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U.S. DEPARTMENT OF
ENERGY

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Bio-C2G Model for Rapid, Agile Assessment of Biofuel and Co-product Routes

April 4, 2023

Data, Modeling, & Analysis

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Lawrence Berkeley National Laboratory

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project Overview

Context: Funding agencies, investors, scientific journals increasingly expect economic and environmental analysis to accompany new technologies. Yet, publicly available end-to-end modeling platforms are largely unavailable.

Goal: Democratize feedstock/site assessment, technoeconomic analysis, & life-cycle assessment through web-based tools to help researchers and startups prioritize efforts and speed up time to deployment for biofuels and bioproducts.

Enter into “siting mode” and select a site, buffer radius and filter feedstocks. Click Run TEA/LCA to carry over to process simulation

Select cost or life-cycle GHG emissions, select pre-defined scenario, or adjust individual parameters manually (~60 total)

Model produces customized process flow diagram, downloadable results & auto-generated documentation

Download Results as CSV Download Documentation as PDF

Manure Point Source
Hogs, 1000+ head: 821.8 dt/year
Milk cows, 500+ head: 264.6 dt/year
Total Manure: 1,086.4 dt/year

Biomass in Buffer Zone:
Forest Residues: 559 dt
Food Waste: 107 dt
MSW: 8,459 dt
Ag Residues: 2,619,589 dt
Energy Crops: 39,880 dt
Manure: 68,906 dt
Total: 2,737,500 dt

Product Properties
Product: Bisabolane
Heating Value: 46.66 MJ/kg
Density: 0.814 kg/L
Boiling Point: 275.4 °C
Additional Properties

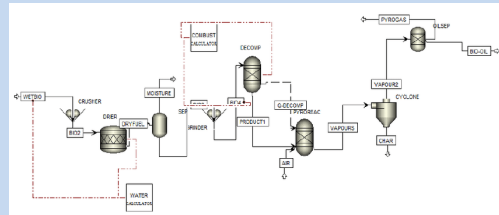
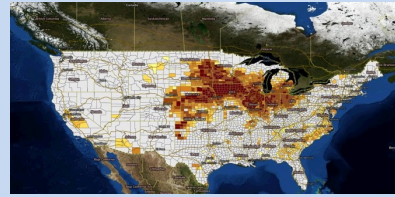
Production Cost of Bisabolane

| Process Stage | Minimum Selling Price (\$/gal) |
|---------------------|--------------------------------|
| Feedstock Supply | 4.08 |
| Pre-treatment | 3.50 |
| Hydrolysis | 3.18 |
| Separation | 2.84 |
| Hydrogenation | 5.15 |
| Acetone Treatment | 1.98 |
| Crude Energy | 2.77 |
| Utilities | 0.88 |
| Total LCA | 24.29 |
| Electricity Credits | 3.04 |
| Net LCA | 22.63 |

1 – Approach

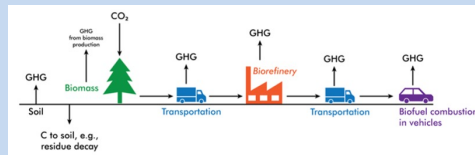
State of the Art

County-level feedstock data



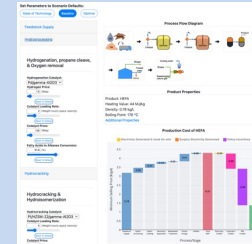
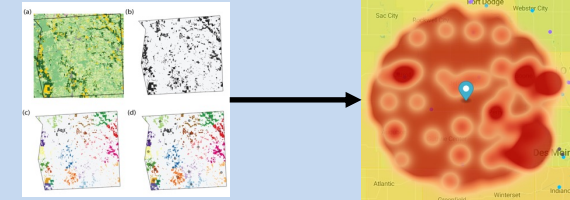
Costly, expert-only process simulation software

Separate LCA models not integrated with, some at substantial cost



This Project

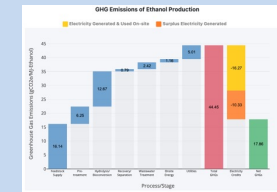
Downscaled feedstocks using satellite data, other sources



Python & machine learning surrogate process models

Physical units-based IO LCA

$$\begin{bmatrix} .50 & 0 & 0 & 0 \\ 0 & 45 & 0 & 0 \\ 0 & 0 & 3.24 & 0 \\ 0 & 0 & 0 & .07 \end{bmatrix} \begin{bmatrix} 1.0 & -10 & -6 & -.45 \\ -.01 & 1.0 & -67 & -8 \\ -.02 & -.45 & 0.9 & -.85 \\ 0.9 & -.34 & -.02 & 1.0 \end{bmatrix}^{-1} \begin{bmatrix} 1.5 \\ .02 \\ 3.0 \\ 45 \end{bmatrix} =$$



Open-source model code targeted at TEA/LCA experts posted on github

Integrated web tool with slider bars, ability to save scenarios

1 – Approach

Management Strategy

- Bi-weekly full team meetings
- Harmonize with others where appropriate (Billion Ton Study, GREET, NREL grid scenarios)
- Extensive testing to ensure accuracy each time new feedstock or process added
- Webtool & ML lead: Huntington
- TEA lead: Baral
- LCA lead: Nordahl
- Feedstocks lead: Nordahl/Hendrickson

