal, TiO_2 support**, and **Pt/TiO_2 interface** based on experimental characterization to elucidate function in key reaction steps

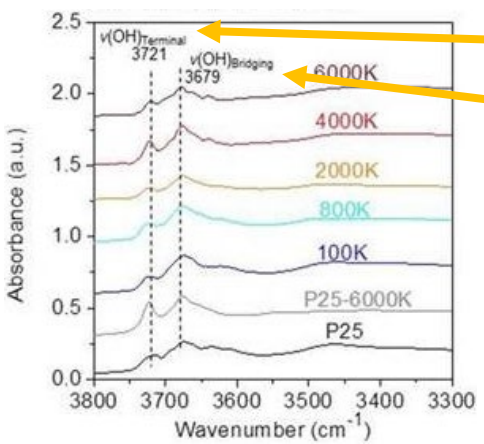
Carboxylic Acid Reactivity on Pt/TiO_2

- Established the **role of metal and interfacial sites** in **carboxylic acid** deoxygenation (desired) and decarbonylation/decarboxylation (undesired) through acetic acid (AA) HDO simulations

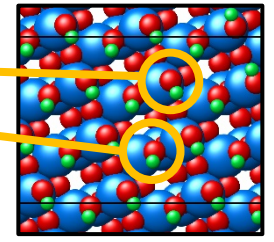
Deactivation of Pt/TiO_2 During HDO

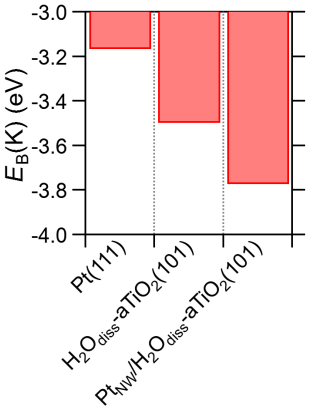
- Determined site-dependent adsorption energetics of K to provide insight into experimental trends for **K-induced deactivation** of model reaction chemistries

Pt/TiO_2 deactivation by K



H_2O_{diss}-aTiO_2(101)



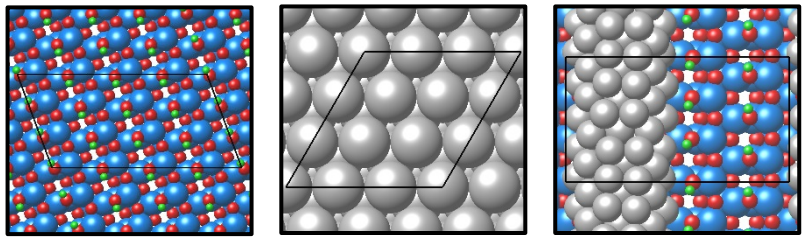


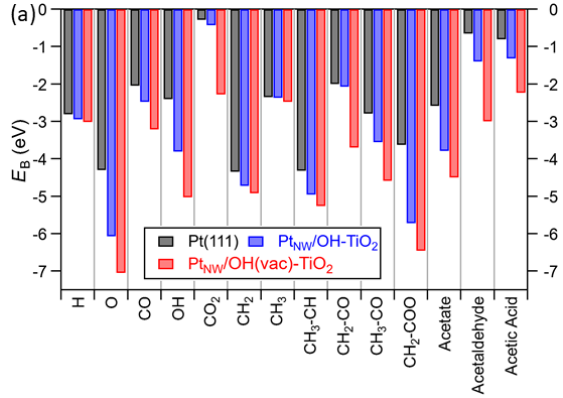
Relevance: Atomic-level **structure-function relationships for the multiple Pt/TiO_2 active sites** informs the **design** of these **catalysts to improve activity and selectivity** and **mitigate deactivation**.

In collaboration with the Catalytic Fast Pyrolysis, Advanced Catalyst Synthesis and Characterization, and Catalyst Deactivation Mitigation Projects

Adsorption of AA HDO Intermediates

OH-aTiO_2(101) Pt(111) Pt_{NW}/OH-aTiO_2(101)





F. Lin, et al. "Deactivation by Potassium Accumulation on a Pt/TiO_2 Bifunctional Catalyst for Biomass Catalytic Fast Pyrolysis ", in preparation

Activity and Water Stability of MgO(111) for 2-pentanone condensation

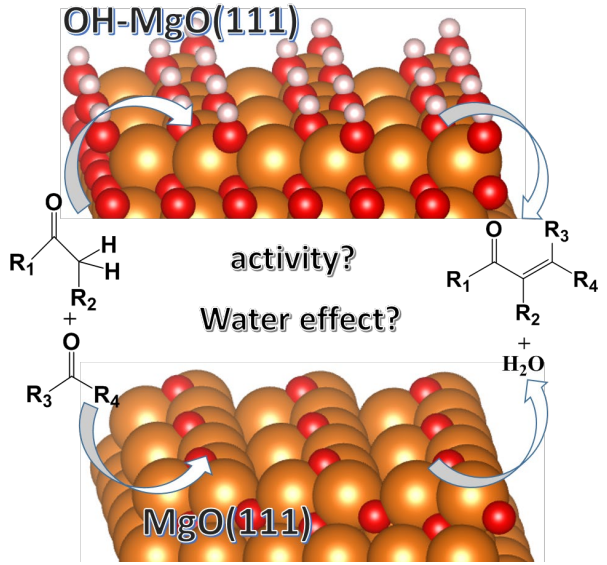
CCPC modeling contributing to broad ChemCatBio R&D on H_2O effects

- Understand the reaction mechanism of 2-pentanone condensation on MgO(111) surface and the role of H_2O in catalytic activity.
- Water molecule dissociate into surface hydroxyls to stabilize the MgO(111) surface and reduce the energy barriers by mediating the proton transfer steps.
- Experimental validation of MgO(111) catalyst reactivity in collaboration CUBI Project

Relevance:
Mechanistic understanding of ketone condensation and catalytic impact of water guides experimental research to design and develop efficient ketones condensation catalyst with high activity and water tolerance.

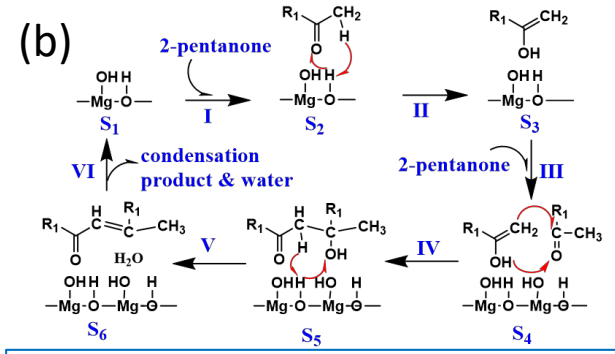
In collaboration with Catalytic Upgrading of Biochemical Intermediates (CUBI) and Advanced Catalyst Synthesis and Characterization (ACSC) and Catalyst Deactivation Mitigation projects

(a)



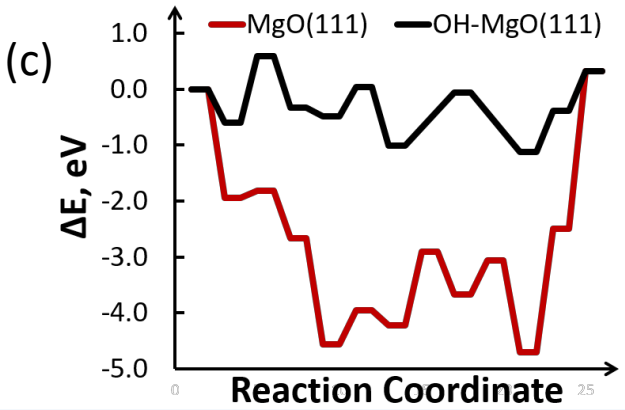
Schematic of condensation reaction on MgO(111) and OH-MgO(111) surfaces

(b)



Reaction scheme of 2-pentanone condensation on OH-MgO(111) surface

(c)



