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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

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# Project Overview

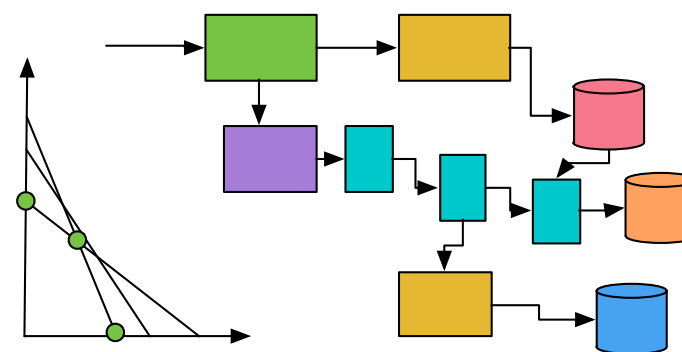
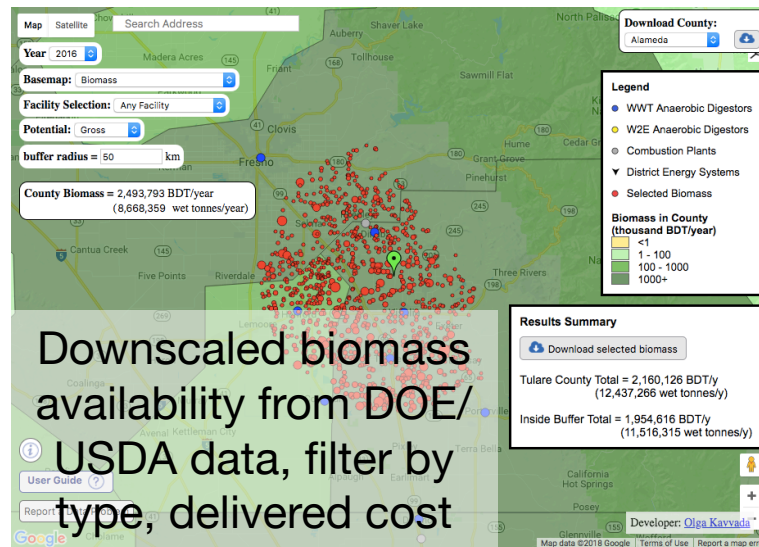
**Challenge:** Feedstock availability, technoeconomic analysis, and life-cycle assessment are modeled on different platforms, difficult to integrate into a single model. Handoffs are clunky and involve proprietary, expensive, expert-only software

