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.

User Facilities

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

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

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

ADVANCED CATALYST CHARACTERIZATION

- Employ i*n 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.

Technique	Outcome
Ex situ	Compare before and after reaction spectra to identify changes in chemical and structural properties
In situ	Assess influence of catalyst pretreatment processes
Operando	Characterize catalyst in process conditions and relate chemical and structural properties to performance

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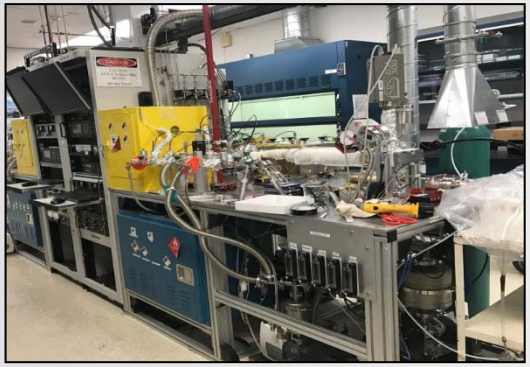
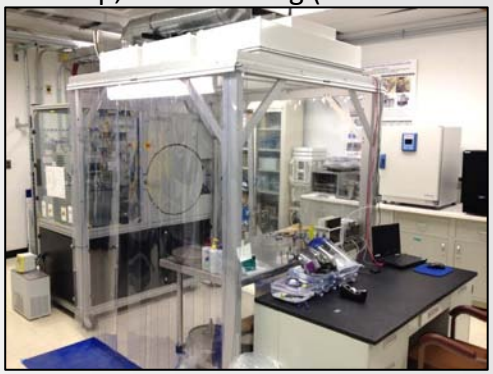
ADVANCED CATALYST SYNTHESIS

ALD Capabilities

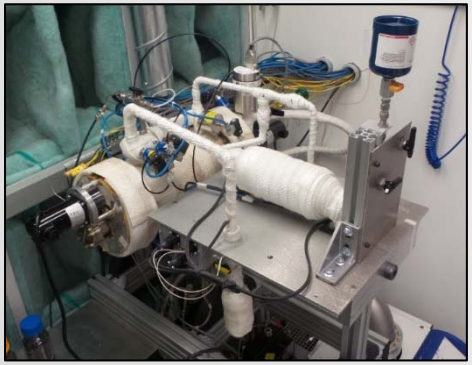
Substrate size (2”x18”), **in situ QCM, QMS, FTIR, I-V**



Beneq TFS500 –3D chamber, large substrates, scale-up, batch coating (15 x 300mm wafers)



(ALD powder coater 1 kg)



60” L x 6” dia. long tube ALD

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)

COMPUTATIONAL MODELING AND ANALYTICAL TOOLS

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 Mo_2C and Ni doped Mo_2C catalytic sites and investigated their affinity towards oxygenated species. Based on the reactivity calculations, the superior stability of Ni doped Mo_2C in the presence of oxygen was predicted. This result has been now been experimentally verified by ChemCatBio.