Energy profile of 2-pentanone condensation on MgO(111) and OH-MgO(111) surfaces

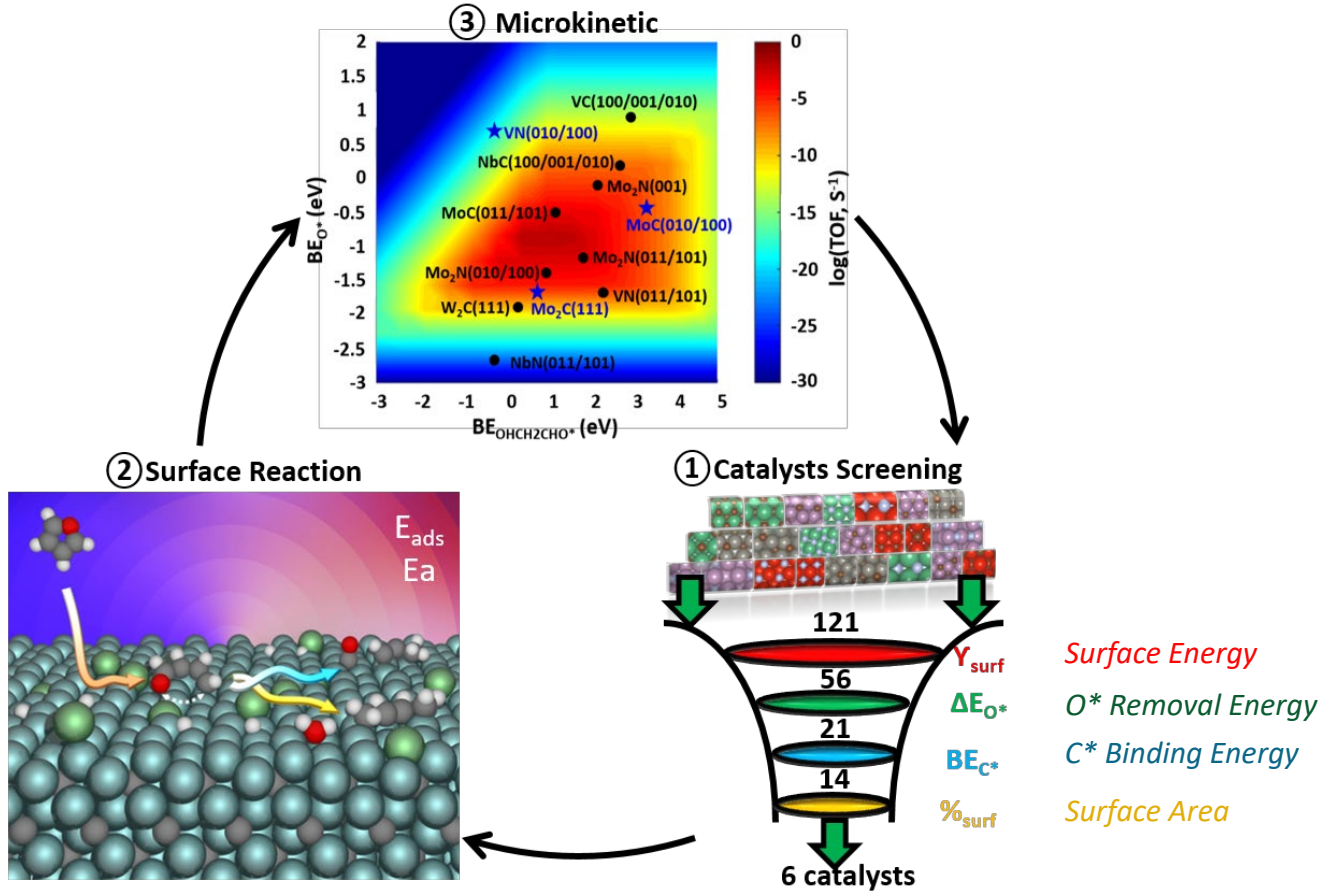
- X. Huo, D. Conklin, M. Zhou, R. S. Assary, S. Purdy, K. Page, Z. Li, K. A. Unocic, R. Balderas, R. Richards, D. Vardon, "Activity and water stability of MgO(111) nanoparticles for 2-pentanone condensation", in preparation.
- M. Zhou, X. Huo, V. Vorotnikov, D. R. Vardon, L. A. Curtiss, R. S. Assary, "A computational investigation of methyl ketones condensation on MgO surfaces: role of water", in preparation

Identification of Active Carbide/ Nitride Catalysts for Hydrodeoxygenation (HDO)

High Performance Computing enables high throughput catalyst screening

- Developed 121 surfaces in eight carbides and nitrides catalysts (Mo_2C, MoC, Mo_2N, W_2C, NbC, VC, VN, and NbN) for HDO reaction.
- Most active surfaces for HDO reactions are $Mo_2C(111)$, MoC(011/101), $Mo_2N(001)$, $Mo_2N(011/101)$, and $Mo_2N(010/100)$.
- Based on the microkinetic modeling, the HDO catalytic activity of carbides and nitrides surfaces are limited. New dopants such as Ni can increase the catalytic activity and decrease the catalyst deactivation.
- 5M CPU-hrs on ANL's Theta High Performance Computer

Relevance:
This *a priori* identification of active catalyst domains for HDO reaction from simulations provide guidelines to improve the optimal catalytic activity and to develop new catalyst designs.



Schematic of catalyst design for HDO reaction

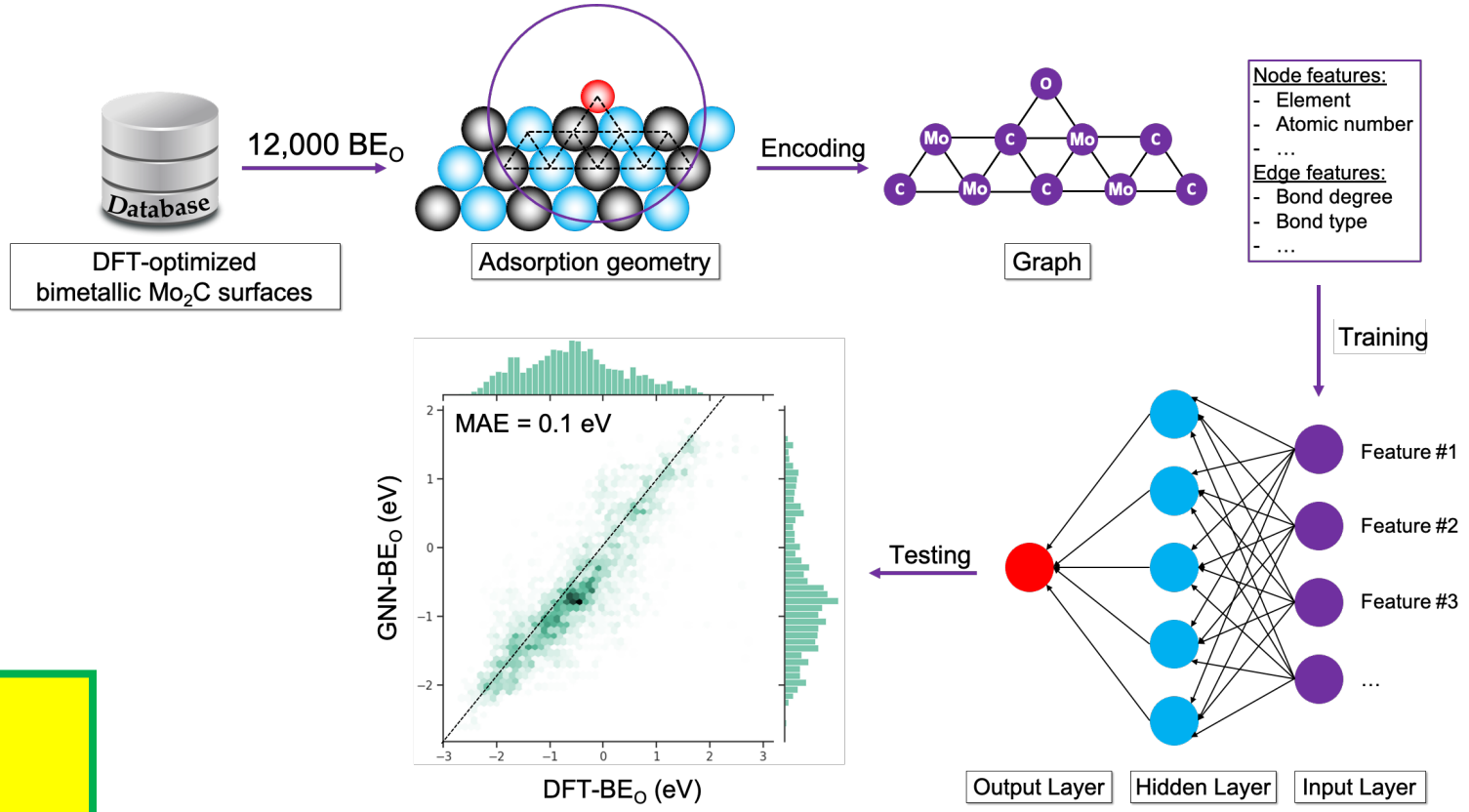
In collaboration with the Catalytic Fast Pyrolysis Project

- M. Zhou, H. A. Doan, L. A. Curtiss, R. S. Assary, "Accelerated discovery of metal carbides and nitrides catalysts for hydrodeoxygenation reaction from high-throughput screening and deep-dive prediction" in preparation
- M. Zhou, H. A. Doan, L. A. Curtiss, R. S. Assary, "Effect of Ni Dopant on Furan Activation over Mo_2C Surface: Insights from First-Principles-Based Microkinetic Modeling", J. Phys. Chem. C, 2020, 5636-5646

Development of Deep Learning Models for Catalytic Reactions

CCPC tool development in area of Machine Learning utilizing High Performance Computing

- Performed high-throughput DFT simulations to build a database of oxygen adsorption on Mo_2C catalysts
- 3500 catalyst sites modeled to obtain oxygen binding energy
- 10M CPU-hrs on ANL's Theta High Performance Computer
- Developed a Graph Neural Network model for predicting oxygen binding energy on bimetallic Mo_2C (MAE = 0.1 eV)



Prediction of oxygen binding energy from the adsorption graph

Relevance:
The GNN model significantly speeds oxygen adsorption energy prediction on any bimetallic Mo_2C facets, thus enabling the computational design of bimetallic Mo_2C nanoparticle catalysts with optimal oxygen binding energy.