**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

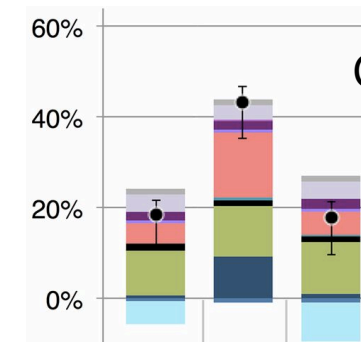
Biorefinery Optimization

Life-Cycle Assessment



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

# 1 – Management



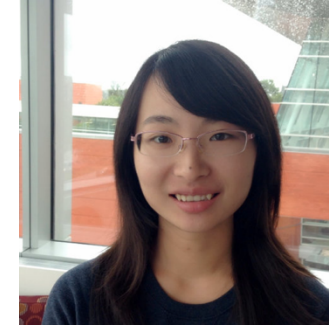
**Corinne Scown (PI)**  
TEA/LCA Expert



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



**Nawa Baral  
(Proj Sci)**  
TEA/LCA



**Minliang Yang  
(Postdoc)**  
TEA/LCA

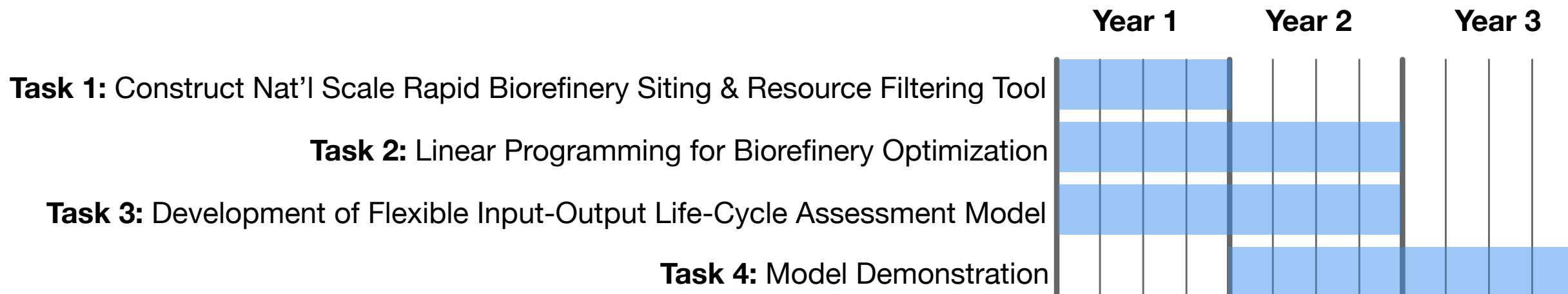


**Sarah Nordahl  
(PhD Student)**  
LCA

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



# 1 – Management

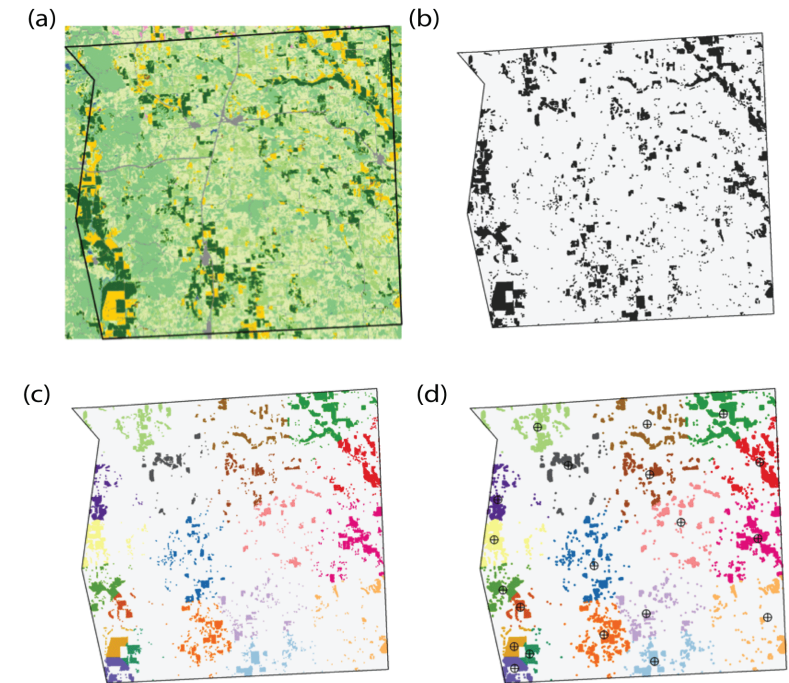


Risk	Mitigation
Limited adoption of tools	Frequent feedback from JBEI users, input from ABPDU and clients, freedom to shift emphasis based on user needs
Model too complex or inaccurate	Staff project with software developer + TEA/LCA experts to ensure robust code and accuracy, publish results in peer-reviewed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

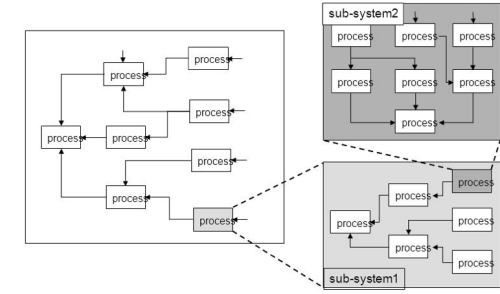
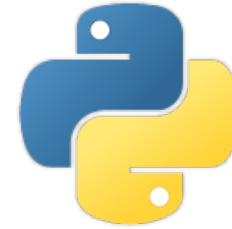
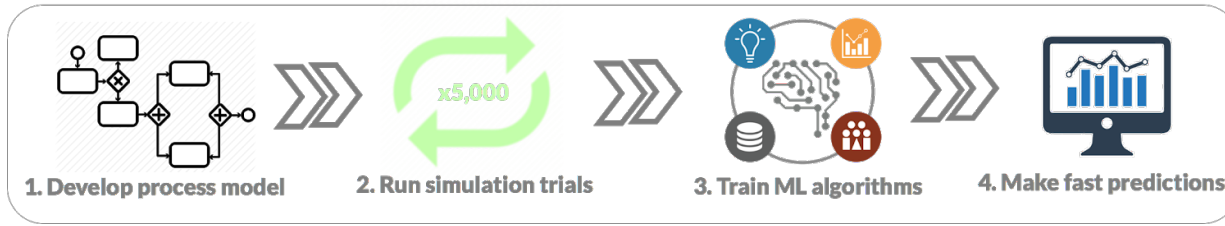
# 2 – Approach