Leadership



**Corinne Scown
(PI)**
TEA/LCA Expert

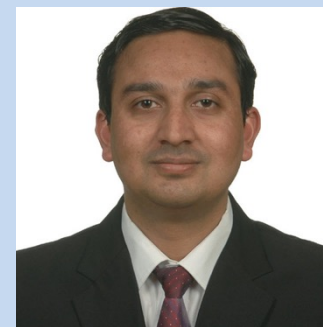
Collaborative Team



**Tyler Huntington
(Software Dev.)**
Tool Development



**Sarah Nordahl
(PhD Student)**
LCA, Feedstocks



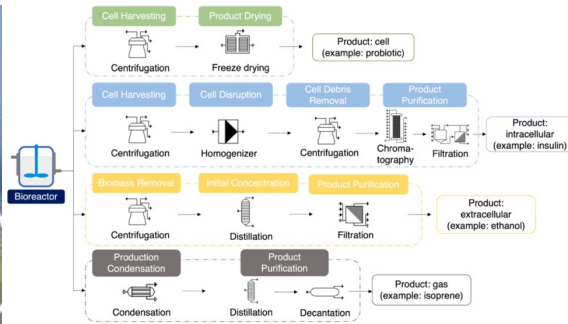
**Nawa Baral
(Proj Sci)**
SuperPro



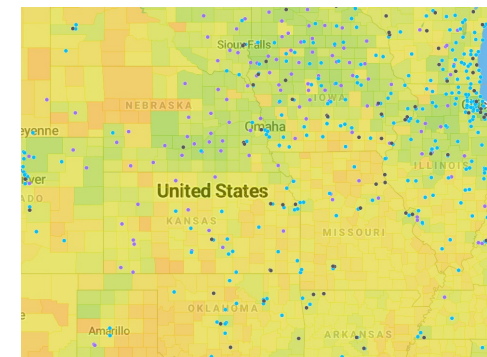
**Tommy Hendrickson
(Proj Sci)**
LCA

1 – Approach

| Risk | Mitigation |
|--|---|
| Algorithm for separations strategy decision tool does not produce reliable recommendations | <ul style="list-style-type: none"> Vetting with ABPDU and industry partners to improve and vet predictions |
| Feedstock availability does not match on-the-ground experience | <ul style="list-style-type: none"> Leverage deep-dive feedstock availability analyses in this and complementary projects Set default to crop residues and wastes only |
| Computational needs exceed the resources we can access for free or minimal costs | <ul style="list-style-type: none"> Adjust resolution of geospatial model Explore use of DOE user facilities |



Separations decision tree algorithm now peer-reviewed, published



Coordinating with Billion Ton team & Roads to Removal report team, doing deep-dive on manure availability

1 – Approach



On schedule – Thanks to NREL colleagues for offering feedback and providing updates on Cambium scenarios that integrate impacts of IRA

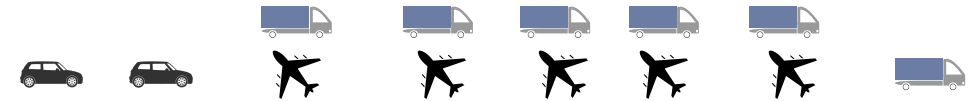
| Milestone Name/Description | Criteria | End Date | Type |
|---|--|-----------|----------------------|
| Build at least 3 grid scenarios into the BioC2G tool using Cambium scenario data from NREL to allow users to explore how grid mixes impact cost and GHG footprint | Add at least 3 alternative future grid scenarios to BioC2G | 9/30/23 | Annual SMART |
| Complete initial expansion of bio-jet fuel modeling capabilities in Bio-C2G. Bio-C2G modeling options must be expanded to incorporate more popular bio-jet fuel routes, such as HEFA and STJ SPK from gen-1.5 feedstocks, such as lipids and starch | At least 2 new bio-jet fuel routes incorporated into Bio-C2G with at least 4 new feedstocks in the siting tool | 9/30/23 | Go/No-Go |
| Complete air pollutant impact vectors and generate geospatially disaggregated environmental impact results for at least 3 biofuel production scenarios | Complete air pollutant impact vectors and generate geospatially disaggregated environmental impact results for at least 3 biofuel production scenarios | 9/30/2024 | End of Project SMART |

1 – Approach

Continual progress toward greater coverage of feedstock-conversion route combinations

