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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

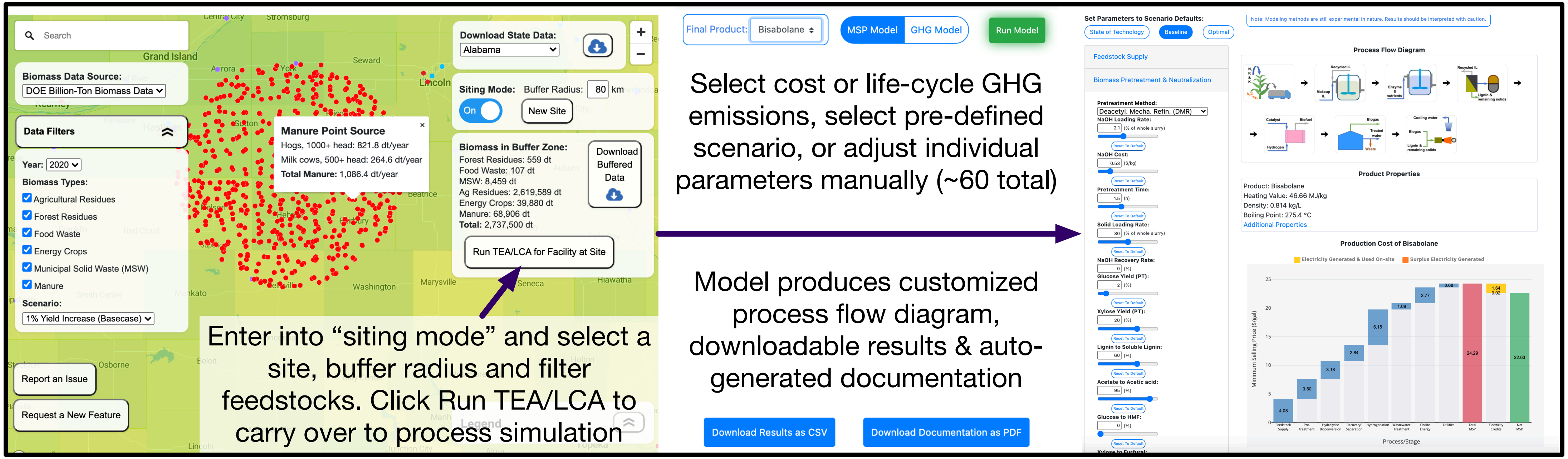
PI: Corinne D. Scown

Lawrence Berkeley National Laboratory

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.

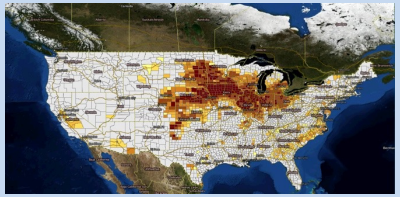
Goal: Democratize feedstock/site assessment, technoeconomic analysis, & life-cycle assessment through web-based tools to help researchers and startups prioritize efforts and speed up time to deployment for biofuels and bioproducts.

