

Design of Sustainable Product Systems and Supply Chains with Life Cycle Optimization Based on Functional Unit: General Modeling Framework, Mixed-Integer Nonlinear Programming Algorithms and Case Study on Hydrocarbon Biofuels

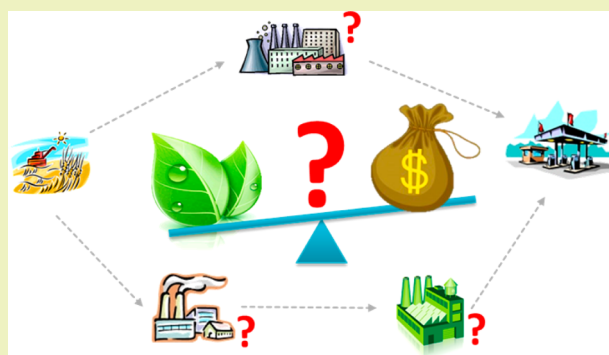
Dajun Yue, Min Ah Kim, and Fengqi You*

Department of Chemical and Biological Engineering, Northwestern University, Evanston, Illinois 60208, United States

Supporting Information

ABSTRACT: We propose a life cycle optimization framework for the design of sustainable product systems and supply chains considering the concept of “functional unit” under economic and environmental criteria. This general modeling framework integrates the life cycle analysis methodology with multiobjective optimization and measures both the economic and environmental performances based on a standard quantity of functional unit associated with final products. The Pareto-optimal frontier returned by the multiobjective optimization problem reveals the trade-off between the economic and environmental objectives. We also present tailored optimization algorithms for efficiently solving the mixed-integer linear fractional programming problems, which result from the life cycle optimization framework. We apply the proposed life cycle optimization framework to a case study on the hydrocarbon biofuels through a spatially explicit model for the county-level supply chain in Illinois. The Pareto-optimal results show that the environmental impact of hydrocarbon biofuels ranges from 10.66 to 23.83 kg CO₂ equiv per gasoline-equivalent gallon (GEG), corresponding to the unit cost ranging from \$4.63 to \$3.58/GEG.

KEYWORDS: Sustainable supply chain, Life cycle optimization, MINLP, Biomass and biofuels



INTRODUCTION

Concerns about climate change, waste pollution, energy security, and resource depletion are driving society to explore a more sustainable way for development and manufacturing. This leads to the question of how to evaluate and improve the sustainability of the product system, which is defined as the method, procedure, or arrangement that includes all functions required to accumulate the inputs, process the inputs, and deliver the marketable outputs.¹ The three core components of a product system are illustrated in Figure 1a. In general, a product system can be treated as a “conversion process” that uses common resources such as labor, capital (machinery and equipment, materials, etc.), and space (land, building, etc.) to convert resources into useful goods and services. From a value-add perspective, all the economic costs and environmental impacts will be accumulated and embedded into the last stage of the product system—final products. The supply chain, as a typical product system with the highest vertical hierarchy,² is a network of facilities and logistic options involving various activities such as procurement of feedstock, transportation and storage of feedstock, conversion of feedstock into finished products, distribution of products to demand zones, and product end use (Figure 1b). In the chemical process industry, there are various supply chains with multiple scales, echelons,

and products. Extensive research both in academia and industry has been done to improve the overall economic performances for the design and operation of supply chains, among which the enterprisewide optimization is considered as a promising frontier in process systems engineering.^{3–5}

Though cost minimizing is critical to the economic viability and profitability of a chemical product system and supply chain, there has been an increasing awareness of the importance to achieve a sustainable design in the recent decade.^{6,7} Srivastava⁸ presented a comprehensive review on the scope of green supply chain management and remarked the importance of a more extensive use of mathematical programming tools that can contribute to a major advance in an environmentally conscious supply chain management. Considering the environmental impact as a design objective rather than merely a constraint on operations would lead to the discovery of novel alternatives with both better economic and environmental performances.^{9–11} However, life-cycle thinking is very critical when measuring the environmental metrics, and the consequences of ignoring impacts over the entire life cycle were illustrated by

