BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

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

March 23, 2021

System Development and Integration

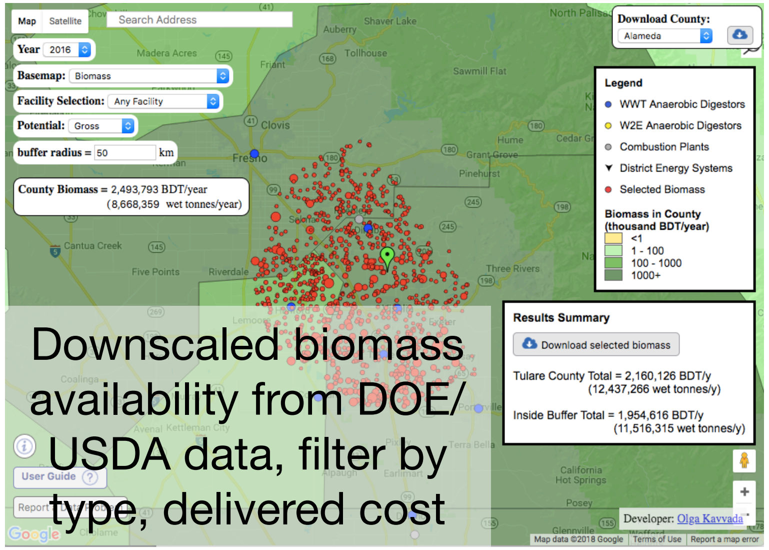
PI: Corinne D. Scown
Lawrence Berkeley National Laboratory

Project Overview

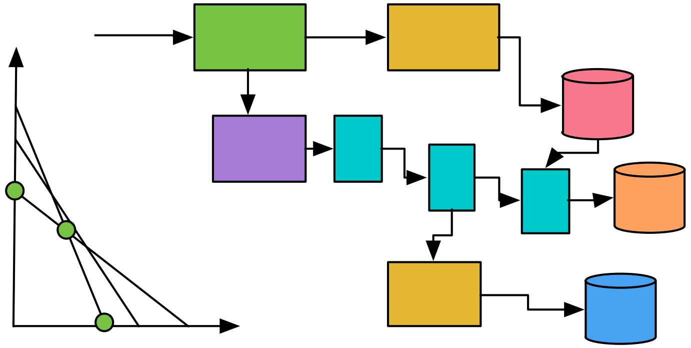
Challenge: Feedstock availability, technoeconomic analysis, and life-cycle assessment are modeled on different platforms, difficult to integrate into a single model. Handoffs are clunky and involve proprietary, expensive, expert-only software

Goal: Develop a lightweight, flexible model capable of quantifying production costs, life-cycle emissions, water use, other relevant metrics for a hypothetical facility with identified organic/biomass feedstocks.

Feedstock Supply ⟷ Biorefinery Optimization ⟷ Life-Cycle Assessment

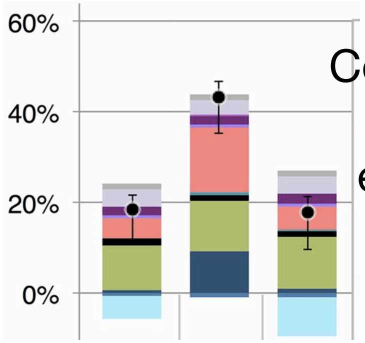


Downscaled biomass availability from DOE/USDA data, filter by type, delivered cost



Optimize for cost, specific outputs, net GHG benefits

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



Compute LC inventory e.g. GHG, water

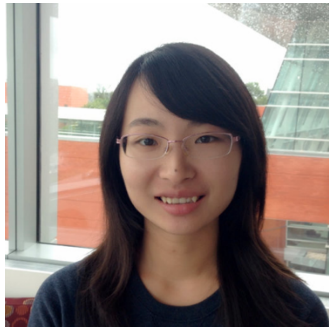
BERKELEY LAB

1 – Management

Corinne Scown (PI)
TEA/LCA Expert

Tyler Huntington (Software Dev.)
Tool Development

Nawa Baral (Proj Sci)
TEA/LCA

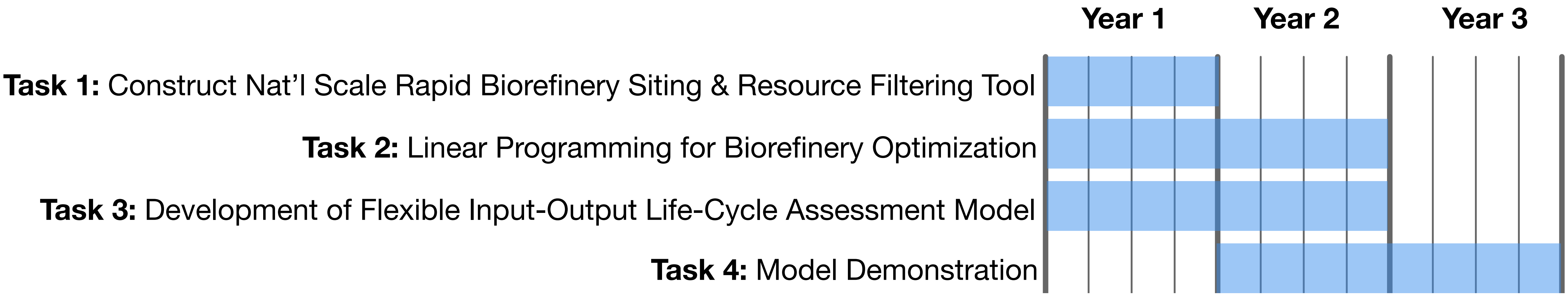


Minliang Yang (Postdoc)
TEA/LCA

Sarah Nordahl (PhD Student)
LCA

All team members at Lawrence Berkeley National Lab
Team located (in non-COVID times) at EmeryStation East, near Joint BioEnergy Institute & ABPDU