CCPC advanced tool development

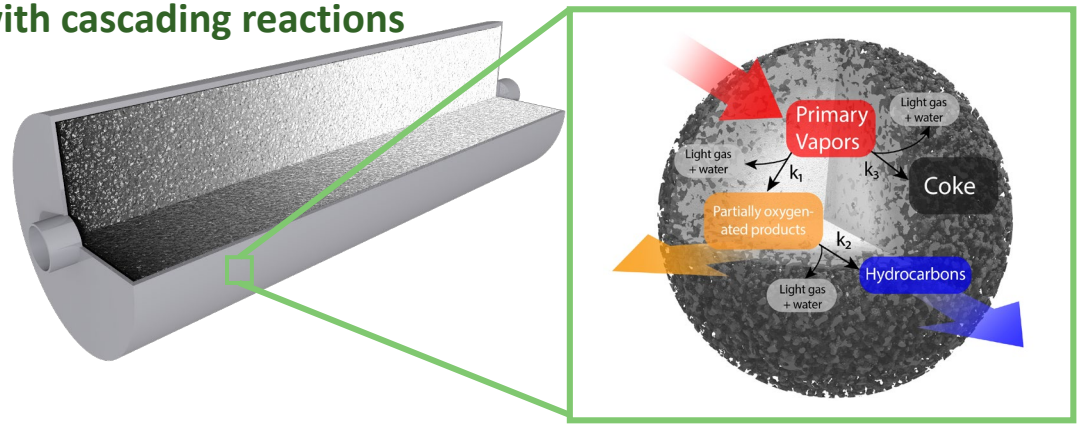
- H. A. Doan, G. Sivaraman, M. Zhou, L. A. Curtiss, R. S. Assary. "Graph neural network for fast and accurate predictions of oxygen binding energies on Mo_2C catalysts". In preparation.

Pyrolysis vapor upgrading over Pt/TiO_2: hierarchical transport modeling and kinetic parameter extraction

Advancements in kinetic parameter extraction enabled by meso-scale catalyst models

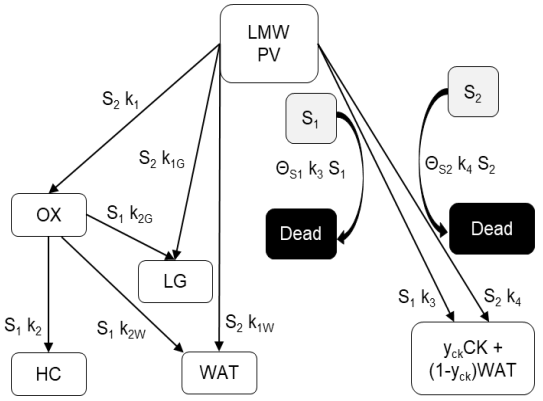
- Enabled by the multicomponent effectiveness vector (MEV), kinetic parameters for upgrading of transport-independent pyrolysis vapors over Pt/TiO_2 were extracted from experimental data.
- Model was used to extract transport-independent kinetic parameters from Catalytic Fast Pyrolysis experiments performed at NREL
- The model was validated against several different sets of experimental conditions with excellent agreement and robust predictive capability
- The validated kinetic model enables broad parametric analysis and enables high-fidelity reactor scale studies of upgrading and regeneration processes

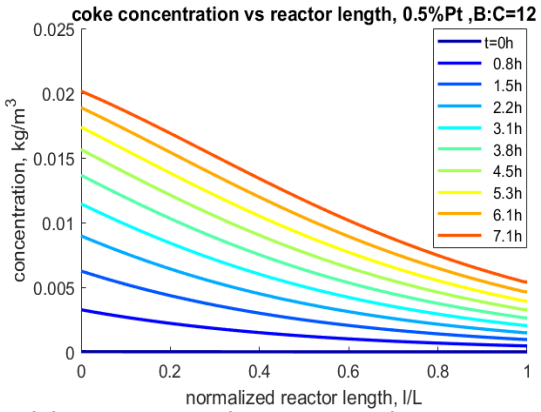
Multiscale Packed Bed Reactor model with cascading reactions



Iterative parameter optimization and experimental validation

Robust kinetic parameters and predictive capability





Relevance: CCPC modeling toolset can extract kinetic parameters from experimental data for use in predictive reactor design R&D.

In collaboration with the Catalytic Fast Pyrolysis Project

Pecha, Iisa, Griffin, Mukarakate, French, Adkins, Bharadwaj, Crowley, Foust, Schaidle, and Ciesielski. *Reaction Chemistry and Engineering*, **2020**

Summary: Consortium for Computational Physics and Chemistry

- **Management**
  - Consortium dedicated to computational science connects across multiple Bioenergy Technologies Office consortia
  - ***New!*** CCPC Direct Funded Assistance Program Approach
- **Approach**
  - Integral component of ChemCatBio ***accelerated catalyst and process development cycle*** together with sister enabling projects Advanced Catalyst Synthesis and Characterization and Catalyst Deactivation Mitigation
  - ***New!*** BETO-HPC: Dedicated High-Performance Computing on Summit (world's #2 fastest computer) and Ridge
- **Impact**
  - Lewis acid and solvent effects on glucose conversion to Hydroxymethylfurfural used to provide predictive guidance for Catalytic Upgrading of Biochemical Intermediates
  - Structure, energetics, and reaction pathways defined for ethanol upgrading over Cu/BETA in collaboration with Advanced Catalyst Synthesis and Characterization and C2+ Upgrading Projects.
  - Kinetics and particle-scale mass/heat transfer effects applied to Pt/TiO_2 packed bed reactor for Catalytic Fast Pyrolysis to cost-effectively inform scale up decisions
- **Progress and Accomplishments**
  - Accomplishments span atomic-, meso-, and reactor-scales with integration of modeling at different scales forming "knowledge train" to advance bioenergy successes at commercial scale

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

www.cpcbiomass.org

A multi-scale problem
… A multi-lab solution

Quad Chart Overview: Consortium for Computational Physics and Chemistry (CCPC)

FY2021 Budget by Task

Task	Budget
1. Coordination	$ 250,000
2. Atomic Scale	$ 801,000
3. Meso Scale	$ 356,000
4. Process Scale	$ 643,000
5. CO2 Conversion	$ 950,000
Total	**$ 3,000,000**

FY2021 Budget by NL

NL [Tasks]	Budget
ORNL [1,4,5]	$ 816,000
ANL [2,5]	$ 457,000
NETL [4]	$ 267,000
NREL [2,3,5]	$ 1,003,000
PNNL [2,5]	$ 457,000
Total	**$ 3,000,000**

*FY2020 funding included $2.0M for ChemCatBio R&D and $0.95M provided by the Systems Development and Integration Program for CCPC participation in the Catalytic Fast Pyrolysis Verification project
**FY2021 funding includes $2.0M for ChemCatBio R&D and $1.0M for CO_2 Conversion R&D

Timeline

- Project start date: October 1, 2019
- Project end date: September 30, 2022

	FY2020*	FY2021**
DOE Funding	$2.95M distributed over 5 NLs [$2.0M ChemCatBio, $0.95M CFP Verification]	$3.0M distributed over 5 NLs (see details at left) [$2.0M ChemCatBio, $1.0M CO_2 Conversion]

Project Partners

- ORNL (lead), ANL, NETL, NREL, PNNL [ChemCatBio Project]
- Note: INL also member of CCPC, but INL R&D in CCPC funded by FCIC*** Project

Barriers Addressed (from MYPP***)

Ct-G. Decreasing the time and cost to developing novel industrially relevant catalysts

Ct-N. Multi-scale computational framework towards accelerating technology development

ADO-D. Technical Risk of Scaling

Project Goal

Enable success of ChemCatBio technology pathways by:

(1) providing actionable surface chemistry information towards accelerating catalyst formulation innovation and development,

(2) providing critical characterization of mass and heat transfer effects to enable optimal design of catalyst particles, and

(3) determining and applying kinetic rates of reactions for catalysts to enable scale-up of catalytic conversion processes

End of Project Milestone

Construct a multi-scale model of the Pt/TiO_2 catalyst for upgrading of fast pyrolysis oil in the Catalyst Fast Pyrolysis (CFP) pathway. The multi-scale model will contain atomic, meso, and reactor-scale elements, and kinetic rates of reaction determined in conjunction with experimentalists will be utilized for modeling conversion at the reactor scale. Catalytic phenomena and parameters characterized and determined by atomic and meso scale models will be incorporated into the reactor scale model in reduced order form. The resulting reactor model will capture both catalytic upgrading and catalyst regeneration (coke oxidation) steps. Cases studied with the model will be analyzed to provide guidance for optimal product yield and information to Techno-Economic Analysis.