Received: March 15, 2013

Revised: May 16, 2013

Published: May 21, 2013

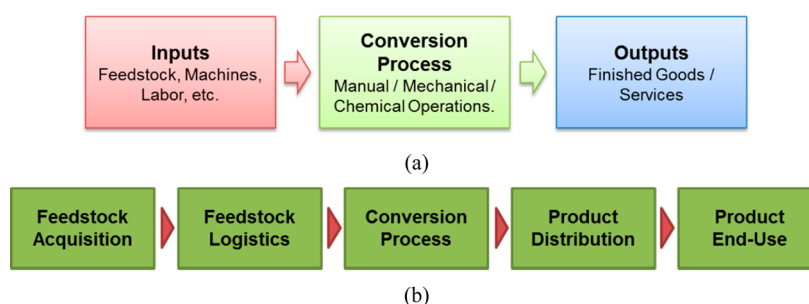


Figure 1. Illustration of general product systems and supply chain networks: (a) general product systems; (b) general structure of supply chain systems.

the works of Fava¹² and Azapagic.^{13,14} Following the idea of incorporating a life-cycle environmental objective into the decision making process, a number of works based on the multiobjective optimization approach emerged to simultaneously improve the economic and environmental performances of the holistic product system and supply chain. Seuring and Müller¹⁵ proposed a conceptual framework for sustainable supply chain management, in which specific features of sustainable supply chains were discussed as well as limitations and challenges in the research. Hugo and Pistikopoulos¹⁶ presented a mathematical programming-based methodology that explicitly includes life cycle assessment criteria as part of the strategic investment decisions related to the design and planning of supply chain networks. Liu et al.¹⁷ incorporated a greenhouse gas emissions indicator as one of the design objectives when studying energy systems engineering problems. Elia et al.¹⁸ proposed an optimization framework for a nationwide energy supply chain network considering CO₂ emissions reduction. Santibañez-Aguilar et al.¹⁹ presented a multiobjective optimization model for the optimal planning of a biorefinery considering both economic and environmental aspects. You et al.²⁰ and You and Wang²¹ proposed a life cycle optimization framework and studied several applications on the optimal design and scheduling on hydrocarbon biofuel supply chains. Giarola et al.²² and Akgul et al.²³ proposed spatially multiobjective models for design and planning of hybrid first/second generation biorefineries and supply chain, which optimized the environmental and financial performances simultaneously. Cucek et al.²⁴ recommended a total footprints-based multicriteria optimization framework for the design of regional biomass energy supply chains. Recently, Santibañez-Aguilar et al.²⁵ studied the synthesis of distributed biorefining networks for sustainable elimination of water hyacinth which would cause severe ecological problems in the infested water bodies. Relevantly, the life cycle optimization framework has also been applied to sustainable design of biorefineries under economic and environmental criteria.^{9,11,26}

All the works reviewed above consider the absolute economic and environmental objectives. However, in a product system, the economic and environmental metrics associated with per functional unit of final products provide further space for improvement regarding economic and environmental concerns, because all the costs and environmental impacts will be embedded and reflected in the functioning outputs of the system: functional unit. In light of this point, we propose two fractional objective functions. The economic objective is defined as total cost divided by total quantity of the functional unit. By using this economic objective, we can determine the optimal sales amount between the demand upper and lower

bounds to guarantee the lowest unit cost per functional unit. This would make the final products more cost-competitive in the marketplace. The environmental objective is defined as total environmental impact divided by total quantity of the functional unit. By using this objective function, we can guarantee the lowest environmental impact per functional unit, which would lead to more environmentally friendly product patterns.

The bicriterion optimization problem is solved using the ϵ -constraint method to obtain a set of Pareto optimal solutions.²⁷ In this work, since both the economic and environmental objective functions are linear fractional functions, each subproblem in the ϵ -constraint method will be formulated as a mixed-integer linear fractional program (MILFP), which is a special class of nonconvex mixed-integer nonlinear programs (MINLPs) that can be computationally intractable for large-size problems due to its combinatorial nature and the pseudoconvexity of its objective function.^{28–30} Though general-purpose MINLP solvers and global optimizers can be utilized, it is demonstrated that the tailored solution approaches for MILFPs are much more efficient and effective, namely the parametric algorithm³¹ and reformulation-linearization method, because these two approaches can take advantage of the efficient mixed-integer linear programming (MILP) methods to globally optimize the MILFP problems with higher computational efficiency and lower memory requirements.

The major novelties of this work are summarized as follows.

