Outline

• Conversion Team Introduction
• Conversion Goals and Approaches
• Portfolio Structure, Challenges, and Budget
• FOA and Other Awards
• Accomplishments and Direction
• New and expanded R&D Areas
• Review Panel Introduction
Conversion R&D Team – DOE and Fellows

Kevin Craig, Program Manager

**DOE Staff**

David Babson
Jay Fitzgerald
Nichole Fitzgerald
Beau Hoffman
Ian Rowe
Liz Moore*

**ORISE Fellows**

Andrea Bailey
Jeremy Leong

*ORISE Fellow
Conversion R&D Team – Support Contractors

Conversion Support Contractors

Josh Messner - AST, Manager
Mark Philbrick – AST
Jessica Phillips – AST
Clayton Rohman – AST
Trevor Smith – AST
Seth Menter - AST
Robert Natelson – AST
Camryn Sorg – The Building People, LLC
• **BETO Strategic Goal:** *Enable use of America’s abundant biomass and waste resources for advanced biofuels, bioproducts, and biopower by:*
  
  – Identifying and developing biofuel pathways and innovative end uses;
  – Lowering the cost of production through increased efficiency, productivity, and yields; and
  – Completing applied research and development on complex, real world systems, and integrating engineering processes for promising new advanced bioenergy technologies

*while maintaining or enhancing economic, environmental, and social sustainability.*
Conversion R&D – Goals and Approaches

• **Conversion R&D Goal:** Develop efficient and economical biological and chemical technologies to convert biomass feedstocks into energy-dense liquid transportation fuels, such as renewable gasoline, diesel, and jet fuel, as well as bioproducts, chemical intermediates, and biopower.

**Approaches:**
• Enhance U.S. industrial competitiveness by reducing time-to-market, improving yields, and increasing selectivity
• Fund research that supports a diversity of biochemical, thermochemical, and hybrid conversion technologies to match the distributed, diverse, domestic resources
• Leverage biological pathway engineering science
• Develop better catalysts and organisms faster through applied science

*Price-competitive technologies for converting biomass into fuels and products*
PORTFOLIO STRUCTURE AND BUDGET
Pathways are collections of technologies and interfaces
Program Structure

Deconstruction & Fractionation
- Feedstock Interface
- High-Temperature Deconstruction
- Low-Temperature Deconstruction
- Fractionation, Cleanup, & Conditioning

Synthesis & Upgrading
- Chemical Conversions to Intermediates & Products
- Biological Conversions to Intermediates & Products
- Cleanup or Finishing
- Hybrid Conversions to Intermediates & Products

Enabling Technologies
- Computational Modeling & Analytical Tools
- Standards & Methods Development
- Systems Biology
- Design & Discovery of New Catalysts/Enzymes
- Advanced Separations
- Novel Technologies

Pathway-focused R&D
The Challenge: How can BETO enable cost-competitive (<$3/GGE) lignocellulosic biofuels in the near term (~5-10 years)?

We annually model and periodically verify 6 lignocellulosic biofuel pathways

The average MSFP at nth plant is $3.36/GGE

Can bioproducts be the thin edge of the wedge?

“An assessment of the potential products and economic and environmental impacts resulting from a billion ton bioeconomy” Biofuels, Bioprod. Bioref. 11:110–128 (2017). Z Haq (BETO) and partners at USDA, Energetics, AST, and ANL
The Challenge: Cost and Time to Market

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Company</th>
<th>Cost</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3-Propanediol (PDO)</td>
<td>DuPont - Tate &amp; Lyle</td>
<td>&gt;&gt;$120M</td>
<td>15 years</td>
</tr>
<tr>
<td>Artemisinin</td>
<td>UC Berkeley, Amyris, Sanofi</td>
<td>&gt;$50M</td>
<td>10 years</td>
</tr>
</tbody>
</table>

Possible savings of billions of dollars by reducing development time of products, reducing energy intensity and increasing carbon efficiency.
Total Conversion Budget by FY for the Review Period

FY17: $80,000,000
FY18: $105,000,000
FY19: $90,000,000
Portfolio Overview – National Lab Work FY17-FY19

<table>
<thead>
<tr>
<th>Enabling Technologies</th>
<th>Pathway Specific</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABF</td>
<td>FCIC</td>
</tr>
<tr>
<td>Analysis + Analytical Methods</td>
<td>PDUs + Co-processing</td>
</tr>
<tr>
<td>Biological Pathways</td>
<td>CO2, WTE, Novel Feedstocks</td>
</tr>
<tr>
<td>CCB</td>
<td>Separations</td>
</tr>
<tr>
<td>CCPC</td>
<td>Lignin</td>
</tr>
<tr>
<td>PABP</td>
<td></td>
</tr>
</tbody>
</table>

ABF: $47,800,000  
Analysis + Analytical Methods: $14,700,000  
Biological Pathways: $24,500,000  
CCB: $32,600,000  
CCPC: $13,250,000  
FCIC: $10,800,000  
PABP: $4,340,000  
CO2, WTE, + Other Novel Feedstocks: $15,000,000  
Lignin: $10,700,000  
Separations: $10,750,000  
PDUs + Co-processing: $12,500,000
Portfolio Overview – Including Awarded Competitive Funds
FY17-FY19