- 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

The screenshot displays the user interface of the lead.jbei.org application. It features a search bar at the top. Below it, there are several filter panels: 'Biomass Data Source' (set to 'USDA NASS Biomass Data'), 'Data Filters' (with an expand/collapse arrow), 'Year' (set to '2017'), 'Biomass Types' (with 'Agricultural Residues' checked), 'Biomass Data Source' (set to 'DOE Billion-Ton Biomass Data'), 'Data Filters' (with an expand/collapse arrow), 'Year' (set to '2020'), 'Biomass Types' (with 'Agricultural Residues', 'Forest Residues', 'Food Waste', 'Energy Crops', 'Municipal Solid Waste (MSW)', and 'Manure' all checked), and 'Scenario' (set to '1% Yield Increase (Basecase)'). A legend panel on the right lists various facility types with checkboxes: Material Recovery Facilities, WWT Anaerobic Digestors, W2E Anaerobic Digestors, Combustion Plants, District Energy Systems, and Biorefineries. Below the legend is a color scale for 'County Biomass (BDT/Year)' ranging from '< 10' (orange) to '> 1,500,000' (dark green), with an 'Opacity: 50%' slider.



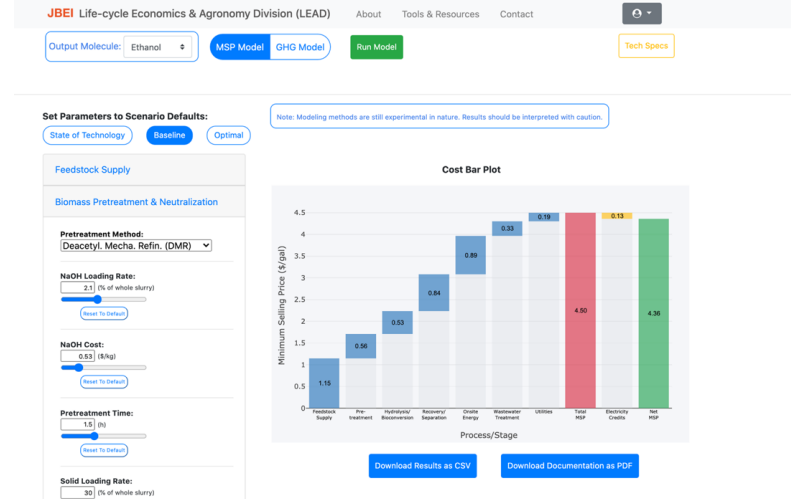
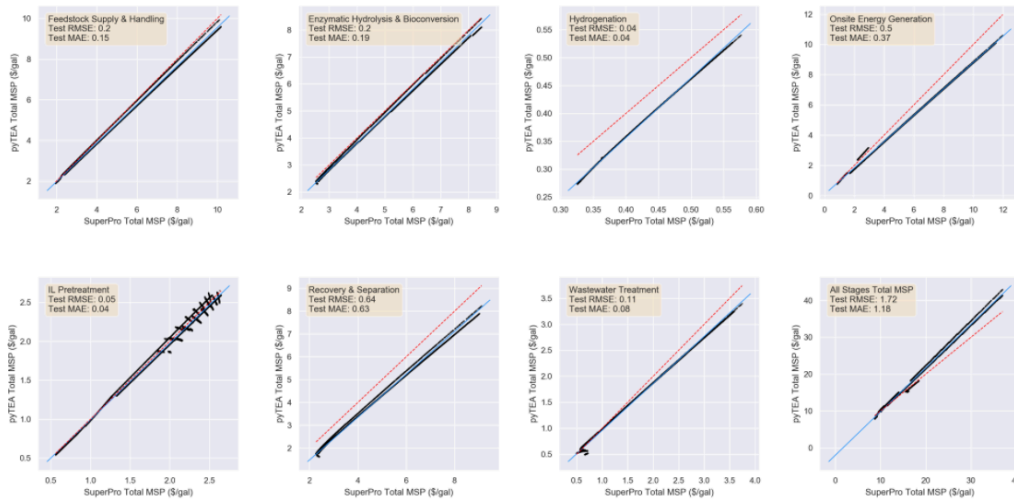
# 2 – Approach



