Biomass Utilization Superstructure Web Application: A Fun Way to Learn the Basics of Superstructure-Based Process Synthesis

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Biomass has the potential to substitute for petroleum as a renewable source of hydrocarbons, helping to meet future energy needs while reducing net carbon emissions as well as dependence on non-renewable and increasingly expensive sources of fossil feedstocks. The conversion of biomass to fuels and chemicals will take place in a facility the National Renewable Energy Laboratory (NREL) has described as a *biorefinery*. However, while basic science advances have resulted in the development of a various promising biomass conversion technologies, how these technologies can be integrated remains unknown. For example, it is unclear what mix of high-value chemicals would make the biorefinery economically viable; and even for a given set of final products, it is unknown which chemistries and conversion technologies should be integrated and how.

To address this challenge, Professor Christos Maravelias and co-workers at the University of Wisconsin – Madison, developed a systems-level methodology for synthesizing and evaluating a wide range of biomass-to-fuels strategies, published in *Energy and Environmental Science* [1]. The methodology is based on a *technology superstructure*, that is, a network that includes multiple conversion technologies and the corresponding feedstocks, intermediates and final products, as shown in Figure 1.

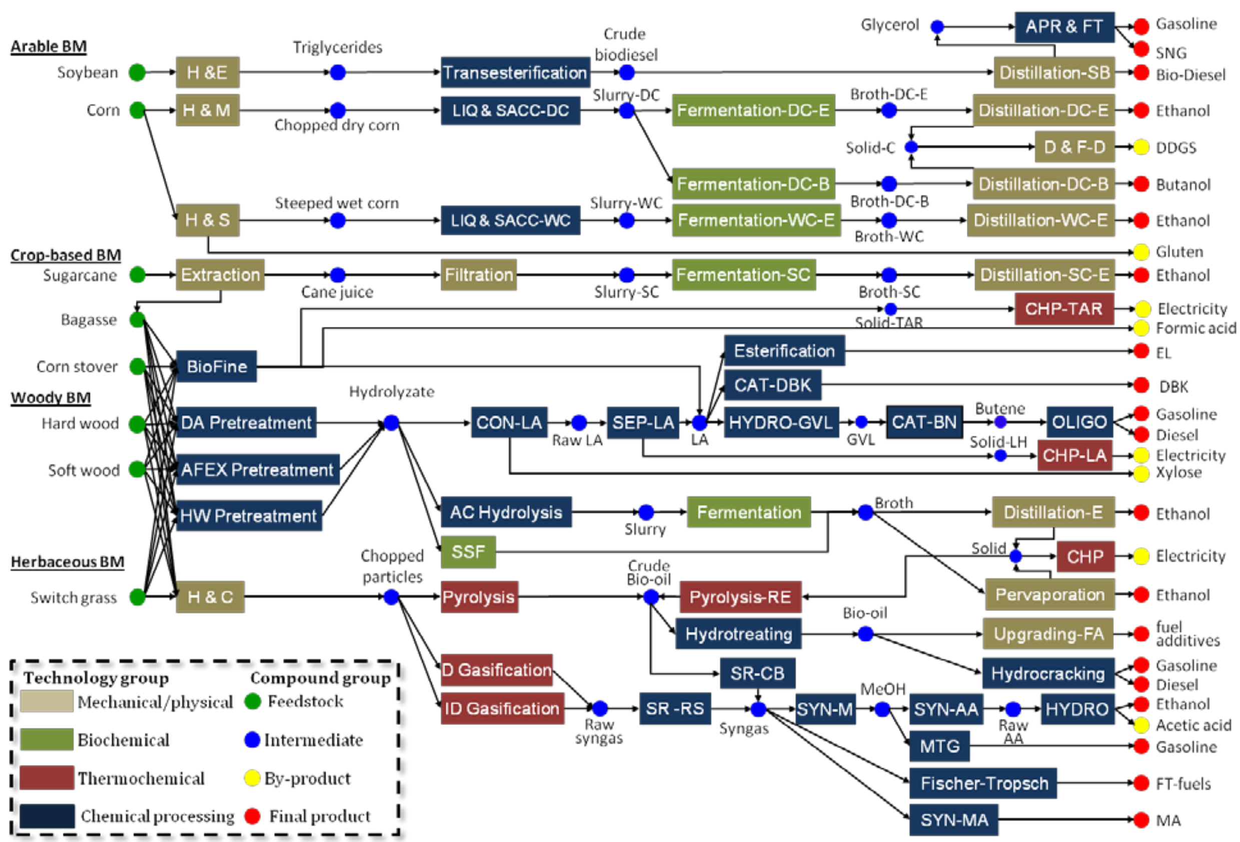

Figure 1. Simplified schematic of Biomass Utilization Superstructure (modified from [1]).