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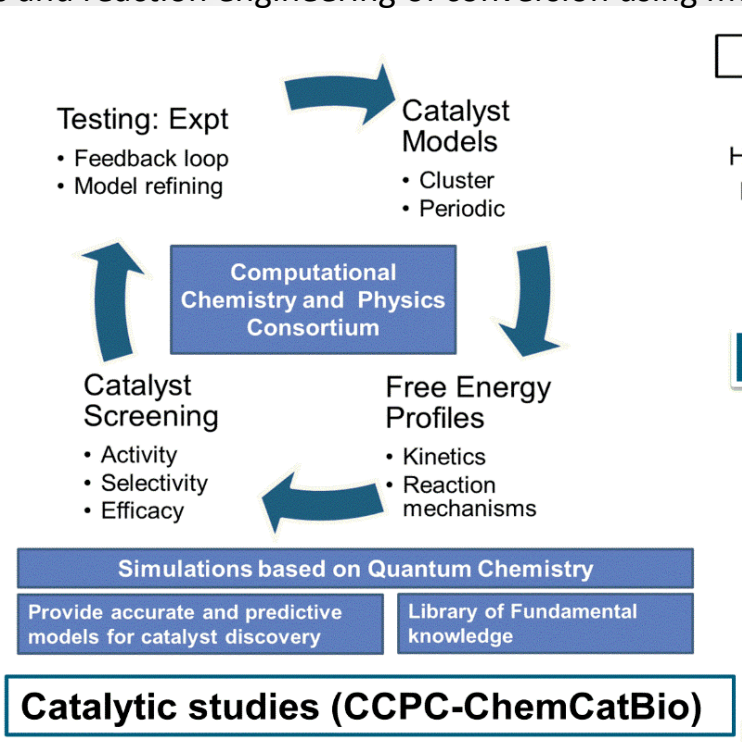
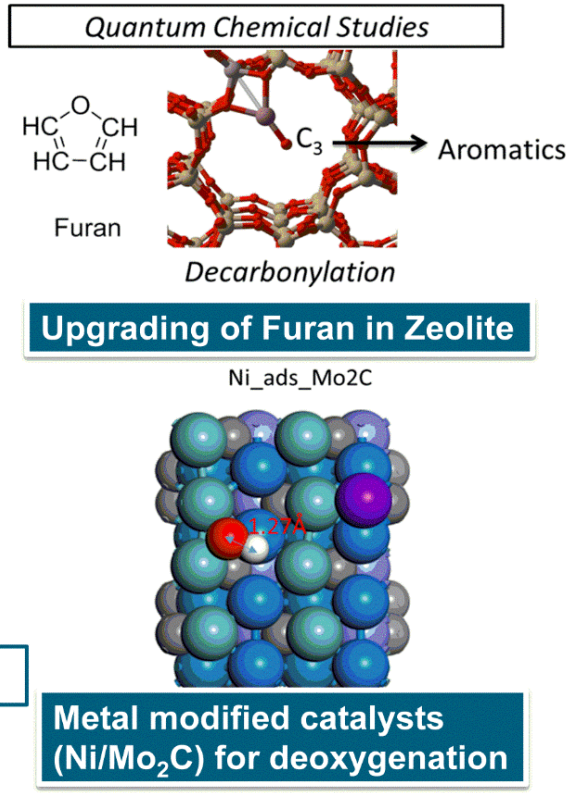




LABSCALE SIMULATION OF TRIBOLOGICAL INTERACTIONS

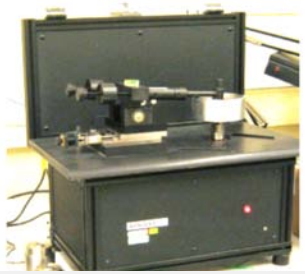
Extensive use of labscale simulation to quantify performance of tribological systems – friction, wear, scuffing, fatigue


PCS Gear/Bearing (micropitting test)

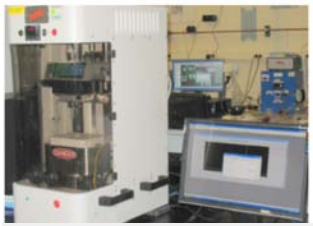

High-temp H_2/N_2/air


Block-on-ring scuffing machine

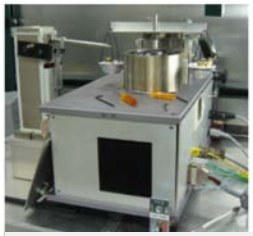

4-Ball EP Test Machine

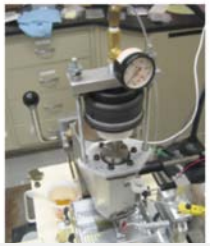

Pin on disk

Tribological Parameters – load, speed, humidity, temperature, environment, motion, materials, ….