- Novel functional-unit-based life cycle optimization modeling framework for the design of general product systems and supply chains.
- Functional unit based economic and environmental models as the optimization objectives and efficient solution strategies.
- Application to sustainable hydrocarbon biofuel supply chain systems.

The rest of the article is organized as follows. We first describe the proposed life cycle optimization modeling framework. Then, an illustrative example is analyzed to demonstrate the trade-offs between various criteria. Later, we present the general problem statement and model formulation, followed by the major solution approaches employed in this work. A county-level case study on the design of hydrocarbon biofuel supply chains is presented to illustrate the application of the modeling framework and solution strategy. The article is concluded in the last section.

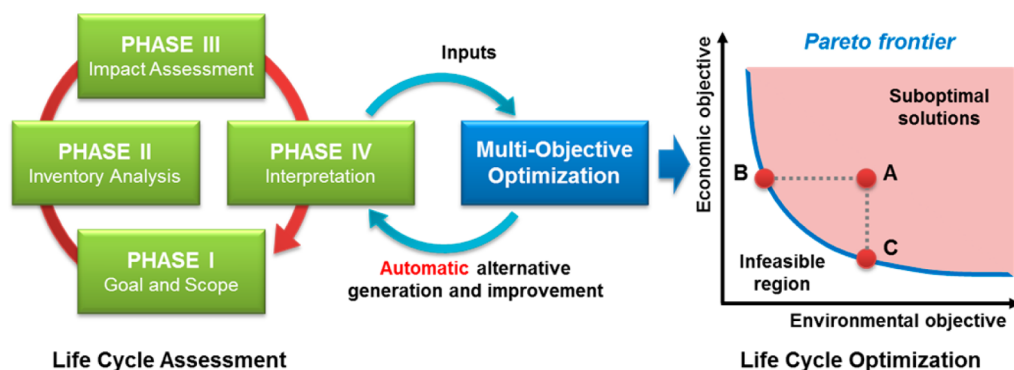


Figure 2. Life cycle optimization modeling framework.

LIFE CYCLE OPTIMIZATION FRAMEWORK

To overcome the drawbacks of classical life cycle assessment (LCA) methodology, we propose a novel life cycle optimization framework which organically integrates the classical four-step LCA methodology with multiobjective optimization method.^{20,21} In the life cycle optimization framework, we will follow the first three phases of the classical LCA, which are goal and scope definition, inventory analysis, and impact assessment. Whereas, the remaining phase—LCA interpretation—will be performed by coupling with multiobjective optimization. The results of life cycle optimization would be presented in the form of a Pareto frontier which reveals the trade-off between the economic and environmental objectives. The life cycle optimization framework is illustrated in Figure 2.

Goal and Scope Definition. This is the first and the most critical phase which defines the main features of the LCA analysis, including the goal of the study, system boundaries, allocation methods, and impact categories, etc. In the study of product systems and supply chains, we restrict the domain of study to all the life cycle stages from “cradle-to-gate”, which include the following activities: feedstock acquisition, feedstock transportation and storage, conversion from feedstock to products, storage and distribution of final products, and product end use. In certain situations, feedstock is not converted directly to finished products but goes through several intermediate processing steps. For example, the biomass-derived gasoline can be converted directly from crop residues at integrated biorefineries or it can be upgraded from bio-oil which is an intermediate product from preconversion facilities using crop residues as feedstock.

The “functional unit” is also defined in the first phase, which is a key element of life cycle analysis. The functional unit provides a reference to which the system’s inputs and outputs can be related, and a logical basis for comparing the sustainability performance for different products. In a product system, it is straightforward to define the functional unit associated to the products. In single-product systems, the quantity of functional unit can simply be the number or weight/volume amount of the product. However, in multi-product systems, the quantity of functional unit is usually calculated based on some functioning properties of the various products (e.g., density, heating value, market value). For example, gasoline-equivalent gallon (GEG) is defined as the amount of alternative fuel it takes to equal the energy content of one liquid gallon of gasoline and, thus, can be considered as the functional unit that characterize different fuel products (e.g., gasoline, diesel, jet fuel). A general formula for the calculation

of standard quantity of total functional unit is given below. An illustration regarding a product system involving 1 unit of product A and 2 units of product B is given in Figure 3.

$$qt^S = \sum_i \lambda_i \cdot qt_i \quad (1)$$

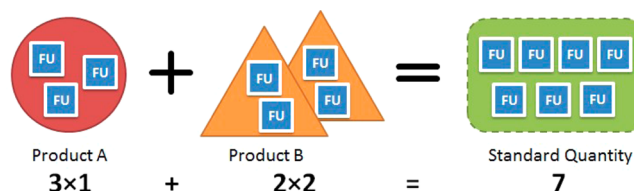


Figure 3. Calculation of the standard quantity for a multiproduct system (FU: functional unit).

where qt^S stands for the quantity of standard functional unit, qt_i is the quantity of product i and λ_i is the function weighting (characterization) factor defined as the amount of functional unit associated with product i .