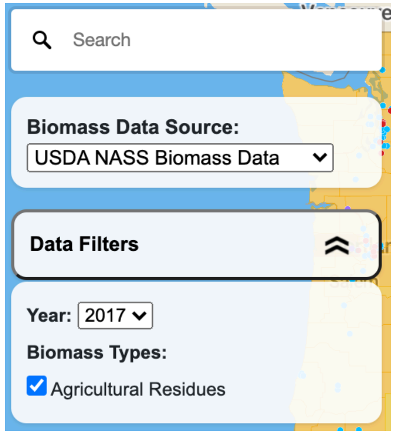
1 – Management

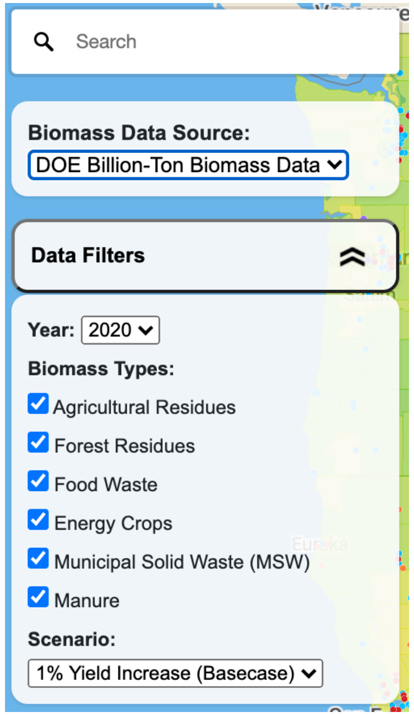


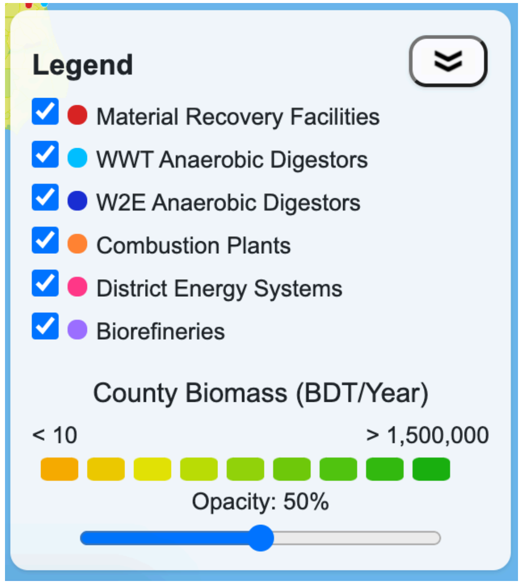
Risk	Mitigation
Limited adoption of tools	Frequent feedback from JBEI users, input from ABPDU and clients, freedom to shift emphasis based on user needs
Model too complex or inaccurate	Staff project with software developer + TEA/LCA experts to ensure robust code and accuracy, publish results in peer-reviewed articles

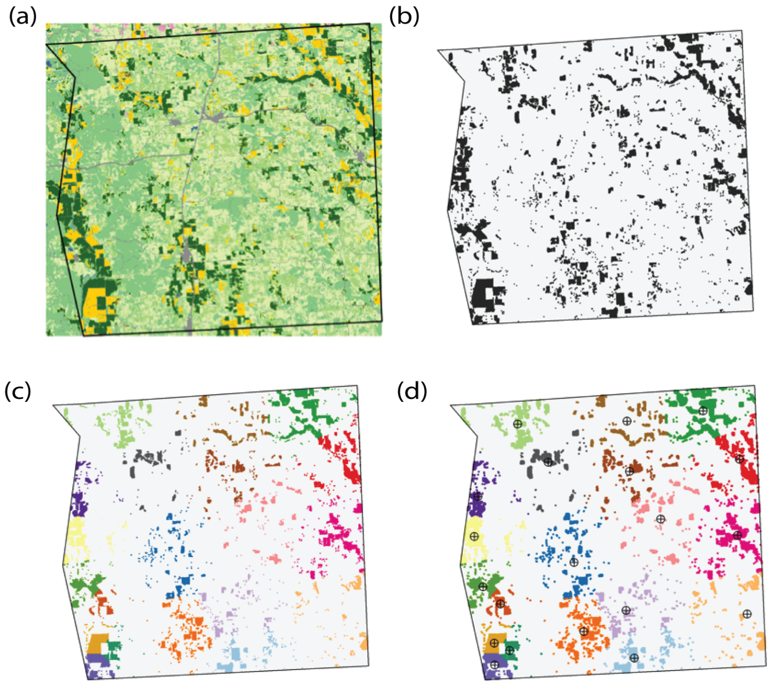
2 – Approach

- Get all biomass data in one place, including current USDA data and projected data from *Billion Ton report*
- Provide users ability to select biomass available around a site of interest, directly feed quantity and composition into a TEA/LCA
- Provide point source locations that may supply feedstocks or compete for types of biomass





