U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Workshop on Predictive Models and High Performance Computing as Tools to Accelerate the Scale-up of New Bio-Based Fuels

June 9, 2020

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US Department of Energy

Bioenergy Technologies Office

Advanced Development and Optimization

Technology Manager

From Challenge to Opportunity

THE CHALLENGE

More than $215 million is spent **every day** on foreign oil **imports ($43/barrel/day in 2016*)**. Dependence on **foreign oil** can leave us vulnerable to disruptions in supplies and contributes significantly to our trade deficit.

Transportation accounts for 67% of petroleum consumption.

THE OPPORTUNITY

More than **1 billion tons of biomass** could be domestically converted into biofuels and products.

Biomass could displace up to **25%** of U.S. petroleum use annually by 2030, **keeping revenues in the United States**, adding **jobs,** and reducing annual CO_2 emissions**.

*Annual Energy Outlook 2017 with projections to 2050
eia.gov/outlooks/aeo/pdf/0383(2017).pdf

** Rogers et al. 2016, An assessment of the potential products and economic and environmental impacts resulting from a billion ton bioeconomy.
onlinelibrary.wiley.com/doi/10.1002/bbb.1728/full

Bioenergy Technologies Office's Mission and Vision

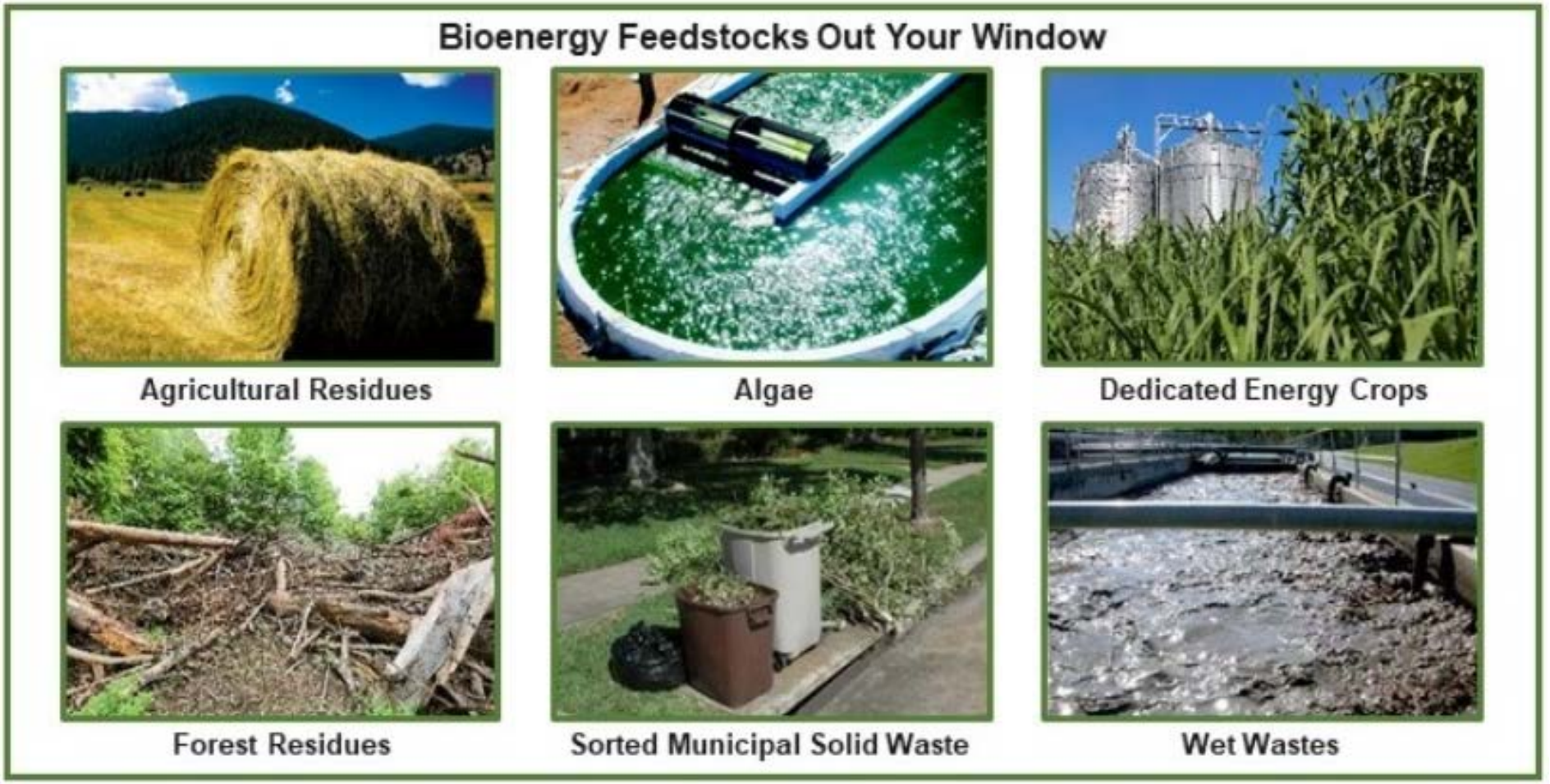
Vision: A thriving and sustainable bioeconomy fueled by innovative technologies

