ENABLING TOOLS AND FACILITIES FOR PRODUCTION OF BIOFUELS AND BIOPRODUCTS

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ADVANCED DEVELOPMENT AND OPTIMIZATION WORKSHOP

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ABOUT ARGONNE

- Argonne is managed by University of Chicago for DOE
- Argonne is a multidisciplinary science and engineering research center, to answer the biggest questions facing humanity from how to obtain affordable clean energy to protecting ourselves and our environment. Our goal has been to make an impact — from the atomic to the human to the global scale.

Lab at a Glance

3,206 total employees (FTEs)
268 postdoctoral scholars
582 graduate and undergrad students
256 joint faculty
7,422 facility users
1,005 visiting scientists

User Facilities

- Advanced Photon Source
- Argonne Leadership Computing Facility
- Argonne Tandem Linear Accelerator System
- Center for Nanoscale Materials
- Transportation Research and Analysis Computing Center

Research

14 research divisions
5 national scientific user facilities
Many centers, joint institutes, program offices
Hundreds of research partners
ADVANCED CATALYST CHARACTERIZATION

- Employ in situ/operando X-ray spectroscopic techniques to provide insight into the chemical and physical properties of catalysts that determine activity and selectivity under working conditions. The knowledge gained enables the catalyst synthetic effort within ACSC to develop new synthesis processes that maximize the critical properties that control catalyst performance.

- Working with other beamlines at the Advanced Photon Source to make new X-ray techniques, such as x-ray tomography and transmission x-ray microscopy, available to answer questions that X-ray absorption spectroscopy can not answer.

<table>
<thead>
<tr>
<th>Technique</th>
<th>Outcome</th>
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<tbody>
<tr>
<td>Ex situ</td>
<td>Compare before and after reaction spectra to identify changes in chemical and structural properties</td>
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<tr>
<td>In situ</td>
<td>Assess influence of catalyst pretreatment processes</td>
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<tr>
<td>Operando</td>
<td>Characterize catalyst in process conditions and relate chemical and structural properties to performance</td>
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POC: Ted Krause
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ADVANCED CATALYST SYNTHESIS

ALD Capabilities

- **Substrate size** (2”x18”), in situ QCM, QMS, FTIR, I-V
- 60” L x 6” dia. long tube ALD
- Beneq TFS500 –3D chamber, large substrates, scale-up, batch coating (15 x 300mm wafers)
- Oxford FlexAL PEALD, 8” wafers, auto-load, in situ ellipsometry and emission spectrometry

For catalysis work

Contact Information: Dr. Jeffrey Elam (jelam@anl.gov); Dr. Anil Mane (amane@anl.gov)
First principles predictive modeling for catalysis

- Provide guidelines for more efficient catalysts based on zeolites and molydenum carbides vapor upgrading of bio-oils
- Provide insights on the feasibility of conversion reactions and the selectivity towards desired intermediates associated with the carbonaceous materials. Uses high performance computing resources at the Argonne Leadership Computing facilities and Center of Nanoscale Materials.
- In silico discovery of catalysts and reaction engineering of conversion using metal clusters and 2-D materials

Developed atomistic models (Density Functional Theory) of Mo2C and Ni doped Mo2C catalytic sites and investigated their affinity towards oxygenated species. Based on the reactivity calculations, the superior stability of Ni doped Mo2C in the presence of oxygen was predicted. This result has been now been experimentally verified by ChemCatBio.

POC: Larry Curtiss
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LABSCALE SIMULATION OF TRIBOLOGICAL INTERACTIONS

Extensive use of labscale simulation to quantify performance of tribological systems – friction, wear, scuffing, fatigue

POC: George Fenske
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Diverse technologies poised to reduce separations costs:
• Functionalized membranes
• Nano-scaled adsorbents
• Resin wafer electrodeionization
MATERIALS ENGINEERING RESEARCH FACILITY (MERF)

- Decrease tech to market time.
- Enables commercial evaluation of new materials and accurate cost modeling.
- Evaluation of emerging manufacturing technologies can help lower costs and improve materials.
- Samples are available.

www.anl.gov/merf
POC: Greg Krumdick
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The GREET® (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model

- A publicly available LCA tool for consistently examining life-cycle energy and environmental effects of vehicle/fuel systems
  - Greenhouse gas emissions
  - Criteria pollutant emissions
  - Water consumptions
  - Energy use

**GREET 1 model:**
Fuel-cycle (or well-to-wheels, WTW) modeling of vehicle/fuel systems

**GREET 2 model:**
Vehicle cycle modeling for vehicles

POC: Michael Wang
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There are 30,000 registered GREET users globally.
An on-line interactive model for water use, water resource, and water quality assessment

**Feature**
- Water footprint at county level for the United States
- Feedstock production and conversion stages; biomass production volume distribution
- Land use: agriculture and forestry
- Metric: product, feedstock, land use

**Application**
- Analyzes multiple feedstock production in a region to support regional water resource planning and management and biorefinery location comparison.
- Enables compatible spatial resolution with POLYSYS, LEAF, FAPRI, and other models/tools, allowing analysis of the interplay of policy, economics, and environmental factors.
- Provides support to bioenergy industry, government, academia, and community for informed decision making.

POC: May Wu
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BETO-DOE

ARGONNE TEAM:
- Michael Wang
- Jeongwoo Han
- George Fenske
- Greg Krumdick
- May Wu
- Ted Krause
- Jeff Elam
ADDITIONAL SLIDES
Goal – develop analytic model of wear (abrasive) with capability to predict component/material wear based on biomass properties and equipment parameters.

**Model Development**

\[
\text{Wear Rate (m/s)} = (\text{Wear Coeff}) \times PV
\]

- **Wear Coefficient** considerations
  - Basic form – dependent on mechanism (abrasive, adhesive, fatigue, corrosion ...)
  - Dependent on elastic properties of ash/debris and stover (moisture)
  - Ash composition - properties
  - Ash debris density & size distribution
- **PV** considerations – contact pressure applied to ash/debris
  - Load and speed – operational parameters
  - Load sharing between stover and ash
  - Effect of moisture (lubricant)

**Abrasion Model Validation**

**Abrasion Test Rig**