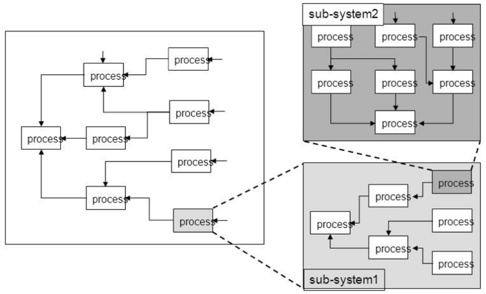




Screenshots from lead.jbei.org

BERKELEY LAB

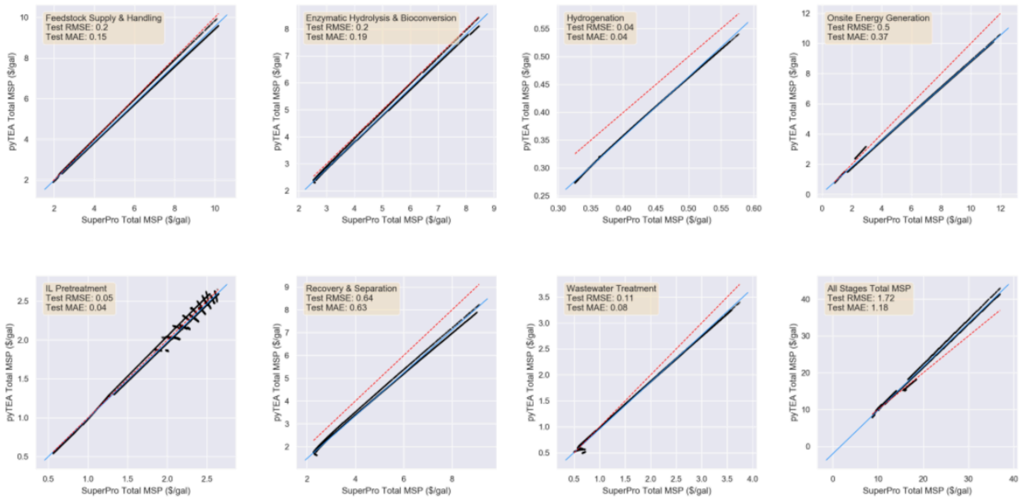
2 – Approach

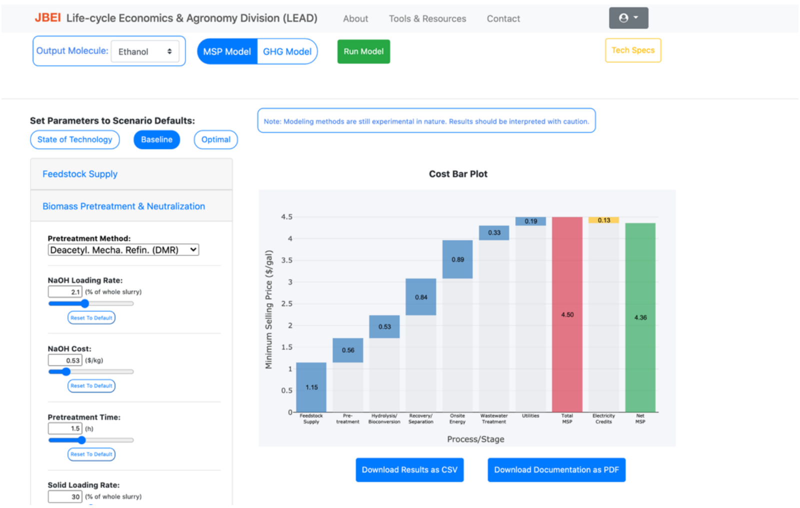


$$b = R(I - A)^{-1}y$$

Surrogate ML modeling, simplified python-based process modeling, & physical units IO LCA modeling

pyTEA





Challenges:

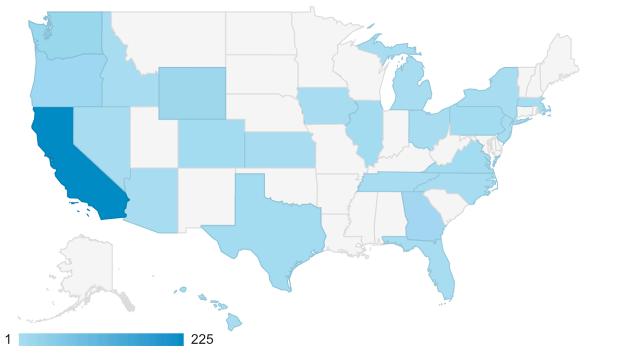
- Accurate energy balance
- Maintaining stable tool
- Relevance for industry w/out much cellulosic biofuel activity