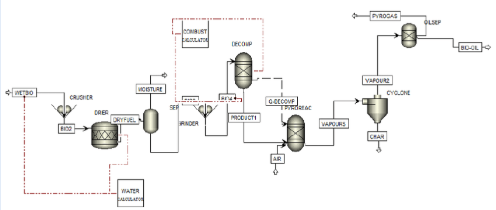


1 – Approach

State of the Art

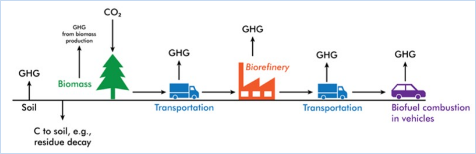
County-level feedstock data

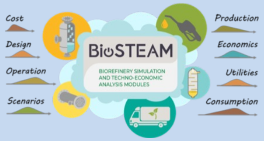


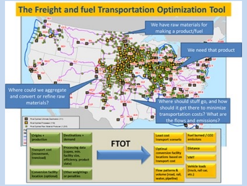


Costly, expert-only process simulation software

Separate LCA models note integrated with, some at substantial cost



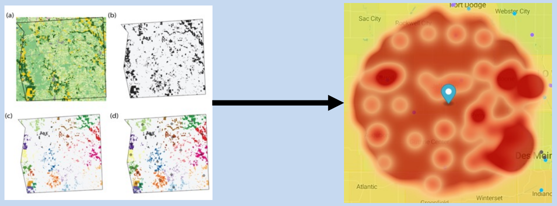


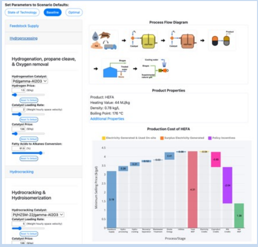


Open-source model code targeted at TEA/LCA experts posted on github

This Project

Downscaled feedstocks using satellite data, other sources

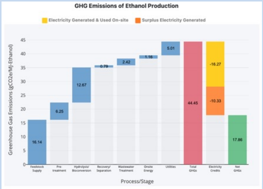


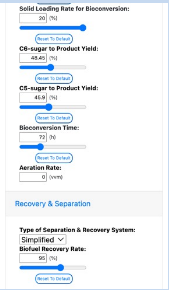


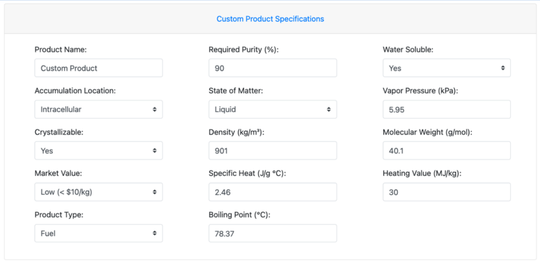
Python & machine learning surrogate process models

Physical units-based IO LCA

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







Integrated web tool with slider bars, ability to save scenarios

Sources: BioenergyKDF / Billion Ton Study; Ward et al. (2014); NASEM LCA Methods report (2022); BioSTEAM model, FTOT; lead.jbei.org

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

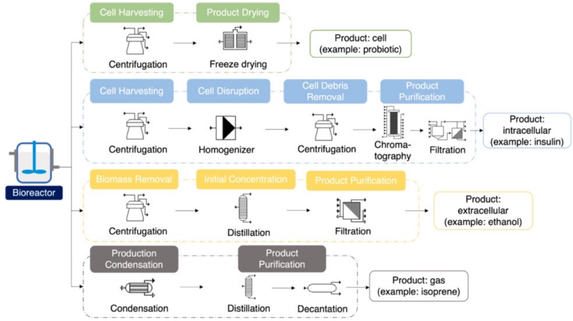
Sarah Nordahl (PhD Student)
LCA, Feedstocks

Nawa Baral (Proj Sci)
SuperPro

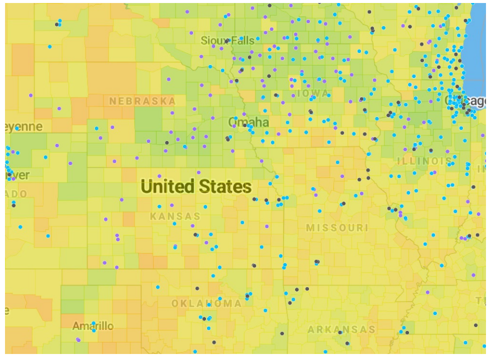
Tommy Hendrickson (Proj Sci)
LCA

1 – Approach

Risk	Mitigation
Algorithm for separations strategy decision tool does not produce reliable recommendations	• Vetting with ABPDU and industry partners to improve and vet predictions
Feedstock availability does not match on-the-ground experience	• 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	• 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

Source: Huntington et al. (2023)

