Agent-based Modeling for the Multi-objective Optimization of Energy Production Pathways: Integrated Techno-economics and Life Cycle Assessment

March 12, 2021
Data Modeling and Analysis

Jason Quinn
Colorado State University
Project Overview

What are the risks:
- Large Scope
- Moving target

How it is done today:
- Evaluate one technology scenario independent of other technologies
- Technology investment and policy are not typically fully informed

What we are doing:
- Support informed research and commercialization direction based on economic and environmental goals
- Developing an integrated modeling framework

Why this is important:
- Sustainable US energy policy
- Biofuels portion of this picture
- Quantitative or measurable % reduction GHG, Cost, etc. of technology

Project Overview:

- First of a Kind analysis project with bold goals
- Project goals: Develop open-source integrated US biofuel model that enables an evaluation from a systems level the ability to meet DOE sustainability goals
1 – Management

CSU Team

PI: Jason Quinn
Co-PI: John Field
Co-PI: Steve Simske
Co-PI: Thomas Bradley
RS I: Evan Sproul
GRA: Jack Smith

B&D LLC

Co-PI: Colin Beal
TL: Nathan Putnam

NCSU Team

Co-PI: Jordan Kern
GRA: Ece Arı Akdemir
UG: Taylor Pack

Advisory Board

Troy Hawkins: ANL
Carlos Quiroz-Arita: SNL
Bill Brandt: ASU
Ryan Davis: NREL
1 – Management

Inclusive Research Environment

The Meeting Details:
• Weekly project meetings
• Quarterly meetings with DOE
• 6 month updates to Advisory board

Research Structure

Collaborative Sub-team Research

Team Research Meetings

Sub-team Research

Risk Management:

Communication

Creative Problem Solving
FOA targets:
• Reducing Consumption Water (10-30%), Energy Consumption (20-60%), GHG Emissions (50-80%), Pollutant Emissions (10-30%)

Program Connections:
• Optimization of the energy bioeconomy
• Defining from a systems level pathways and investments that lead to sustainable bio-economy
2 – Approach

DayCent: Geospatial Agricultural Modeling

Spatially-resolved data generated from DayCent model

- Process-based simulation of crop yields, soil carbon changes, other soil GHG emissions as affected by soil, climate, and land management

Python-based spatial modeling workflow:

1. Identification of target land base (e.g., existing annual cropland, marginal or abandoned land, etc.)

2. Specification of management scenarios (e.g., fertilizer application rates, stover removal, etc.) & associated pseudo field-scale model runs

3. Automated simulation execution (CSU cluster) and results analysis

abandoned land

switchgrass yield

annual production

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© OpenStreetMap

© OpenStreetMap
Fundamental Process Models

1st Generation Feedstocks (Corn, Sugar Crops, Oil Crops)

Crop Residues (Corn Stover, Sorghum, Bagasse)

Dedicated Cellulosics (Switchgrass, Miscanthus, Straw, Woody Biomass)

Microalgae and Macroalgae

Municipal Solid Wastes

Lipid Extraction

Fermentation

Pyrolysis

Gasification

Hydrothermal Liquefaction

Anaerobic Digestion

Ethanol to Jet Fuel

Distillation

Fischer-Tropsch

Gas Fermentation

Transesterification

Hydroprocessing

Renewable Diesel

Butanol

Jet Fuel

Ethanol

Non-Fuel BP; protein/meal...

Biodiesel

Refined Hydrocarbons

Methane

Numerous Pathways – Consistent Methodology
Defines Potential Solution Space (Enables Project)
LCA and TEA Results
MFSP
Greenhouse Gas Impact
Water Use
Criteria Pollutants
Consumes Rich Spatial Data (DayCent)
Feeds Optimization Algorithm

B&D LLC
2 – Approach
Modular Process Modeling

Fundamental Process Models

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Ethanol to Jet Fuel
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Gas Fermentation
Transesterification
Hydroprocessing

Renewable Diesel
Butanol
Jet Fuel
Ethanol
Non-Fuel BP; protein/meal...
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2 – Approach
Multi-objective Optimization
Embed LCA/TEA within Multi-objective optimization of Biofuel Supply Chain (farm to fuel)

Optimize County-to-Hub Supply Chain Network

**Decision variables:**
- County level cultivation choices (feedstock, volume)
- Flow of biomass between preprocessing hubs and biorefineries
- Biorefinery design, size and location
- End product choice

**Constraints:**
- Production quotas, resource usage (land, water), supply vulnerability (weather)

Navigating Tradeoffs in Cost and Greenhouse Gas Emissions (what if there’s no silver bullet?)

Better understand design choices that lead to:

- Higher cost + lower emission  vs  Lower cost + higher emission
2 – Approach
Agent Based Modeling

Agents in US Bioeconomy

**Framework Capacity:**
- Farmer/Biorefinery/Consumer Interaction and Behavior
- Predict Pathway Adoption Rates and Mechanisms
- Identification of Levers in Industry
- Informs Behavior of Proposed Policy

**Characteristics:**
- Yearly Time-Steps (Analysis of Intermediate States)
- Preserves Heterogeneity
- Potential to Model Adaptive Behavior
3 – Impact

• **Goal of the project is IMPACT**
  – Identifying technologies and pathways that meet DOE sustainability targets
  – Identify performance (R&D) targets for DOE and Industry

• **System level assessment**
  – Not individual technologies

• **Department of Energy is Dynamic**
  – Modeling work is intended to be re-active and adjustable
    • Current administration is focusing on the environment
    • Future of biofuels (heavy fuels and jet)