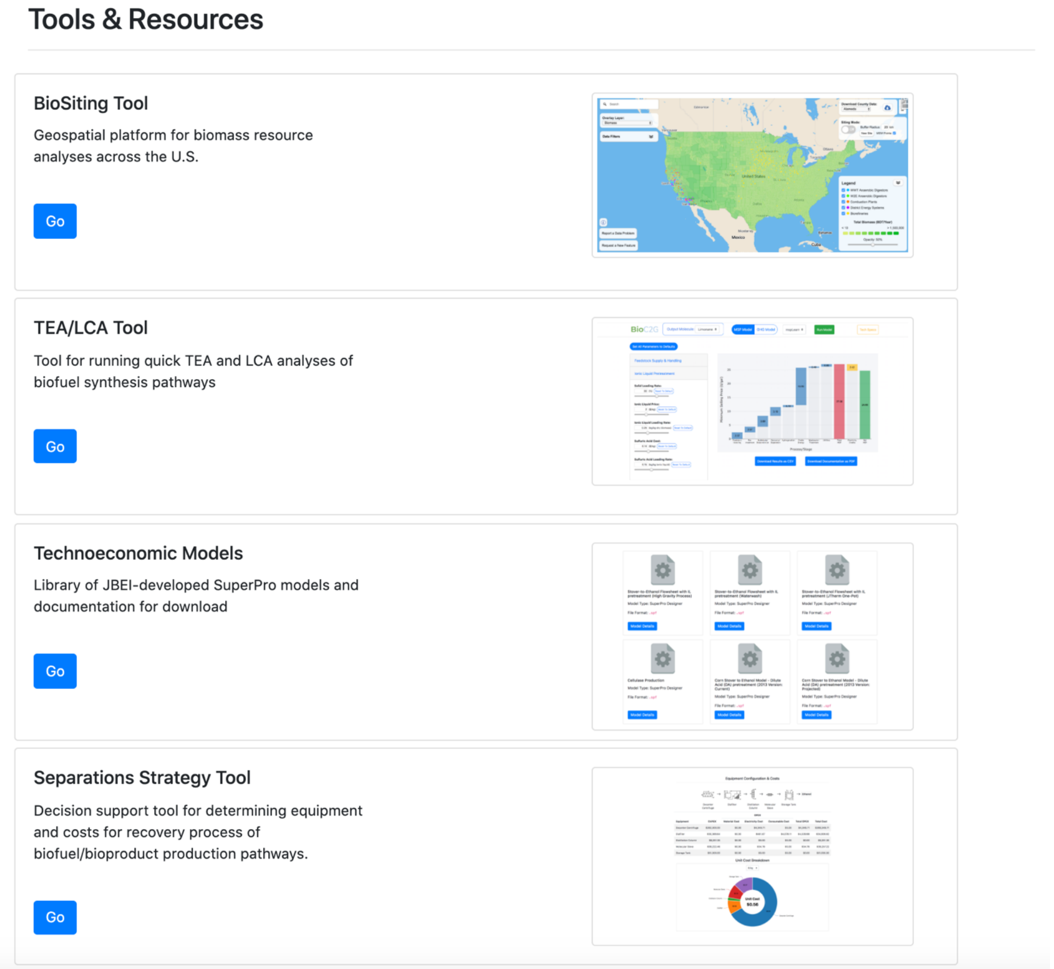
Metrics: # users, accuracy (R^2), completeness, geographic coverage, # production routes built in

BERKELEY LAB

3 – Impact

- Puts TEA and LCA in the hands of non-experts (but with “guardrails”)
- Provides insight into how varying different parts of the process impacts overall cost and environmental impact results – enables lab scientists to see what matters, what doesn’t
- 4 publications published in *ES&T* (IF=7.9), *Current Opinions in Biotechnology* (IF=8.5), *ACS Sustainable Chemistry & Engineering* (IF=7.6)
- 6,825 visits
- 370 unique visitors
- ~10 min per visit





