An optimization-based web application for synthesis and analysis of biomass-to-fuel strategies

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Abstract: We develop an optimization-based web application for assessing biomass-to-fuels strategies based on the Biomass Utilization Superstructure (BUS) framework. This web application allows researchers with limited knowledge of optimization to assess different technologies employed at different strategies and identify the major cost drivers. The user must only provide the necessary parameters and create an optimization run after identifying the question to be addressed and the assessment metric. The web application generates visual representations of the results once the optimal solution is obtained. Finally, we demonstrate the applicability of the web application through an example. © 2017 The Authors. Biofuels, Bioproducts and Biorefining published by Society of Chemical Industry and John Wiley & Sons, Ltd.

Supporting information may be found in the online version of this article.

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Introduction

Biomass is a renewable energy source that can potentially mitigate global climate change linked to greenhouse gas (GHG) emissions. Advances in fundamental research have resulted in the development of numerous biomass-to-fuels strategies. The abundant biomass, including energy crops and biomass wastes, can be deconstructed and converted to biofuels biochemically, catalytically, or thermo-chemically. Evaluation of these strategies is key in identifying major cost drivers and bottlenecks for biofuel production. The major challenge in this type of analysis is that feedstocks can be converted to biofuels in multiple ways and, in
general, a biofuel can be produced by multiple feedstocks. An effective way to evaluate multiple options simultaneously is superstructure optimization,13–16 which is a model-based approach that considers alternative strategies simultaneously. Based on this approach, Kim et al.17 developed a Biomass Utilization Superstructure (BUS) framework, which incorporates a wide range of conversion technologies along with the corresponding feedstocks, intermediates, and final products. This framework allows the identification of new biofuel production strategies, and the simultaneous assessment and comparison of alternative strategies.

Nonetheless, generating a superstructure, and developing and solving the resulting optimization model are complicated and can be especially challenging for researchers without domain expertise. Therefore, to facilitate the implementation of the BUS framework, which allows researchers to generate key insights into the use of newly developed technologies, we develop a web application for assessing biomass-to-fuels strategies, which is accessible to the public through https://bus.glbrc.org/. This web application offers the user the flexibility to select different products or feedstocks of interest and assessment metrics (e.g., cost minimization or profit maximization).

In the remaining text, we first present the problem statement and model formulation. Then we describe the different types of questions that can be addressed using this web application and its basic structure. Finally, we demonstrate how it can be used to address a range of problems.

### Optimization problem

#### Problem statement

Figure 1 shows a biomass utilization superstructure which consists of potential deconstruction and conversion technologies, and the corresponding compounds. We treat technologies and compounds as nodes, and compound flows as arcs. We classify compounds into four categories: feedstocks, intermediates, products, and by-products. A strategy consists of a subset of technologies and the associated compounds, and it is obtained as a solution of the superstructure model. For example, in a biochemical conversion strategy, corn stover is pre-treated and converted to ethanol via dilute acid pre-treatment, enzymatic hydrolysis, and co-fermentation, followed by product purification.18

We use lowercase Greek letters for parameters, uppercase italic Latin letters for variables, lowercase italic Latin letters for indices, and uppercase bold Latin letters for sets.

The general problem is stated as follows: We are given a set of compounds \( i \in \mathbf{I} \) with availability \( \alpha_i \), minimum purchase \( \beta_i \), minimum and maximum demands \( \underline{d}_i/\overline{d}_i \), and price \( \lambda_i \). The subsets of feedstock, intermediate, product, and by-product are denoted by \( i \in \mathbf{I}_F/\mathbf{I}_I/\mathbf{I}_P/\mathbf{I}_B \), respectively. We are also given a set of technologies \( j \in \mathbf{J} \) with capacity \( \delta_j \), unit production cost \( \mu_j \), and conversion coefficient \( \eta_{ij} \). The subsets of technologies that produce and consume compounds are denoted by \( j \in \mathbf{J}_P/\mathbf{J}_I \), respectively.

We aim to identify an optimal strategy to meet feedstock consumption or final product demand targets using various metrics.

