

## Process Systems Engineering for Biofuels and Bio-based Chemicals

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<https://www.glbrc.org/research/deconstruction>

**Project Goals: The goal of our research is to develop methods and tools for the synthesis and evaluation of biomass-to-fuels strategies employing pretreatment and conversion technologies developed within the Great Lake Bioenergy Research Center (GLBRC). Specifically, we design new processes, develop models for their evaluation, and eventually identify technological bottlenecks and economic drivers that have to be addressed. Additionally, we develop a general framework for the synthesis of separation and purification networks for bio-based products based on their physical properties. Finally, we explore optimization methods for the design and operation of biofuel supply chain networks with regional depots.**

***Process Synthesis and Analysis.*** We develop an integrated strategy that utilizes a mixture of  $\gamma$ -valerolactone (GVL), water, and toluene as a solvent containing dilute sulfuric acid as a catalyst for the production of ethanol from lignocellulosic biomass<sup>1</sup>. Specifically, cellulose and hemicellulose fractions are first hydrolyzed into sugars using solvent mixtures and catalyst, and the sugars are then co-fermented into ethanol over engineered yeast strains. We design separation subsystems to (1) effectively recover GVL and toluene for reuse in biomass hydrolysis, (2) recover sugars and GVL from the residual biomass, and (3) recover lignin and humins for heat and power generation. To minimize utility requirements, we conduct heat integration, which allows us to meet all heating requirement using biomass residues. Then, we perform a range of system-level analyses to identify the major cost and technological drivers. We found that the proposed strategy results in lower minimum ethanol selling price ((\$ 2.95 per gallon of gasoline equivalent (GGE<sup>-1</sup>)) than those for the GVL/water-based non-enzymatic ethanol production (\$3.37 GGE<sup>-1</sup>)<sup>2</sup> and the enzymatic/biochemical ethanol production (\$ 3.27 GGE<sup>-1</sup>)<sup>3</sup> strategies.

***Design of Separation Networks for Bioproducts.*** Separation of bioproducts is a major challenge that can contribute to more than 70% of the total production costs<sup>4,5</sup>. Based on the physical properties of the desired chemical and other components in the bioreactor effluent, there can be multiple feasible options for product recovery<sup>6,7</sup>. These options are composed of several alternative technologies performing similar tasks and their suitability for a particular chemical varies based on the difference in key parameters such as separation efficiency, cost or amount of added separating agents, biomass titer, and desired product purity. To develop new separation strategies, we propose an optimization-based framework that allows us to identify the key cost drivers and critical technologies. This framework provides significant insights for technology selection and

assists in making an informed decision regarding technologies that should be used for a given set of input/output specifications.

***Biofuel Supply Design and Operation.*** To ensure biomass supply meets biofuel demand, it is necessary to have an effective supply network. Towards this end, the concept of regional biomass processing depot<sup>8</sup>, where biomass is pretreated and/or densified to a higher density intermediate, has been introduced to improve the performance of supply network in terms of costs and emissions. We develop optimization models for the design and operation planning of biofuel supply chains with regional depots that account for seasonal biomass supply<sup>9,10</sup>. Unlike previous approaches which assume predetermined depot and biorefinery locations, we treat the locations of depots and/or biorefineries as continuous optimization decisions. The proposed models account for technology selection and capacity planning decisions, as well as auxiliary decisions such as harvesting site and biomass feedstock selection, biomass allocation to depots and biorefineries, and inventory planning. Furthermore, the proposed models can be extended to handle different features and practical considerations.

## References

- (1) Motagamwala, A. H.; Won, W.; Maravelias, C. T.; Dumesic, J. A. An Engineered Solvent System for Sugar Production from Lignocellulosic Biomass Using Biomass Derived  $\gamma$ -Valerolactone. *Green Chem.* **2016**, *18* (21), 5756.
- (2) Han, J.; Luterbacher, J. S.; Alonso, D. M.; Dumesic, J. A.; Maravelias, C. T. A Lignocellulosic Ethanol Strategy via Nonenzymatic Sugar Production: Process Synthesis and Analysis. *Bioresour. Technol.* **2015**, *182*, 258.
- (3) Humbird, D.; Davis, R.; Tao, L.; Kinchin, C.; Hsu, D.; Aden, A.; Schoen, P.; Lukas, J.; Olthof, B.; Worley, M. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover.
- (4) Kiss, A. A.; Grievink, J.; Rito-Palomares, M. A Systems Engineering Perspective on Process Integration in Industrial Biotechnology. *J. Chem. Technol. Biotechnol.* **2015**, *90* (3), 349.
- (5) Brandt, K.; Schembecker, G. Production Rate-Dependent Key Performance Indicators for a Systematic Design of Biochemical Downstream Processes. *Chem. Eng. Technol.* **2016**, *39* (2), 354.
- (6) Wu, W.; Yenkie, K.; Maravelias, C. T. A Superstructure-Based Framework for Bio-Separation Network Synthesis. *Comput. Chem. Eng.* **2017**, *96*, 1.
- (7) Yenkie, K. M.; Wu, W.; Clark, R. L.; Pflieger, B. F.; Root, T. W.; Maravelias, C. T. A Roadmap for the Synthesis of Separation Networks for the Recovery of Bio-Based Chemicals: Matching Biological and Process Feasibility. *Biotechnol. Adv.* **2016**.
- (8) Eranki, P. L.; Bals, B. D.; Dale, B. E. Advanced Regional Biomass Processing Depots: A Key to the Logistical Challenges of the Cellulosic Biofuel Industry. *Biofuels, Bioprod. Biorefining* **2011**, *5*, 621.
- (9) Ng, R. T. L.; Maravelias, C. T. Design of Cellulosic Ethanol Supply Chains with Regional Depots. *Ind. Eng. Chem. Res.* **2016**, *55* (12), 3420.
- (10) Ng, R. T. L.; Maravelias, C. T. Design of Biofuel Supply Chains with Variable Regional Depot and Biorefinery Locations. *Renew. Energy* **2017**, *100*, 90.

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