Case studies on bio-derived blue dyes

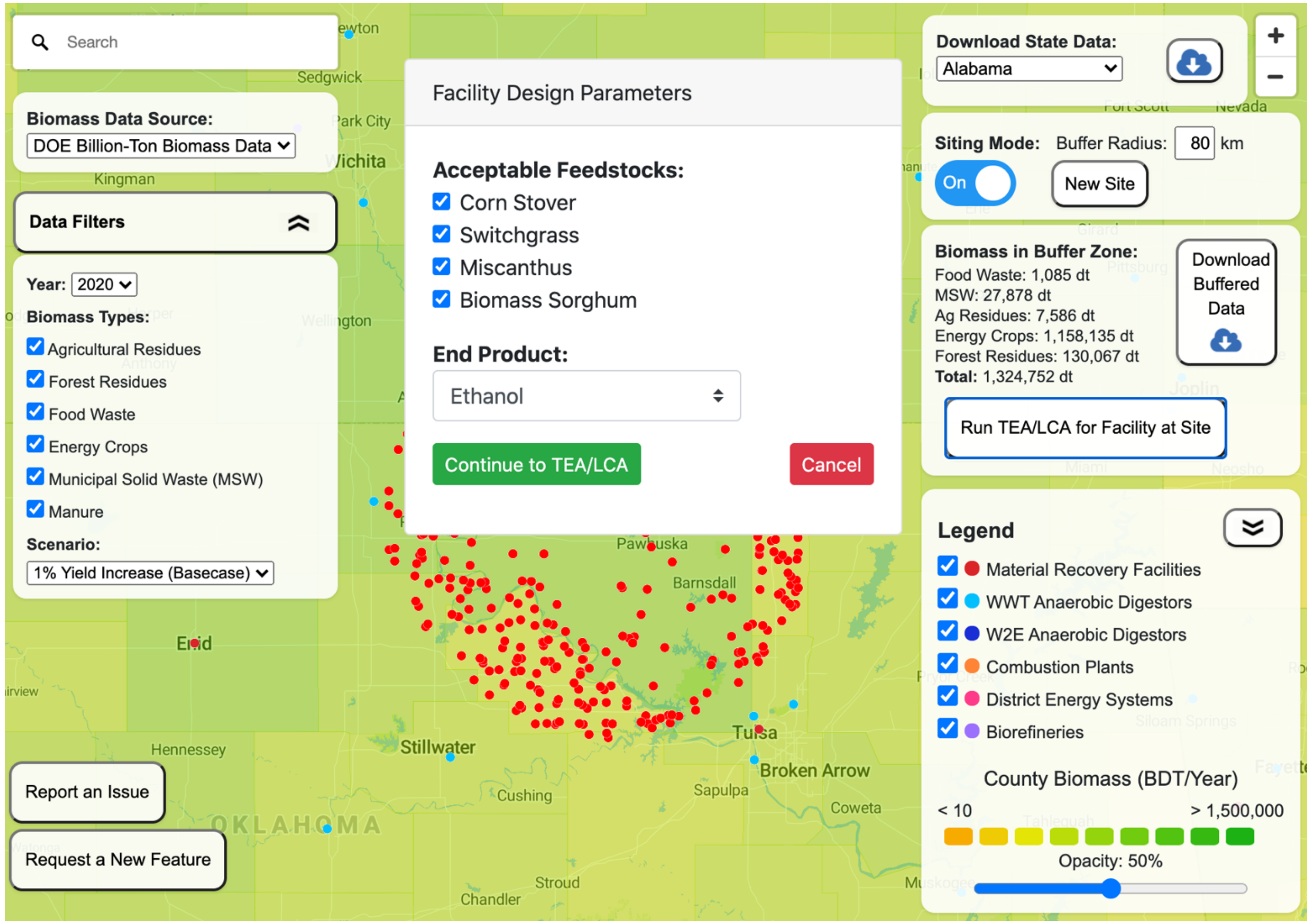
Screenshots from lead.jbei.org

4 – Progress & Outcomes

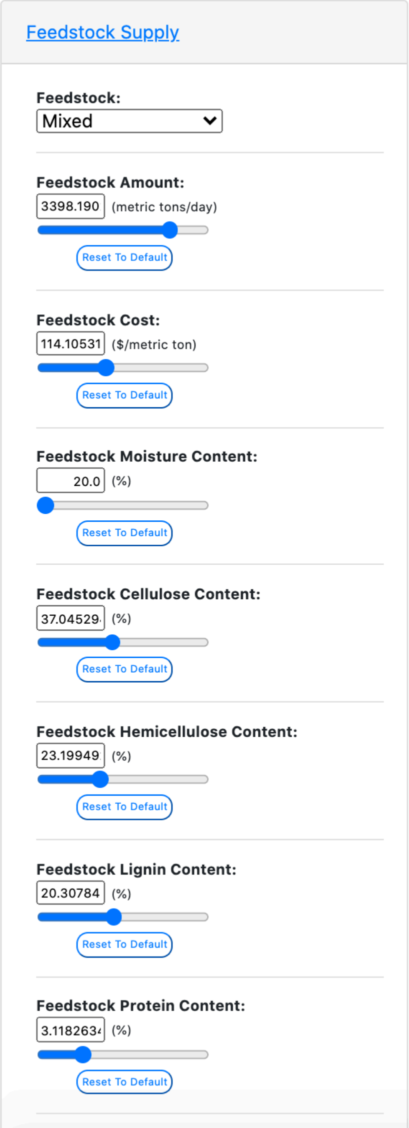
Milestone Name/Description	Criteria	End Date
Finalize and demonstrate automated documentation feature for integration of all 3 tools: Biositing (feedstock filtering) tool, TEA, and LCA	Live demonstration of workflow to run model and auto-generate documentation file	12/31/2020
Complete integration of separations tool and demonstrate for 3 products not pre-built into the BioC2G tool	Case study documentation and preparation of journal article	3/31/2021
Build capability in Biositing tool to select at least 3 different types of plastics as a feedstock for conversion from MRFs	Live demonstration	6/30/2021
Complete demonstration case study (defined in Task 4) for cost and at least 2 environmental metrics (e.g. GHG emissions, water consumption), and deliver completed updating and maintenance plan for Bio-C2G including harmonization with other BETO-sponsored tools/models.	Preparation of journal article	9/30/2021

- **Pretreatment:**
  - Ionic Liquid ([Ch][Lys])
  - Dilute Acid
  - AFEX
  - DMR
- **Products:**
  - Ethanol
  - Limonene + Limonane
  - Bisabolene + Bisabolane
  - Isopentenol (posted soon)
  - DMCO (posted soon)
- **Scenarios:**
  - State of Technology (today)
  - Baseline (50% theoretical yield)
  - Optimal (90% theoretical yield)