Inventory Analysis. In the second phase of LCA, the life cycle inventory is analyzed related to each process/activity in the life cycle stages confined within the system boundary. Mass and energy balances are required to identify and quantify the most relevant inputs and outputs of materials and energy use associated with the process/activity. Note that the life cycle inventory mentioned here is a different concept from the physical inventory kept in stock keeping units, which is an important part of the supply chain management.

Impact Assessment. In this phase, the inventory entries can be translated into impacts using impact factors, and then, the impacts can be aggregated into a single metric. The most widely used LCA metrics include GWP (global warming potential), EI-99 (Eco-indicator 99), etc. GWP measures how much heat could be trapped by greenhouse gas (GHG) emissions relative to CO₂. EI-99 evaluates the environmental impacts in more comprehensive categories (e.g., human health, ecosystem quality, and resources) and provides an environmental indicator point. The damage and environmental impacts is determined based on the life cycle inventory by multiplying each life cycle inventory entry with the corresponding impact factor specified by the damage assessment model.

Interpretation. In the fourth phase, the LCA results are analyzed to provide a set of conclusions and recommendations. In this regard, the goal of LCA is to provide criteria and quantitative measurements for comparing different supply chain

design and operation alternatives. However, one of the critical drawbacks of classical LCA framework is that it lacks a systematic approach for generating such alternatives and identifying the best one in terms of environmental performance. To circumvent these limitations, we couple optimization tools with environmental impact assessment. This integrated framework would allow us to evaluate the environmental impacts of diverse process alternatives and identify the optimal solution via multiobjective optimization. Note that various impact metrics can be employed as the environmental objective. A set of Pareto-optimal solutions can be obtained by solving the multiobjective optimization problem. These Pareto solutions form a Pareto curve which reveals the trade-off between the economic objective and environmental objective, thus allowing for a better decision-making for the design and operation of sustainable product systems and supply chains.

■ ILLUSTRATIVE EXAMPLE

To reveal the trade-offs between the economic and environmental objectives, we present an illustrative example for a simplified supply chain optimization problem in this section. The structure of the supply chain is given in Figure 4. As can be

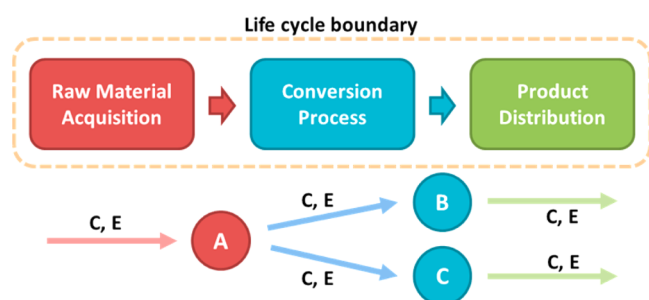


Figure 4. Superstructure of the illustrative example.

seen, we consider a cradle-to-gate life cycle boundary in this problem. This product system includes three life cycle stages, which are raw material acquisition, conversion process, and product distribution, respectively. Specifically in this product system, raw material A is collected from the supplier; then raw material A will be converted into product B or product C at a given production ratio in the conversion process; and at the last stage product B and product C are distributed to the market to meet the demand requirements. At every stage of the product system, costs and environmental impacts would occur, which would eventually be embedded and reflected in the final products as economic and environmental footprints.

On the basis of the structure given in Figure 4, we present the economic and environmental data of this simplified supply chain model as follows. We first assume that the cost is measured by monetary units (e.g., USD) and the environmental impact is measured in terms of damage factors (e.g., Eco-

Indicator 99³² points). The costs and impact data are given in Table 1. The fixed costs and environmental impact account for the setup and infrastructure. The production ratio of raw material A to product B is 1:1. The production ratio of raw material A to product C is also 1:1. The processing capacity of the conversion process is 3 ton of raw material A per day. The minimum demand is 1 ton per day for both product B and product C, assuming there is no upper limit for the demands of the market. The amount of provision of functions (e.g., electricity) is 1 functional unit (e.g., kW h) for per ton of product B and 1.5 functional unit for per ton of product C.