<table>
<thead>
<tr>
<th>Category</th>
<th>Awarded Funds</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABF</td>
<td>$60,300,000</td>
</tr>
<tr>
<td>Analysis + Analytical Methods</td>
<td>$14,700,000</td>
</tr>
<tr>
<td>Biological Pathways</td>
<td>$24,500,000</td>
</tr>
<tr>
<td>CCB</td>
<td>$40,400,000</td>
</tr>
<tr>
<td>CCPC</td>
<td>$13,250,000</td>
</tr>
<tr>
<td>FCIC</td>
<td>$10,800,000</td>
</tr>
<tr>
<td>PABP</td>
<td>$13,340,000</td>
</tr>
<tr>
<td>CO2, WTE, + Other Novel Feedstocks</td>
<td>$26,000,000</td>
</tr>
<tr>
<td>Lignin</td>
<td>$15,200,000</td>
</tr>
<tr>
<td>Separations</td>
<td>$10,750,000</td>
</tr>
<tr>
<td>PDUs + Co-processing</td>
<td>$12,500,000</td>
</tr>
</tbody>
</table>

Enabling Technologies
Pathway Specific

$1M
Portfolio Structure

149 total Conversion portfolio projects to be reviewed over the next four days:

- 27 in the Biochemical Review Session
- 10 in the ABF Review Session
- 24 in the Catalysis Review Session
- 11 in the Waste to Energy (WTE) Session
- 14 in the PABP/Seps Review Session
- 11 in the Lignin Review Session
- 7 in the CO2 Review Session
- 32 in the Poster Session
- 12 in additional review sessions from other programs
Portfolio Structure and Budget

Amount Appropriated During Review Period by Recipient Type (numbers rounded)

FY15-16
- National Labs, $126,491,000
- Industry, $19,200,000
- Research Institutes, $1,900,000
- Academia, $4,000,000

FY17-18
- Directly Funded Lab/Industry Agreements, $11,300,000
- National Labs - Direct Funding, $131,630,000
- Industry, $14,000,000
- Academia, $17,000,000
- National Labs - Subrecipients to Competitive Awards, $8,000,000

Industry, $19,200,000
Research Institutes, $1,900,000
Academia, $4,000,000
National Labs, $126,491,000
Ex-situ CFP

% Change to MFSP from the ex situ base case ($3.31/GGE)
### Ex-situ CFP

<table>
<thead>
<tr>
<th>Rank</th>
<th>Description</th>
<th>Max Impact (negative)</th>
<th>Max Impact (positive)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Total Capital Investment</td>
<td>-8.0%</td>
<td>16.1%</td>
</tr>
<tr>
<td>2</td>
<td>Feedstock Cost $/dry US ton</td>
<td>-7.8%</td>
<td>15.7%</td>
</tr>
<tr>
<td>3</td>
<td>Internal IRR</td>
<td>-14.8%</td>
<td>15.4%</td>
</tr>
<tr>
<td>4</td>
<td>HGF Capital Cost</td>
<td>-0.0%</td>
<td>15.2%</td>
</tr>
<tr>
<td>5</td>
<td>Ex-Situ Organic Liq Yield</td>
<td>-8.1%</td>
<td>11.6%</td>
</tr>
<tr>
<td>6</td>
<td>Plant Size</td>
<td>-10.0%</td>
<td>8.1%</td>
</tr>
<tr>
<td>7</td>
<td>Vapor Upgrading Catalyst Unit Cost</td>
<td>-6.4%</td>
<td>9.6%</td>
</tr>
<tr>
<td>8</td>
<td>Fast Py &amp; Ex Situ Reactor Capital</td>
<td>-4.6%</td>
<td>9.2%</td>
</tr>
<tr>
<td>9</td>
<td>Hydroprocessing C Efficiency</td>
<td>-0.0%</td>
<td>9.0%</td>
</tr>
<tr>
<td>10</td>
<td>Interest Rate on Debt</td>
<td>-5.3%</td>
<td>5.6%</td>
</tr>
<tr>
<td>11</td>
<td>Vapor Upgrading Catalyst Replacement</td>
<td>-2.7%</td>
<td>5.3%</td>
</tr>
<tr>
<td>12</td>
<td>Plant Life</td>
<td>-0.0%</td>
<td>4.1%</td>
</tr>
<tr>
<td>13</td>
<td>Ex Situ Catalyst Biomass with Circulation</td>
<td>-0.0%</td>
<td>3.9%</td>
</tr>
<tr>
<td>14</td>
<td>Hot Gas Filter, Capital Cost</td>
<td>-0.0%</td>
<td>3.2%</td>
</tr>
<tr>
<td>15</td>
<td>Hydrogen Plant Capital</td>
<td>-2.0%</td>
<td>3.0%</td>
</tr>
<tr>
<td>16</td>
<td>Time on Stream</td>
<td>-2.5%</td>
<td>2.7%</td>
</tr>
<tr>
<td>17</td>
<td>Steam and Power Plant Capital</td>
<td>-1.5%</td>
<td>2.3%</td>
</tr>
<tr>
<td>18</td>
<td>Hydrotreating Catalyst Unit Cost</td>
<td>-0.6%</td>
<td>2.2%</td>
</tr>
<tr>
<td>19</td>
<td>Hydroprocessing and Separation Capital</td>
<td>-1.0%</td>
<td>2.1%</td>
</tr>
<tr>
<td>20</td>
<td>C Loss as Coke with Constant Organic Liquid Yield</td>
<td>-0.4%</td>
<td>1.2%</td>
</tr>
<tr>
<td>21</td>
<td>Wastewater Management Capital</td>
<td>-0.4%</td>
<td>1.0%</td>
</tr>
<tr>
<td>22</td>
<td>No Vapor Heat Recovery Below Temp</td>
<td>-0.0%</td>
<td>0.9%</td>
</tr>
<tr>
<td>23</td>
<td>Electricity Credit Impact</td>
<td>-0.0%</td>
<td>0.8%</td>
</tr>
<tr>
<td>24</td>
<td>Hydroprocessing Catalyst Unit Cost</td>
<td>-0.2%</td>
<td>0.7%</td>
</tr>
<tr>
<td>25</td>
<td>Number of HT Reactors x %Capacity</td>
<td>-0.0%</td>
<td>0.7%</td>
</tr>
<tr>
<td>26</td>
<td>Heat Loss During Pyrolysis Vapor Upgrading</td>
<td>-0.0%</td>
<td>0.4%</td>
</tr>
<tr>
<td>27</td>
<td>Hydrotreating Pressure</td>
<td>-0.0%</td>
<td>0.1%</td>
</tr>
</tbody>
</table>