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

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

pyTEA



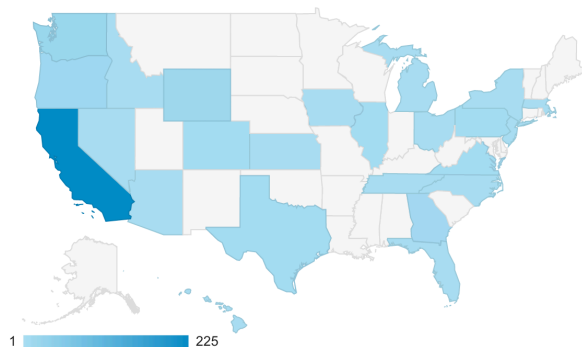
Challenges:

- 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

# 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

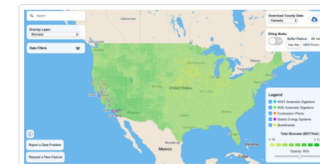


## Tools & Resources

### 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

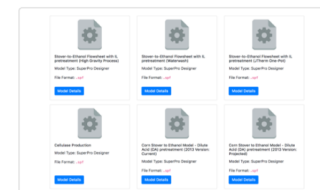
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### Technoeconomic Models

Library of JBEI-developed SuperPro models and documentation for download

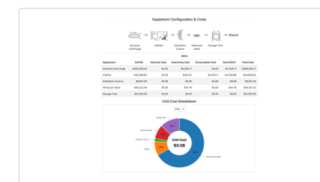
Go



### Separations Strategy Tool

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

Go



## Case studies on bio-derived blue dyes



# 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

The screenshot displays the lead.jbei.org web application interface. It features a map of Oklahoma with various facility locations marked by colored dots. The interface includes several panels and controls:

- Search:** A search bar at the top left.
- Biomass Data Source:** A dropdown menu set to "DOE Billion-Ton Biomass Data".
- Data Filters:** A panel with a "Year" dropdown set to "2020" and "Biomass Types" checkboxes for Agricultural Residues, Forest Residues, Food Waste, Energy Crops, Municipal Solid Waste (MSW), and Manure. A "Scenario" dropdown is set to "1% Yield Increase (Basecase)".
- Facility Design Parameters:** A central panel with "Acceptable Feedstocks" (Corn Stover, Switchgrass, Miscanthus, Biomass Sorghum) and "End Product" (Ethanol). It includes "Continue to TEA/LCA" and "Cancel" buttons.
- Download State Data:** A dropdown menu set to "Alabama" with a download icon.
- Siting Mode:** A panel with "Buffer Radius" set to "80 km" and "On" radio button selected. A "New Site" button is present.
- Biomass in Buffer Zone:** A panel showing biomass data for the buffer zone: Food Waste: 1,085 dt, MSW: 27,878 dt, Ag Residues: 7,586 dt, Energy Crops: 1,158,135 dt, Forest Residues: 130,067 dt, Total: 1,324,752 dt. A "Download Buffered Data" button is present.
- Run TEA/LCA for Facility at Site:** A prominent button at the bottom of the Siting Mode panel.
- Legend:** A panel with checkboxes for Material Recovery Facilities, WWT Anaerobic Digestors, W2E Anaerobic Digestors, Combustion Plants, District Energy Systems, and Biorefineries. It also includes a "County Biomass (BDT/Year)" legend with a color scale from < 10 to > 1,500,000 and an "Opacity: 50%" slider.
- Report an Issue** and **Request a New Feature** buttons are located at the bottom left.

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

The screenshot shows the "Feedstock Supply" configuration panel. It includes several settings with sliders and "Reset To Default" buttons:

- Feedstock:** A dropdown menu set to "Mixed".
- Feedstock Amount:** A slider set to 3398.190 (metric tons/day).
- Feedstock Cost:** A slider set to 114.10531 (\$/metric ton).
- Feedstock Moisture Content:** A slider set to 20.0 (%).
- Feedstock Cellulose Content:** A slider set to 37.04529 (%).
- Feedstock Hemicellulose Content:** A slider set to 23.19949 (%).
- Feedstock Lignin Content:** A slider set to 20.30784 (%).
- Feedstock Protein Content:** A slider set to 3.118263 (%).