4 – Progress & Outcomes

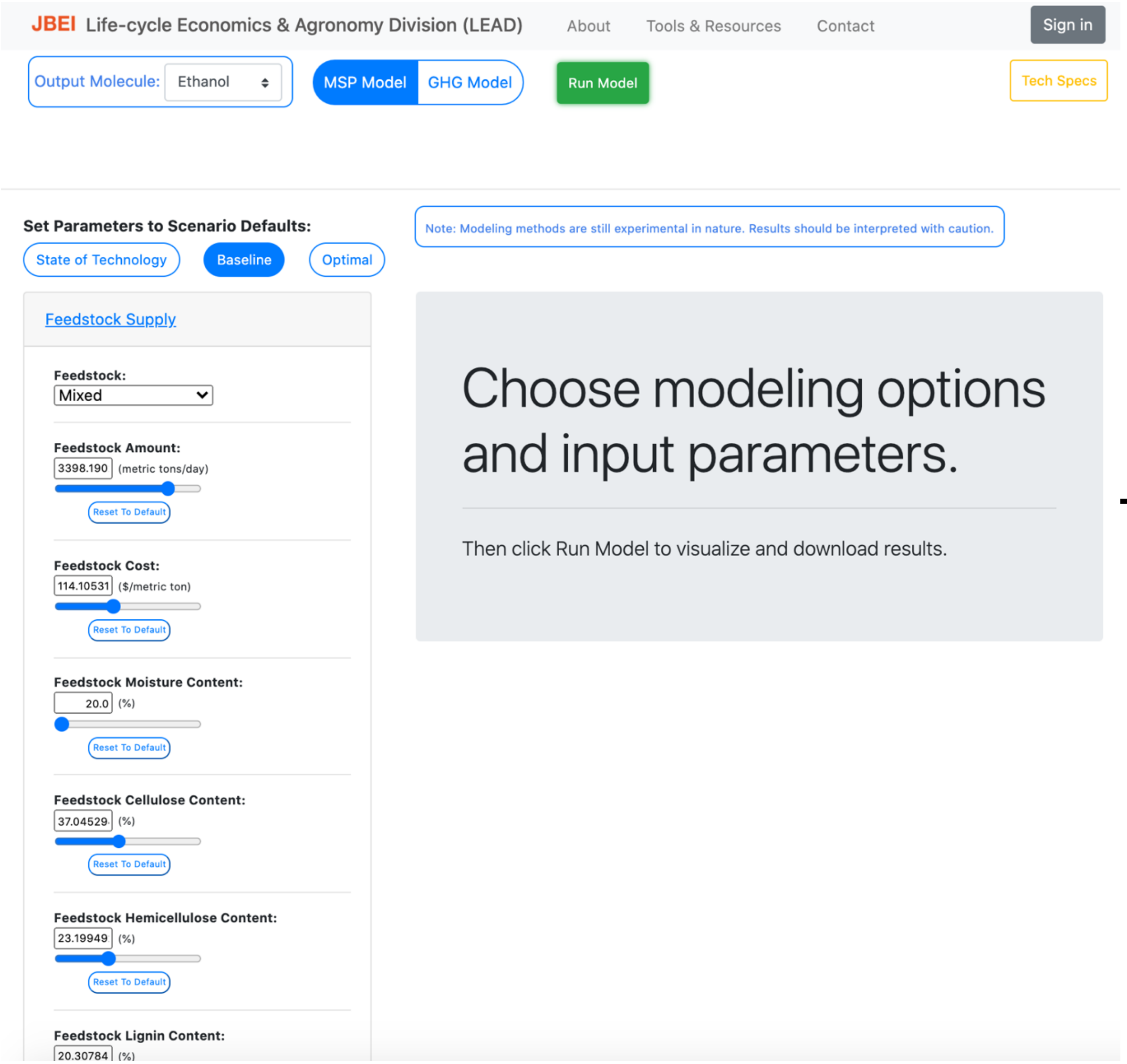


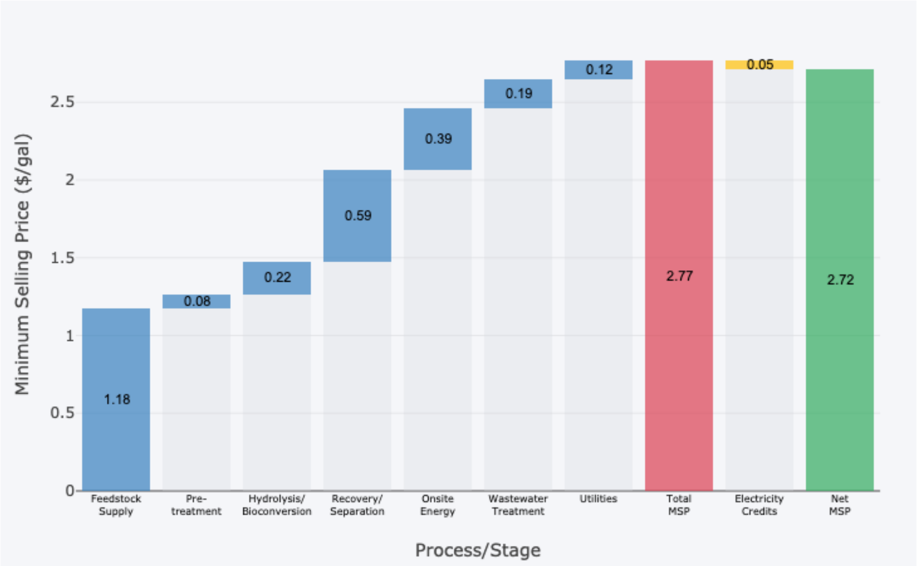
- Tool allows users to define location, radius, and feedstock scenario
- Filter feedstock tyles of interest
- Carry over feedstock mix & quantity to TEA/LCA tool