Top priority: aviation fuels

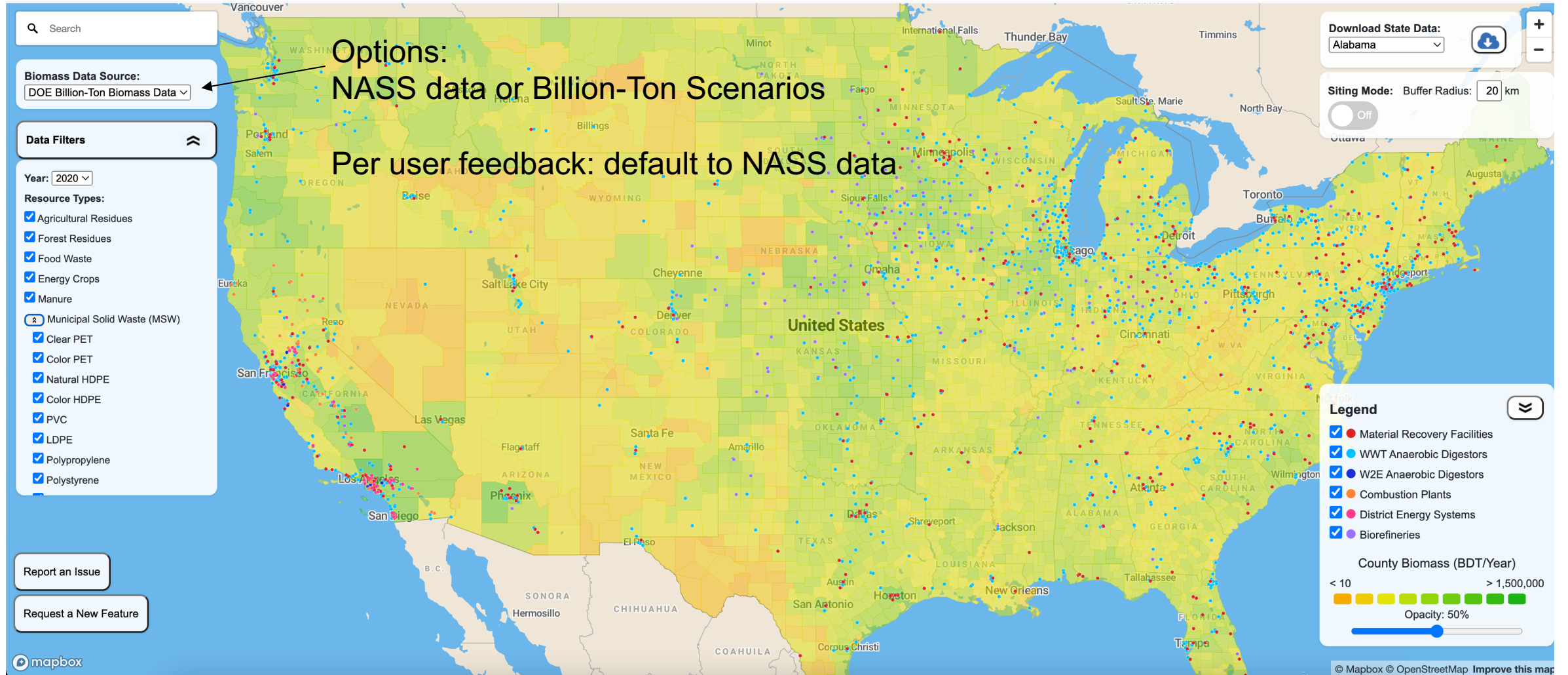
Serving on SAF Grand Challenge Supply Chain group



| Feedstocks / Sources | Ethanol | Isoprenol | Limonene/ Limonane | Bisabolene/ Bisabolane | DMCO | HEFA | ATJ SPK | Biodiesel |
|-------------------------------------|---------|-----------|-----------------------|---------------------------|-------|---------|--------------|-----------|
| Biomass sorghum | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Corn stover | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Miscanthus | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Switchgrass | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Self-defined custom biomass | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Forest residues | Blue | Blue | Blue | Blue | Blue | Grey | via alcohols | Grey |
| Lignocellulosic sugar | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Glucose | Blue | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Dextrose | Blue | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Corn syrup | Blue | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Cane sugar | Blue | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Beet sugar | Blue | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Self-defined custom sugar | Green | Green | Green | Green | Green | Grey | via alcohols | Grey |
| Municipal solid waste | Grey | Grey | Grey | Grey | Grey | via AAD | Grey | Grey |
| Cow manure | Grey | Grey | Grey | Grey | Grey | via AAD | Grey | Grey |
| Hog manure | Grey | Grey | Grey | Grey | Grey | via AAD | Grey | Grey |
| Food processor waste | Grey | Grey | Grey | Grey | Grey | via AAD | Grey | Grey |
| Ethanol biorefineries | Green | Grey | Grey | Grey | Grey | Grey | Blue | Grey |
| Anaerobic digesters | Grey | Grey | Grey | Grey | Grey | via AAD | via alcohols | Grey |
| Wastewater treatment facilities | Grey | Grey | Grey | Grey | Grey | via AAD | via alcohols | Grey |
| Material recovery facilities (MRFs) | Grey | Grey | Grey | Grey | Grey | Grey | Grey | Grey |
| Syngas / industrial gases | Blue | Grey | Grey | Grey | Grey | Grey | via alcohols | Grey |
| Fats, oils, & greases (FOG) | Grey | Grey | Grey | Grey | Grey | Blue | Grey | Blue |
| Soybeans | Grey | Grey | Grey | Grey | Grey | Blue | Grey | Blue |
| Corn grain | Blue | Blue | Blue | Blue | Blue | Grey | via alcohols | Grey |

Included in siting tool
 To be added to siting tool
 Included in TEA/LCA tool
 To be added to TEA/LCA tool