Funding Mechanism

Annual Operating Plan (core BETO project)

Consortium for Computational Physics and Chemistry (CCPC)

OAK RIDGE National Laboratory

Jim Parks
Gavin Wiggins
Bruce Adkins
Zach Mills
Canan Karakaya
Oluwafemi Oyedeji
Charles Finney
John Turner
Ashley Barker

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Peter Ciesielski
Seonah Kim*
Lintao Bu
Carrie Farberow
Aaron Lattanzi**
Mark Nimlos
Brandon Knott
Brennan Pecha
Vivek Bharadwaj
Meagan Crowley
Yeonjoon Kim*
Sean Tacey
Matt Jankousky****

Pacific Northwest NATIONAL LABORATORY

Roger Rousseau
Vanda Glezakou
Asanga Padmaperuma
Gregory Collinge
Mal-Soon Lee
Difan Zhang
Pradeep Gunarathan
Sneha Akhade***

NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

Bill Rogers
Madhava Syamlal
Xi Gao
Liqiang Lu
Deepthi Chandramouli
Mehrdad Shahnam
Rupen Panday
Huda Ashfaq
Cheng Li
Subhodeep Banerjee
Bryan Hughes
Tim Floyd
Steve Rowan

Argonne NATIONAL LABORATORY

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Larry Curtiss
Mingxia Zhou
Hieu Doan
Lei Cheng
Cong Liu

INL Idaho National Laboratory

Yidong Xia
Wencheng Jin
Jordan Klinger
Tiasha Bhattacharjee
Robert Seifert

Special thanks to DOE BETO Technology Managers:
Trevor Smith, Andrea Bailey, Sonia Hammache, and Kevin Craig

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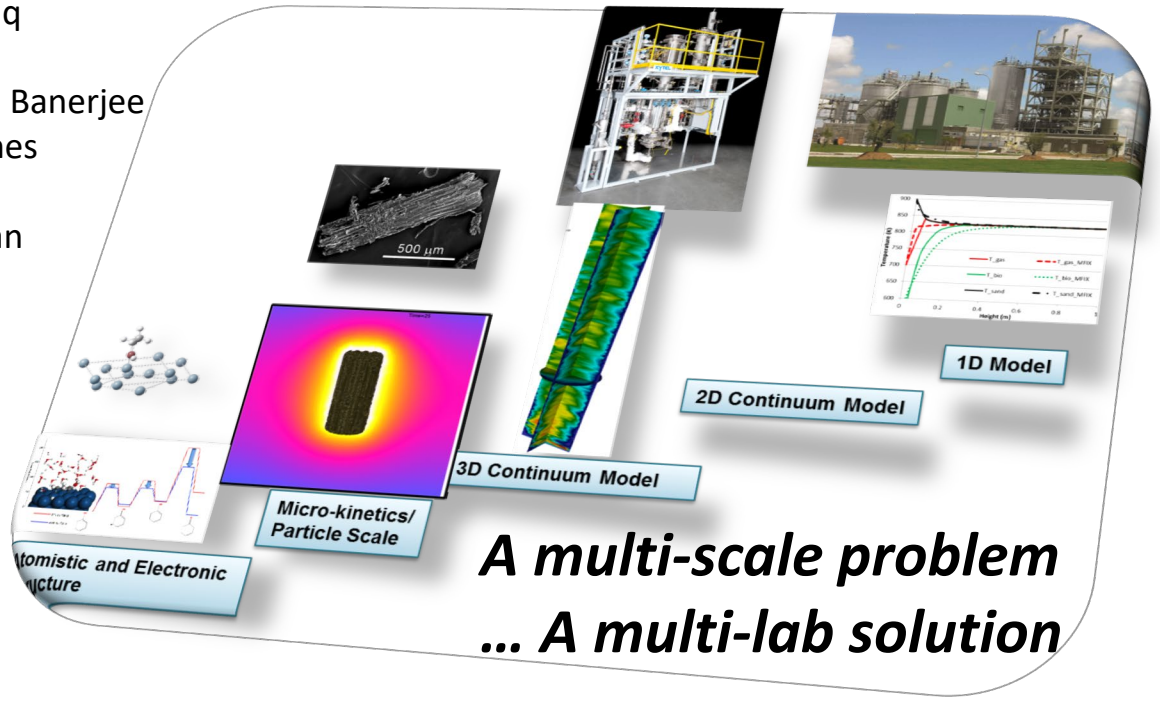
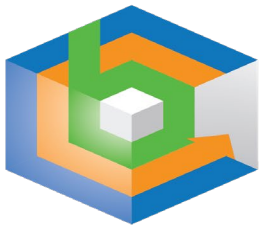


*Seonah Kim and Yeonjoon now at Colorado State University; **Aaron Lattanzi now at University of Michigan; ***Sneha Akhade now at LLNL; ****Matt Jankousky now at Colorado School of Mines

Additional Slides



ChemCatBio
Chemical Catalysis for Bioenergy

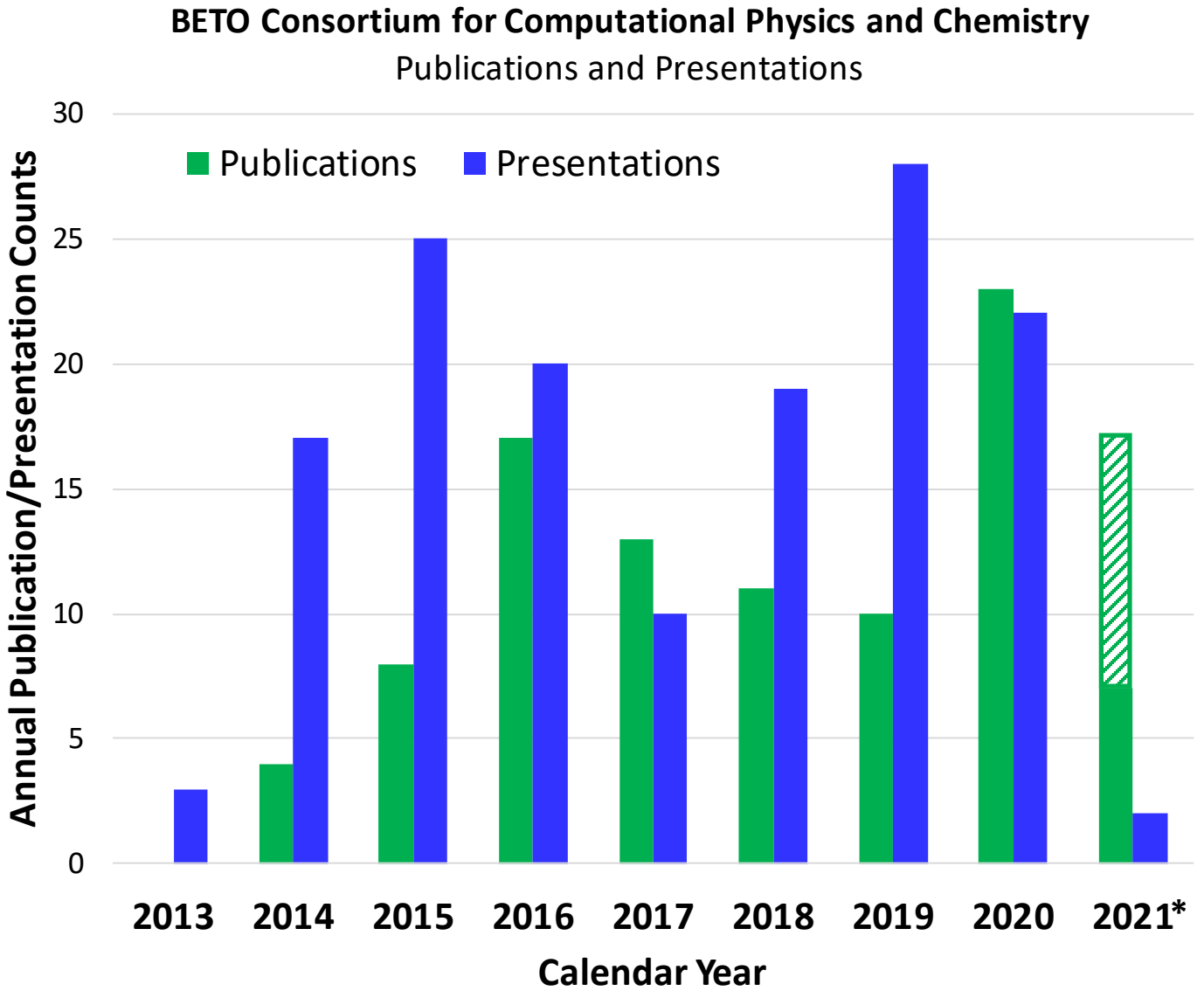
Responses to Previous Reviewers' Comments (FY2019 Peer Review)

- **Positive Feedback:**
  - *"…a **very impressive effort that covers many scales** of catalyst/reactor performance."*
  - *"A well organized, expansive center level effort which did an excellent job of demonstrating its **pervasive value throughout CCB [ChemCatBio]**."*
  - *"The approaches taken by computational physics and chemistry team are the **scientifically sound application of mathematical models** to problems arise from biomass conversion technologies."*
  - *"The operation of the CCPC is to what all the Enabling Capability projects might aspire. What a **solid, helpful, impactful consortium.**"*
- **Advice and Constructive Criticism:**
  - *"**Experimental validation will always continue to be the key** to computational programs building both the researchers and process deign engineer's confidence as reasonable agreement is reached at all scales."*
    - ***Response:** We agree and continue to observe the critical need for high quality experimental validation. We continue to improve in our interactions with experimentalists toward this key.*
  - *"Atomic scale activities should continue to show clearly how the computer experimental results will be incorporated in reaction engineering models for MFiX and the anticipated implications of these new simulations." & "CCPC has an opportunity to demonstrate how all of these efforts mathematically fit together at least at a simple first approach **to establish the "knowledge train" for a commercial design basis**."*
    - ***Response:** Yes, we like the "knowledge train" objective to bridge our multi-scale models. We have made progress in linking kinetics and meso-scale models to fixed bed reactor models. We have more progress to complete our "train" from atomic to reactor.*
  - *"…the group is encouraged to **pursue leverage with the existing basic science programs**."*
    - ***Response:** We agree. We have leveraged basic energy sciences programs specifically related to atomic-scale catalysis modeling techniques.*
  - *"…**machine learning algorithms might be a great fit** for these multiscale reactor models…."*
    - ***Response:** We agree. We have leveraged machine learning tools and continue to pursue this approach along with high-performance computing.*