Items either not directly tied to BETO R&D or influenced by progress in the bioenergy industry as a whole were eliminated.
### Ex-situ CFP

**Top 10 remaining areas by current active project:**

<table>
<thead>
<tr>
<th>Rank</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Feedstock Cost $/dry US ton</td>
</tr>
<tr>
<td>4</td>
<td>HGF Capital Cost + Yield C Efficiency</td>
</tr>
<tr>
<td>5</td>
<td>Ex-Situ Organic Liquid Yield</td>
</tr>
<tr>
<td>7</td>
<td>Vapor Upgrading Catalyst Unit Cost</td>
</tr>
<tr>
<td>8</td>
<td>Fast Py &amp; Ex Situ Reactor Capital</td>
</tr>
<tr>
<td>9</td>
<td>Hydroprocessing C Efficiency</td>
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<tr>
<td>11</td>
<td>Vapor Upgrading Catalyst Replacement</td>
</tr>
<tr>
<td>13</td>
<td>Ex Situ Catalyst Biomass with Circulation</td>
</tr>
<tr>
<td>15</td>
<td>Hydrogen Plant Capital</td>
</tr>
<tr>
<td>16</td>
<td>Time on Stream</td>
</tr>
</tbody>
</table>

- **FSL Core Work (INL, ORNL)**
- **Ex-Situ CFP (NREL, PNNL)**
- **Advanced Catalyst Synthesis and Characterization (NREL, ORNL, ANL)**
- **CCPC (ORNL, NREL, ANL, PNNL, NETL)**
- **TCPDU (NREL)**
- **Corrosion Studies (ORNL)**
- **Bio-Oil Standardization (NREL, PNNL)**
- **Potential Biopower Selections**
## Ex-situ CFP

### Top 10 remaining areas by FY17 investment:

<table>
<thead>
<tr>
<th>Rank</th>
<th>Description</th>
<th>FY17 Investment ($K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Feedstock Cost $/dry US ton</td>
<td>$1,600</td>
</tr>
<tr>
<td>4</td>
<td>HGF Capital Cost + Yield C Efficiency</td>
<td>$4,000</td>
</tr>
<tr>
<td>5</td>
<td>Ex-Situ Organic Liquid Yield</td>
<td>$4,750</td>
</tr>
<tr>
<td>7</td>
<td>Vapor Upgrading Catalyst Unit Cost</td>
<td>$7,925</td>
</tr>
<tr>
<td>8</td>
<td>Fast Py &amp; Ex Situ Reactor Capital</td>
<td>$7,550</td>
</tr>
<tr>
<td>9</td>
<td>Hydroprocessing C Efficiency</td>
<td>$4,750</td>
</tr>
<tr>
<td>11</td>
<td>Vapor Upgrading Catalyst Replacement</td>
<td>$7,925</td>
</tr>
<tr>
<td>13</td>
<td>Ex Situ Catalyst Biomass with Circulation</td>
<td>$7,925</td>
</tr>
<tr>
<td>15</td>
<td>Hydrogen Plant Capital</td>
<td>$0</td>
</tr>
<tr>
<td>16</td>
<td>Time on Stream</td>
<td>$7,550</td>
</tr>
</tbody>
</table>
FOA and Direct Funding Opportunities
On May 5, 2018 the U.S. Department of Energy (DOE) announced a FOA to support R&D to develop highly efficient conversion processes for improving the affordability of fuels and products from biomass and waste streams.