2 – Progress & Outcomes



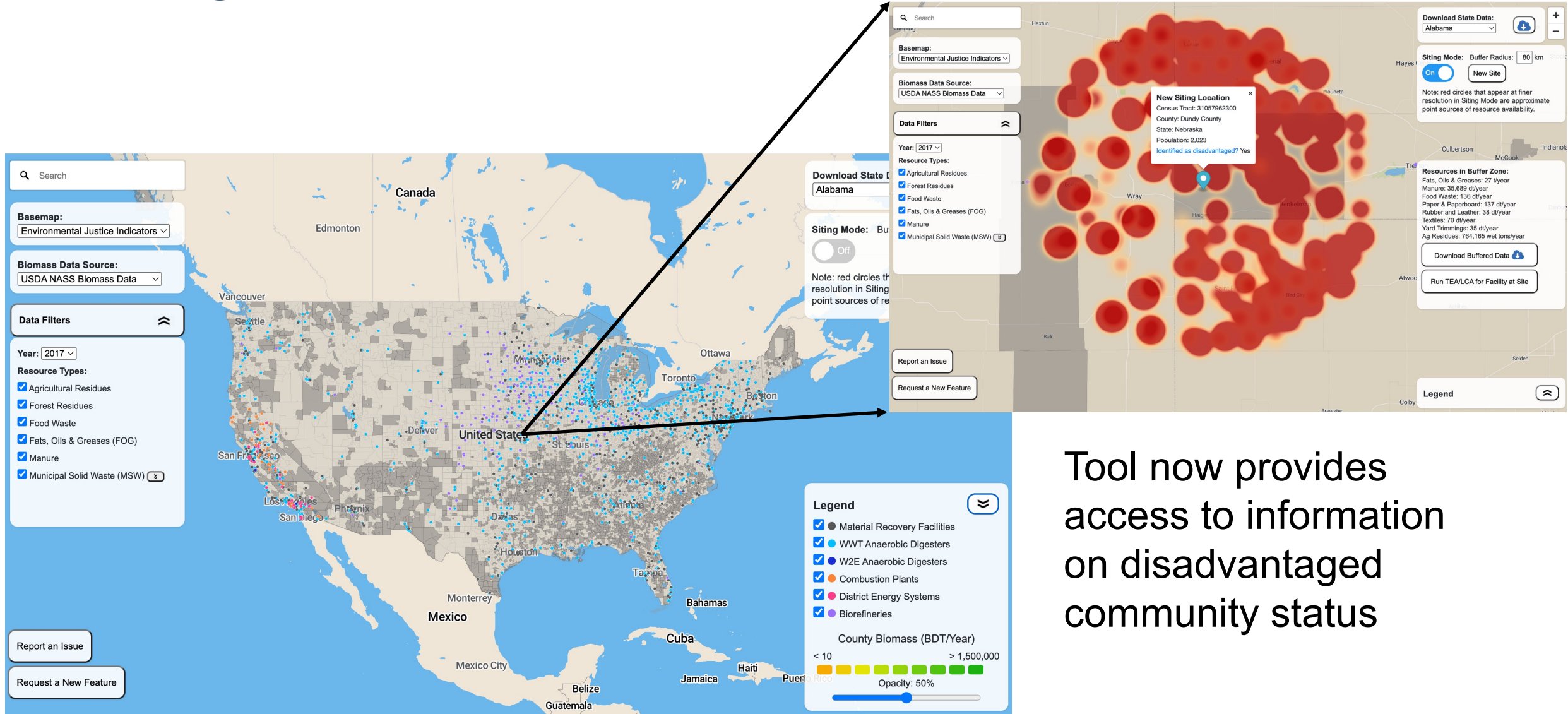
2 – Progress & Outcomes

The screenshot displays the JBEI BioSiting Webtool interface. At the top, the navigation bar includes "JBEI BioSiting Webtool", "Map", "Data Downloads", "Data Sources", and "Contact". On the right, it shows the email "tylerhuntington222@lbl.gov", "Log out", and "Admin" links. A search bar is located in the top left. The main map area shows the United States with a color-coded geologic storage potential overlay. A text box with an arrow points to the "Geologic Storage Layer" dropdown, which is set to "RCSP Saline" and has a "More Info" link. Other dropdowns include "Basemap: Bioeconomy Resources" and "Biomass Data Source: USDA NASS Biomass Data". A "Data Filters" button is also present. On the right side, there are controls for "Download State Data:" (set to Alabama) and "Siting Mode: Buffer Radius: 20 km" (with an "Off" toggle). A note below these controls states: "Note: red circles that appear at finer resolution in Siting Mode are approximate point sources of resource availability." A "New Siting Location" popup is visible over Texas, showing details for Census Tract 48139061700, County Ellis County, State Texas, and Population 5,289. It also indicates "Identified as disadvantaged? No" and "Geologic Storage Potential? Yes". At the bottom left, there are buttons for "Report an Issue" and "Request a New Feature".