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

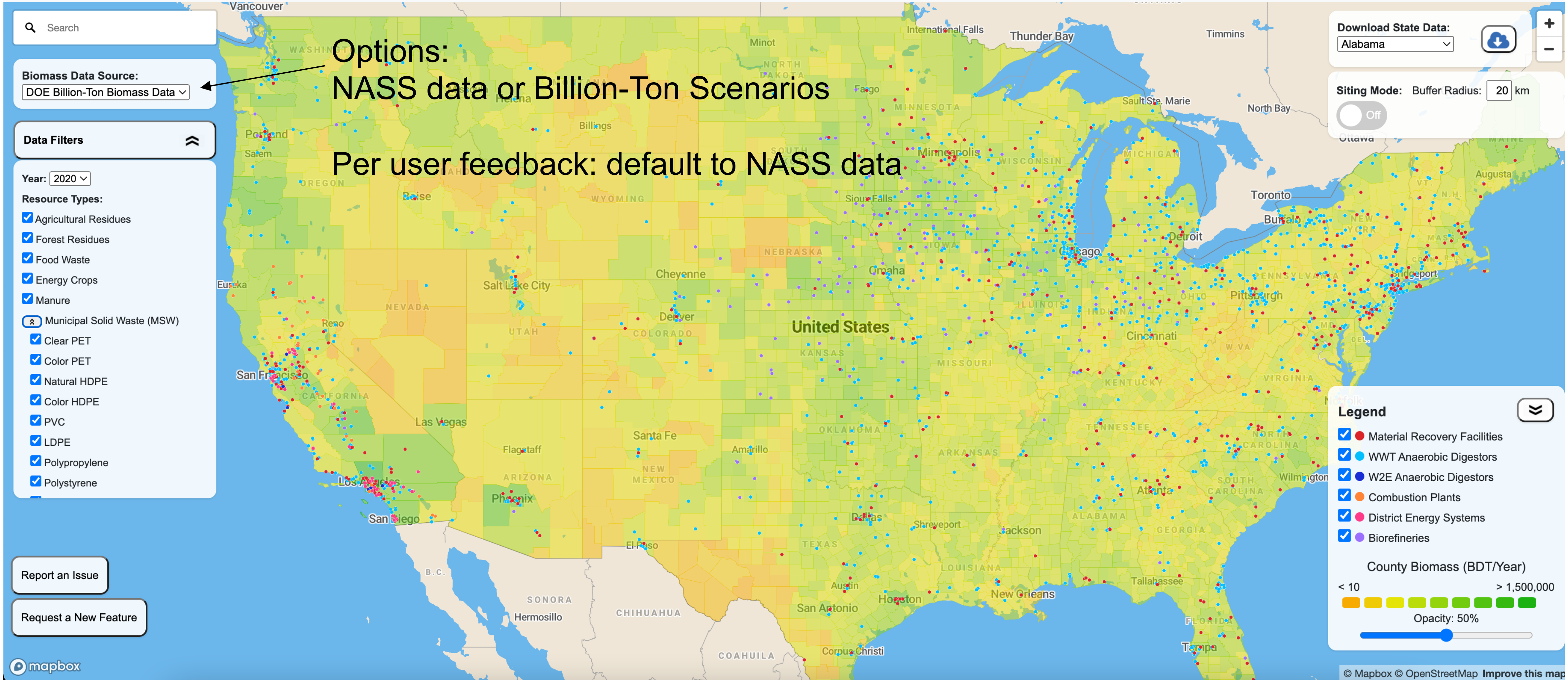
Top priority: aviation fuels

Serving on SAF Grand Challenge Supply Chain group