# 4 – Progress & Outcomes

JBEI Life-cycle Economics & Agronomy Division (LEAD)    About    Tools & Resources    Contact    Sign in

Output Molecule: Ethanol    MSP Model    GHG Model    Run Model    Tech Specs

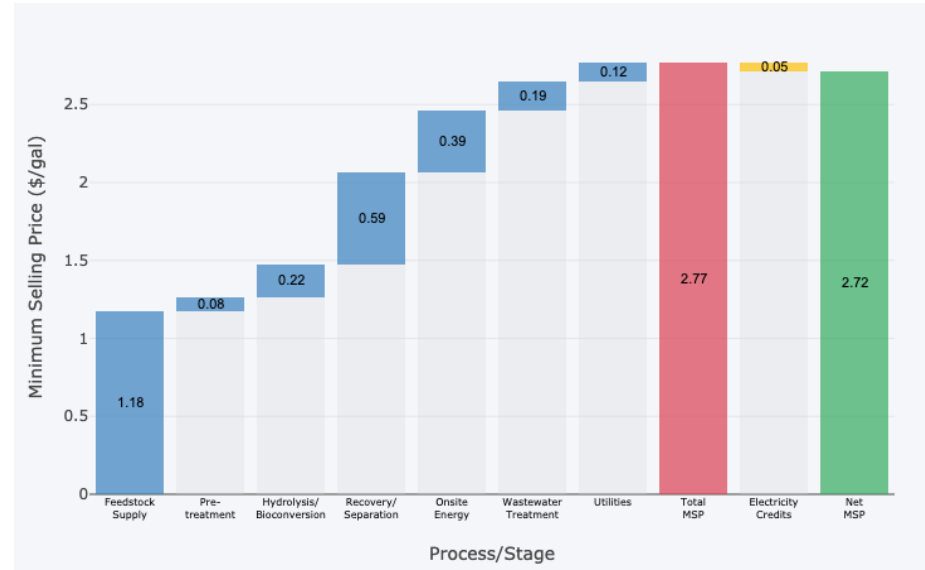
Set Parameters to Scenario Defaults:

State of Technology    Baseline    Optimal

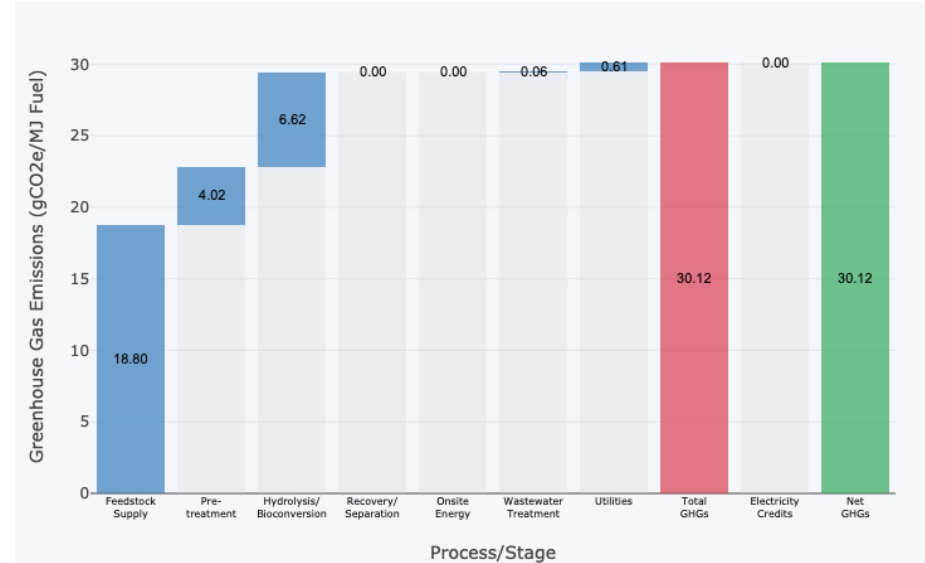
Note: Modeling methods are still experimental in nature. Results should be interpreted with caution.

## Choose modeling options and input parameters.

Then click Run Model to visualize and download results.