Options for geologic storage potential (NETL Atlas):
RCSP Saline or USGS Coal

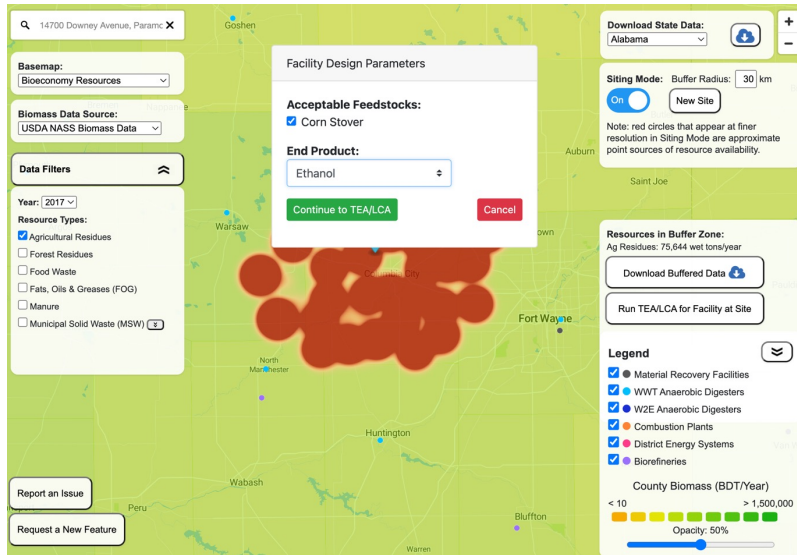
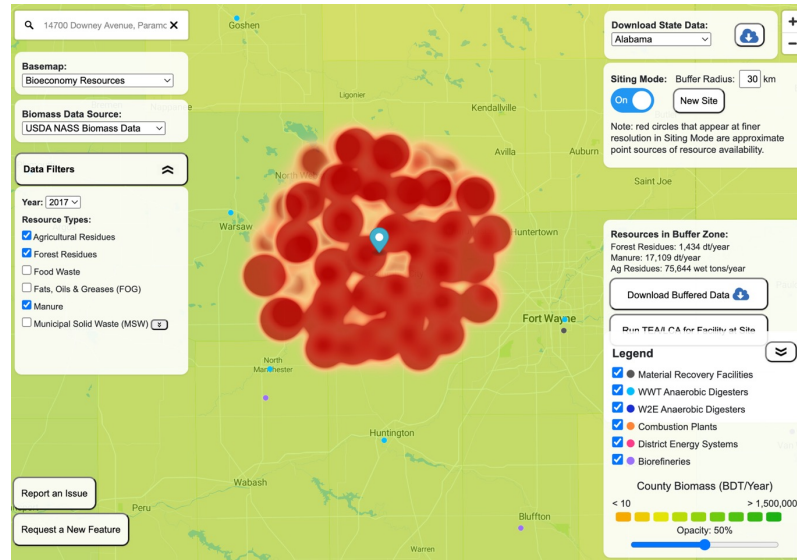
Screenshots from lead.jbei.org

2 – Progress & Outcomes



Tool now provides access to information on disadvantaged community status

2 – Progress & Outcomes



- Tool allows users to define location, radius, and feedstock scenario
- Filter feedstock types of interest
- Carry over feedstock mix & quantity to TEA/LCA tool



Feedstock Supply

Feedstock: Mixed

Feedstock Amount: 3398.190 (metric tons/day)

Feedstock Cost: 114.10531 (\$/metric ton)

Feedstock Moisture Content: 20.0 (%)

Feedstock Cellulose Content: 37.04529 (%)

Feedstock Hemicellulose Content: 23.19949 (%)

Feedstock Lignin Content: 20.30784 (%)

Feedstock Protein Content: 3.1182634 (%)

2 – Progress & Outcomes

HEFA Simulation Interface:

- Final Product: HEFA
- Buttons: MSP, Water Consumption, GHGs, Run Model, Tech Specs
- Set Parameters to Scenario Defaults: State of Technology, Baseline, Optimal
- Process Flow Diagram: Shows feedstocks (Oil, Fat, Grass) entering a reactor with H₂ and Catalyst, followed by another reactor with H₂ and Catalyst, leading to Product. Includes side streams for Biogas, Cooling water, Treated water, Waste, and Supplemental natural gas.
- Product Properties:
 - Product: HEFA
 - Heating Value: 44 MJ/kg
 - Density: 0.78 kg/L
 - Boiling Point: 176 °C
 - Additional Properties
- Production Cost of HEFA:

| Category | Value (\$/gal) |
|----------------------|----------------|
| Feedstock Supply | 3.19 |
| Hydro-processing | 0.28 |
| Hydro-cracking | 0.21 |
| Recovery Separation | 0.12 |
| Wastewater Treatment | -0.03 |
| On-site Energy | 0.41 |
| Utilities | 0.06 |
| Total MSP | 4.31 |
| Electricity Credits | -0.04 |
| Coproduct Credits | -0.85 |
| RIN Credits | -2.04 |
| Net MSP | 1.38 |

Ethanol Simulation Interface:

- Final Product: Custom
- Buttons: MSP, GHGs, Water Consumption, Run Model, Tech Specs
- Set Parameters to Scenario Defaults: State of Technology, Baseline, Optimal
- Note: Modeling methods are still experimental. Results should be interpreted with caution.
- Process Flow Diagram: Shows feedstocks (N, P, K, F, A) entering a reactor with Recycled IL and Makeup IL, followed by a reactor with Enzymes and nutrients, leading to Product. Includes side streams for Biogas, Cooling water, Treated water, Waste, Lignin & remaining solids, and Recycled IL.
- Production Cost of Ethanol:

| Category | Value (\$/gal) |
|----------------------|----------------|
| Feedstock Supply | 4 |
| Hydro-processing | 0.15 |
| Hydro-cracking | 0.17 |
| Recovery Separation | 0.12 |
| Wastewater Treatment | -0.03 |
| On-site Energy | 0.41 |
| Utilities | 0.06 |
| Total MSP | 4.31 |
| Electricity Credits | -0.04 |
| Coproduct Credits | -0.85 |
| RIN Credits | -2.04 |
| Net MSP | 1.38 |

Custom Product Specifications:

| | | |
|--------------------------------------|-----------------------------------|--------------------------------|
| Product Name: Custom Product | Required Purity (%): 90 | Water Soluble: Yes |
| Accumulation Location: Intracellular | State of Matter: Liquid | Vapor Pressure (kPa): 5.95 |
| Crystallizable: Yes | Density (kg/m ³): 901 | Molecular Weight (g/mol): 40.1 |
| Market Value: Low (< \$10/kg) | Specific Heat (J/g °C): 2.46 | Heating Value (MJ/kg): 30 |
| Product Type: Fuel | Boiling Point (°C): 78.37 | |

Feedback examples:

ORNL input

Added graphical PFD w/ key parameters popup when mouse hovers over

Industry feedback

Added RIN values
Added 1st-gen feedstocks

ABPDU & industry

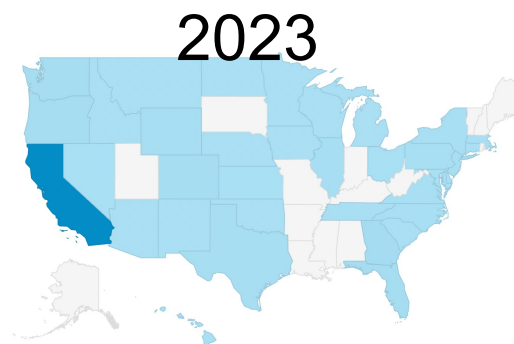
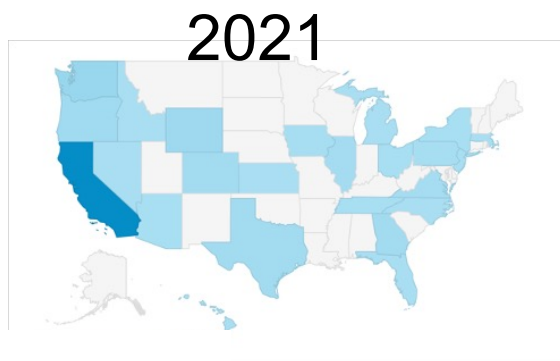
Added custom products & separations tool

BETO feedback

Added plastic waste to biositing tool

3 – Impact

- If successful:
 - All researchers and startups develop better intuition for key cost and environmental impact drivers
 - Preliminary TEA, LCA, siting analyses for grant proposals, papers, early commercialization can be (partially) automated
- 9 publications published in high-impact journals including *Joule*, *Nature Biotechnology*, *Environmental Science & Technology*, *ACS Sustainable Chemistry & Engineering*
- 9,567 visits; 833 unique visitors; expanding reach

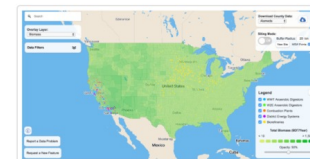


Tools & Resources

BioSiting Tool

Geospatial platform for biomass resource analyses across the U.S.

Go



TEA/LCA Tool

Tool for running quick TEA and LCA analyses of biofuel synthesis pathways

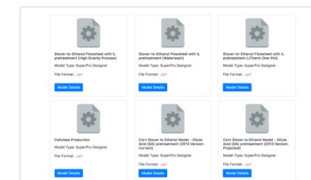
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Technoeconomic Models

Library of JBEI-developed SuperPro models and documentation for download

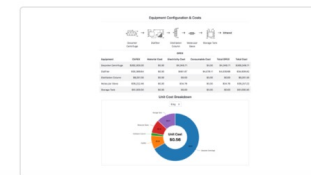
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Separations Strategy Tool

Decision support tool for determining equipment and costs for recovery process of biofuel/bioproduct production pathways.