Note: select reviewer comments shown. For full reviewer assessment, see 2019 BETO Peer Review Report at www.energy.gov/eere/bioenergy/2019-project-peer-review-report

Publications, Patents, Presentations, Awards, and Commercialization:
Summary *(following slides contain more detail and full list of publications and presentations)*

- **Publications:**
  - 40 journal publications since Jan. 1, 2019
  - 10 additional submissions under review
- **Patents:**
  - No patents
- **Presentations:**
  - 52 presentations since Jan. 1, 2019
- **Awards:**
  - 2 Conference Best Poster Awards
  - 3 Journal Cover Features
- **Commercialization:**
  - *Note: a primary method of technology transfer for the CCPC is the release of open-source code (cited here).*
  - 12 Repositories of CCPC open-source code on CCPC GitHub site at:
    - github.com/ccpcode



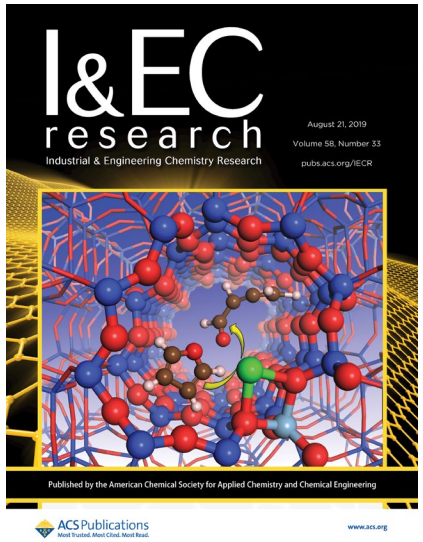
Note: Publications and presentations in this section represent CCPC publications associated with R&D with ChemCatBio, FCIC, and Bioprocessing Separation consortia

*For 2021 data, solid bar represents accepted publications through Feb. 17, 2021; cross-hatch bar represents publications submitted that are currently under review and revision.

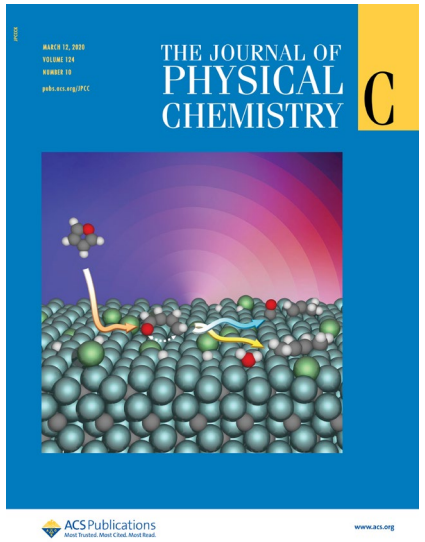
Awards and Notable Recognition

Awards:

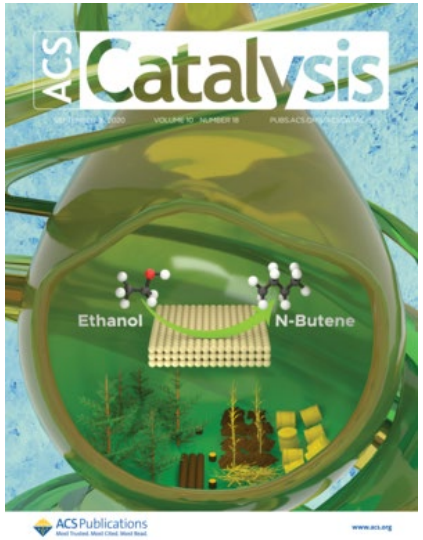
- Best Poster Award @ 2020 Virtual AIChE Annual Meeting, November 16-20, 2020.
  - Bhattacharjee, T. et al. “Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine”.
- Best Poster Award @ 2019 AIChE Annual Meeting, November 10-15, 2019, Orlando, FL.
  - Bhattacharjee, T. et al. “Mechanical Properties and Bulk Flow Characterization of Loblolly Pine.”



Journal Article Featured on Cover of *Industrial & Engineering Chemistry Research*:
M. Zhou, L. Cheng, B. Liu, L. A. Curtiss, and R. S. Assary, A First-Principles Investigation of Gas-phase Ring-Opening Reaction of Furan over HZSM-5 and Ga-Substituted ZSM-5, *Ind. Eng. Chem. Res.* 2019, **58**, 15127-15133.



Journal Article Featured on Cover of *The Journal of Physical Chemistry C*:
M. Zhou, H. A. Doan, L. A. Curtiss and R. S. Assary, Effect of Ni Dopant on Furan Activation over Mo_2C Surface: Insights from First Principles-Based Microkinetic Modeling, *J. Phys. Chem. C.* 2020, **124**, 5636-5646.



Journal Article Featured on Cover of *ACS Catalysis*:
Vanessa Lebarbier Dagle, Austin D. Winkelman, Nicholas R. Jaegers, Johnny Saavedra-Lopez, Jianzhi Hu, Mark H. Engelhard, Susan E. Habas, Sneha A. Akhade, Libor Kovarik, Vassilliki-Alexandra Glezakou, Roger Rousseau, Yong Wang, and Robert A. Dagle, Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO_2/SiO_2 Catalysts, *ACS Catalysis*, **10**(18), 10602-10613.

Publications [Page 1 of 4]

Publications in Peer-Reviewed Journals:

1. Pecha, M.B., Iisa, K., Griffin, M., Mukarakate, C., French, R., Adkins, B., Bharadwaj, V.S., Crowley, M., Foust, T.D., Schaidle, J.A. and Ciesielski, P.N., 2021. Ex situ upgrading of pyrolysis vapors over PtTiO2: extraction of apparent kinetics via hierarchical transport modeling. *Reaction Chemistry & Engineering*, *6*(1), pp.125-137. DOI: 10.1039/D0RE00339E (2021, ChemCatBio)
2. P. D. Coan, C. A. Farberow, M. B. Griffin, and J. W. Medlin, "Organic modifiers promote furfuryl alcohol ring hydrogenation via surface hydrogen-bonding interaction," *ACS Catalysis* 2021 (accepted). (2021, ChemCatBio)
3. Lu, Y., Jin, W., Klinger, J., Westover, T., Dai, S. "Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model", *Powder Technology*, Vol, 383, pp. 396-409, 2021. https://doi.org/10.1016/j.powtec.2021.01.027 (2021, FCIC)
4. L. Lu, X. Gao, M. Shahnam, W.A. Rogers, Open Source Implementation of Glued Sphere Discrete Element Method and Non-spherical Biomass Fast Pyrolysis Simulation, *AIChE* J. n/a (n.d.) e17211. https://doi.org/10.1002/aic.17211. (2021, FCIC)
5. Jia Yu, Xi Gao, Liqiang Lu, Yupeng Xu, Cheng Li, Tingwen Li, William A.Rogers, Validation of a filtered drag model for solid residence time distribution (RTD) prediction in a pilot-scale FCC riser, *Powder Technology*, Volume 378, Part A, 22 January 2021, Pages 339-347, https://doi.org/10.1016/j.powtec.2020.10.007. (2021, FCIC)
6. Xi Gao, Jia Yu, Liqiang Lu, William A. Rogers, Coupling particle scale model and SuperDEM-CFD for multiscale simulation of biomass pyrolysis in a packed bed pyrolyzer. *AIChE Journal*, 2021, e17139. https://aiche.onlinelibrary.wiley.com/doi/abs/10.1002/aic.17139 (2021, FCIC)
7. Xi Gao, Jia Yu, Ricardo J.F.Portal, Jean-François Dietiker, Mehrdad Shahnam, William A. Rogers, Development and validation of SuperDEM for non-spherical particulate systems using a superquadric particle method, *Particuology*, January 2021. https://www.sciencedirect.com/science/article/abs/pii/S1674200121000146 (2021, FCIC)
8. Yuk, Simuck F., Mal-Soon Lee, Greg Collinge, Junyan Zhang, Asanga B. Padmaperuma, Zhenglong Li, Felipe Polo-Garzon, Zili Wu, Vassiliki-Alexandra Glezakou, and Roger Rousseau. "Mechanistic Understanding of Catalytic Conversion of Ethanol to 1-Butene over 2D-Pillared MFI Zeolite." *The Journal of Physical Chemistry C*. 124, 52, 28437–28447. https://doi.org/10.1021/acs.jpcc.0c05585 (2020, ChemCatBio)
9. Dagle, Vanessa Lebarbier, Austin D. Winkelman, Nicholas R. Jaegers, Johnny Saavedra-Lopez, Jianzhi Hu, Mark H. Engelhard, Susan E. Habas et al. "Single-Step Conversion of Ethanol to n-Butene over Ag-ZrO2/SiO2 Catalysts." *ACS Catalysis* 10, no. 18 (2020): 10602-10613. https://doi.org/10.1021/acscatal.0c02235 (2020, ChemCatBio)
10. Akhade, Sneha A., Austin Winkelman, Vanessa Lebarbier Dagle, Libor Kovarik, Simuck F. Yuk, Mal-Soon Lee, Jun Zhang et al. "Influence of Ag metal dispersion on the thermal conversion of ethanol to butadiene over Ag-ZrO2/SiO2 catalysts." *Journal of Catalysis* 386 (2020): 30-38. https://doi.org/10.1016/j.jcat.2020.03.030 (2020, ChemCatBio)

Publications [Page 2 of 4]

Publications in Peer-Reviewed Journals:

11. K. Iisa, Y. Kim, K. A. Orton, D. J. Robichaud, R. Katahira, M. J. Watson, E. C. Wegener, M. R. Nimlos, J. A. Schaidle, C. Mukarakate, and S. Kim, "Ga/ZSM-5 catalyst improves hydrocarbon yields and increases alkene selectivity during catalytic fast pyrolysis of biomass with co-fed hydrogen," *Green Chemistry* 2020, 22, 2403-2418. DOI: 10.1039/C9GC03408K (2020, ChemCatBio)
12. C. Mukarakate, K. Orton, Y. Kim, S. Dell'Orco, C. A. Farberow, S. Kim, M. J. Watson, R. M. Baldwin, and K. A. Magrini, "Isotopic studies of tracking biogenic carbon during co-processing of biomass and vacuum gas oil," *ACS Sustainable Chemistry and Engineering* 2020, 8, 2652-2664. DOI: 10.1021/acssuschemeng.9b05762 (2020, ChemCatBio)
13. Y. Kim, A. Mittal, D. J. Robichaud, H. Pilath, B. D. Etz, P. C. St. John, D. K. Johnson, and S. Kim, "Prediction of hydroxymethylfurfural yield in glucose conversion through investigation of lewis acid and organic solvent effects". *ACS Catalysis* 2020, 10, 14707-14721. DOI: 10.1021/acscatal.0c04245 (2020, ChemCatBio)
14. Lattanzi, A.M., Pecha, M.B., Bharadwaj, V.S. and Ciesielski, P.N., 2020. Beyond the effectiveness factor: Multi-step reactions with intraparticle diffusion limitations. *Chemical Engineering Journal*, *380*, p.122507. https://doi.org/10.1016/j.cej.2019.122507 (2020, ChemCatBio)
15. Zhang, Difan, Pradeep Gurunathan, Lauren Valentino, Yupo Lin, Roger Rousseau, and Vanda Glezakou. "Atomic scale understanding of organic anion separations using ion-exchange resins." *Journal of Membrane Science* (2020): 118890. https://doi.org/10.1016/j.memsci.2020.1188900 (2020, SepCon)
16. M. Zhou, S. Krishna, M. De bruyn, B. Weckhuysen, L. Curtiss, J. Dumesic, G. Huber, R. Assary, Mechanistic Insight into the Conversion of Bio-renewable Levoglucosanol to Dideoxysugars, *ACS. Sustain. Chem. Eng.* 2020, 8, 43, 16339-16349. (2020, ChemCatBio)
17. M. Zhou, H. A. Doan, L. A. Curtiss and R. S. Assary, Effect of Ni Dopant on Furan Activation over Mo_2C Surface: Insights from First Principles-Based Microkinetic Modeling, *J. Phys. Chem. C.* 2020, 124, 5636-5646 (2020, ChemCatBio) ***[Note: Featured Cover of 10th issue in 2020]***
18. Xi Gao, Tingwen Li, William A. Rogers, Kristin Smith, Katherine Gaston, Gavin Wiggins, James E. Parks II, Validation and application of a multiphase CFD model for hydrodynamics, temperature field and RTD simulation in a pilot-scale biomass pyrolysis vapor phase upgrading reactor, *Chemical Engineering Journal*, Volume 388, 15 May 2020, 124279, https://doi.org/10.1016/j.cej.2020.124279. (2020, ChemCatBio)
19. Jin, W., Klinger, J. Westover, T. and Huang, H. "A density dependent drucker-prager/cap model for ring shear simulation of ground loblolly pine: advantages and limitations". *Powder Technology*, Vol. 368, pp. 45-58, 2020. https://doi.org/10.1016/j.powtec.2020.04.038 (2020, FCIC)
20. Xia, Y., Stickel, J., Jin, W., Klinger, J. "A review of computational models for the flow of milled biomass I: Discrete-particle models". *ACS Sustainable Chemistry & Engineering*, 2020, 8, 16, pp. 6142-6156. https://doi.org/10.1021/acssuschemeng.0c00402 (2020, FCIC)

Publications [Page 3 of 4]

Publications in Peer-Reviewed Journals:

21. Jin, W., Stickel, J., Xia, Y., Klinger, J. "A review of computational models for the flow of milled biomass II: Continuum-mechanics models". *ACS Sustainable Chemistry & Engineering*, 2020, 8, 16, pp. 6157-6172. https://doi.org/10.1021/acssuschemeng.0c00412 (2020, FCIC)
22. Guo, Y., Chen, Q., Xia, Y., Westover, T., Eksioglu, S. Roni, M. "Discrete element modeling of switchgrass particles under compression and rotational shear". *Biomass & Bioenergy*, 2020. https://doi.org/10.1016/j.biombioe.2020.105649 (2020, FCIC)
23. Thornburg, N.E., Pecha, M.B., Brandner, D.G., Reed, M.L., Vermaas, J.V., Michener, W.E., Katahira, R., Vinzant, T.B., Foust, T.D., Donohoe, B.S. and Román-Leshkov, Y., Mesoscale Reaction–Diffusion Phenomena Governing Lignin-First Biomass Fractionation. *ChemSusChem*, *13*(17), pp.4495-4509. https://doi.org/10.1002/cssc.202000558 (2020, FCIC)
24. Ciesielski, P.N., Pecha, M.B., Lattanzi, A.M., Bharadwaj, V.S., Crowley, M.F., Bu, L., Vermaas, J.V., Steirer, K.X. and Crowley, M.F., Advances in multiscale modeling of lignocellulosic Biomass. *ACS Sustainable Chemistry & Engineering*, *8*(9), pp.3512-3531. https://doi.org/10.1021/acssuschemeng.9b07415 (2020, FCIC)
25. L. Lu, X. Gao, A. Gel, G. Wiggins, M. Crowley, B. Pecha, M. Shahnam, W.A. Rogers, J. Parks, P.N. Ciesielski, Investigating Biomass Composition and Size Effects on Fast Pyrolysis using Global Sensitivity Analysis and CFD Simulations, *Chem. Eng. J.* (2020) 127789. https://doi.org/10.1016/j.cej.2020.127789. (2020, FCIC)
26. L. Lu, X. Gao, M. Shahnam, W.A. Rogers, Bridging particle and reactor scales in the simulation of biomass fast pyrolysis by coupling particle resolved simulation and coarse grained CFD-DEM, *Chem. Eng. Sci.* 216 (2020) 115471. https://doi.org/10.1016/j.ces.2020.115471. (2020, FCIC)
27. L. Lu, X. Gao, M. Shahnam, W.A. Rogers, Coarse grained computational fluid dynamic simulation of sands and biomass fluidization with a hybrid drag, *AIChE J.* 66 (2020) e16867. https://doi.org/10.1002/aic.16867. (2020, FCIC)
28. L. Lu, J. Yu, X. Gao, Y. Xu, M. Shahnam, W.A. Rogers, Experimental and numerical investigation of sands and Geldart A biomass co-fluidization, *AIChE J.* 66 (2020) e16969. https://doi.org/10.1002/aic.16969. (2020, FCIC)
29. Xi Gao, Tingwen Li, William A Rogers, Kristin Smith, Katherine Gaston, Gavin Wiggins, James E Parks II, "Validation and application of a multiphase CFD model for hydrodynamics, temperature field and RTD simulation in a pilot-scale biomass pyrolysis vapor phase upgrading reactor", *Chemical Engineering Journal* **388**, 124279 (2020). doi.org/10.1016/j.cej.2020.124279 (2020, FCIC)
30. Xi Gao, Jia Yu, Liqiang Lu, Cheng Li, William A. Rogers, Development and validation of SuperDEM-CFD coupled model for simulating non-spherical particles hydrodynamics in fluidized beds, *Chemical Engineering Journal*, November 2020, 127654. https://www.sciencedirect.com/science/article/abs/pii/S1385894720337761 (2020, FCIC)

Publications [Page 4 of 4]

Publications in Peer-Reviewed Journals:

31. L. Y. Kunz, L. Bu, B. C. Knott, C. Liu, M. R. Nimlos, R. S. Assary, L. A. Curtiss, D. J. Robichaud, and S. Kim, "Theoretical determination of size effects in zeolite-catalyzed alcohol dehydration," *Catalysts* 2019, 9, 700. DOI: 10.3390/catal9090700 (2019, ChemCatBio)
32. A. E. Settle, N. S. Cleveland, C. A. Farberow, D. R. Conklin, X. Huo, A. A. Dameron, R. W. Tracy, R. Sarkar, E. J. Kautz, A. Devaraj, K. K. Ramasamy, M. J. Watson, A. M. York, R. M. Richards, K. A. Unocic, G. T. Beckham, M. B. Griffin, K. E. Hurst, E. C. D. Tan, S. T. Christensen, and D. R. Vardon, "Enhanced catalyst durability for bio-based adipic acid production by atomic layer deposition," *Joule* 2019, 3, 2219-2240. DOI: 10.1016/j.joule.2019.06.022 (2019, ChemCatBio)
33. Bharadwaj, V.S., Pecha, M.B., Bu, L., Dagle, V.L., Dagle, R.A. and Ciesielski, P.N., 2019. Multi-scale simulation of reaction, transport and deactivation in a SBA-16 supported catalyst for the conversion of ethanol to butadiene. *Catalysis Today*, *338*, pp.141-151. https://doi.org/10.1016/j.cattod.2019.05.042 (2019, ChemCatBio)
34. Moyer, K., Conklin, D.R., Mukarakate, C., Vardon, D.R., Nimlos, M.R. and Ciesielski, P.N., 2019. Hierarchically structured CeO2 catalyst particles from nanocellulose/alginate templates for upgrading of fast pyrolysis vapors. *Frontiers in chemistry*, *7*, p.730. https://doi.org/10.3389/fchem.2019.00730 (2019, ChemCatBio)
35. Coan, P.D., Griffin, M.B., Ciesielski, P.N. and Medlin, J.W., 2019. Phosphonic acid modifiers for enhancing selective hydrodeoxygenation over Pt catalysts: The role of the catalyst support. *Journal of Catalysis*, *372*, pp.311-320. https://doi.org/10.1016/j.jcat.2019.03.011 (2019, ChemCatBio)
36. Yang, Guoju, Sneha A. Akhade, Xi Chen, Yue Liu, Mal-Soon Lee, Vassiliki-Alexandra Glezakou, Roger Rousseau, and Johannes A. Lercher. "The nature of hydrogen adsorption on platinum in the aqueous phase." *Angewandte Chemie International Edition* 58, no. 11 (2019): 3527-3532. https://doi.org/10.1002/anie.201813958 (2019, ChemCatBio)
37. M. Zhou, L. Cheng, B. Liu, L. A. Curtiss, and R. S. Assary, A First-Principles Investigation of Gas-phase Ring-Opening Reaction of Furan over HZSM-5 and Ga-Substituted ZSM-5, *Ind. Eng. Chem. Res.* 2019, 58, 15127-15133. (2019, ChemCatBio) ***[Note: Featured Cover of August 21st issue in 2019]***
38. Xia, Y., Lai, Z., Westover, T., Klinger, J., Huang, H., Chen, Q. "Discrete element modeling of deformable pinewood chips in cyclic loading test", *Powder Technology*, Vol 345, 1, pp. 1-14, 2019. https://doi.org/10.1016/j.powtec.2018.12.072 (2019, FCIC)
39. Pecha, M.B., Arbelaez, J.I.M., Garcia-Perez, M., Chejne, F. and Ciesielski, P.N., 2019. Progress in understanding the four dominant intra-particle phenomena of lignocellulose pyrolysis: chemical reactions, heat transfer, mass transfer, and phase change. *Green chemistry*, *21*(11), pp.2868-2898. DOI: 10.1039/C9GC00585D (2019, FCIC)
40. Xi Gao; Jia Yu; Cheng Li; Rupen Panday; Yupeng Xu; Tingwen Li; Huda Ashfaq; Bryan Huges; William A. Rogers, "Comprehensive experimental investigation on biomass-glass beads binary fluidization: A data set for CFD model validation", *AIChE Journal*, Oct. 18, 2019 https://aiche.onlinelibrary.wiley.com/doi/abs/10.1002/aic.16843 (2019, FCIC)

Recent Publications Submitted (under review or revision)

Recent Publications Submitted to Peer-Reviewed Journals in Various Stages of Review and Revision:

1. M. Cordon, J. Zhang, S. Purdy, E. Wegener, K. Unocic, L. Allard, M. Zhou, R. Assary, J. Miller, T. Krause, A. Kropf, C. Yang, D. Liu, Z. Li. Selective Butene Formation in Direct Ethanol C_{3+} Olefin Valorization over Zn-Y/Beta and Single-atom Alloy Composition Catalysts Using in situ Generated Hydrogen, *ACS Catalysis*, 2021 submitted. (2021, ChemCatBio)
2. M. Zhou, A. Church, R. Hunt, J. Choi, L. Bai, Z. Li, J. Park, M. Hu, L. Curtiss, R. Assary, A Combined Experimental and Computational Investigation of Acetic Acid Ketonization over Ca-doped CeO_2 catalyst, *Appl. Catal. A*, 2021 submitted. (2021, ChemCatBio)
3. X. Huo, D. Conklin, M. Zhou, V. Vorotnikov, R. Assary, S. Purdy, K. Page, Z. Li, K. Unocic, R. Balderas, R. Richards, D. Vardon, Catalytic Activity and Water Stability of the MgO(111) Surface for 2-Pentanone Condensation, *Appl. Catal. B*, 2021, submitted. (2021, ChemCatBio)
4. M. Zhou, H. Doan, L. Curtiss, R. Assary, Identification of Active Metal Carbides and Nitrides Catalytic Facets for Hydrodeoxygenation Reactions, *ACS Catalysis*, 2021, submitted. (2021, ChemCatBio)
5. Bruce D. Adkins, Zach Mills, James Parks II, M. Brennan Pecha, Peter N. Ciesielski, Kristiina Iisa, Calvin Mukarakate, David Robichaud, Kristin Smith, Katherine Gaston, Michael Griffin and Josh Schaidle, "Predicting thermal excursions during in-situ oxidative regeneration of packed bed catalytic fast pyrolysis catalyst", submitted to *Reaction Chemistry and Engineering* (under revision). (2021, ChemCatBio)
6. Guo, Y., Chen Q., Xia, Y., Klinger, J. Thompson, V., "A nonlinear elasto-plastic bond model for the discrete element modeling of woody biomass particles," *Powder Technology*, 2021 (revision under review). (2021, FCIC)
7. Sun, Q., Xia, Y., Klinger, J. Seifert, R., Kane, J., Thompson, V., Chen, Q. "X-ray computer tomography-based porosity analysis: Algorithms and application for porous woody biomass", submitted to *Bioresource Technology*, 2021 (under review). (2021, FCIC)
8. Cheng, Z., Leal, J., Hartford, C., Carson, J., Donohoe, B., Craig, D., Xia, Y., Daniel, R., Ajayi, O., Semelsberger, T. "Flow behavior characterization of biomass feedstocks", *Powder Technology*, 2021 (under review). (2021, FCIC)
9. Xia, Y. Chen, F., Klinger, J. Kane, J., Bhattacharjee, T., Seifert, R., Ajayi, O., Chen, Q. "Assessment of a tomography-informed polyhedral discrete element modeling approach for complex-shaped granular woody biomass in stress consolidation", *Biosystems Engineering*, 2021 (under review). (2021, FCIC)
10. Xi Gao, Liqiang Lu, Mehrdad Shahnam, William A. Rogers, Kristin Smith, Katherine Gaston, David Robichaud, Brennan Pecha, Meagan Crowley, Peter N. Ciesielski, Gavin Wiggins, Charles Finney, James E Parks II, Assessment of a detailed biomass pyrolysis kinetic scheme in multiscale simulations of a single-particle pyrolyzer and a pilot-scale entrained flow pyrolyzer, *Chemical Engineering Journal*, 2021, In revision. (2021, FCIC)

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Presentations [ChemCatBio]:

1. C. A. Farberow, C. Nash, J. Hall, and J. Schaidle. “On the role of surface adsorbed oxygen in ethanol reaction pathways on Mo2C.” ACS Spring National Meeting, April 2019, Orlando, FL, (Invited).
2. C. A. Farberow, S. R. J. Likith, S. Manna, A. Abdulslam, V. Stevanovic, D. A. Ruddy, J. A. Schaidle, D. J. Robichaud, and C. V. Ciobanu, “Thermodynamic Stability of Molybdenum Oxycarbides Formed from Orthorhombic Mo2C in Oxygen-Rich Environments,” NAM26, June 2019, Chicago, IL.
3. L. Bu, C. Mukarakate, J. Hensley, D. A. Ruddy, D. Robichaud and S. Kim, “Methanol and Dimethyl Ether Conversion over Zeolites By Reactive Molecular Dynamics Simulations,” NAM26, June 2019, Chicago, IL (Poster).
4. S. Kim, “Design Principles for Sustainable Chemistry: from Biomass to Renewable Biofuel and Biomaterial,” Colorado State University, Department of Chemistry, Nov. 14, 2019, Fort Collins, CO (Invited).
5. Y. Kim, H. M. Pilath, D. J. Robichaud, D. K. Johnson, and S. Kim, “Predicting Hydroxymethylfurfural (HMF) Formation Rate in Sugar Upgrading through Investigation of Lewis Acid and Organic Solvent Effects,” ACS Fall National Meeting, August 2019, San Diego, CA.
6. Y. Kim, C. Mukarakate, and S. Kim. “Theoretical and experimental developments of catalytic partial oxidation of lignin to simple phenols.” ACS Fall National Meeting, August 2019, San Diego, CA.
7. Y. Kim “Towards improvement of hydroxymethylfurfural yield in glucose conversion: considering the effect of solvent systems through multivariate analysis.” ACS Fall Virtual Meeting, August 2020.
8. M. Zhou, L. Curtiss, R. Assary, Catalytic Design Guidelines from Atomistic Simulations for Vapor Phase Reactions, Thermal & Catalytic Sciences Virtual Symposium, **2020**.
9. M. Zhou, L. Curtiss, R. Assary, First-Principle-Based Microkinetic Study of Water Effect in Aldol Condensation Reaction on MgO(111) Surface, ACS National Meeting & Exposition, San Diego, California, United States, **2019**.
10. M. Zhou, L. Curtiss, R. Assary, Density Functional Theory Study of Ca Dopant Effect on Acetic Acid Ketonization over CeO_2(111) surface, North American Catalysis Society Meeting, Chicago, Illinois, United States, **2019**.
11. M. Zhou, L. Curtiss, R. Assary, Computational Studies of Aldol Condensation over MgO Catalyst Surface, ACS National Meeting & Exposition, **2019**, Orlando, Florida, United States.
12. H. A. Doan, M. Zhou, R.S. Assary. “Computational Screening of Molybdenum Carbide Catalysts for Biomass Conversion”. ACS Spring. March **2020**. Philadelphia PA. Canceled.
13. H. A. Doan, M. Zhou, R.S. Assary . “Toward the Optimal Design of Molybdenum Carbide Catalysts for Biomass Conversion” (invited). ACS Fall. August **2019**, San Diego CA.
14. Rajeev Assary, Reactivity of model oxygenates on heterogeneous catalysts: Insights from first principles Simulations (PAPER ID: 3113726, paper number: CATL 569), American Chemical Society Meeting, April 4, 2019, Orlando, FL.
15. Rajeev S. Assary, Atomistic modeling of vapor phase catalysis in H-ZSM5 (PAPER ID: 3113997), American Chemical Society Meeting, April 2, 2019, Orlando, FL.