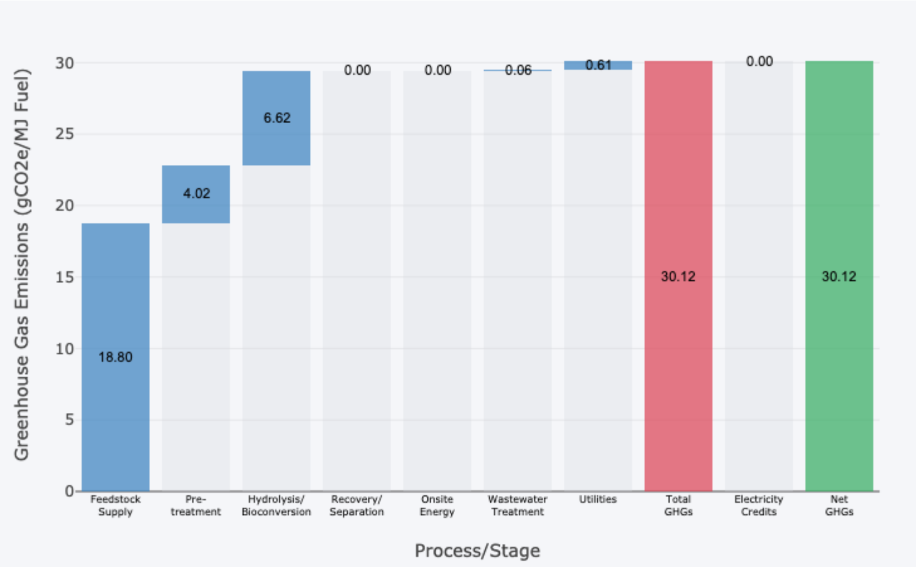
Screenshots from lead.jbei.org

4 – Progress & Outcomes





Sample results



Screenshots from lead.jbei.org

4 – Progress & Outcomes

Separation tool built to give more flexibility specifically for sugar-based routes

Choose your end-product

Ethanol

Select 'other' if product is not listed.

Next

Product Specifications & Microbe Properties

Product Specifications

Product Type/Application: Fuel

Boiling Point: 78.37 °C

Specific Heat Capacity: 2.46 J/g °C

Market Value: Moderate ($10 - $100/kg)

Vapor Pressure: 5.95 kPa

Solubility in Water: Soluble | Insoluble

State of Matter: Liquid

Solid Content: 29.7 %

Crystallizable: Yes | No

Density: 789 g/mL

Required Purity: 97 %

Product Accumulation: Intracellular | Extracellular

Microbe Properties

Microbial Host: *E. coli*

Cell Diameter: 1.69 microns

Process Parameters

Upstream Process Parameters

Facility Working Time: 7920 hr/yr

Flow Rate from Fermentation Broth: 380000 kg/hr

Recovery Process Parameters

Solvent/Extractant Price: 0.4 $/kg

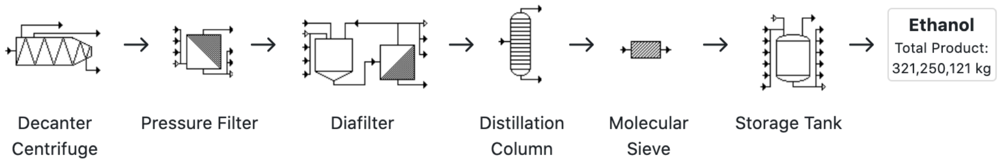
Electricity Price: 0.0572 $/kWh

Solvent/Extractant Density: 655 %

Onsite Storage Time: 7 days

Solvent/Extractant Boiling Point: 68.73 °C

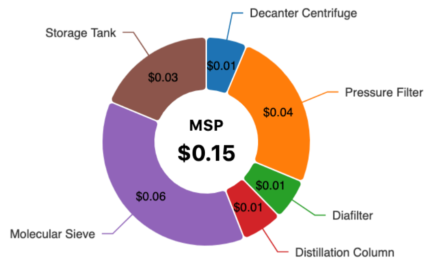
Equipment Configuration & Costs



Equipment	Installed Cost	CAPEX	OPEX: Materials	OPEX: Energy	OPEX: Consumables	OPEX: Total OPEX
Decanter Centrifuge	$524,000.00	$2,576,993.00	$0.00	$25,076.00	$0.00	$25,076.00
Pressure Filter	$6,502,170.00	$10,985,140.00	$0.00	$0.00	$0.00	$0.00
Diafilter	$56,000.00	$1,918,763.00	$0.00	$176.00	$1,556.00	$1,732.00
Distillation Column	$34,318.00	$1,888,268.00	$0.00	$3,905.00	$0.00	$3,905.00
Molecular Sieve	$9,013,122.00	$14,516,731.00	$0.00	$94,392.00	$0.00	$94,392.00
Storage Tank	$4,099,966.00	$7,606,500.00	$0.00	$0.00	$0.00	$0.00
Totals	**$20,229,577.00**	**$39,492,395.00**	**$0.00**	**$123,549.00**	**$1,556.00**	**$125,104.00**