**FOA Topic Areas:**
- **Topic Area 1:** ChemCatBio Industrial Partnerships (CCB)
- **Topic Area 2:** Agile BioFoundry Industry Partnership Initiative (ABF)
- **Topic Area 3:** Performance Advantaged Bioproducts (PABP)
- **Topic Area 4:** Biofuels and Bioproducts from Wet Organic Waste Streams
- **Topic Area 5:** Rewiring Carbon Utilization (Rewiring)
- **Topic Area 6:** Lignin Valorization (Lignin)

**Funding Amount:** Up to $28,000,000

**Contributions to BETO’s mission:**
- R&D to increase efficiency of conversion to drive down cost of biofuels and bioproducts
- Increases industry access to capabilities to improve biofuel and bioproduct production and management through partnerships with DOE’s Agile BioFoundry and ChemCatBio
- R&D in valorizing residual side streams through lignin valorization
- R&D on leveraging waste as an untapped resource with economic advantages
Bioprocessing Separations Consortium CRADA/DFO Partnerships

- Separations for Biochemical Conversion – Developed in situ product recovery system to extract carboxylic acids from fermentation broth utilizing solvent/membrane systems and increased acid product concentration ~6x
- Separations for Thermochemical Conversion – Developed functionalized resins and molecular sieves that exceeded FY18 target of 25% carbonyl reduction in liquid pine bio-oils

- Directed Funding Opportunity

<table>
<thead>
<tr>
<th>Company w/ Labs</th>
<th>Feedstock</th>
<th>Separations</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Visolis w/ ANL &amp; LBNL</td>
<td>Cellulosic Sugar</td>
<td>RW-EDI, wiped film distillation</td>
<td>fatty acid</td>
</tr>
<tr>
<td>Kalion w/ ORNL, ANL &amp; NREL</td>
<td>Cellulosic Sugar</td>
<td>pervaporation, RW-EDI, nano-adsorbents</td>
<td>Glucaric acid</td>
</tr>
<tr>
<td>Mango Materials w/ LBNL</td>
<td>Biogas</td>
<td>Tangential Flow Filtration</td>
<td>PHAs from methanotrophs</td>
</tr>
<tr>
<td>DMC Biotechnologies w/ ANL</td>
<td>Cellulosic Sugar</td>
<td>Nano-adsorbents</td>
<td>Farnesene, liquid hydrocarbons</td>
</tr>
<tr>
<td>HelioBioSys w/ LANL &amp; LBNL</td>
<td>Atmospheric CO₂</td>
<td>Ultrasonic Separations</td>
<td>Extracellular polysaccharides from cyanobacterial consortium</td>
</tr>
</tbody>
</table>
## Agile BioFoundry CRADA/DFO Partnerships

<table>
<thead>
<tr>
<th>Company</th>
<th>Labs</th>
<th>Feedstock</th>
<th>Organism</th>
<th>Capabilities</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kiverdi</td>
<td>NREL, LBNL, ORNL</td>
<td>CO₂ and H₂</td>
<td><em>Cupriavidus necator</em></td>
<td>Design: DIVA, Test: targeted –omics and biocatalyst optimization</td>
<td>Fatty-acid derived molecule</td>
</tr>
<tr>
<td>LanzaTech</td>
<td>ANL &amp; NREL</td>
<td>Syngas &amp; Waste Gas</td>
<td><em>Clostridium autoethanogenum</em></td>
<td>Learn: machine learning and deep learning</td>
<td>Various chemicals and fuels</td>
</tr>
<tr>
<td>Lygos</td>
<td>SNL, LBNL, PNNL</td>
<td>Cellulosic Sugar</td>
<td><em>Pichia kudriavzeii</em></td>
<td>Design: DIVA, Build, Test: Proteomics, Metabolomics, Experiment Data Depot</td>
<td>Organic acid</td>
</tr>
<tr>
<td>TeselaGen</td>
<td>LBNL, PNNL, SNL</td>
<td>NA</td>
<td>NA</td>
<td>Design: BOOST, BLISS; Test: Experiment Data Depot</td>
<td>NA</td>
</tr>
<tr>
<td>Visolis</td>
<td>NREL, ORNL</td>
<td>Cellulosic Sugar and Waste Gas</td>
<td><em>Clostridium ljungdahli</em></td>
<td>Build: Genetic Transformation and Tool Development</td>
<td>Hydroxyacid intermediate</td>
</tr>
<tr>
<td>University of Georgia</td>
<td>LANL, NREL</td>
<td>Cellulosic Sugar</td>
<td><em>Acinetobacter baylyi ADP1</em></td>
<td>Test: Biocatalyst Optimization, High Throughput Screening</td>
<td>Terephthalic acid</td>
</tr>
</tbody>
</table>
## ChemCatBio CRADA/DFO Partnerships