Sample results



# 4 – Progress & Outcomes

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

State of Matter: Liquid

Solid Content: 29.7 %

Crystallizable: Yes

Density: 789 g/mL

Required Purity: 97 %

Product Accumulation: Intracellular

### 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

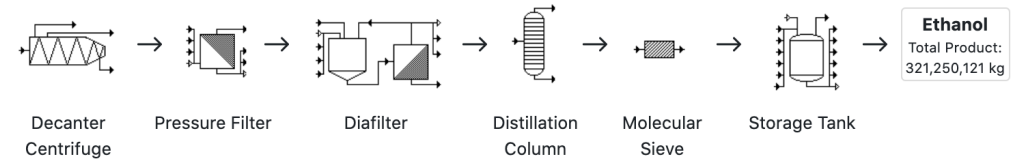
Solvent/Extractant Density: 655 %

Onsite Storage Time: 7 days

Solvent/Extractant Boiling Point: 68.73 °C

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

## Equipment Configuration & Costs

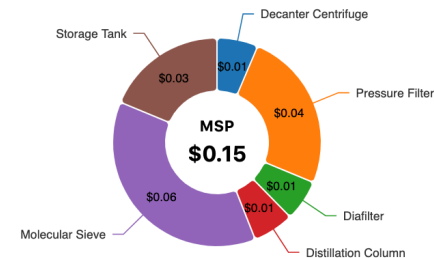


### OPEX

Equipment	Installed Cost	CAPEX	Materials	Energy	Consumables	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
<b>Totals</b>	<b>\$20,229,577.00</b>	<b>\$39,492,395.00</b>	<b>\$0.00</b>	<b>\$123,549.00</b>	<b>\$1,556.00</b>	<b>\$125,104.00</b>

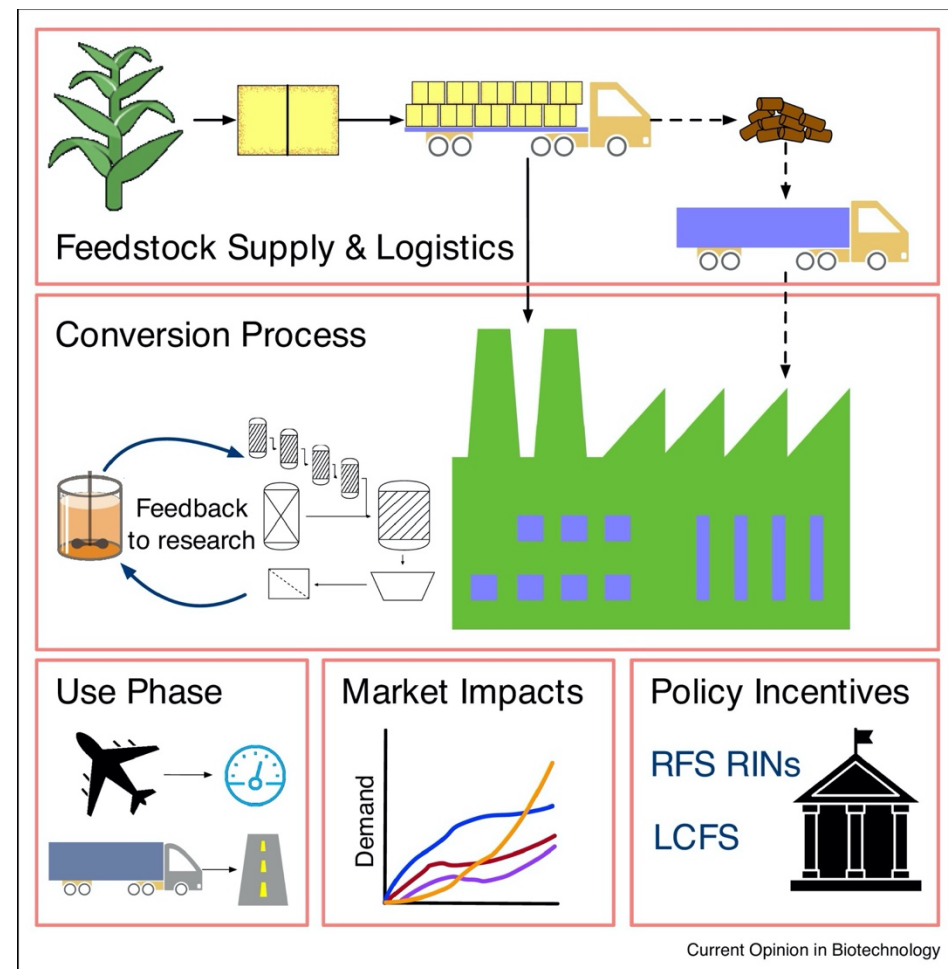
## Minimum Selling Price Analysis

Units: \$/gal



# 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

## Project Goal

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

FY20

Active Project

DOE  
Funding

(10/01/2020 –  
9/30/2021)

\$325K

## 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.

## Barriers addressed

Technology Uncertainty of Integration and Scaling

Process Integration

## Funding Mechanism

BETO Lab Call, FY19

# 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.