Universal Tribometer


Ball-on-disk


High-temp ball-on-disk


Ring-on-liner


High-temp reciprocating

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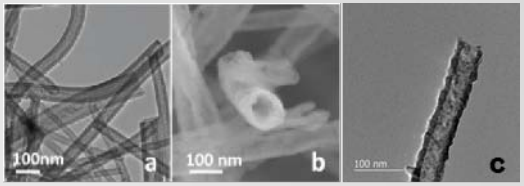
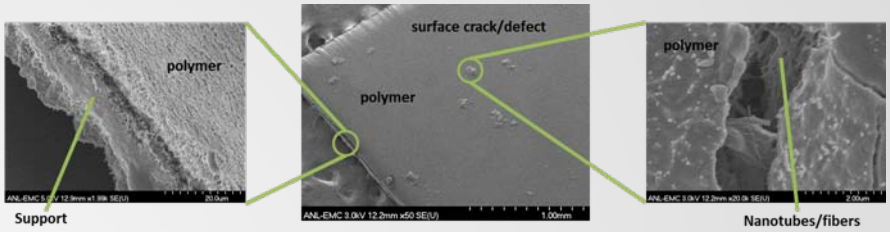
ADVANCED SEPARATIONS

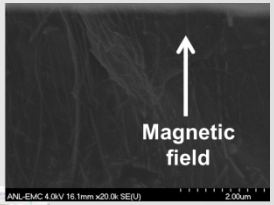
Diverse technologies poised to reduce separations costs:

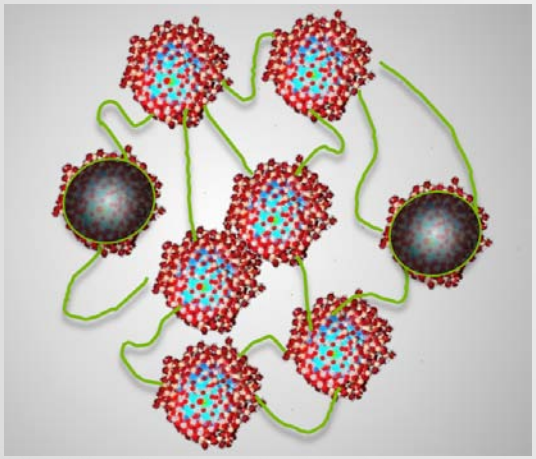
- Functionalized membranes
- Nano-scaled adsorbents
- Resin wafer electrodeionization

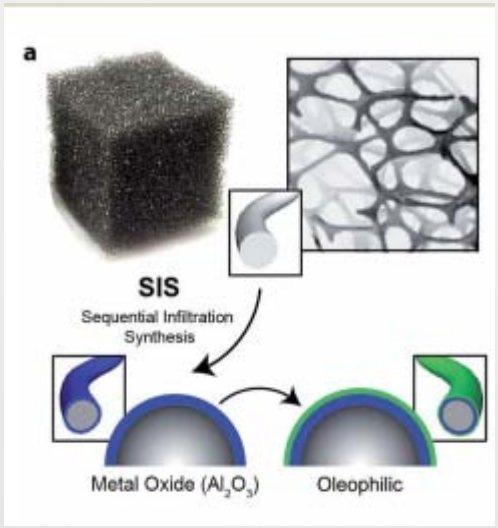


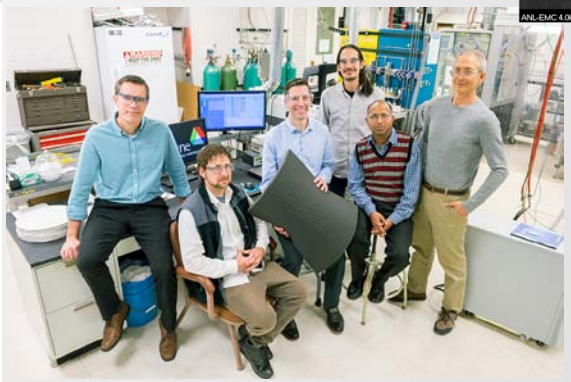
a) α-Fe_2O_3 b) Co and c) Fe_2CoO_4 NTs











R&D 100 2017 Winner

Oleo Oil Adsorbents

Nanosorbents

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
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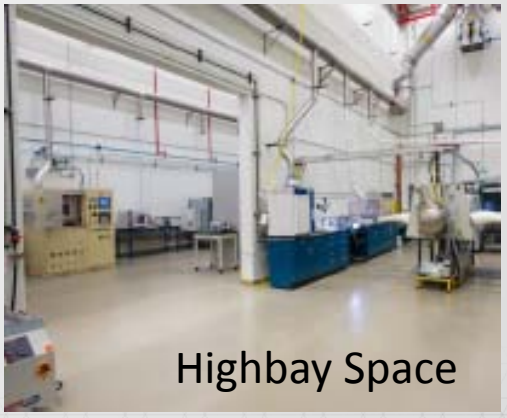
Bench Labs