<table>
<thead>
<tr>
<th>Company</th>
<th>Labs</th>
<th>CCB Capabilities</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>GEVO (mixed oxide)</td>
<td>NREL, ANL, ORNL</td>
<td>Characterization</td>
<td>C₃-C₄ olefins</td>
</tr>
<tr>
<td>Visolis</td>
<td>NREL</td>
<td>Synthesis, Evaluation</td>
<td>Diols</td>
</tr>
<tr>
<td>Vertimass</td>
<td>NREL, ANL, ORNL</td>
<td>Characterization</td>
<td>Hydrocarbon fuels</td>
</tr>
<tr>
<td>Lanzatech (Terephthalic Acid)</td>
<td>PNNL</td>
<td>Synthesis, Characterization, Evaluation, Modeling</td>
<td>Terephthalic acid</td>
</tr>
<tr>
<td>GEVO (Tactical Aviation Fuels)</td>
<td>LANL</td>
<td>Synthesis, Characterization, Evaluation, Modeling</td>
<td>Cyclobutanes</td>
</tr>
<tr>
<td>ALD Nanosolutions and JM</td>
<td>NREL</td>
<td>Synthesis, Characterization, Evaluation, Modeling</td>
<td>Hydrocarbons</td>
</tr>
<tr>
<td>Lanzatech (Fuel Fractions)</td>
<td>PNNL</td>
<td>Evaluation, Modeling</td>
<td>Jet fuel</td>
</tr>
<tr>
<td>Opus-12</td>
<td>NREL</td>
<td>Synthesis, Characterization, Evaluation</td>
<td>Alcohols</td>
</tr>
<tr>
<td>Sironix Renewables</td>
<td>LANL</td>
<td>Synthesis, Characterization, Evaluation, Modeling</td>
<td>Oleo-furan surfactants</td>
</tr>
</tbody>
</table>
Accomplishments & Direction
Achieved FY2017 Office Performance Metric

• $3/gge Modeled, Mature-plant Fuel Price (plant gate)
• Unanticipated problems with Fast Pyrolysis & Upgrading
• Pivoted to analysis of Lanzatech alcohol-to-jet process utilizing PNNL catalyst
  – PNNL received “Excellence in Technology Transfer Award” for this work with LanzaTech
• Highlights importance of co-products
FY18 Office GPRA Target: For at least one approach (e.g., in situ, ex situ, dual bed, co-processing/hydrotreating),

- Carbon efficiency greater than 36% to fuel blendstocks. Final result: **39.7%**
- Reduction in the modeled MFSP by $0.25/GGE compared to the FY17 SOT. Final result: **-$0.59/GGE**

Target MFSP of $3.84/GGE

Actual achieved MFSP of $3.50 (total reduction of $0.59/GGE, $0.34/GGE below the target)
Replacing the Whole Barrel – A Shift Toward Drop-ins and Bioproducts

- Only ~40% of a barrel of crude oil is used to produce petroleum gasoline. Reducing oil dependence requires replacing diesel, jet fuel, heavy distillates, and other products.
- EERE successfully achieved modeled mature cost goals for cellulosic ethanol in 2012 and shifted its R&D to focus on hydrocarbon “drop-in” biofuels, jet fuels, and bio-based products.
- Fuel makes up 76% of the volume of U.S. oil products and is worth $935B.
- Products make up 17% of the volume of U.S. oil products and are worth $812B.
Potential Pathways of Interest to BETO

- **Fuel alone.** Traditional approach which was highly successful for cellulosic ethanol

- **Platform chemical.** (e.g. Vertimass EtOH to jet, levulinic acid)

- **Coproduct.** May utilize waste stream/slip stream conversion (e.g. C5 to succinic, lignin utilization, starch ethanol, etc.)

- **Product alone.** De-risks upstream unit operations, builds supply infrastructure, builds investor confidence
Biobased products contain oxygen... like biomass

Crude oil
Avg. wt%:
C 83-87%
H 10-14%
O 0.1-1.5%

Biomass
Avg. wt%:
C 36-53%
H 5-7%
O 31-48%

Consider the oxidation state of chemicals – retain what nature provides

Scalability of Bioproducts

Chemicals from Biomass: A Market Assessment of Bioproducts with Near-Term Potential, Mary Biddy (NREL) and colleagues. Available at: http://www.nrel.gov/docs/fy16osti/65509.pdf
Bioproducts uniformly showed emission reductions compared to their fossil-derived counterparts.
Consortia
FY18 began $1.9M mini consortium at NREL to identify novel, performance advantaged bioproducts; FY19 introduced LANL + NREL partnership

Three focus areas that represent workshop stakeholder concerns:
  - Computational modeling to predict how biobased compounds will behave
  - High throughput screening of biobased compounds to understand what can be easily made and what
  - End-Use Needs- can we look at existing products and assess what is ripe for innovation?