Mission: Developing transformative and revolutionary sustainable bioenergy and bioproducts technologies for a prosperous nation

Strategic Goals: Develop industrially relevant technologies to enable domestically produced biofuels, biopower, and bioproducts

BETO Reduces Technology Uncertainties and Enables Affordability Through R&D

Definition of Biomass



Bioenergy Technologies Office's Critical Program Areas

Production & Harvesting

Feedstock Supply & Logistics

Works to reduce the cost, improve the quality, and increase the volume of sustainable feedstocks available for delivery to a conversion process.

Advanced Algal Systems

Focuses on improving the productivity of algal biomass and enhancing the efficiency of cultivation and harvesting.

Conversion & Refining

Conversion

Develops technologies to convert non-food feedstocks into biofuels, bioproducts, and biopower.

Conducts feedstock blend testing, separations, materials compatibility evaluations, and techno-economic analyses to focus research on highest impacts.

Distribution & End Use

Advanced Development and Optimization

Aims to reduce technology uncertainty in bioenergy by integrating individual technologies into a system/process and provides vital knowledge fed back to research programs.

Crosscutting

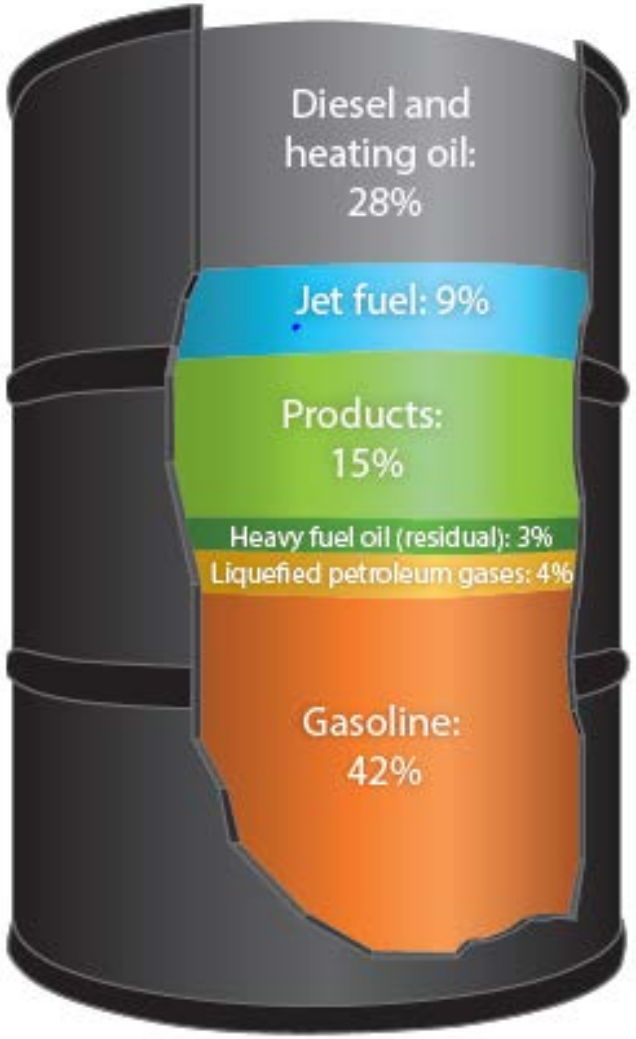
Sustainability and Strategic Analysis

Supports program decision-making and develops science-based strategies to understand and enhance the economic and environmental benefits of advanced bioenergy.