Pilot Labs

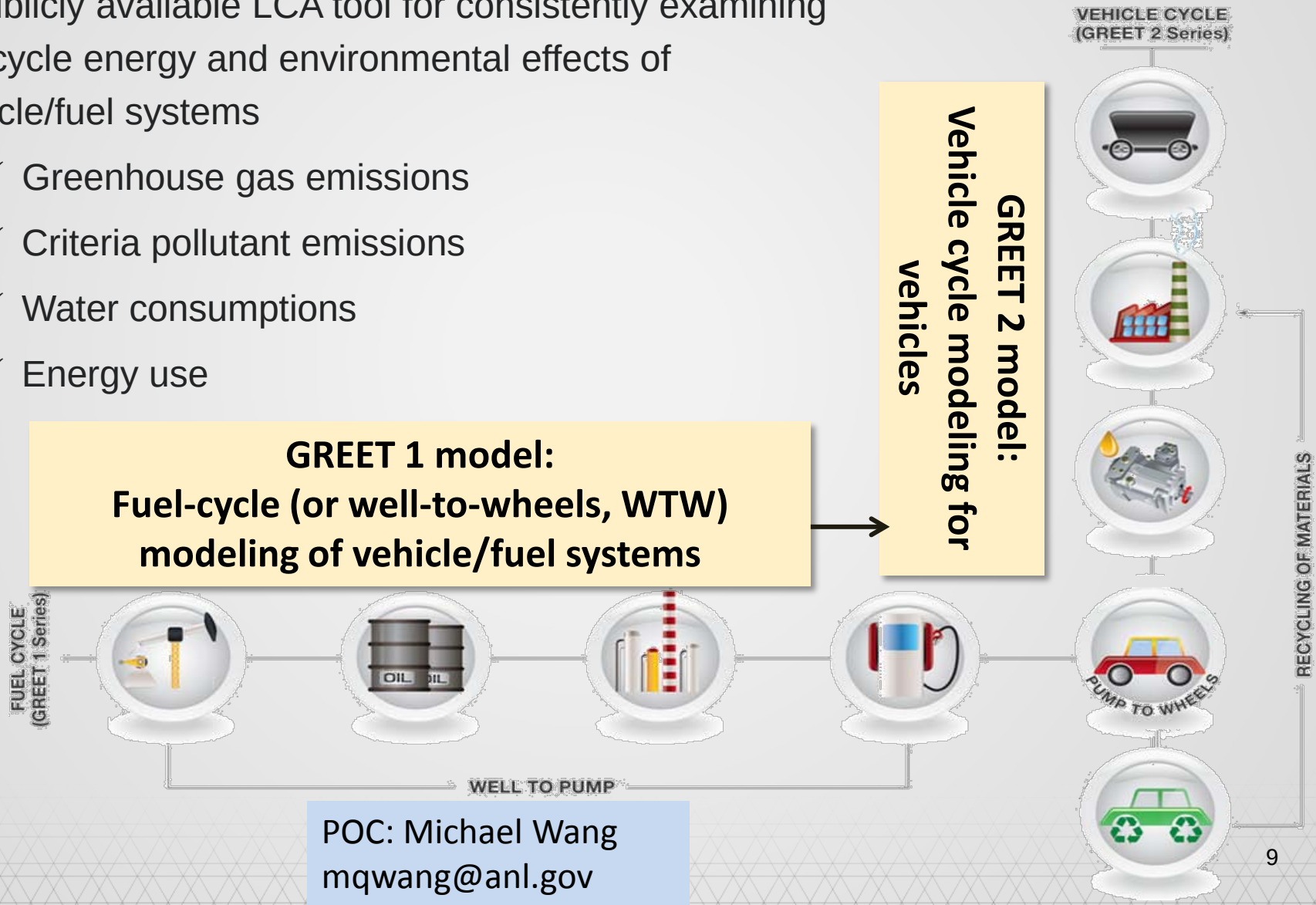

Highbay Space

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



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