1. Introduction and Objective

Biomass-derived liquid transportation fuels and energy products have been proposed as part of the solution to climate change and our heavy dependence on fossil fuels, because the biomass feedstock can be produced renewably from a variety of domestic sources, and the production and use of bioenergy/biofuel products have potentially lower environmental impacts than their petroleum counterparts. Consequently, many countries have set national biofuels targets and provide incentives and supports to accelerate the growth of bioenergy industry. For example, in the U.S. the Renewable Fuels Standard (RFS), part of the Energy Independence and Security Act (EISA) of 2007, establishes an annual production target of 36 billion gallons of biofuels by 2022. Currently most biofuels in the U.S. are made from corn starch that might have negative implications in terms of both food prices and production. To avoid adverse impacts on food supply, EISA further specifies that 16 out of the 36 billion gallons of renewable fuels produced in 2022 should be advanced biofuels made from non-starch feedstocks, such as cellulosic or algal biomass. Yet, the current annual production capacity of advanced biofuels is less than 1 billion gallon worldwide. It is foreseeable that the bioenergy industry will be undergoing a rapid expansion in the coming decade. Many sustainable and robust biomass-to-bioenergy supply chains, which link the sustainable biomass feedstock and the final fuel/energy products, need to be designed and developed for lower costs, less environmental impacts and more social benefits. To accelerate the transition towards the large-scale and sustainable production and use of biofuels and bioenergy products, a significant challenge in research is to systematically design and optimize the entire bioenergy supply chains from the biomass feedstock production to the biofuel/bioenergy end-use across multiple spatial scales, from unit operations to biorefinery processes and to the entire value chain, as well as across multiple temporal scales, from strategic to operational levels, in a cost-effective, robust and sustainable manner. It is the objective of this project to identify the key research challenges and opportunities in modeling and optimization of biomass-to-bioenergy supply chains, and to chart a path for addressing these challenges.
2. Summary of Results in Year 1

During the first year of this project, the research team concentrated our efforts on developing a novel multi-scale modeling and optimization framework for sustainable biofuel supply chains. Some results of this study are summarized into a journal article, which has been published recently [Yue, D., You, F.,* & Snyder, S.W. (2014). Biomass-to-Bioenergy and Biofuel Supply Chain Optimization: Overview, Key Issues and Challenges. *Computers & Chemical Engineering*, 66, 36–56].

*Figure 1 Illustration of multi-scale modeling and optimization of biofuel supply chains*
While most works on biofuel supply chains provide a great insight to specific fields, they may fall into a narrow perspective and do not cover sufficiently all the aspects of the biofuel supply chain. Therefore, we need a multi-scale modeling and optimization framework to provide a holistic view and organically integrate the different components of the biofuel supply chain. In this work described in the published paper, we portray a schematic framework of multi-scale modeling and optimization for biofuel supply chains in Figure 1. From bottom to top, four system layers regarding different temporal and spatial scales typify the level of ecosystem, supply chain, process, and molecule, respectively.

At the ecosystem layer, the ecosystem and human society constitute the environment where various activities in biofuel supply chains take place. All these activities would cause impacts and footprints on the ecosystem throughout the life cycle and value chain of the biofuel products, involving biomass cultivation, biomass harvesting and logistics, biomass pretreatment and fuel production in conversion facilities, and fuel distribution and end-use. Modeling and optimization tools can be applied to simultaneously evaluate and identify the sustainable solutions with minimum adverse impacts on the environment and maximum benefits to the society. Since multiple conflicting objectives are often involved when optimizing the sustainability of biofuel supply chains, a number of multi-objective optimization techniques can be applied, such as epsilon-constraint method, goal programming method, etc. Triangle charts can be used for comparison between different solutions with different economic, environmental, and social performances. Pareto frontiers obtained from multi-objective optimization can reveal the tradeoffs between conflicting objectives and provide a set of Pareto-optimal solutions for decision-making.

At the supply chain layer, modeling and optimization tools can play an important role in optimizing the supply chain network structure and improving the various activities involved in the installation and operation of biofuel supply chains. A biofuel supply chain usually consists of multiple sites and multiple echelons, which requires coordination across the entire supply chain network. At the design stage, superstructure optimization allows the decision maker to determine the optimal network design from a number of choices among candidate suppliers, facility locations, technology options, transport modes, etc. By using mathematical programming approaches, description of the various activities, even across multiple sectors, can be easily interpreted into equations in the constraints or objective functions. However, a comprehensive and detailed superstructure, though appealing, may be computationally intractable. Therefore, when modeling the biofuel supply chain systems, we should take advantage of the properties of the supply chain system (e.g., network structure, spatial scale) and drop off the components that have negligible influences on the optimization objectives to trade off the modeling resolution and computation efficiency.

At the process layer, the processes and units at a production facility are studied in a more detailed manner. Superstructure-based optimization can again be employed for the design, synthesis, and retrofit of conversion processes, involving the selection among candidate processing methods, equipment units, catalysts, resource supply scenarios, etc. Regarding the operation at a biorefinery, three levels of decisions need to be optimized, namely planning, scheduling, and control. Optimization for planning involves the development of robust forecasting model, multi-year strategy for capacity expansion and process retrofit,
multi-period targets for purchase, sales and production, etc. Optimization for scheduling involves the efficient and timely allocation of equipment units, raw materials, and human labors to fulfill the external and internal orders. Optimization for control involves real-time monitoring and adjustment of process parameters to meet the required quantity and quality of the products. The three decision levels are closely related, thus also providing enormous opportunities for vertical integration.

At the molecule level, modeling and optimization tools can be employed by researchers with diverse background to facilitate their studies on biomass-to-biofuel conversion technologies, both theoretical and experimental. Optimization tools can help to identify the promising reaction pathways that are cost-effective and sustainable, thus saving unnecessary efforts in experimental trials. Furthermore, studies in molecular engineering, bioengineering, and multi-physics simulation can be guided by the system engineering approaches, while in return serve as the practical basis for upper-level modeling and optimization.

As illustrated by the arrows on the left of Figure 1, the system scale addressed in the model grows from top to bottom, whereas the practical details considered in the model increases from bottom to top. The double-headed arrows between adjacent layers indicate that the modeling layers are never isolated but closely inter-connected. Generally speaking, the lower layer conveys target or requirement to the higher layer, whereas the higher layer provides detailed data which serve as building blocks for the modeling and optimization of the lower layer.

Our on-going effort on this project is to investigate future biofuel supply chains that integrate with petroleum refinery systems and/or carbon capture and sequestration systems. We are also working on addressing issues on modeling of sustainability and the treatment of uncertainties in biofuel supply chains.

3. Outcomes

The project produces 4 journal publications listed below. They all cite ISEN and Argonne’s support.


In the past year, the project also leads to 3 proposals to National Science Foundation; 2 Proposals to Department of Energy (funded); and 2 Proposals to Minnesota Corn Research & Promotion Council.