Here in this problem, we consider four metrics, namely the absolute total cost, absolute total environmental impact, cost per functional unit, and environmental impact per functional unit. Let x_B and x_C stand for the produced quantity of product B and product C, respectively. The acquisition amount of raw material A can be calculated according to its production ratios with product B and product C, namely $x_A = x_B + x_C$. For clarity, we show here how the total cost is calculated. The total acquisition cost is $20x_A = 20(x_B + x_C)$; the total production cost equals to the variable part $70x_B + 520x_C$ plus the fixed part 250; The total distribution cost is $10x_B + 60x_C$. By summing up all the cost components, we can derive

$$\text{total cost} = 250 + 100x_B + 600x_C \quad (2)$$

Similarly, the other metrics can be derived and given as follows.

$$\text{total environmental impact} = 300 + 400x_B + 200x_C \quad (3)$$

$$\text{unit cost} = \frac{250 + 100x_B + 600x_C}{x_B + 1.5x_C} \quad (4)$$

$$\text{unit environmental impact} = \frac{300 + 400x_B + 200x_C}{x_B + 1.5x_C} \quad (5)$$

The total production amount of product B and product C cannot exceed the capacity of the conversion process, which suggests

$$x_B + x_C \leq 3 \quad (6)$$

Also, minimum demands from the market have to be met, which leads to

$$x_B \geq 1, \quad x_C \geq 1; \quad x_B \in \mathbb{R}, \quad x_C \in \mathbb{R} \quad (7)$$

We perform a scenario analysis for this illustrative example. Four scenarios producing different amounts of product B and product C are considered. By evaluating the objective functions above, we summarized the results in Table 2. Scenario 1 produces minimum amount of product B and product C to satisfy the minimum demand from the market. It is obvious that this scenario leads to the lowest total cost as well as the lowest total environmental impact. However, the unit cost and unit environmental impact are also important for a product system

Table 1. Inputs of the Illustrative Example

| processes | material | variable cost (\$/ton) | variable environmental impact (points/ton) | fixed cost (\$) | fixed environmental impact (points) |
|--------------------------|----------|------------------------|--|-----------------|-------------------------------------|
| raw material acquisition | A | 20 | 40 | | |
| conversion process | B | 70 | 300 | 250 | 300 |
| | C | 520 | 140 | | |
| product distribution | B | 10 | 60 | | |
| | C | 60 | 20 | | |

Table 2. Results of Scenario Analysis

| scenarios | product B (ton) | product C (ton) | total cost (\$) | total impact (points) | unit cost (\$/FU) | unit impact (points/FU) |
|-----------|-----------------|-----------------|-----------------|-----------------------|-------------------|-------------------------|
| 1 | 1 | 1 | 950 | 900 | 380 | 360 |
| 2 | 1.5 | 1.5 | 1300 | 1200 | 347 | 320 |
| 3 | 2 | 1 | 1050 | 1300 | 300 | 371 |
| 4 | 1 | 2 | 1550 | 1100 | 387 | 275 |

and supply chain in practice. We can see that the unit cost of scenario 1 is much higher than that of scenario 3, while the unit environmental impact of scenario 1 is much higher than that of scenario 4. In other words, scenario 3 appears to be the most cost-effective design, while scenario 4 produces the products in the most environmentally friendly way. Scenario 2 has mediate unit cost and unit environmental impact and, thus, can be treated as a balance solution between cost-reduction and green manufacturing. Besides, note that scenarios 2–4 fully utilize the production capacity while scenario 1 does not. Therefore, we conclude that employing the functional-unit-based economic and environmental objectives allows us to take full advantage of the process capacities of the product system and demand potentials in the marketplace.

■ GENERAL PROBLEM STATEMENT

In the design of general product systems and supply chains, the parameters below are given.