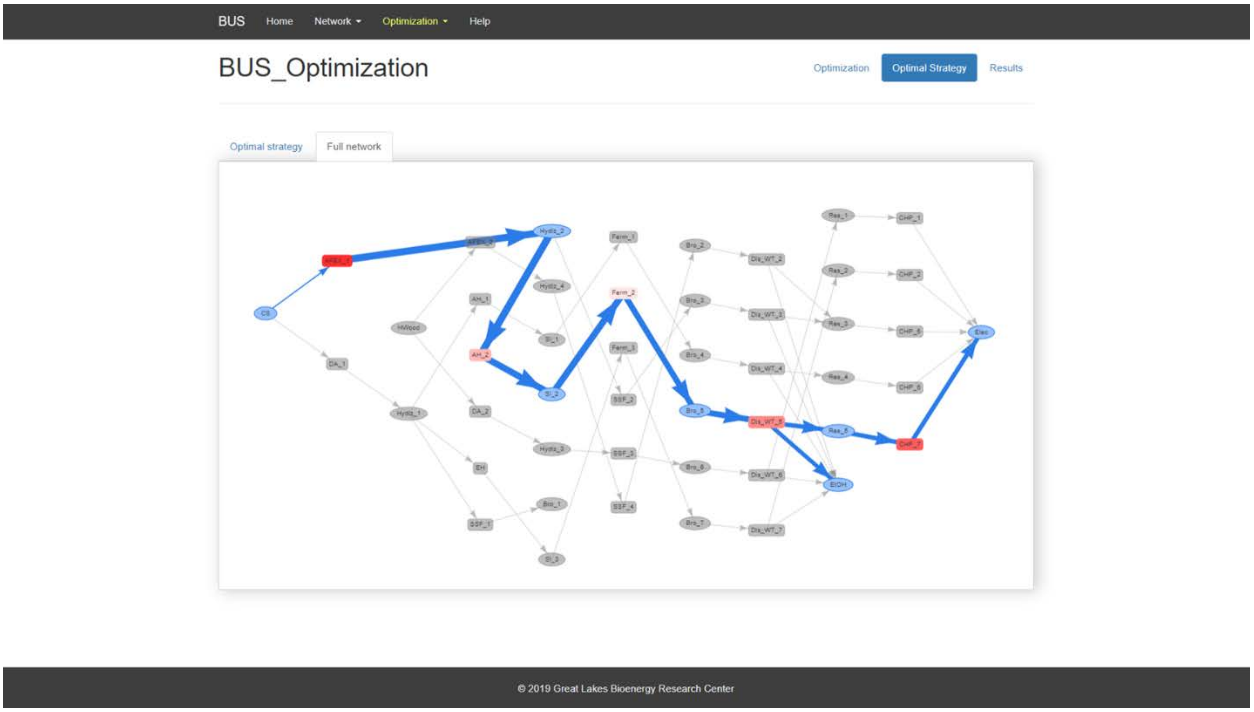

Figure 2. Web app screenshot showing the selected strategy; arc thickness represents flow magnitude of key components (flows of components such as water not shown); block color represents cost of selected technology.

Using literature results and simple process models, the authors estimate a set of key technology parameters (yields of major products, unit production cost, and energy requirements), and then formulated optimization models for the synthesis and analysis of new systems. The proposed framework, the authors coined *Biomass Utilization Superstructure* (BUS), can be used to identify the limitations of existing strategies and generate promising alternatives, as well as study a range of interesting questions, such as: What is the best feedstock and combination of technologies for the production of a specific fuel?