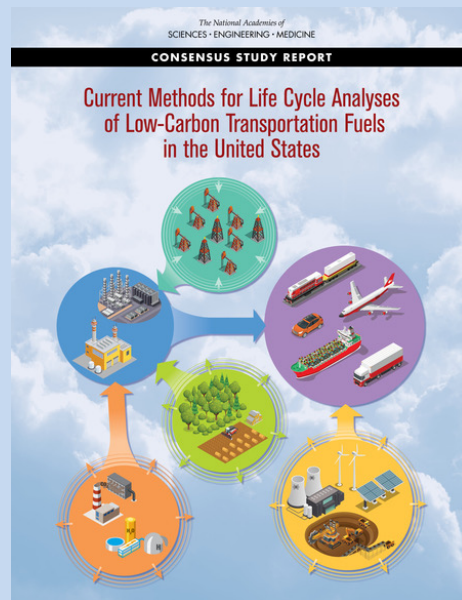
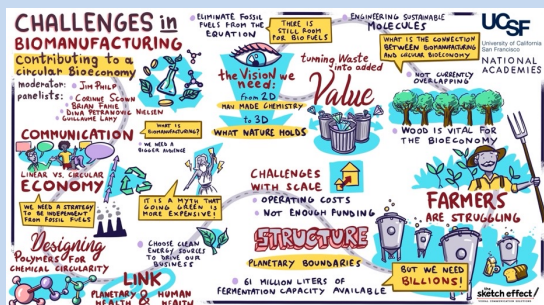
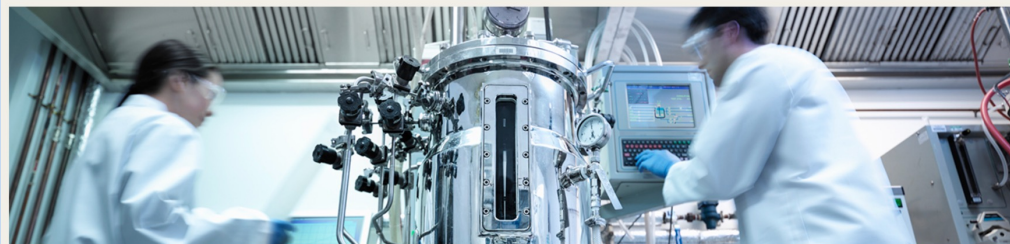
Go



3 – Impact

National Academies Workshops & Reports

Successes and Challenges in Biomanufacturing – A Workshop



Impactful Alumni



Minliang Yang, NC State Faculty

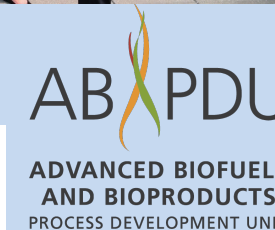


Nemi Vora, Sustainability Science @ Amazon



Olga Kavvada, Comp. Sci. & AI Lab, ENGIE

Collaborations & Dissemination



3 – Impact

- Looking forward
 - Leverage experience working with industry to focus tools on most pressing barriers
 - Work more closely with key stakeholders to design tools and resources that **de-risk deployment and ensure facilities are good neighbors**
- Adding location-specific considerations to biositing
 - Pre-existing environmental/health burdens
 - Pre-existing resource constraints (e.g., water)
- Integrating potential local impacts
 - Traffic (noise, truck traffic volume)
 - Noise (facility)
 - Freshwater consumption
 - Nutrient discharge/runoff
 - Air pollutant emissions: NO_x , SO_x , $\text{PM}_{2.5}$, VOCs, NH_3
 - Odor (e.g., H_2S , some VOCs)



Summary

- **Goal:** Democratize end-to-end feedstock assessment, TEA, & LCA by creating robust, publicly accessible webtools.
- **Approach:** Combine fast, high-resolution feedstock mapping with Python-based process-based model and surrogate ML modeling, add physical units-based input-output life-cycle assessment model.
- **Progress:** User feedback-informed interface updates. HEFA and microbial production routes integrated into the tool with 4 pretreatment options for biomass. Separations decision tool linked with core TEA/LCA tool. Wide variety of feedstocks and disadvantaged community data added to biositing tool.
- **Potential Impact:** Critical information to help researchers develop early-stage TEA/LCA and enable startups to identify key cost, GHG, water use drivers and screen potential sites
- **Future Work:** Complete siting updates to incorporate CO₂ sequestration potential, disadvantaged communities, and air pollution. Continue expanding fuel production pathways with a focus on aviation fuels.

Quad Chart Overview

Timeline

- Start: 10/01/2021
- End: 09/30/2024

Project Goal

Continue development and expansion a lightweight, flexible model capable of iterative quantification of production costs, life-cycle emissions, and water use: Bio-C2G

FY20

Active Project

DOE
Funding

(10/01/2021 –
9/30/2024)

\$300K/year

End of Project Milestone

Complete air pollutant impact vectors and generate geospatially disaggregated environmental impact results for at least 3 biofuel production scenarios