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

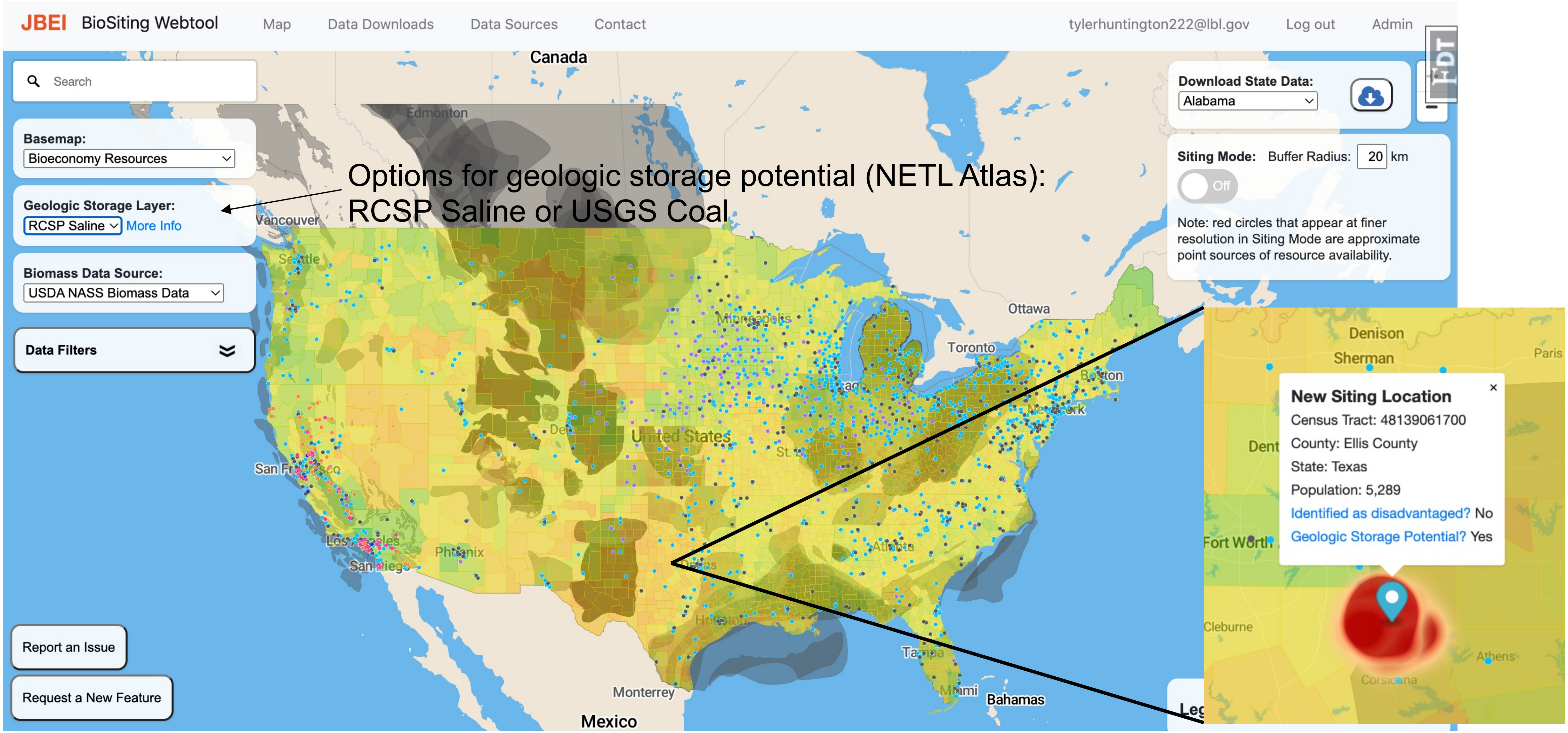
Included in siting tool | To be added to siting tool | Included in TEA/LCA tool | To be added to TEA/LCA tool