Building upon this framework, the Maravelias group in collaboration with the information services of the Great Lakes Bioenergy Research Center (https://www.glbrc.org/), developed a web application that allows users with limited knowledge of optimization to assess different biorefinery configurations and identify the major cost drivers [2]. The user must only provide the necessary parameters and create an optimization run after identifying the type of question to be addressed and the specific assessment metric. The application generates a visual representation of the optimal strategy (see Figure 2), and charts with breakdowns of the major cost and revenue components as well as other variables (see Figure 3). <u>Importantly, the BUS application is a great way for instructors to teach the basic ideas underpinning superstructure-based process synthesis.</u>

The BUS web application, which is accessible through https://bus.glbrc.org/, is built on the Ruby on Rails framework. After creating an account, the user is required to enter the necessary parameters in the Network page and identify the question and the assessment metric in the Optimization page. If there are any errors, warnings will appear. There are two methods to insert compounds and technologies: (i) manual entry and (ii) spreadsheet upload. In the former, data are filled out manually. If the network involves large numbers of compounds and technologies, users are encouraged to use the latter method where the server will automatically process the uploaded data (a spreadsheet template is readily downloadable for users to fill in all data). Finally, the application allows the user to save the inserted data and the optimization results, and share them with other users.

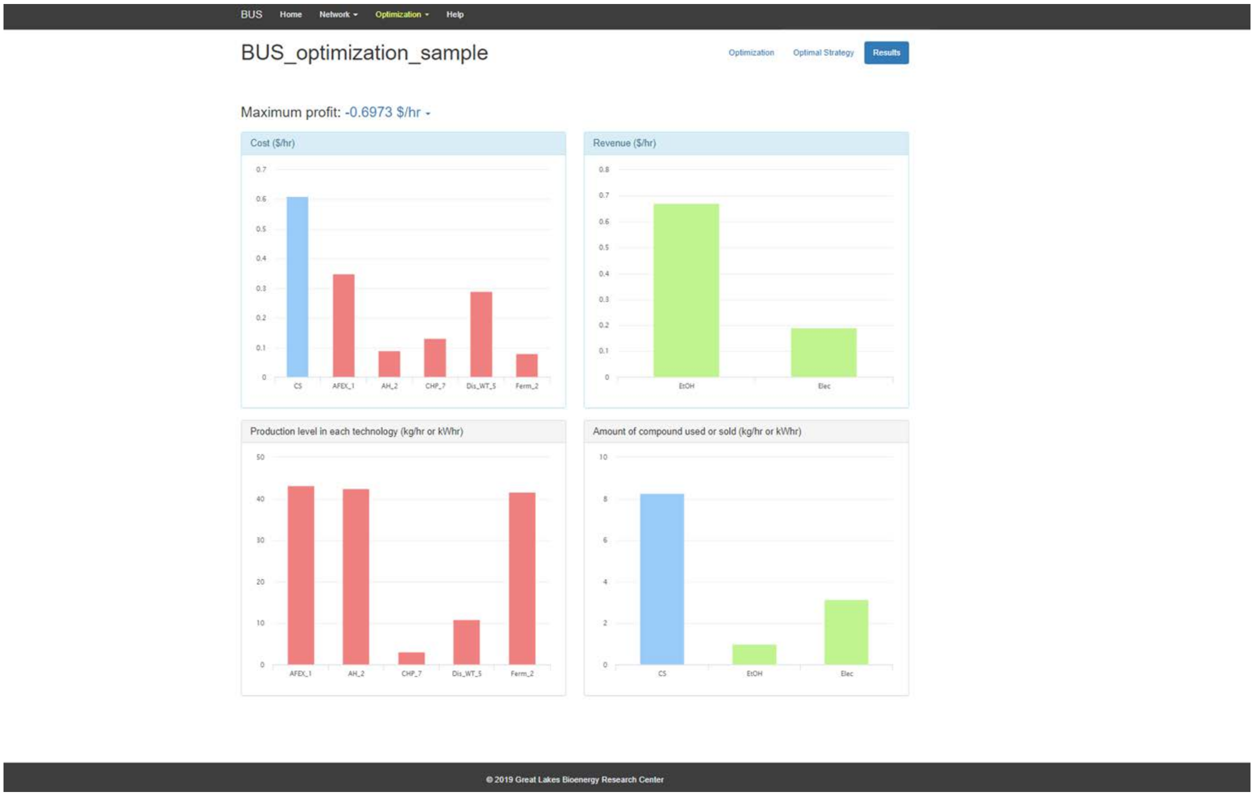

Figure 3. Web app screenshot showing charts for different optimization decisions.

References

[1] Kim J, Sen SM, Maravelias CT. An optimization-based assessment framework for biomass-to-fuel conversion strategies. Energy Environ Sci. 2013;6(4):1093-104.

[2] Ng RTL, Patchin S, Wu WZ, Sheth N, Maravelias CT. An optimization-based web application for synthesis and analysis of biomass-to-fuel strategies. Biofuels Bioprod Biorefining. 2018;12(2):170-6.