LANL: glycerol-based polyesters

Synthesis and Testing

Target Identification

Computational Prediction of Structure-Function Relationships

End-Use Needs

PET

PEF

\[
\text{O}_2 \text{ diffusion coefficient (cm}^2\text{)} \]

- PET crystal
- PEF crystal

lattice dimension

Workshop in June, 2017; report PUBLISHED (check BETO website)
Agile BioFoundry

Structure:
• Virtual consortium of 8 national laboratories

Goal:
• Public infrastructure to enable 50% reductions in time and cost to bring a new bio-derived chemical to market through enhance conversion efficiency

Outcomes:
• 10X improvement in Design-Build-Test-Learn cycle efficiency, new host organisms, new IP and manufacturing technologies effectively translated to U.S. industry ensuring market transformation.

Recent Accomplishments:
• Three FY18 FOA selections awarded for Agile BioFoundry Industry Partnerships
• Constructed advanced machine learning models to improve pathway design
• 4X increase in DNA sequence validation speed (384 -> 1536 samples/week)
• PNNL/LBNL designed and built 3-hydroxpropionic acid pathway and transformed it into Aspergillus pseudoterreus
  • 1st cycle demonstrated 2-3 g/L titer, and doubled the titer in 2nd cycle
• NREL/ORNL/ANL reached near-theoretical yields of muconate from glucose-fed Pseudomonas putida (41.3% mol/mol)
• SNL produced up to ~200 mg/L 1,8-cineole on modified Rhodospiridium toruloides
Establish an integrated and collaborative portfolio of catalytic technologies and enabling capabilities

Foundational Science

Advanced Synthesis and Characterization

Theory

Hydrotalcites

Cu/BEA

Product analysis

Bench-scale reactions

Performance Evaluation

Catalyst Cost Estimation

Catalyst Scaling and Integrated Testing

Applied Engineering
NREL has developed atomic layer deposition (ALD) coatings that improve catalyst stability during the production of biobased chemicals, with potential to favorably impact process economics. Through the ChemCatBio DFA, these ALD coatings were recently tailored to improve catalyst performance in the presence of biogenic impurities.

Impact in the words of industry:

“The work being done by the NREL team in the ChemCatBio project is of significant value in being able to understand the potential of ALD coating as a tool for next generation catalysts in biomass processing.”
-Mike Watson
Technology Manager at Johnson Matthey

“The collaboration with NREL is an extremely valuable method to get industrial validation to the emerging applications for advanced catalyst thin film coatings.”
-Karen Buechler,
CTO of ALD NanoSolutions
The project team at ORNL, NREL and ANL utilized unique characterization techniques to study catalysts used in ethanol upgrading process at Vertimass LLC.

- **Deep characterization is helping optimize the catalysts and process, lower cost**
  - Identified catalyst changes at various operation conditions
    - Certain operational parameters can effect catalyst performance
    - Characterization provides structure-performance relationship, allowing for process and catalyst optimization

*Impact in the words of industry:*

*“The ChemCatBio program has provided excellent catalyst characterization insights allowing us to optimize performance and lower conversion costs.”*

- John Hannon, Chief Operating Officer at Vertimass LLC
Consortium for Computational Chemistry and Physics (CCPC): Mesoscale Modeling in Biomass Pyrolysis

- The CCPC has developed coupled particle and reactor scale models that have been extensively validated at NREL.
- Recently, these models were leveraged in a collaboration with Forest Concepts to predict required thermochemical conversion times and expected product yields as a function of specific feedstock attributes.

Impact in the words of industry:

“The work that you are doing has two direct benefits to our company and the industry. First, the simulations and associated graphics help us understand and explain how the ‘dials we turn in production’ affect feedstock functional performance. Second, we may want to add new ‘label information’ to our production reports related to functional performance as well as the physical properties measurements that we currently provide our customers and clients.”

-Jim Dooley
CTO of Forest Concepts

Problem: High commercialization risk
• Catalyst cost is a major contributor to commercialization risk for catalytic processes
• Up to 10% of capital cost and ±10% uncertainty in MFSP for biomass conversion
• No publicly available tools to evaluate cost

Solution: “CatCost” Catalyst Cost Estimation Tool
• Enables early-stage comprehensive cost analysis
• No process design / TEA experience needed
• Improves cost-responsiveness of catalyst R&D

Developed at NREL and PNNL with guidance of industry experts

Free and public release: 01 October 2018 (debuted at AIChE meeting’s dedicated session)
catcost.chemcatbio.org
Excel- and web-based versions available
Separations strategies for biofuels via acid intermediates (BC)

- Evaluating TEA/LCA for 3 different technologies for acid intermediates extraction (planning for 2022 BC Verifications)

**Techno-economic analysis**
- **Separations Cost**
  - Off The Shelf: Simulated Moving Bed
  - SepCon: Electro-deionization
  - SepCon: Pertractive