2 – Progress & Outcomes



Screenshots from lead.jbei.org

2 – Progress & Outcomes



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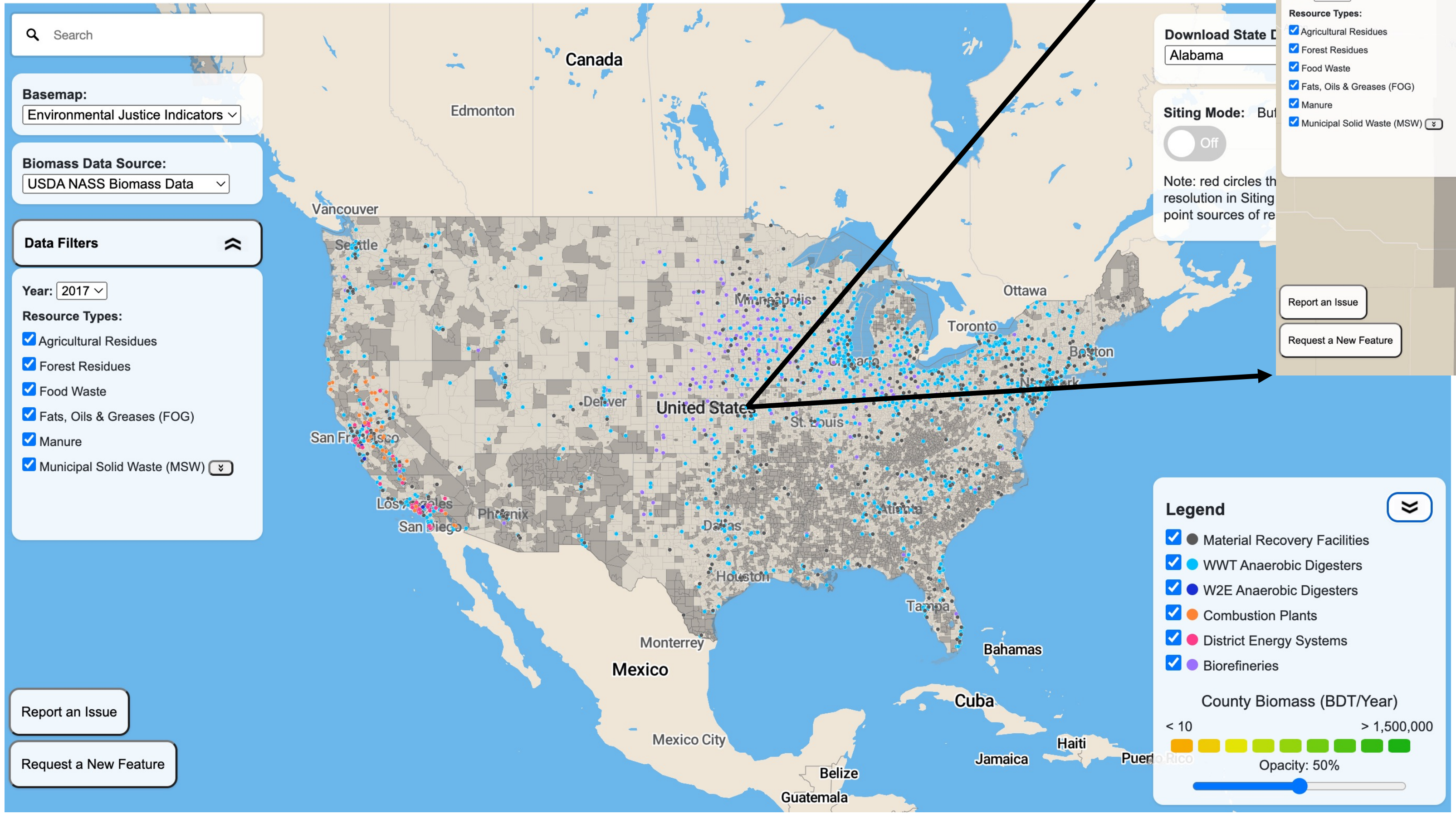
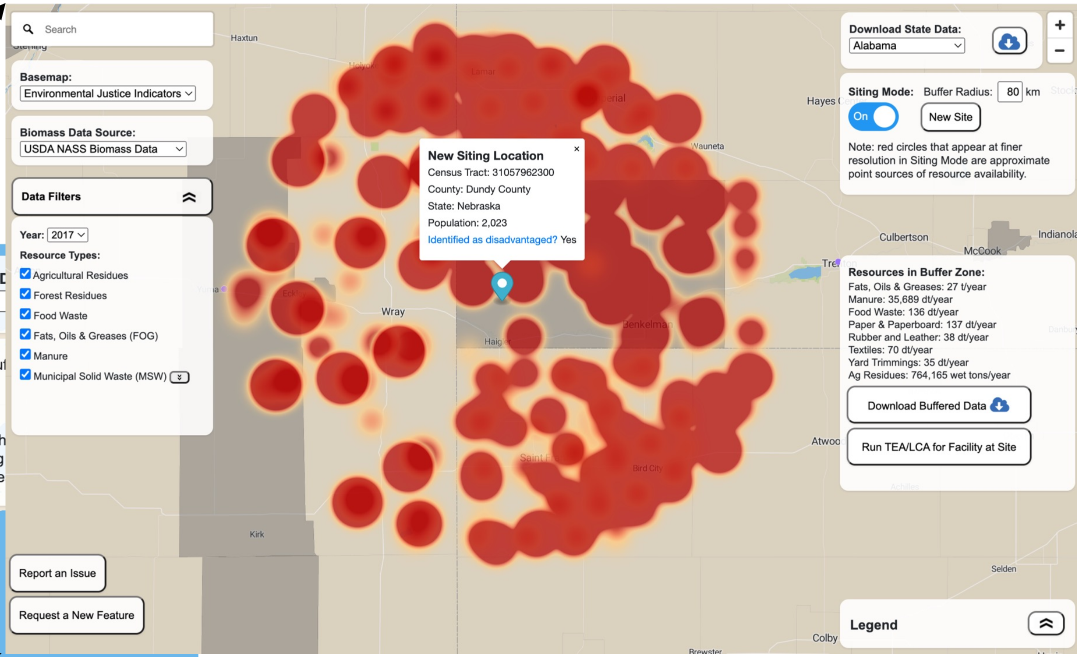
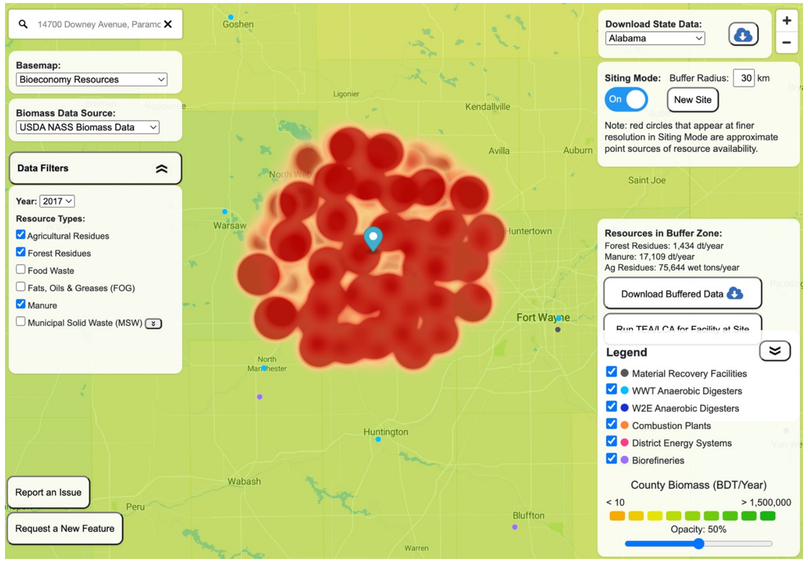