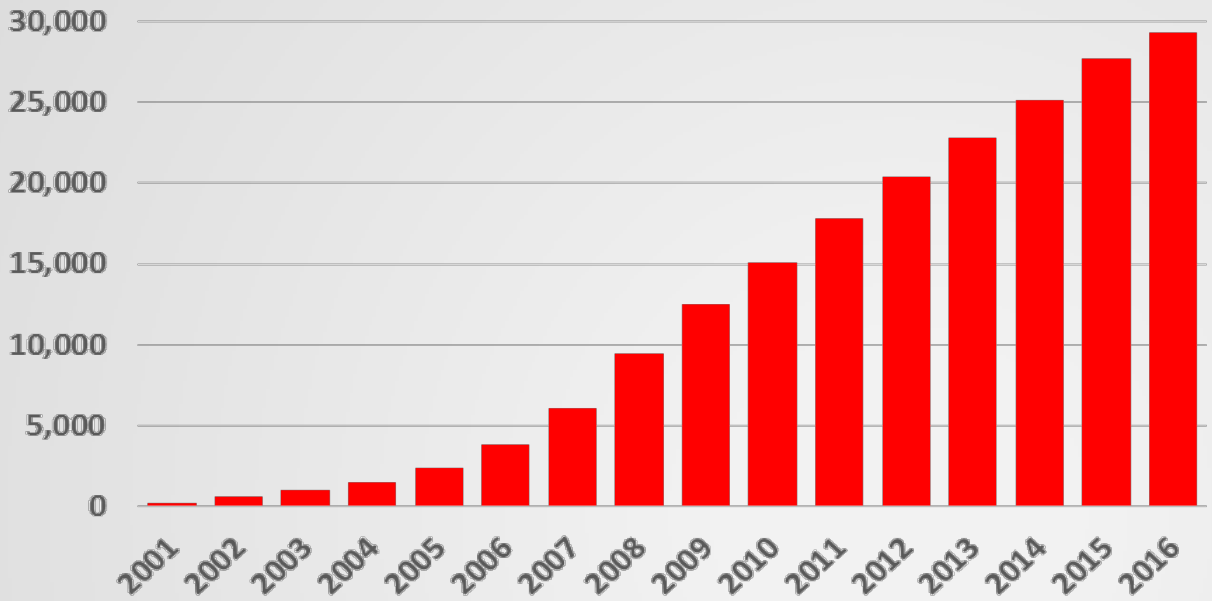
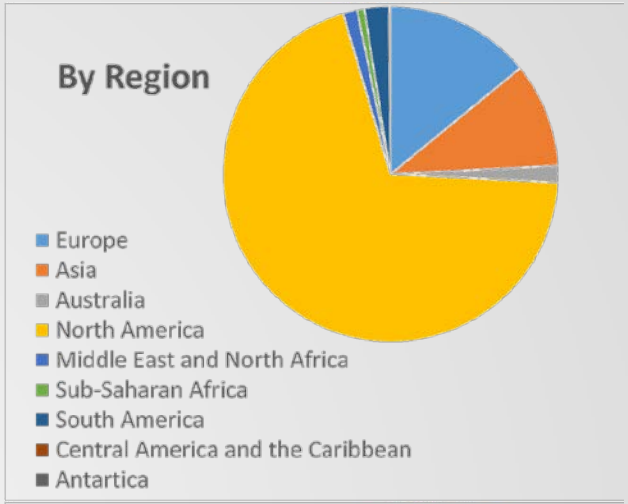
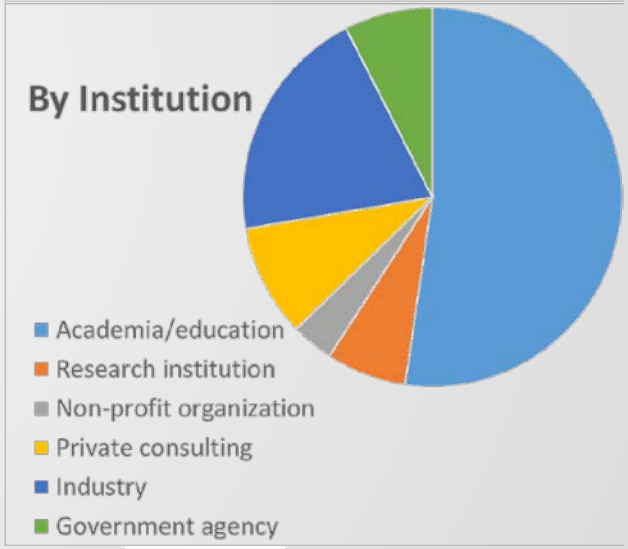
There are 30,000 registered GREET users globally