- A set of locations, including feedstock harvesting sites, conversion facility candidates, storage sites, and demand zones.
- Technical and logistic options, including alternative conversion technologies, types of storage, and transportation modes.
- Capacity limitations, including availability of feedstock at harvesting sites, demands of final products at demand zones, and production as well as inventory capacity at conversion facilities and storage sites.
- Timing parameters, including planning horizon, lead times of production and transportation.
- Costs data, including feedstock acquisition costs, transportation costs, capital investments, operation and maintenance (O&M) costs, storage holding costs, final product distribution costs, and government incentives.
- Environmental impact data, including impacts for feedstock acquisition, transportation, material processing, storage, final product distribution, and environmental credits.
- Problem specific conditions, including material degradation, seasonality, setup costs, backlogging and lost sale penalties, etc.

Major decision variables for the design of sustainable product systems and supply chains are summarized as follows.

- Selection of feedstock suppliers, conversion facilities, and storage sites.
- Selection of conversion technologies, storage types, and transportation modes.
- Feedstock procurement amounts, product sales, production targets, inventory levels, and inter-region material flow amounts.

There are two objectives as discussed in the section above: the economic objective is to minimize the unit cost per

functional unit and the environmental objective is to minimize the environmental impact per functional unit.

■ GENERAL MODEL FORMULATION

According to the general problem statement mentioned in the previous section, we present the general life cycle optimization model for the design of sustainable product systems and supply chains in this section. The bicriterion optimization problem is given below and denoted as problem (P0).

$$(P0) \min ftc = \sum_g cost_g / \sum_i \lambda_i \cdot qt_i \quad (8)$$

$$\min fte = \sum_g env_g / \sum_i \lambda_i \cdot qt_i \quad (9)$$

$$s. t. C0 + C1 \cdot \bar{x} + C2 \cdot \bar{y} = 0 \quad (10)$$

$$\bar{x} \in \mathbb{R}^n \quad \text{and} \quad \bar{y} \in \{0, 1\}^m \quad (11)$$

where i is the set of products; qt_i is the quantity of products i ; λ_i is the amount of functional unit associated with product i . For a given system, once defined, a functional unit is used for all the objectives and constraints, thus the weighting factors λ_i are constants. g is the set of process stages (e.g., procurement, production, transportation, and storage), \bar{x} is the vector of the continuous variables, \bar{y} is the vector of binary 0–1 variables, and $C0$, $C1$, and $C2$ are parameters in matrix format. Note that, the vector \bar{x} includes all the continuous variables, such as $cost_g$, env_g , qt_i , etc. Distinguishing them from \bar{x} is merely for better understanding of the physical meaning of the model. Equation 8 defines the economic objective, where ftc is the unit cost per functional unit, and $cost_g$ is the total cost associated with stage g . Equation 9 defines the environmental objective, where fte is the environmental impact per functional unit, and env_g is the total environmental impact associated with stage g . All the constraints (e.g., mass balance relationship, capacity constraints, and availability constraints) are written in a compact format given as eq 10. Without loss of generality, all the inequalities are converted into equations via the use of slack variables.

As can be seen, we assume that all the constraints in eq 10 are linear, which is usually the case in supply chain design problems.^{4,33,34} The economic objective 8 and environmental objective 9 are formulated as linear fractional functions, where both the numerator and denominator are linear functions. Continuous variables \bar{x} model the purchase amounts, sales amounts, production amounts, transportation amounts, etc. Binary 0–1 variables \bar{y} represent the discrete decisions for the selection of facility location, technology, capacity level, etc.

■ SOLUTION APPROACHES

In this section, we briefly introduce the major solution approaches that can be applied to the bicriterion optimization problem (P0) formulated in the previous section.

ϵ -Constraint Method. Due to its efficiency and simplicity, the ϵ -constraint method is widely used to obtain Pareto-optimal solutions for multiobjective optimization problems. Considering our two-dimensional case, the Pareto frontier will be a Pareto curve. We convert the environmental objective in problem (P0) into the ϵ -constraint while leaving the economic objective in the resulting single-objective ϵ -constraint subproblems (P1). Certainly, the other way around is also valid. Also, because the standard quantity of functional unit is always

positive, we can derive the following general model formulation (P1).

$$(P1) \min ftc = \sum_g cost_g / \sum_i \lambda_i \cdot qt_i \quad (12)$$

$$\text{s. t. } \sum_g env_g \leq \varepsilon \cdot \sum_i \lambda_i \cdot qt_i \quad (13)$$

$$C0 + C1 \cdot \bar{x} + C2 \cdot \bar{y} = 0 \quad (14)$$

$$\bar{x} \in \mathbb{R}^n \quad \text{and} \quad \bar{y} \in \{0, 1\}^m \quad (15)$$

As can be seen, in formulation (P1), all the constraints are linear. The only nonlinearity is at the objective function, which is a linear fractional term. This problem belongs to MILFP, which is a special class of nonconvex MINLP. In order to globally optimize the MILFP problem (P1) efficiently, we present two tailored MILFP algorithms in the following sections.