Minimum Selling Price Analysis

Units: $/gal

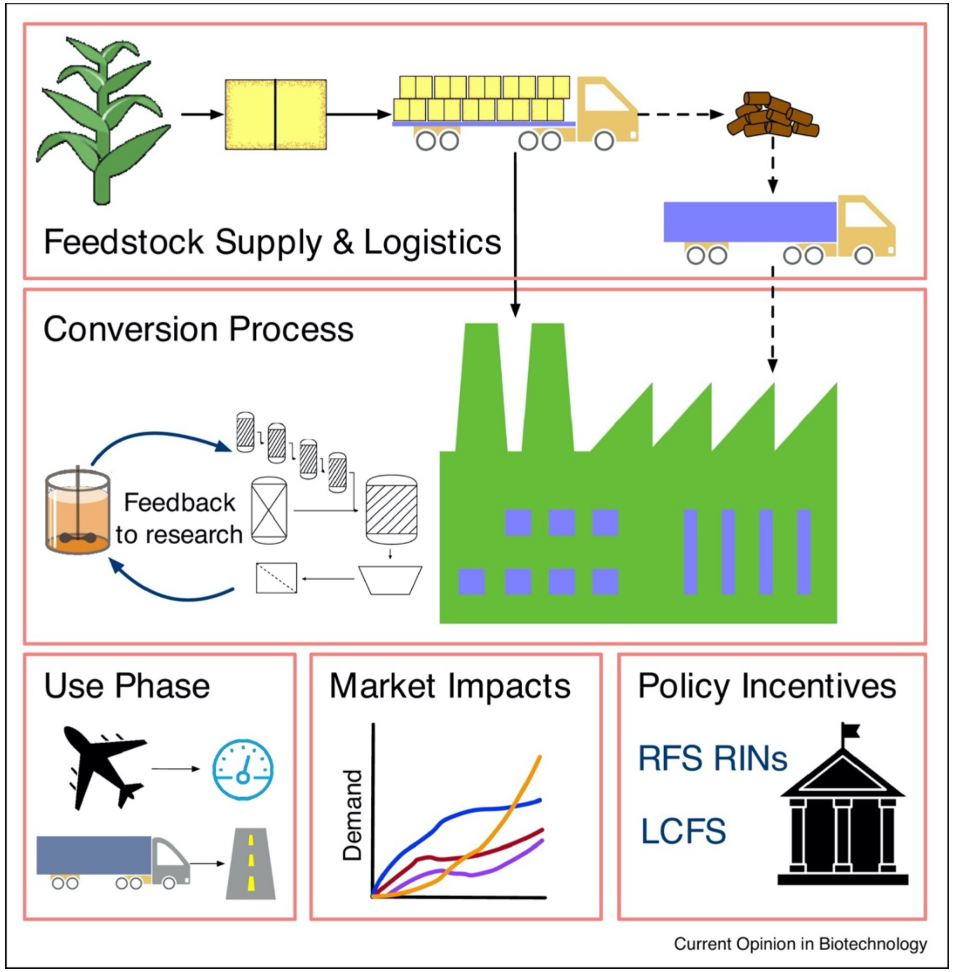


Screenshots from lead.jbei.org

BERKELEY LAB

Summary

- **Goal:** Create an end-to-end feedstock assessment, TEA, & LCA tool usable by non-experts but still functional for experts.
- **Approach:** Combine fast, high-resolution feedstock mapping with lightweight process-based model and surrogate ML modeling, add physical units-based input-output life-cycle assessment model.
- **Progress:** Demonstrated for IL, DA, AFEX, DMR pretreatment methods, > 5 biofuels. Completed linked biositing tool, TEA, and LCA tool.
- **Potential Impact:** Early feedback for non-experts on key cost and environmental impact drivers, as well as screening of potential biorefinery sites.
- **Future Work:** Finish linking separations tool with conventional TEA/LCA and continue adding more routes and built-in products. Build user base and iterate on interface based on user feedback.



Source: Scown et al. 2021

Quad Chart Overview

Timeline
- Start: 10/01/2018
- End: 09/30/2021

	FY20	Active Project
DOE Funding	(10/01/2020 – 9/30/2021)	$325K

Barriers addressed

Technology Uncertainty of Integration and Scaling

Process Integration

Project Goal

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

End of Project Milestone

Complete demonstration case study (defined in Task 4) for cost and at least 2 environmental metrics (e.g. GHG emissions, water consumption), and deliver completed updating and maintenance plan for Bio-C2G including harmonization with other BETO-sponsored tools/models.

Funding Mechanism

BETO Lab Call, FY19

*Only fill out if applicable.

Additional Slides

Publications, Patents, Presentations, Awards, and Commercialization

- Yang, M., Baral, N. R., Anastasopoulou, A., Breunig, H. M., & Scown, C. D. (2020). Cost and Life-Cycle Greenhouse Gas Implications of Integrating Biogas Upgrading and Carbon Capture Technologies in Cellulosic Biorefineries. *Environmental Science & Technology*, 54(20), 12810-12819.
- Baral, N. R., Dahlberg, J., Putnam, D., Mortimer, J. C., & Scown, C. D. (2020). Supply Cost and Life-Cycle Greenhouse Gas Footprint of Dry and Ensiled Biomass Sorghum for Biofuel Production. *ACS Sustainable Chemistry & Engineering*, 8(42), 15855-15864.
- Nordahl, S. L., Devkota, J. P., Amirebrahimi, J., Smith, S. J., Breunig, H. M., Preble, C. V., ... & Scown, C. D. (2020). Life-Cycle Greenhouse Gas Emissions and Human Health Trade-Offs of Organic Waste Management Strategies. *Environmental science & technology*, 54(15), 9200-9209.
- Scown, C. D., Baral, N. R., Yang, M., Vora, N., & Huntington, T. (2021). Technoeconomic analysis for biofuels and bioproducts. *Current Opinion in Biotechnology*, 67, 58-64.