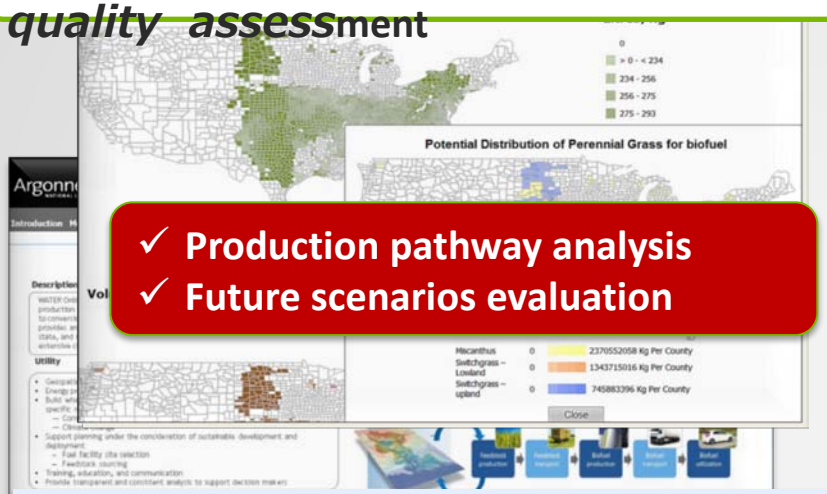




WATER (Water Analysis Tool for Energy Resources)

http://WATER.es.anl.gov

An on-line interactive model for water use, water resource, and water quality assessment



✓ **Production pathway analysis**
✓ **Future scenarios evaluation**

- Corn grain & stover, soy bean, wheat straw
- Switchgrass and Miscanthus
- Forest wood (hard, soft) resource
- SRWC (willow, hybrid poplar, pine)
- Ethanol, biodiesel, renewable diesel blend, mixed alcohol blend
- *Electricity (fossil, renewable)*
- *Petroleum (conventional, oil sands)*
- *Natural gas*

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.

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OFFICE OF SCIENCE-DOE

BETO-DOE

ARGONNE TEAM:

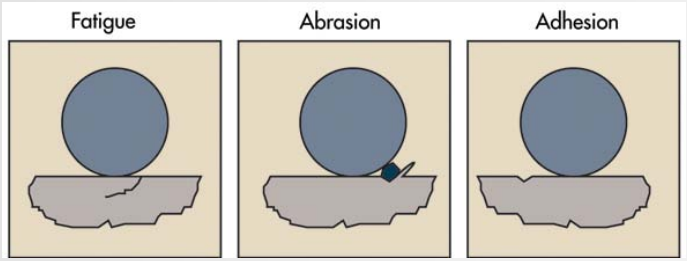
- Michael Wang
- Jeongwoo Han
- George Fenske
- Greg Krumdick
- May Wu
- Ted Krause
- Jeff Elam

ADDITIONAL SLIDES

PROCESS MODELLING AND SIMULATION

Goal – develop analytic model of wear (abrasive) with capability to predict component/material wear based on biomass properties and equipment parameters

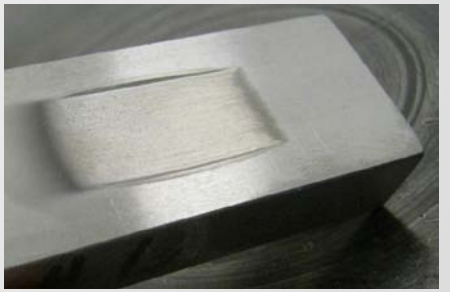
Model Development



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

- **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