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Presentations [ChemCatBio]:

16. Gao, X., Li, T., Rogers W.A., Panday, R., Li, Cheng., Ashfaq, Huda., Hughes, Bryan. Computational fluid dynamic modeling and simulation of biomass pyrolysis vapor-phase upgrading process at reactor scale. COMP: Advances in Multiscale Computational Modeling of Biomass Conversion Processes (Invited Talk). ACS Fall 2019 National Meeting & Exposition, San Diego, Sept 2019.
17. Gao, X., Li, T., Rogers W.A. CFD simulation of hydrodynamics, RTD, heat transfer and chemical reaction in a pilot-scale biomass pyrolysis vapor-phase upgrading (VPU) reactor. ChemCatBio session (Invited Talk) . ACS Spring 2019 National Meeting & Exposition, Orlando, April 2019.
18. James E. Parks II, Zach Mills, Gavin Wiggins, Bruce Adkins, Charles Finney, Vivek Bharadwaj, Brennan Pecha, Meagan Crowley, Anne Starace, Calvin Mukarakate, Peter Ciesielski, David Robichaud, Kristin Smith, Katherine Gaston, Kristiina Iisa, Xi Gao, Tingwen Li, and William Rogers, “Development and Validation of a Lumped Kinetic Model for Catalytic Fast Pyrolysis Upgrading Over a ZSM-5 Catalyst”, The International Conference on Thermochemical Conversion Science: Biomass & Municipal Solid Waste to RNG, Biofuels & Chemicals (TCBiomassPlus), Chicago, IL, October 2019.
19. Bruce Adkins, James Parks II, Kristiina Iisa, Kristin Smith, “Computational Scale-Up of Packed Bed Reactor and Process for Catalytic Upgrading of Pyrolysis Vapors Using COMSOL”, American Chemical Society Fall Meeting 2019, San Diego, CA, August 2019.
20. Bruce Adkins, James Parks II, Kristiina Iisa, Kristin Smith, ”COMSOL Model for Optimizing Regeneraion of CFP Catalyst in Packed-Bed Reactors”, COMSOL Users Conference, Boston, MA, October 2019.
21. Bruce Adkins et al., “Computational Scale-up of packed bed reactors for ex-situ catalytic fast pyrolysis”, TCS2020 (Virtual).
22. Oluwafemi Oyedeji et al., “Multiscale modeling of autothermal pyrolysis of corn stover”, TCS2020 (Virtual).
23. Brennan Pecha et al., “High fidelity multiscale modeling of fast pyrolysis of woody feedstock blends in a fluidized bed reactor and entrained flow reactor”, TCS2020 (Virtual).
24. Banerjee, S., Shahnam, M., Rogers, W., “Transient Reacting Flow Simulation of Biomass Combustion in a Pilot-Scale Circulating Fluidized Bed Combustor’, 2020 Virtual AIChE Annual Meeting, November 16-20, 2020.
25. Mike Griffin, Brennan Pecha and Bruce Adkins, “Advancing Catalytic Fast Pyrolysis through Integrated Experimentation and Mulit-Scale Computational Modelling”, ChemCatBio Webinar, Jan 13, 2021.

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Presentations [Feedstock Conversion Interface Consortium]:

- **FCIC Webinar series**
  - Xia, Y. & Ciesielski, P. “FCIC Modeling 1”, February 11, 2021.
- **2020 Virtual AIChE Annual Meeting, November 16-20, 2020**
  - Rahimi, M. et al. "Computational modeling of a biomass screw-feeder with compressible non-Newtonian rheology".
  - Chen, F. et al. “A Hysteretic Nonlinear Elastoplastic Contact Model for Discrete Element Modeling of Milled Woody Biomass”.
  - Jin, W. et al. “A Multi-Regime Continuum Approach for Modeling Flow of Granular Pine Chip”.
  - Jin, W. et al. “Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine”.
  - Ahsan, S. et al. “Computational Fluid-Dynamics Modeling of Biomass-Feedstock Flow Using a Non-Local Granular-Fluidity Constitutive Model”.
  - Bhattacharjee, T. et al. “Effects of Preprocessing Parameters on Material Attributes and Flow Behavior of Loblolly Pine”.
- **International Powder & Bulk Solids Conference & Exhibition, The Powder Show Digital Flow (virtual), October 1, 2020.**
  - Xia, Y. “Limitations and Best Practice for DEM Modeling of Biomass”.
- **ASABE Annual Meeting 2020 (virtual), July 13-15, 2020**
  - Xia, Y. et al. “FCIC Materials Handling Project Overview and R&D Highlights”.
  - Klinger, J. et al. “Bulk Physical, Mechanical, and Shear Properties of Loblolly Pine and Flow Characterization in Variable Wedge Hopper Geometries”.
  - Jin, W. et al. “Multi-scale Computational Modeling of Milled Biomass Flow with Multi-regime Constitutive Model”.
  - Xia, Y. et al. “Discrete Element Modeling for the Flow of Milled Biomass: Current State of the Art and Applications”.
  - Ahsan, S. et al. “Non-local granular fluidity based constitutive modeling of woody biomass feed flow”.
- **2019 AIChE Annual Meeting, November 10-15, 2019, Orlando, FL.**
  - Jordan, K. et al. “Experimental Study of Intermediate Storage and Discharge of Compressible Biomass Particulate Solids in a Wedge-Shaped Hopper of Changing Geometry”.
  - Bhattacharjee, T. et al. “Mechanical Properties and Bulk Flow Characterization of Loblolly Pine.”
  - Xia, Y. “Discrete Element Modeling of Granular Flow of Flexible Woody Biomass Particles”.
- **2019 The Society of Rheology Annual Meeting**
  - Stickel J. et al. “Parameter determination of the non-local granular fluidity model for wood chips by comparison to well-defined experimental flow systems.”
- **Engineering Mechanics Institute Conference 2019, June 18-21, 2019, Pasadena, CA.**
  - Xia, Y. et al. “Discrete Element Modeling of Granular Flow of Flexible Woody Biomass Particles”.
  - Jin, W. et al. “On the Implementation and Application of a Critical State Particle Mechanics Enhanced Drucker-Prager/Cap Model for Biomass Flow”.
- **2019 AIChE Annual Meeting, October 28 – November 2, 2018, Pittsburg, PA.**
  - Westover, T. et al. “Flow Behavior of Particulate Pine Forest Residues and Corn Stover: A Comparison of Experiments and Simulations”.

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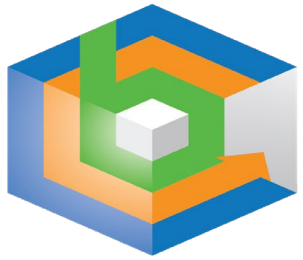
Presentations [Feedstock Conversion Interface Consortium]:

1. Xi Gao, Jia Yu, Liqiang Lu, Cheng Li, William A. Rogers. SuperDEM-CFD: Open Source Parallel Solver for Non-Spherical Particle-Fluid Fluidization Systems. 2020 Virtual AIChE Annual Meeting.
2. Xi Gao, Liqiang Lu, James E. Parks, Mehrdad Shahnam, Madhava Syamlal, Simulation-Based Engineering of Biomass Fast Pyrolysis Reactors, Session: Fluidization: In Honor of Stuart Daw (Invited Talks), 2020 Virtual AIChE Annual Meeting.
3. Xi Gao, Jia Yu, Ricardo J.F.Portal, William A.Rogers, Superquadric particle method for non-spherical DEM simulation in open source MFiX: development, implementation and verification. AIChE 2019 Annual Meeting, Orlando, Nov 2019.
4. Liqiang Lu, Xi Gao, Aytekin Gel, Mehrdad Shahnam, William A. Rogers. Influences of Biomass Compositions, Particle Sizes, and Fluidization Gases on Fast Pyrolysis. 2020 Virtual AIChE Annual Meeting.
5. Liqiang Lu, Xi Gao, Mehrdad Shahnam, William A. Rogers, Hybrid drag model for the simulation of biomass fast pyrolysis. AIChE 2019 Annual Meeting, Orlando, Nov 2019.
6. Gavin Wiggins, “Using Python to Model Biomass Pyrolysis Reactors”, SciPy 2019, Austin, TX, July 2019.
7. Zachary Mills, Xi Gao, Liqiang Lu, Gavin Wiggins, Charles Finney, Jim Parks, “Influence of Operating Parameters on Mixing and Elutriation in Fluidized Bed Pyrolysis Reactors”, 2019 Multiphase Flow Science Workshop, Morgantown, WV, August 2019.



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