**Life cycle analysis**
- Off The Shelf: Simulated Moving Bed
- SepCon: Electro-deionization
- SepCon: Pertractive

Low Sulfur Diesel baseline: 94 g CO₂e/MJ

If solar power used

**NOTE:** Results reflect scenario in which lignin combusted, resulting energy consumed in process.
CUBI and ACSC collaboration: key to identifying catalyst structure and informing better operation for 2,3-BDO Upgrading

**CUBI**

- Cu/zeolite synthesis (ORNL)

**ACSC**

- STEM/EDS analysis (ORNL)
- X-ray absorption near edge structure (ANL)

**Fresh catalysts**

**Used catalysts**

2,3-BDO conversion to butenes (ORNL)

**ACSC helped understand catalyst structure and inform better catalyst operations**

- **STEM/EDS**: uniform Cu distribution, no large agglomeration
- **XAS**: metallic Cu (majority), particle size \(\approx 0.7-1.2 \text{ nm}\)
- Frequent catalyst regeneration (<90 h each cycle): avoid hard coke formation

**Major impact**: better catalyst design to increase higher olefins yield and lower MFSP
Biological Deconstruction

• At NREL, moved from batch to continuous countercurrent deacetylation

• NREL’s Low Temperature Advanced Deconstruction studied how DMR (deacetylation and mechanical refining: the planned pathway for 2022 verification) impacts lignin
  • Used NMR, GPC, and TOF MS to demonstrate that DMR black liquor stream contains large amounts of lignin monomers/dimers along with aryl-ether bonds (β-O-4 linkages intact)

• NREL’s Enzyme Engineering and Optimization (EEO) developed an artificial multifunctional cellulase with improved performance over native enzyme mixture
  • NREL has been shifting from DDA to DMR for 2022 cost targets, because DMR’s lignin is more readily converted to products
    • But DMR cellulose is more recalcitrant than DDA cellulose
    • So EEO has been developing new cellulases to handle DMR cellulose
Biological Upgrading

- NREL - Bench Scale Integration’s (BSI) end of year SMART milestone goal was to produce 75 g/L of 2,3-butanediol (BDO) from recombinant *Zymomonas mobilis* strain fed biomass sugars. **BSI exceeded this goal, producing an average of 83 g/L BDO from triplicate fermentations, using a combination of concentrated hydrolysate liquor from deacetylated disc refined (DDR) corn stover, using a fed-batch fermentation strategy, and lowering the aeration rate during xylose metabolism to maximize BDO production.**

  - Knockout of pyruvate decarboxylase gene enabled eliminating ethanol pathway
  - Data was produced too late in year to be included in FY18 SOT, but moves BETO closer to the 102 g/L that is targeted in the design case (as a route to $2.5/gge) and nearly a 2X increase from the end of FY17.
  - Yield was ~86% of theoretical (ultimate project goal is 125 g/L @ 85% yield).
  - In Q1, NREL will deliver 100 L of this fermentation broth to the CUBI teams

- NREL’s Biological Upgrading of Sugars (BUS) worked with BioESep to develop in situ product recovery of butyric acid produced from Clostridium, as the Clostridium produces the acid but before cytotoxicity kicks in at high titer

  - Fermentation broth continuously pumped to membrane contactors; cells recycled
  - Extractant in contactors extracts acids; acids then distilled and extractant recycled
  - 300-hr continuous run → +22% productivity and +7% yield of butyric acid
Motivation: Lignin constitutes 15-40% of biomass carbon but it is currently considered a waste-stream in biorefineries, generally burned for heat and power.

Techno-economic modeling at NREL has indicated that lignin valorization to high-value products may reduce lignocellulosic biofuel cost by ~$1-2/gge.

FY18 FOA Selections on conversion of lignin to higher-value products:
- Two awards, $3.4 million
- Carbon fiber and spray insulation, thermoset polymers used for fiberglass and automotive applications

DOE/USDA Biomass Research and Development Initiative (BRDI) awarded and started to develop a solvent liquefaction process for feedstock deconstruction and lignin upgrading.
Recent Wins in Lignin

Chemical Breakdown
New flow system gives >35% yield of upgradable monomers with >90% enzymatic hydrolysis yields for monomers

Biological Funneling
Model feed: 50 g/L titer, 100% yield, 0.5g/L/hr productivity
Real Lignin Baseline First Test: 4 g/L, 15% yield by mass (137% yield from 2 major monomers in stream)

Catalytic Upgrading
>99% yield of adipic acid from biologically produced muconic acid in flow system
New/Expanded Areas Since Last Peer Review
Cell-Free Synthetic Biology and Biocatalysis

• **Cell-Free Synthetic Biology as an Enabling Tool for the Bioeconomy**
  – Utilizing cell-free synthetic biology as a prototyping tool to rapidly discover the most carbon-efficient and energy-efficient routes from biomass to chemicals

• **Cell-Free Synthetic Biology as a New Conversion Platform for the Bioeconomy**
  – **Free Enzyme Biocatalysis**
    • Mix of only the needed enzymes in a reactor could allow better titers, rates, and yields, plus easier product separation
  – **Scaffold/Stabilized Biocatalysis**
    • Potential novel bioreactor designs such as the “printed tube reactor” (right) for improved mass transfer and heat transfer, compared to traditional designs such as the Continuous Stirred-Tank Reactor

Image courtesy Sarah Baker, Lawrence Livermore National Laboratory.