#### Mathematical formulation

We introduce the following non-negative continuous variables: \( P_i \) denotes the amount of feedstock \( i \in \mathbf{I}_F \), purchased; \( S_i \) denotes the amount of product or by-product \( i \in \mathbf{I}_P/\mathbf{I}_B \), sold; \( X_j \) denotes the production level of technology \( j \).

The material balance is given as:

\[
P_i + \sum_{j \in \mathbf{J}_P} \eta_{ij} X_j = S_i - \sum_{j \in \mathbf{J}_I} \gamma_{ij} X_j \quad \forall i
\]  

(1)

Note that \( \eta_{ij} < 0 \) for inputs and \( \eta_{ij} > 0 \) for outputs. For each technology, we fix the conversion coefficient for the main product to 1, and normalize the coefficients for the remaining components that enter or exit the technology (Supporting Information).

The feedstock consumption is bounded by its minimum purchase and availability:

\[
\beta_i \leq P_i \leq \alpha_i \quad \forall i \in \mathbf{I}_F
\]  

(2)

The production level of each technology is bounded by its allowable capacity.

\[
X_j \leq \delta_j \quad \forall j
\]  

(3)

The sales of products and by-products are bounded by their minimum and maximum demands.

\[
\gamma_i \leq S_i \leq \overline{\gamma}_i \quad \forall i \in \mathbf{I}_P/\mathbf{I}_B
\]  

(4)
The evaluation can be performed using various metrics. For example, we can use minimum cost, which includes the feedstock purchase and the production costs, minus the sales of by-products.

\[
\text{Min } Z_1 = \sum_{i \in I} \lambda_i P_i + \sum_{j} \mu_j X_j - \sum_{i \in I_B} \lambda_i S_i
\]  

(5)

We can also use maximum profit as an objective function, which includes the sales of products and by-products, minus the feedstock purchase and the production costs.

\[
\text{Max } Z_2 = \sum_{i \in I} P_i \cup I_B \lambda_i S_i - \sum_{i \in I_F} \lambda_i P_i - \sum_{j} \mu_j X_j
\]  

(6)

The linear programming (LP) model is coded in General Algebraic Modeling System (GAMS)\(^{19}\) and solved using CPLEX solver.

### Types of questions

We can use the proposed model to address different types of questions, such as:

- **Question 1**: What is the optimal strategy for a specific feedstock?
- **Question 2**: What is the optimal strategy for a specific product?
- **Question 3**: What is the optimal strategy for specific feedstock and product?

The details on how the models must be modified to address these questions are given in the Supporting Information. Once a question is chosen, we formulate a problem by selecting the metric (e.g. cost minimization or profit maximization) to be used to find the optimal strategy. The problem is represented as Q.Z, where Q is the question and Z is the assessment metric (Fig. 2). For example, we define problem Q1.Z2 if we aim to find the optimal strategy for a given feedstock (Q1) using profit maximization as the metric (Z2).

### Web application interface

The BUS web application is built on the Ruby on Rails\(^{20}\) web application framework and hosted at the Great Lake Bioenergy Researcher Center (GLBRC). To begin using the application, the user must first create an account. Figure 3 depicts the general workflow within the web application. The user is only required to enter the necessary parameters in the **Network** page, and identify the question to be addressed and the assessment metric in the **Optimization** page. If there are any errors, warnings will appear to alert the user. The details on **Network** and **Optimization** pages will be discussed in the following sub-sections. All stored parameters will be exported to the optimization tool and the LP model will be solved. The application then stores optimization results and generates visual representations. The user can view and clone the existing network or optimization results as well as share it with other users.

### Network

There are three main elements in the **Network** page: **Compounds**, **Technologies**, and **Links**. The user first defines the technologies of interest and their corresponding compounds and then provides the necessary parameters (e.g. price, availability, demand). It is then followed by inserting...
conversion coefficients to connect the compounds and the technologies. There are two methods to insert compounds and technologies within a network: (i) manual entry and (ii) spreadsheet upload. The former can be implemented by creating compounds and technologies and filling out the data manually. If the network involves large numbers of compounds and technologies, users are encouraged to use the latter method. A spreadsheet template is readily downloadable for users to fill in all data. The server will automatically process the uploaded data in the database. Finally, the user will be able to see a visual representation of the network that connects all technologies and compounds.