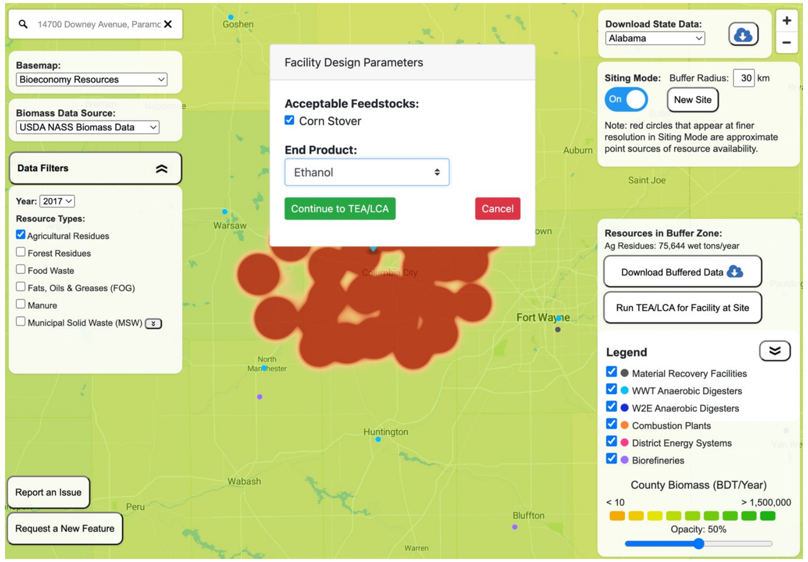


Tool now provides access to information on disadvantaged community status

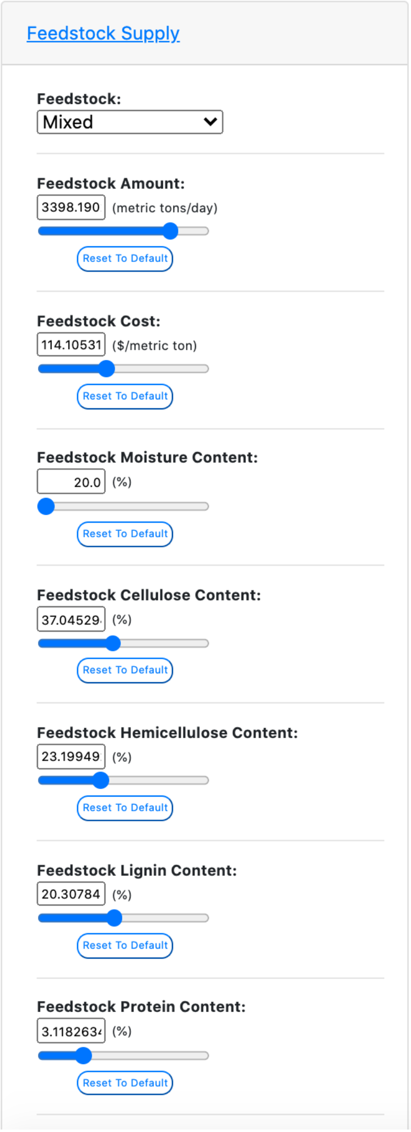
Screenshots from lead.jbei.org

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



Screenshots from lead.jbei.org

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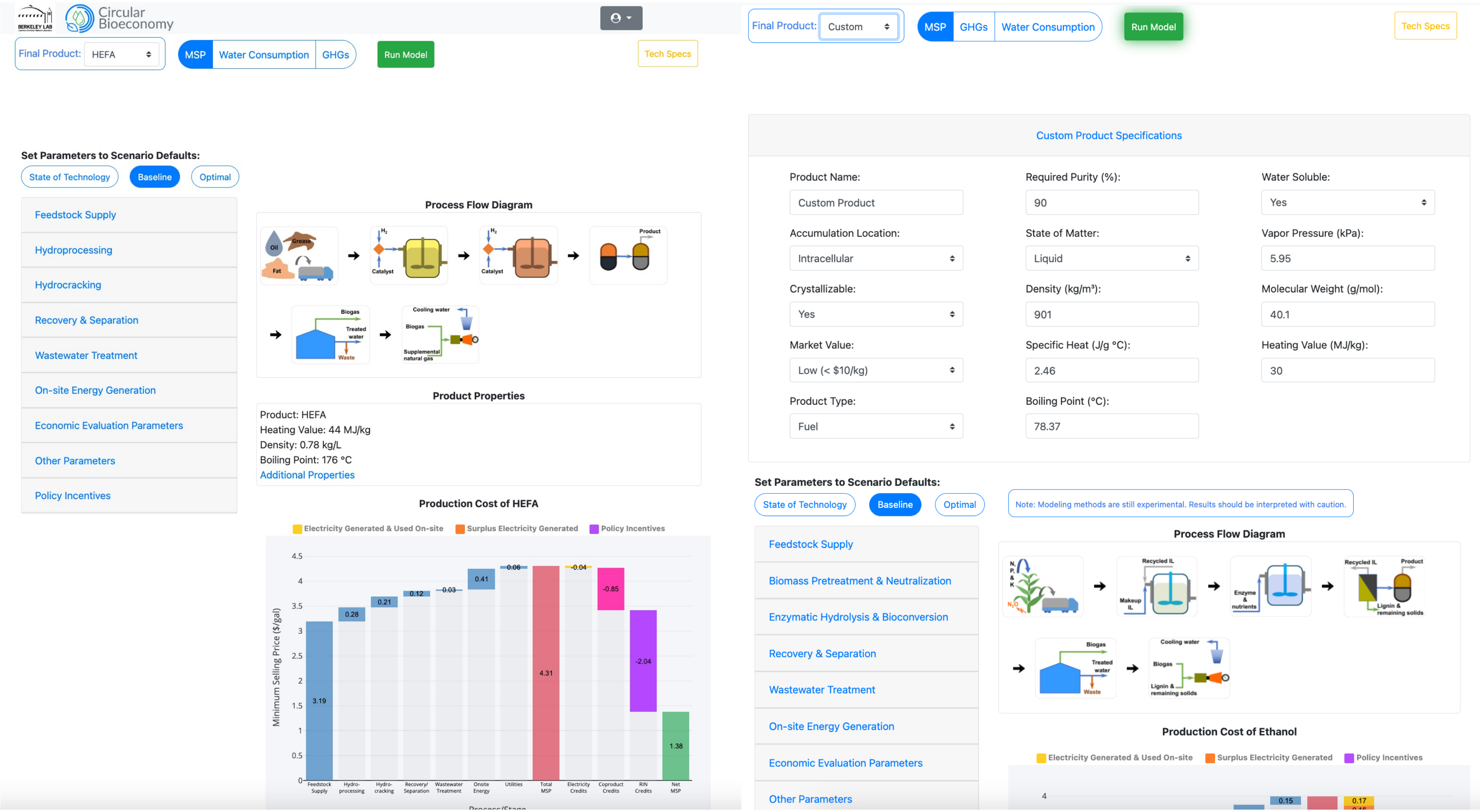
2 – Progress & Outcomes