Replacing the Whole Barrel – Fuels & Products

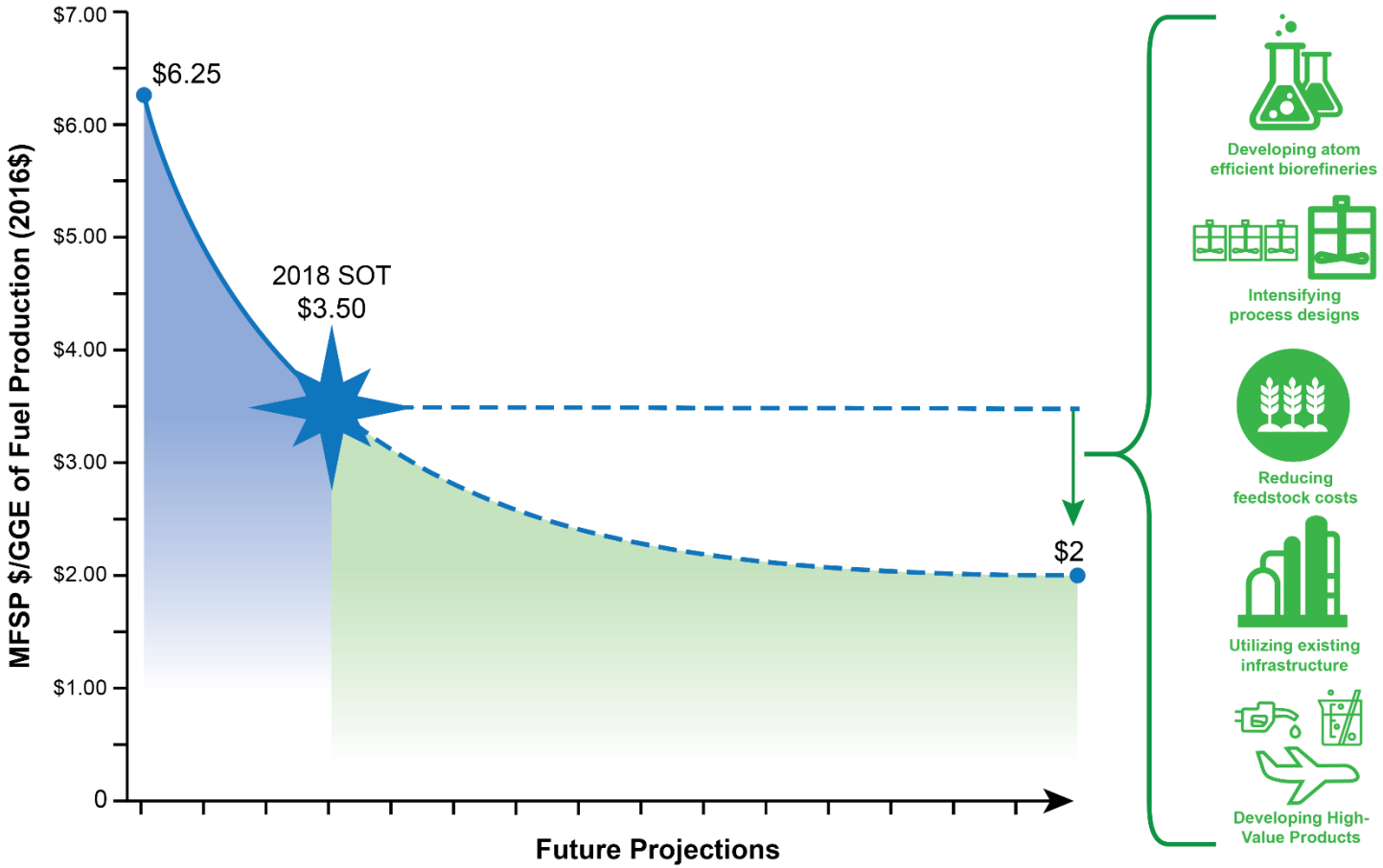
BETO R&D focuses on:

- Drop-in hydrocarbon biofuels
  - Gasoline
  - Diesel
  - Jet
- Bio-based products
  - Chemicals
  - Plastics
  - Waxes
  - Lubricants



Opportunities to Reach BETO Price Goals

BETO's goal $2.50/Gasoline Gallon Equivalent (GGE) by 2030



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Workshop Introduction

Over the past decade:

- Total investments in the scale-up of integrated biorefineries have exceeded $2 billion.
- Majority of these facilities are shut down or struggling
- Mathematical models representing the end-to-end process flow of an integrated biorefinery do not exist currently.
- BETO's past observations
  - Feedstocks are not well understood
  - Solids handling is not well understood
  - Understanding equipment is essential
  - Understanding integration of equipment is essential

Past BETO Observation

Feedstock variation should not be under estimated, associated quality and system specifications should all be understood prior to design:

"One of the single most important lessons learned from the project was the data gathered from compositional [analysis] of the feedstocks. The key message regarding feedstock composition is that it will vary. It will vary over the course of the growing season; it will vary due to harvest method; it will vary due to on-site staging/storage methods; and finally, it will change due to handling methods immediately prior to the conversion process."

– Verenium BioFuels Jennings Demonstration Plant Final Technical Report (EtOH from bagasse)

Past BETO Observation

Solids handling should not be under estimated and should be understood prior to design:

abrasion, flowability, bridging, channeling, particle size distribution, affects on rate of reaction, ash content, neutralization effects, etc.

Wear on SS316 auger from corn stover
(light wear – left & significant wear – right) FCIC peer review image

Channeling of corn stover
FCIC image

Past BETO Observation

Understanding equipment is essential

"Commercially available" equipment needs to be treated as if it is **new technology** if has not been demonstrated in the new function or at the new scale

Greater emphasis needs to be placed on the **risks associated** with **scaling up critical unit operations** and equipment from proof of concept/lab scale to 'next' scale designs

Select BETO Identified Lessons Learned

Understanding integration of equipment is equally essential

pressure differentials, entrance velocities, particle size distributions, rheology, reaction kinetics, materials of construction, etc.

Combining two well know unit operations in a new way can increase complexity and lead to operational issues

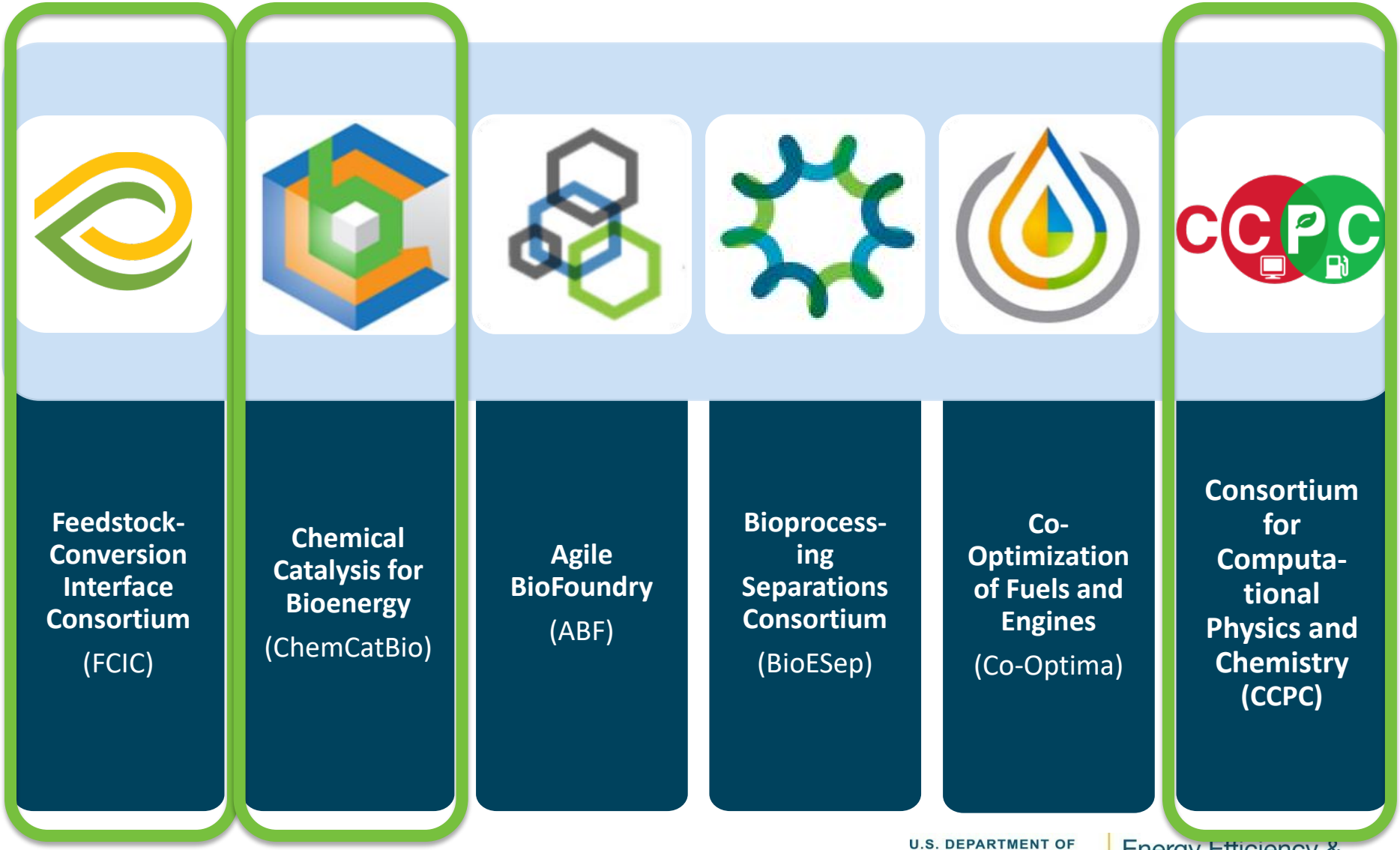
Systems Readiness Level (SRL), which quantifies maturity of technology integration in a system & overall system readiness should be at an adequate level prior to design