**Optimization**

Following the creation of a network, the user proceeds to the Optimization page to create a new optimization run. The user selects the question to be addressed and the compounds of interest, as well as the assessment metric. The optimal strategy is found once the optimization model is solved. The Optimal Strategy tab shows the selected technologies and compounds. The arcs vary in width based on the flows of compounds, and the technology nodes vary in shades of red based on their production costs. A darker color indicates higher production cost while thicker arcs indicate larger compound flow. The user can see the numerical values (e.g. production cost, compound flow, etc.) by hovering over the nodes and arcs. The Results tab shows the detailed results of the optimal strategy (e.g. production level of selected technologies, amounts of compounds sold and consumed, cost contributions) in bar charts.

**Application**

**Example**

We consider the utilization of corn stover and hardwood to produce gasoline, diesel, and ethanol. Figure 4 shows the corresponding simplified superstructure, where we group similar technologies or compound into one node. For example, there are two different dilute acid pre-treatment technologies that consume corn stover and hardwood, respectively. We group both technologies into one node, which denoted as ‘DA.’ The full superstructure is given in the Supporting Information. In thermochemical-based conversion strategies, corn stover and hardwood are chopped prior to pyrolysis or gasification. We consider two pyrolysis technologies\(^1\) (in situ and ex situ upgrading of fast pyrolysis vapors) and two gasification technologies\(^2\) (indirect and direct gasification). Crude bio-oil and char are produced from pyrolysis. The former is then converted to gasoline and diesel via hydrotreating and hydrocracking, while the latter is sent to combined heat and power plant for electricity generation. The raw syngas produced from gasification is sent for steam reforming, followed by methanol synthesis. Methanol is either sent

![Figure 4. Corn stover and hardwood utilization superstructure. Orange, gray, green, and yellow circles represent feedstocks, intermediates, products, and by-products, respectively. Abbreviations: Compounds – AA: acetic acid, BO: bio-oil, Bro: broth, CBO: crude bio-oil, CS: corn stover, Dies: diesel, Elec: electricity, EtOH: ethanol, Gas: gasoline, HWood: hardwood, Hydz: hydrolyzate, MeOH: methanol, Parti: chopped particles, RawAA: raw acetic acid, RawSG: raw syngas, Res: residue, SG: syngas, Sl: slurry. Technologies – AAS: acetic acid synthesis, AFEX: ammonia fiber expansion pre-treatment, AH: acidic hydrolysis, CHP: combined heat and power generation, DA: dilute acid pre-treatment, DG: direct gasification, Dis-WT: distillation and wastewater treatment, EH: enzymatic hydrolysis, Ferm: fermentation, H-C: handling and chopping, Hycrack: hydrocracking, Hygen: hydrogenation, Hytreat: hydrotreating, IDG indirect gasification, MS: methanol synthesis, PyrIn: in situ pyrolysis, PyrEX: ex situ pyrolysis, SR: steam reforming, SSF: simultaneous saccharification and fermentation.](image-url)
to acetic acid synthesis and hydrogenation for ethanol production. Acetic acid can be sold as a by-product. In biochemical-based conversion strategies, corn stover and hardwood can be pre-treated using dilute acid\textsuperscript{18,23} or ammonia fiber expansion\textsuperscript{6,17} pre-treatments. The hydrolyzate is either sent to separate acidic or enzymatic hydrolysis and followed by fermentation; or simultaneous saccharification and fermentation. The culture broth is then separated using distillation to obtain high purity ethanol. The remaining residue can be utilized in combined heat and power plant to generate electricity, which can be sold to the market.