Image courtesy James Bowie, University of California, Los Angeles.
Potentially Untapped Carbon Resources

Leveraging DOE’s National Laboratories expertise in polymer deconstruction in biomass and applying it to distributed sources of waste carbon to make molecular building blocks for fuels, products, and energy.

- **Wet Wastes:** Biosolids, Food Wastes, Manures
- **Gaseous Wastes:** CO and CO$_2$
- **Solid Wastes:** Sorted Municipal Solid Waste including Plastics

Economically Advantageous Feedstocks
• BETO-supported National Academies of Sciences study on “Developing a research agenda for utilization of gaseous carbon waste streams”

• CO₂ Valorization via Rewiring Carbon Metabolic Network in bacterial cells
  • NREL tailored bacteria as a model for direct biochemical CO₂ utilization, reaching 150 mg/L titer of 3-hydroxybutyrate (3-HB, a polyester precursor) and developing CRISPR-Cas9 gene editing tools

• Three FY18 FOAs awarded in Topic Area 5: Rewiring Carbon Utilization

• Formate Lab Call – new AOPs in early stage R&D for biological platforms capable of upgrading formate, which can be efficiently generated from CO₂
  • NREL – Improving formate upgrading via bacterial conversion
  • NREL – Enhancing CO₂ conversion to value-added products via formate
  • NREL/LBNL – Synthetic cycle for electrosynthesis of products and fuels from formate

Re-Evaluating the Value of CO₂ as a Resource
Plastics are ubiquitous in modern society

~300 MM tonnes per year produced worldwide
Plastics are also creating an environmental catastrophe

~8 MM tonnes per year of plastics enter the ocean

**2014**
- Plastics Production: 311 MT
- Ratio of Plastics to Fish in the Ocean: 1:5
- Plastics' Share of Global Oil Consumption: 6%
- Plastics' Share of Carbon Budget: 1%

**2050**
- Plastics Production: 1,124 MT
- Ratio of Plastics to Fish in the Ocean: >1:1
- Plastics' Share of Global Oil Consumption: 20%
- Plastics' Share of Carbon Budget: 15%
Moving beyond PET/PE recycling
Most plastic waste is not currently recycled – New methodologies hold promise for recycling a wider range of plastics, including mixtures.

Today’s Waste = Tomorrow’s Untapped Resources
Introductions – Biochemical Conversion

<table>
<thead>
<tr>
<th>Name</th>
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<td>iBiocat</td>
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- Charles
- Steve
- Ben
- Chris
- Farzaneh
# Introductions – Agile BioFoundry Reviewers

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**Photographs:**

- Ben
- Matt
- Farzaneh
- Chris
- Steve
# Introductions – Catalysis Reviewers

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<tr>
<td>Lorenz (Larry) Bauer</td>
<td>Consultant</td>
<td>TC Reviewer 2017</td>
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<tr>
<td>Jesse Bond</td>
<td>Syracuse University</td>
<td>New, w/MR experience</td>
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<tr>
<td>Chris Bradley</td>
<td>DOE, Office of Science</td>
<td>New, w/MR experience</td>
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<tr>
<td>Viviane Schwartz</td>
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<tr>
<td>Cory Phillips</td>
<td>Phillips 66</td>
<td>New</td>
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<tr>
<td>John Regalbuto</td>
<td>University of South Carolina</td>
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## Introductions – CO2 Reviewers

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<tr>
<td>Alissa Park</td>
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<tr>
<td>Jason Ren</td>
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<tr>
<td>Matthew Lucas</td>
<td>Carbon180</td>
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<tr>
<td>Igor Bogorad</td>
<td>Amyris</td>
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<td>Matthew Kanan</td>
<td>Stanford University</td>
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# Waste to Energy Reviewers

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<tr>
<td>Phil Marrone</td>
<td>Leidos, Inc.</td>
<td>Reviewer</td>
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<tr>
<td>Tim Olson</td>
<td>California Energy Commission</td>
<td>New to BETO peer review, has reviewed for DOE</td>
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<tr>
<td>Gary Vanzin</td>
<td>Colorado School of Mines</td>
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</tr>
<tr>
<td>Luca Zullo</td>
<td>VerdeNero, Inc.</td>
<td>Lead Reviewer</td>
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![Phil](image1.jpg)  
Phil  

![Tim](image2.jpg)  
Tim  

![Gary](image3.jpg)  
Gary  

![Luca](image4.jpg)  
Luca
## Introductions – Separations/Performance

Advantaged Bioproducts

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<td>Peter Keeling</td>
<td>Purdue University</td>
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<tr>
<td>Melissa Klembara</td>
<td>U.S. Department of Energy – Advanced Manufacturing Office</td>
<td>New to reviewing this year, formerly BETO staff</td>
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Melissa  
Jeff  
Matt
## Introductions – Lignin

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