Barriers addressed

Technology Uncertainty of Integration and Scaling

Process Integration

Funding Mechanism

BETO Lab Call, FY22

Additional Slides

Responses to 2021 Peer Review Feedback

- The approach was good except for the very narrow limits placed on feedback (Joint BioEnergy Institute, ABPDU)
 - **Action: Gathered feedback from startups, investors, and researchers (non-JBEI/ABPDU) who were using the tools. Expanded reach of collaborations dramatically, to including ORNL, LLNL, NREL**
- Restriction to specific products perhaps is not as valuable as a parameterized description (select the most likely from a set of generic product recovery processes, etc.) as opposed to needing a fresh set of detailed simulations for each case.
 - **Action: Added a “custom” product option by implementing a separations and recovery decision tree algorithm. This quickly became the most popular option in the TEA/LCA portion of the tool.**
- The focus on cellulosic sugars limits the scope to processes that will not exist for years, if ever. That said, the end product has the potential to be an extraordinary tool for a very wide range of “customers,” and the progress so far has been excellent.
 - **Action: We added a range of first-generation sugars, which have also become a popular functionality. We learned that users prefer to self-define sugar feedstocks rather than model a full lignocellulosic biorefinery.**
- This will allow the startups to apply for grants, to sell their technology to potential investors, and to better understand their overall impact. The tool should be modified to consider significant figures. Costs to the dollar are not reasonable. They should be rounded to no more precise than \$1,000.
 - **Action: We agree, and for publications, we limit the precision, but we provide exact results based on carefully documented inputs to avoid unnecessary rounding errors.**
- There does not appear to have been any planning or evaluation of design options for the front-end user interface. It appears to be the result of one team’s idea of what would make a good software platform, and the team did not plan to execute a formal customer research study. If it is targeted at the C-suite, high schools, or industry people, it would be important to know what forms and format they would like.
 - **Action: Intended audience is researchers and industry, and we have made substantial improvements to the interface based on direct feedback from both groups**
- This project is too large and broad to be achievable with impactful results if the intent is to model all conversion approaches. The use case for this project is very unclear. It is not clear whether the modeling is the equivalent of what can readily be done in an Excel file, is more in line with Aspen, or is somewhere in between. The idea of combining three different modeling tools is a good idea.
 - **Action: We gathered input from users to understand what features they are finding useful and how they are using it. It is clear that many users are making use of the custom sugar feedstock and custom product to rapidly evaluate different microbial production processes so we have worked on improving those functionalities and adding features as they are requested. It is true that so far, we do not model thermochemical processes.**

Publications, Patents, Presentations, Awards, and Commercialization

Publications

- Huntington, T., Baral, N.R., Yang, M., Sundstrom, E. and Scown, C.D., 2023. Machine learning for surrogate process models of bioproduction pathways. *Bioresource Technology*, 370, p.128528.
- Nordahl, S.L., Preble, C.V., Kirchstetter, T.W. and Scown, C.D., 2023. Greenhouse Gas and Air Pollutant Emissions from Composting. *Environmental Science & Technology*.
- Liu, D., Baral, N.R., Liang, L., Scown, C.D. and Sun, N., 2023. Torrefaction of almond shell as a renewable reinforcing agent for plastics: techno-economic analyses and comparison to bioethanol process. *Environmental Research: Infrastructure and Sustainability*.
- Scown, C.D., 2022. Prospects for carbon-negative biomanufacturing. *Trends in Biotechnology*.
- Cruz-Morales, P., Yin, K., Landera, A., Cort, J.R., Young, R.P., Kyle, J.E., Bertrand, R., Iavarone, A.T., Acharya, S., Cowan, A. and Chen, Y., 2022. Biosynthesis of polycyclopropanated high energy biofuels. *Joule*, 6(7), pp.1590-1605.
- Yang, M., Liu, D., Baral, N.R., Lin, C.Y., Simmons, B.A., Gladden, J.M., Eudes, A. and Scown, C.D., 2022. Comparing in planta accumulation with microbial routes to set targets for a cost-competitive bioeconomy. *Proceedings of the National Academy of Sciences*, 119(30), p.e2122309119.
- Comesana, A.E., Huntington, T.T., Scown, C.D., Niemeyer, K.E. and Rapp, V.H., 2022. A systematic method for selecting molecular descriptors as features when training models for predicting physiochemical properties. *Fuel*, 321, p.123836.
- Scown, C.D. and Keasling, J.D., 2022. Sustainable manufacturing with synthetic biology. *Nature Biotechnology*, 40(3), pp.304-307.
- Wang, Y., Huntington, T. and Scown, C.D., 2021. Tree-based automated machine learning to predict biogas production for anaerobic co-digestion of organic waste. *ACS Sustainable Chemistry & Engineering*, 9(38), pp.12990-13000.

Publications, Patents, Presentations, Awards, and Commercialization

Presentations

- "Biomanufacturing to Address Near-Term Climate Goals", Invited Panel Discussion, National Academies Biomanufacturing Workshop, Washington, DC, March 3, 2023. [virtual]
- "Challenges in Biomanufacturing Contributing to a Circular Bioeconomy", Invited Panel Discussion, National Academies Biomanufacturing Workshop, Washington, DC, October 24, 2022. [virtual]
- "Designing the bioeconomy for deep decarbonization", Keynote Talk, Annual Green Chemistry & Engineering Conference, June 3, 2022. [virtual]
- "Overcoming the Engineering and Environmental Challenges of Achieving a More Circular Economy", Invited Talk, CUWP Seminar Series, University of Wisconsin-Madison, April 14, 2022. [virtual visit]
- "Overcoming the Engineering and Environmental Challenges of Achieving a More Circular Economy", Invited Talk, Ezra's Systems Roundtable Seminar, Cornell University, February 4, 2022. [virtual due to COVID]
- "Weighing Life-Cycle Climate and Health Tradeoffs in the Push Toward Zero Waste", Invited Talk, EEE Research Seminar, Purdue University, January 18, 2022. [virtual]
- "Designing the Bioeconomy for Deep Decarbonization: Opportunities and impacts for the agricultural sector", Invited Conference Presentation, Society for Industrial Microbiology and Biotechnology Annual Meeting, Austin, TX, August 9, 2021. [virtual]

Awards

- ACS Sustainable Chemistry & Engineering Lectureship, 2022