We assume that the prices\textsuperscript{6,17,18,20–22} of corn stover, hardwood, acetic acid, and electricity are 0.074 $ dry kg\textsuperscript{-1}, 0.074 $ dry kg\textsuperscript{-1}, 0.789 $ kg\textsuperscript{-1}, and $0.059 $ kWh\textsuperscript{-1}, respectively. All technical and economic parameters are provided in the Supporting Information. All costs are indexed to 2016 dollars. Note that the consumption of utilities and auxiliary inputs, (e.g. make-up water, solvents, catalysts) are included in the calculation of costs but they do not appear as compounds in the superstructure.

Next, we solve the following problems using the web application:

- **Q1.Z2**: most profitable utilization strategy for corn stover.
- **Q2.Z1**: most cost-effective production strategy for ethanol.
- **Q3.Z1**: most cost-effective production strategy for hardwood-to-gasoline.

We show the results and discuss the key cost drivers in the next sub-section.

**Results and discussions**

In Problem Q1.Z2, we assume the market price of ethanol to be 0.67 $ kg\textsuperscript{-1} (3 $ GGE\textsuperscript{-1}). The maximum profit is –0.04 $ kg\textsuperscript{-1} corn stover consumed. The negative profit value means that the revenue from ethanol (0.26 kg kg\textsuperscript{-1} corn stover) and electricity sales (0.16 kWh kg\textsuperscript{-1} corn stover) are lower than the sum of feedstock and production costs. The optimal strategy includes dilute acid pre-treatment, enzymatic hydrolysis, fermentation, distillation and waste-water treatment, and combined heat and power (Fig. 5(a)). Note that the flow of hydrolyzate is larger than the flow of corn stover due to water, which is not defined as a compound here, is added in the pre-treatment. We calculate the breakeven price to cover the cost of this strategy, which includes feedstock purchase and production costs, minus the sales of by-products. The breakeven price is 3.78 $ per gallon gasoline equivalent (GGE). The main cost driver is feedstock cost (34% of breakeven cost) (Fig. 6(a)). In terms of production costs, distillation, and waste-water treatment (20% of breakeven cost) is the major cost contributor and it is followed by enzymatic hydrolysis (17% of breakeven cost).

In Problem Q2.Z1, the minimum cost is 0.80 $ kg\textsuperscript{-1} ethanol (minimum selling price, MSP = 3.64 $ GGE\textsuperscript{-1}). This strategy shows 2.86 kg of hardwood is consumed to produce 1 kg ethanol, and 0.33 kg acetic acid is produced as by-product. The selected technologies are handling and chopping, direct gasification, steam reforming, methanol synthesis, acetic acid synthesis, and hydrogenation (Fig. 5(b)). Hydrogenation (1.50 $ GGE\textsuperscript{-1}) and acetic acid synthesis (1.45 $ GGE\textsuperscript{-1}) are the major cost drivers, accounting for 41% and 40% of MSP, respectively (Fig. 6(b)). This

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**Figure 5.** Screenshots of optimal strategies for Problems (a) Q1.Z2, (b) Q2.Z1, and (c) Q3.Z1. Circles denote compounds and rectangles denote technologies. A darker color indicates higher production cost of technology while a thicker arc indicates larger compound flow.
user-friendly application allows researchers with no background on optimization to easily assess strategies employing technologies of interest. The user only needs to insert the technologies and compounds data since the application integrates data processing, optimization, and visual representation. Furthermore, this application allows the user to save the inserted data and the optimization results, and share them with other users. Beyond the user-friendly interface, the application has the flexibility to address different questions using various metrics. We hope this web application will help researchers in identifying economic drivers of their strategies, thereby guiding their future research efforts.