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

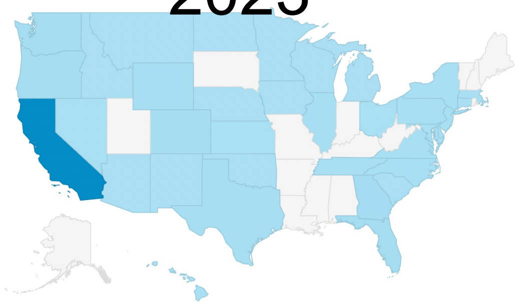
Screenshots from lead.jbei.org

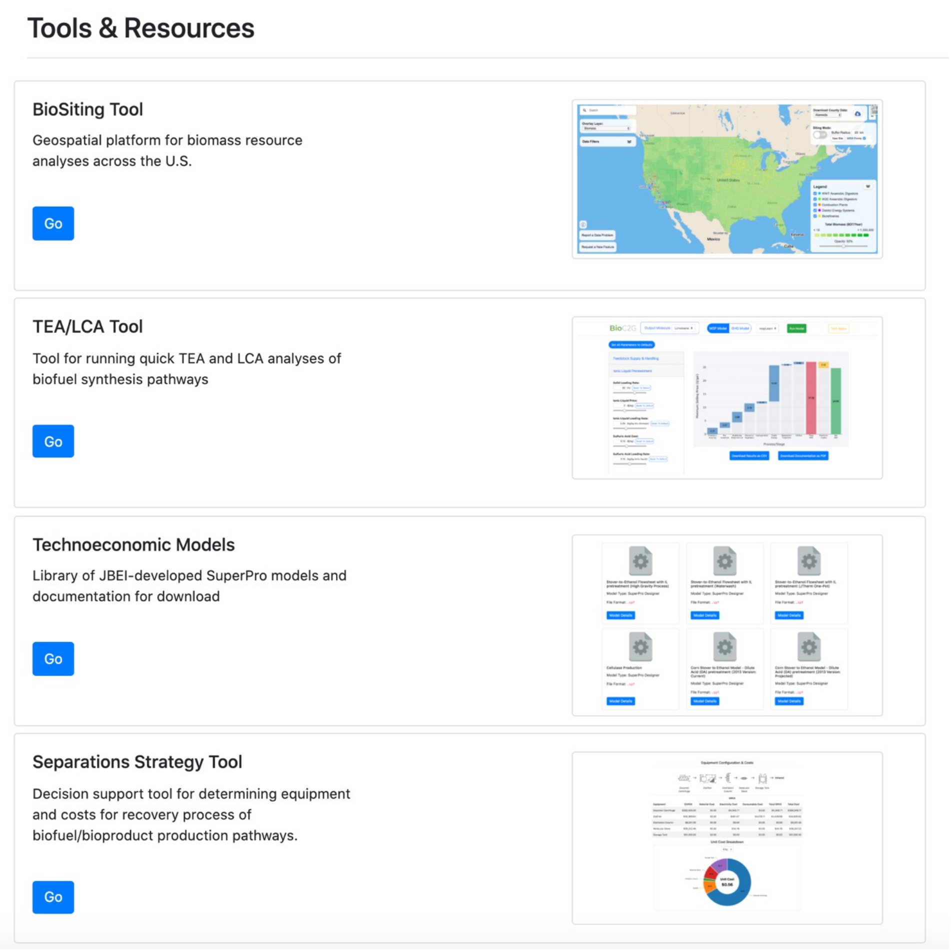
3 – Impact

- 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

2021

2023

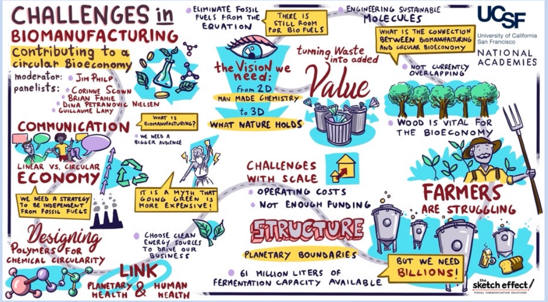


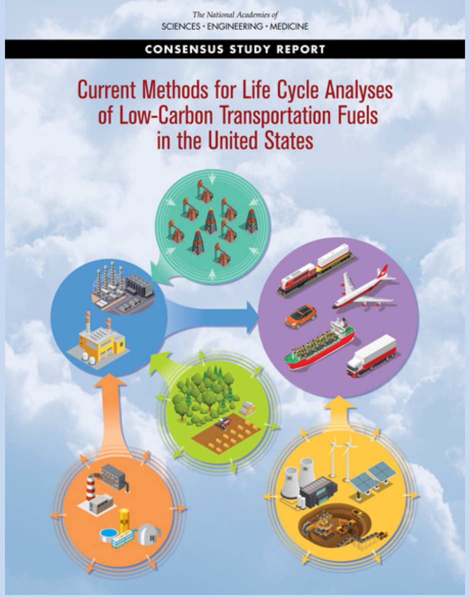


Screenshots from lead.jbei.org

3 – Impact

National Academies Workshops & Reports





Impactful Alumni

Minliang Yang, NC State Faculty

Nemi Vora, Sustainability Science @ Amazon

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

Collaborations & Dissemination

cbi THE CENTER FOR BIOENERGY INNOVATION

CABBI CENTER FOR ADVANCED BIOENERGY AND BIOPRODUCTS INNOVATION

GREAT LAKES BIOENERGY RESEARCH CENTER

JBEI Joint BioEnergy Institute

ABPDU ADVANCED BIOFUELS AND BIOPRODUCTS PROCESS DEVELOPMENT UNIT

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, $PM_{2.5}$, VOCs, NH_3
  - Odor (e.g., H_2S, some VOCs)

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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 CO_2 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

	FY20	Active Project
DOE Funding	(10/01/2021 – 9/30/2024)	$300K/year

Barriers addressed

Technology Uncertainty of Integration and Scaling

Process Integration

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

End of Project Milestone

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

Funding Mechanism

BETO Lab Call, FY22

*Only fill out if applicable.

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