Workshop Introduction

Workshop on Predictive Models and High Performance Computing as Tools to Accelerate the Scaling-up of New Bio-Based Fuels

- The purpose of this workshop is to understand how modeling tools can be effectively utilized in conjunction with operational data to augment and accelerate scale-up and integration efforts and reduce scaling risk.
- Through the use of highly instrumented bench-, pilot-, and demonstration-scaled facilities along with high performance computing, artificial intelligence, and machine learning it may be possible to reduce technology uncertainty and accelerate scale-up.

Bioenergy Technologies Office's Consortia



Feedstock Conversion Interface Consortium (FCIC)

Quantify, understand, and manage variability in biomass from field through downstream conversion and to understand how biomass composition, structure, and behavior impacts system performance

Provide First Principles based knowledge related to unit operations

Provide transfer functions to bridge scales from bench to pioneer biorefinery

Provide valuation of intermediate streams which can be commoditized

TOOLS FOR TECHNOLOGY DEVELOPERS AND BIOREFINERY DESIGNERS

Sandia National Laboratories
BERKELEY LAB
Argonne NATIONAL LABORATORY
NREL NATIONAL RENEWABLE ENERGY LABORATORY
OAK RIDGE National Laboratory
INL Idaho National Laboratory
Pacific Northwest NATIONAL LABORATORY
Los Alamos NATIONAL LABORATORY EST. 1943
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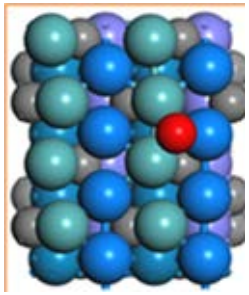
Chemical Catalysis for Bioenergy (ChemCatBio)

Research and development consortium dedicated to identifying and overcoming catalysis challenges for the conversion of biomass and waste resources into fuels, chemicals, and materials.

Accelerates the development of catalysts and related technologies for the production of fuels and chemicals derived from biomass and waste feedstocks.

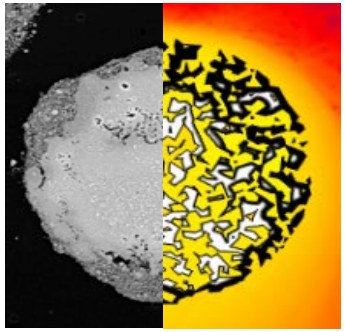
Consortium for Computational Physics and Chemistry (CCPC)

Atomic Scale Catalysis Modeling



Accelerating ChemCatBio catalyst development *by investigating novel catalyst material combinations and understanding surface chemistry phenomena to guide experimentalists*

