Sustainability through Biofuels and Bioproducts R&D

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The Circular Economy

- Intersects with the **Bioeconomy**
- Accelerating innovative technologies that harness the nation’s biomass resources for affordable biofuels, bioproducts, and biopower
- Create new possibilities for renewable product supply-chains, jobs, and economic opportunities while benefiting the environment
Sustainability R&D Highlights

Replace fossil fuels, chemicals, and materials with bio-based, sustainable alternatives

• Chemical upgrading of bio-building blocks

• Algae biology

• Synthetic biology

• Biopolymer design using machine learning

• Waste CO₂ capture and sequestration software tool
BioFuels for a Range of Transportation Modes

- **Light-Duty**
  - Octane Number - how resistant a fuel is to auto-ignition
  - Research Octane Number (RON)
  - Motor Octane Number (MON)
  - Anti-Knock Index (AKI) = (MON + RON)/2

- **Medium/Heavy-Duty**
  - Cetane Number (CN) - how readily a fuel auto-ignites

- **Aviation**
  - Compatibility and operability i.e. SAFETY!
  - Energy density, specific energy and thermal stability key metrics
  - No heteroatoms
Guerbet reaction couples alcohols: dehydrogenation, aldol condensation, hydrogenation

Dehydrogenation endergonic and other reactions exergonic

Can we alleviate the thermodynamic constraints by separating the dehydrogenation and condensation step?

\[
\text{OH} - \text{H}_2 \quad \xrightarrow{\text{Amberlyst 15, Pd/C}} \quad \text{O} \quad \xrightarrow{\text{Ar/H}_2 (94/6, 200 \text{ psi})} \quad \text{cyclohexane} \\
\text{1. 60 °C, 1 h} \quad \text{2. 100 °C, 3 h}
\]

\[
\text{H}_2 \text{O} + \text{H}_2 \text{O} + \text{H}_2 \text{O} \\
\text{<1%} \quad 79\% \quad 13\% \\
\text{Total yield = 92%}
\]

Diesel

Gasoline

Chemicals

Staples, Moore, Leal, Semelsberger, McEnally, Pfefferle, Sutton, Sustainable Energy & Fuels, 2018, 2(12), 2742
Upgrading Acetone

Gasoline

- DCN = 19, RON = 91
- DCN = 24, RON = 83
- DCN = 25, RON = 80
- DCN = 31, RON = 68

Gasoline

- DCN = 12, RON = 100
- DCN = 20, RON = 89
- DCN = 17, RON = 93
- DCN = 21, RON = 88

Diesel

- DCN = 32, RON = 66
- DCN = 45, RON = 31
- DCN = 42, RON = 39
- DCN = 51, RON = 9

Chemicals

Reaction catalyzed by light!

High Energy Jet Fuel

12% higher energy content than Jet-A

Ryan, Moore, Cherry, McEnally, Pfefferle, Leal, Semelsberger, Sutton, *2019 Submitted*
Recyclable Polymers from Bioderived Monomers

Polymers can be synthesized from environmentally benign building blocks, deconstructed using very simple approaches and repolymerized.
Agile BioFoundry (ABF)

This consortium of U.S. DOE national laboratories is dedicated to developing an agile biomanufacturing platform that features:

- Industrially-relevant production microbes
- Advanced tools for biological engineering and data analysis
- Process integration and scale-up
- Techno-economic analysis and life-cycle assessment

The ABF goals are to:
- Reduce risks in bringing bio-based products to market
- Develop performance-advantaged bioproducts
- Reduce biomanufacturing carbon footprints and energy intensities
LANL ABF Project: Improving Enzyme Efficiency

- Enzymes can catalyze reaction with utmost precision and finesse
- Natural enzymes may not be suitable for industrial application or to work on anthropogenic molecules
- Need for evolution in the lab
  - Enhanced stability
  - Reduced product inhibition
  - Improved catalytic efficiency
“Smart” Microbial Cell Technology: Catalyze & Sense

Needle-in-a-haystack

Gene diversification

Sensor Plasmid

Transcription factor

ampR
gfp

(Enzyme)

(custom)

(Enzyme Plasmid)

Enzyme

Plasmid

Laser

~10^8 cells / day

Sort by flow cytometry


Los Alamos National Laboratory
Result: *P. putida* High Muconate Producing Strain

50 mM Glucose

Muconate (mM) vs. Time (h)

- Mutant UbiC (12%)
- WT UbiC (7%)
- No UbiC (5%)

HPLC histogram for muconate

- 6.944
- 7.003
- 6.931

130% increase in muconate yield

Jha et al, ACS Syn Biol, 2019

Muonic acid: Global market > $40 B, used for nylon, plastics
Algae Biology at LANL

• “Algae might be a secret weapon for combating climate change”
• A source of fuel, food, materials, and more
  – Wastewater treatment; CO₂ capture and sequestration

Ben Lamm, Quartz, October 1, 2019

https://www.epa.gov/
Algae Productivity Studies

Multiscale cultivation capabilities

Strain Improvement tools: genetic and non-genetic

Greenhouse
An omics knowledgebase for algal feedstocks

Regulators of productivity

Salt-adapted C. sorokiniana 1228 grows well outdoors

Los Alamos National Laboratory
Algae Gene X Environment Studies

The paradigm for understanding gene by environment interactions to control phenotype

- GENETICS
  - Genes
  - SNPs
  - Mutations

- ENVIRONMENT
  - Toxins
  - Nutrition
  - Experience

- PHENOTYPE
  - DNA methylation
  - Histone modifications
  - ncRNA

- EPIGENETICS
BioManufacturing with Intelligent Adaptive Control

Los Alamos Maniac: Developed to perform more exact and extensive calculations of the thermonuclear process

BioManIAC: Discover, design, and develop a new generation biopolymers from microalgae that will help solve the plastic pollution problem

- Mine the rich landscape of biology, finding new chemistries to develop into biopolymers with target properties of *durability and faster degradability in the environment*

- Novel application of **machine learning** to predict and classify biosynthetic polymers and precursor monomers

*Reinvent the plastics lifecycle*
BioManIAC Machine Learning activities

Major Effort Directions

Chemistry Loop
ML and electronic structure calculations to guide chemical synthesis

Biology Loop
ML for biology-based pattern recognition problems

Dual Loop
Development and implementation of the dual-loop adaptive framework

An integrated and synergistic effort
Biology ↔ ML/Theory ↔ Chemistry

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.
Unique new software delivers real-world routes for reducing carbon footprints

- **SimCCS$$^2$$.0** is the only tool to simultaneously consider where, how much and when to capture, transport and store CO$_2$. It can identify effective energy, economic, and environmental solutions that no other tool can find.
**SimCCS** addresses emerging CCS issues for industry, government, & policy makers

- For its infrastructure designs, the software identifies real-world routes for CO$_2$ pipeline networks and links. It estimates the costs of pipeline construction based on an extensive list of factors, including topography, water bodies, land cover, existing rights of way, and social constraints such as population density, federal lands, and environmental impact.

- Addresses all critical parts of the CCS supply chain simultaneously, allowing identification of key cost savings, revenue streams, and risks to help reduce industry carbon footprints and maximize revenue.

- Access
  - Desktop: [https://github.com/SimCCS/SimCCS](https://github.com/SimCCS/SimCCS)
  - Gateway: [https://beta.simccs.org](https://beta.simccs.org)
Thank you!

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