• **Generation of open-source toolset**
4 – Progress and Outcomes
DayCent: Geospatial Agricultural Modeling

• Completed curation of modeling results for current-day corn–soybean cultivation in US Corn Belt, incl. stover harvest
  – Highest density of production in Iowa, Illinois
  – Quantified soil carbon penalty of different rates of stover harvest rates

• Preliminary results for switchgrass cultivation on abandoned cropland across same region
  – Abandoned land down-scaled from historical county land use records
  – Different spatial pattern, with abandoned land most concentrated at periphery of the Corn Belt
  – Ongoing modeling effort to capture baseline for business-as-usual management of abandoned lands
4 – Progress and Outcomes
Process Modeling

Completed Pathways
- Corn Grain to EtOH
- Corn Stover to EtOH
- Soy to Biodiesel
- Switchgrass to Jet
- Corn Stover to Jet

Flexible Structure – Facilitates Added Pathway Steps
4 – Progress and Outcomes

Multi-objective Optimization

Initial proof-of-concept for 5 national jet fuel pathways: Balance cost, GHGs, and land use, produce 12M gallons

Multi-objective optimization of Biofuel Supply Chain (farm to fuel)

<table>
<thead>
<tr>
<th>Source</th>
<th>Cost ($/gge)</th>
<th>Post-Combustion GHG (g CO2e/MJ)</th>
<th>Arable Land (m2/GJ/yr)</th>
<th>Nitrogen (g/GJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soybean HEFA</td>
<td>$14.85</td>
<td>20.94</td>
<td>370.75</td>
<td>102.08</td>
</tr>
<tr>
<td>Corn AF</td>
<td>$6.66</td>
<td>40.92</td>
<td>85.52</td>
<td>1,186.38</td>
</tr>
<tr>
<td>Forestry Biomass FT</td>
<td>$7.11</td>
<td>70.88</td>
<td>99.64</td>
<td>354.82</td>
</tr>
<tr>
<td>Grasses FT</td>
<td>$8.24</td>
<td>41.87</td>
<td>128.17</td>
<td>1,512.40</td>
</tr>
<tr>
<td>Marine Microalgae HTL</td>
<td>$16.79</td>
<td>108.90</td>
<td>0.00</td>
<td>226.60</td>
</tr>
</tbody>
</table>

Lowest Price

1. Lowest Price

2. Lowest Price

3. Lowest Price

Highest land, Lowest GHG

1. Highest land, Lowest GHG

Lowest land, Highest GHG

2. Lowest land, Highest GHG

3. Lowest land, Highest GHG
Scenarios:

1) Only profitability
2) Only familiarity
3) Only environmental
4) Equal weighting
5) Random weighting

4 – Progress and Outcomes
Agent Based Modeling

![Diagram showing progress and outcomes with bar charts and a pie chart.](image-url)
Note future potential
• >1 billion tons biomass in 2040
• ~35% from dedicated energy crops

Identify promising case studies

Near Term

Long Term

Integrated Assessment Model
• Dynamic assessment tool
• Holistic tool set that investigates non-trivial trade-offs
• Enables informed policy decisions
• Leverages multiple optimization techniques

Open-source model for the community
## 4 – Progress and Outcomes

<table>
<thead>
<tr>
<th></th>
<th>Development of modular engineering process models</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>Development of concurrent and spatially explicit sustainability models</td>
</tr>
<tr>
<td>3.0</td>
<td>External Review</td>
</tr>
<tr>
<td>Go/No-go</td>
<td>Modeling of 6 production pathways with results quantifying water consumption, energy consumption, greenhouse gas emissions, and pollutant emissions for fuel products on the metrics of MJ MJ-1, g-CO2-eq MJ-1, and g MJ-1, respectively</td>
</tr>
<tr>
<td>4.0</td>
<td>Development of modular engineering process models</td>
</tr>
<tr>
<td>5.0</td>
<td>Optimization and evaluation of favorable configurations</td>
</tr>
<tr>
<td>6.0</td>
<td>External review</td>
</tr>
</tbody>
</table>

**Progress:**
- On schedule with process modeling
- Ahead of Schedule on optimization work
Summary

• **Demonstrated capabilities**
• **Adapting to Directions of the DOE**
• **Established an effective working team**
• **Technical achievements**
  – Modular Process modeling
  – Demonstrated proof of concept on MOO and ABM
  – Geospatial data modeling and integration
• **Defining near term directions with the DOE**
Quad Chart Overview

Timeline
- 10/01/2019
- 09/30/2021

<table>
<thead>
<tr>
<th>FY20 Costed</th>
<th>Total Award</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10/01/2019 – 9/30/2020) $15,703.51</td>
<td>$1,000,000</td>
</tr>
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</table>

DOE Funding

Project Goal
Develop an open-source sustainability model that supports the strategic investment of research by the DOE to achieve renewable fuel goals.

End of Project Milestone
- Develop an open source bioenergy tool to support strategic investments by DOE.
- Identify optimum bioenergy pathways through Agent Based Modeling (ABM) and multi-objective optimization to meet sustainability goals: reduction in water consumption, energy consumption, greenhouse gas emissions, and/or pollutant emissions.
- Couple economic modeling and life cycle assessment to understand the impact of carbon accounting on technology investments.

Project Partners*
- North Carolina State University
- B&D Consulting

Funding Mechanism
DE-FOA-0002029

*Only fill out if applicable.
DOE Bioenergy Technologies Office (BETO)
2021 Project Peer Review

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