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References
1. Reed M, Increasing Security and Reducing Carbon Emissions of the U. S. Transportation Sector: A Transformational Role for Coal with Biomass. National Energy Technology Laboratory, Albany, OR (2007).
2. Coyle W, Dohlman E and Elbheri A. The economics of biomass feedstocks in the United States: A review of the literature. 101 (2008) [Online]. Available at: https://biomassboard.gov/pdfs/feedstocks_literature_review.pdf [June 15, 2017].
3. James LK, Swinton SM, and Thelen KD, Profitability analysis of cellulosic energy crops compared with corn. Agron J 102(2):675–687 (2010).
4. Larson ED, Consonni S, Katofsky RE, Iisa K and James Fredrick Jr W. A Cost-Benefit Assessment of Gasification-Based Biorefining in the Kraft Pulp and Paper Industry Volume 1 Main Report, Princeton University (2006).
5. Naik SN, Goud VV, Rout PK and Dalai AK, Production of first and second generation biofuels: A comprehensive review. Renew Sustain Energ Rev 14:578–597 (2010).
6. Kazi FK, Fortman J, Anex R, Kothandaraman G, Hsu D, Aden A, et al., Techno-Economic Analysis of Biochemical Scenarios for Production of Cellulosic Ethanol. National Renewable Energy Laboratory (NREL), Golden, CO, USA (2010).
7. Stoklosa RJ, del Pilar Orjuela A, da Costa Sousa L, Uppugundla N, Williams DL, Dale BE, et al., Techno-economic comparison of centralized versus decentralized biorefineries for two alkaline pretreatment processes. Bioresour Technol 226:9–17 (2017).
8. Tao L, Markham JN, Haq Z and Biddy MJ, Techno-economic analysis for upgrading the biomass-derived ethanol-to-jet blendstocks. Green Chem 19(4):1082–1101 (2017).
9. Brown TR, Zhang Y, Hu G and Brown RC, Techno-economic analysis of biobased chemicals production via integrated catalytic processing. Biofuels Bioprod Bioref 6(1):73–87 (2012).
10. Han J, Murat Sen S, Luttbacher JS, Alonso DM, Dumescic JA and Maravelias CT. Process systems engineering studies for the synthesis of catalytic biomass-to-fuels strategies. Comput Chem Eng 81:57–69 (2015).
11. Anex RP, Aden A, Kazi FK, Fortman J, Swanson RM, Wright MM, et al., Techno-economic comparison of biomass-to-transportation fuels via pyrolysis, gasification, and biochemical pathways. Fuel 89(S29-S35) (2010).
12. Haro P, Ollero P, Villanueva Perales ÁL and Vidal-Barrero F, Potential routes for thermochemical biorefineries. Biofuels Bioprod Bioref 7(5):551–572 (2013).
13. Nishida N, Stephanopoulos G and Westerberg AW, A review of process synthesis. AIChE J 27(3):321–351 (1981).
14. Biegler LT, Grossmann IE and Westerberg AW, Systematic Methods for Chemical Process Design. Prentice Hall, Old Tappan, NJ, USA (1997).
15. Barnicki SD and Sirola JJ, Process synthesis prospective. Comput Chem Eng 28(4):441–446 (2004).
16. Pham V and El-Halwagi M, Process synthesis and optimization of biorefinery configurations. AIChE J 58(4):1212–1221 (2012).
17. Kim J, Sen SM and Maravelias CT, An optimization-based assessment framework for biomass-to-fuel conversion strategies. Energy Environ Sci 6(4):1093–1104 (2013).
18. Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, et al., Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover. National Renewable Energy Laboratory (NREL), Golden, CO, USA (2011).
19. GAMS Development Corporation, GAMS - A User’s Guide. Washington, DC, USA (2017).
20. Ruby on Rails. Website. [Online]. Available at: http://rubyonrails.org/ [June 15, 2017].
21. Dutta A, Sahir A, Tan E, Humbird D, Snowden-Swan LJ, Meyer P, et al., Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels - Thermochemical Research Pathways with In Situ and Ex Situ Upgrading of Fast Pyrolysis Vapors. National Renewable Energy Laboratory (NREL), Golden, CO (2015).
22. Zhu Y and Jones S, Techno-economic Analysis for the Thermochemical Conversion of Lignocellulosic Biomass to Ethanol via Acetic Acid Synthesis. Pacific Northwest National Laboratory, Richland, WA (2009).
23. Zhu JY, Pan X and Zalesny RS, Pretreatment of woody biomass for biofuel production: energy efficiency, technologies, and recalcitrance. Appl Microbiol Biotechnol 87(3):847–857 (2010).

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