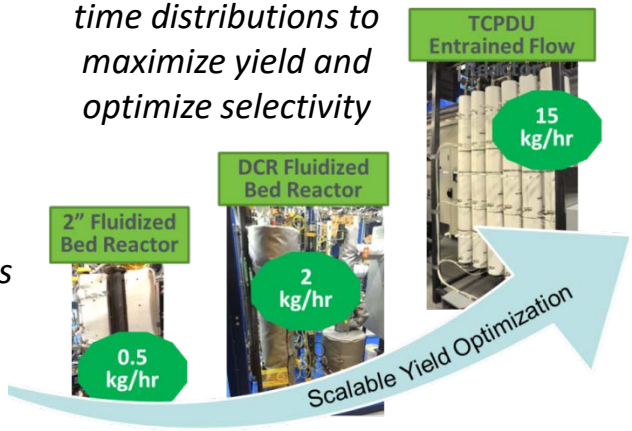
Meso Scale Particle Modeling



Addressing bio-complexity challenges *by understanding mass transport of reactants/products, reaction kinetics, and coking and deactivation processes*

Process Scale Reactor Modeling

Enabling scalability of ChemCatBio technology *via process residence time distributions to maximize yield and optimize selectivity*



OAK RIDGE National Laboratory · NREL National Renewable Energy Laboratory · National Energy Technology Laboratory · Argonne National Laboratory · Pacific Northwest National Laboratory · INL Idaho National Laboratory

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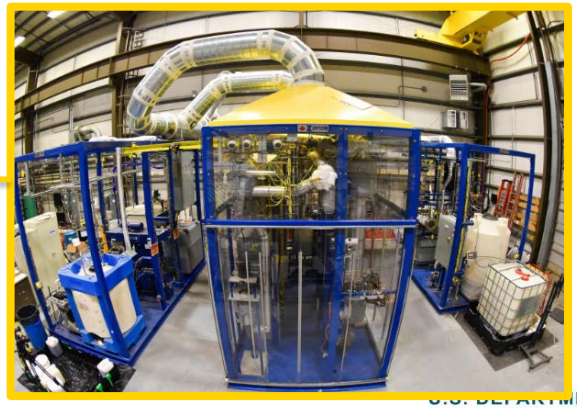
Bioenergy Technologies Office's PDUs

Process Development Units (PDUs)

- Integrated Biorefinery Research Facility (IBRF) - NREL
- Thermal and Catalytic Process Development Unit (TCPDU) – NREL
- Biomass Feedstock National User Facility (BFNUF) - INL
- Advanced Biofuels Process Demonstration Unit (ABPDU) - LBNL
- Modular Hydrothermal Liquefaction System (MHLS or HTL skid) - PNNL



BETO High Performance Computing

BETO has access to stacks within

- NREL's EAGLE
  - 8 petaflops
  - EERE specific High Performance Computer

- ORNL's Summit
  - 200 petaflops
  - Most powerful and smartest scientific supercomputer in the world

Workshop High Level Agenda

Tuesday, June 9

- Plenary 1 (10:30 ET – 1:30 ET): Webex
- Breakout Session 1 (2:00 ET – 4:30 ET): MeetingSphere

Wednesday, June 10

- Breakout Session 2, part 1 (10:30 ET – 1:00 ET): MeetingSphere
- Breakout Session 2, part 2 (2:00 ET – 4:00 ET): MeetingSphere

Thursday, June 11

- Breakout Session 3, (10:30 ET – 1:30 ET): MeetingSphere
- Plenary 2 (2:30 ET – 3:45 ET): Webex

Workshop Logistics

	Group A	Group B	Group C	Group D
Moderator	Marykate O'Brien	Mark Shmorhun	Liz Moore	Josh Messner
Facilitator	Remy Biron	Lauren Illing	Jeff Hood	Kelly Yee
Scribe	Ben Simon	Liz Burrows	Camryn Sorg	Colleen Tomaino
Volunteer Rapporteurs	Zia Abdullah, NREL	Mariefel Olarte, PNNL	Jim Parks, ORNL	Michael Thorson, PNNL

Questions

- Please type your question in the Chat box and we will try and get to as many as we can with the time remaining.

Speaker Introductions

Dr. Peter Ciesielski

- Principal Scientist
- Biosciences Center at the National Renewable Energy Laboratory

Modeling and Simulation for Bioenergy Applications: Challenges, Successes, and Lessons Learned

Speaker Introductions

Dr. Steven Lee

- Program Manager in Applied Mathematics and AI
- DOE's Advanced Scientific Computing Research (ASCR) program

Scientific Artificial Intelligence/Machine Learning

Workshop Logistics – Lauren Illing

- MeetingSphere Introduction.