Parametric Algorithm. We first introduce the parametric algorithm which relies on the solution of a sequence of MILP subproblems iteratively to obtain the global optimal solution of the original MILFP problem.³¹ The MILP subproblems of the parametric algorithm corresponding to (P1) are given as follows and denoted as (P1-D).

$$(P1-D) \min ftc = \sum_g cost_g - Q \cdot \sum_i \lambda_i \cdot qt_i \quad (16)$$

$$\text{s. t. } \sum_g env_g \leq \varepsilon \cdot \sum_i \lambda_i \cdot qt_i \quad (17)$$

$$C0 + C1 \cdot \bar{x} + C2 \cdot \bar{y} = 0 \quad (18)$$

$$\bar{x} \in \mathbb{R}^n \quad \text{and} \quad \bar{y} \in \{0, 1\}^m \quad (19)$$

where Q is the critical parameter that will be updated iteratively and eventually approach the optimal value of the original objective function.^{34,35} The flowchart of the parametric algorithm is given in Figure 5.

The MILP subproblem (P1-D) has exactly the same constraints as the original MILFP problem (P1), but it is a linear parametric objective function, instead of a nonlinear one.

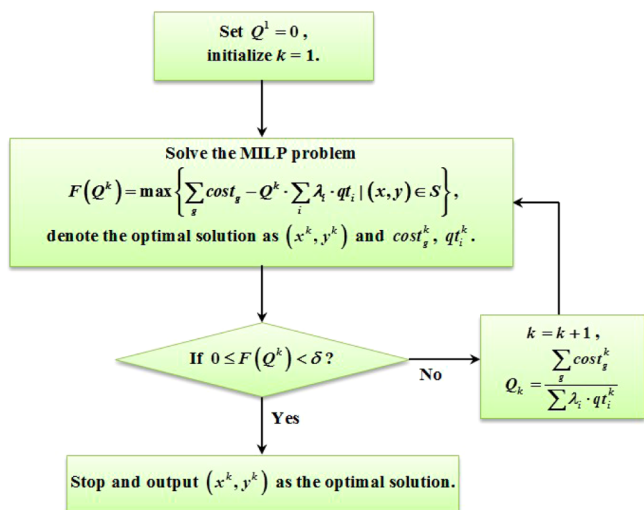


Figure 5. Flowchart of the parametric algorithm.

A drawback of this approach is that the number of iterations is unpredictable and no absolute gap information is returned.

Reformulation-Linearization Method. Another alternative, the reformulation-linearization method, transforms the original MILFP problem into its exact equivalent MILP problem, so that we can take advantage of the powerful MILP optimization algorithms, such as the branch-and-cut methods. The reformulation-linearization method integrates the Charnes–Cooper transformation and Glover’s linearization scheme, and the equivalent MILP formulation of (P1) is given below and denoted as (P1-R).

$$(P1-R) \min Ufct = \sum_g Ucost_g \quad (20)$$

$$\text{s. t. } \sum_g Uenv_g \leq \varepsilon \quad (21)$$

$$C0 \cdot u + C1 \cdot \bar{z} + C2 \cdot \bar{w} = 0 \quad (22)$$

$$\sum_i \lambda_i \cdot Uqt_i = 1 \quad (23)$$

$$\bar{w} \leq u \quad (24)$$

$$\bar{w} \leq M \cdot \bar{y} \quad (25)$$

$$\bar{w} \geq u - M(1 - \bar{y}) \quad (26)$$

$$u \in \mathbb{R}, \quad \bar{z} \in \mathbb{R}^n, \quad \bar{w} \in \mathbb{R}^m, \quad \text{and} \quad \bar{y} \in \{0, 1\}^m \quad (27)$$

An important property of (P1-R) is that there exists a one-to-one correlation between the reformulated variables and variables in the original formulation as shown in Figure 6.

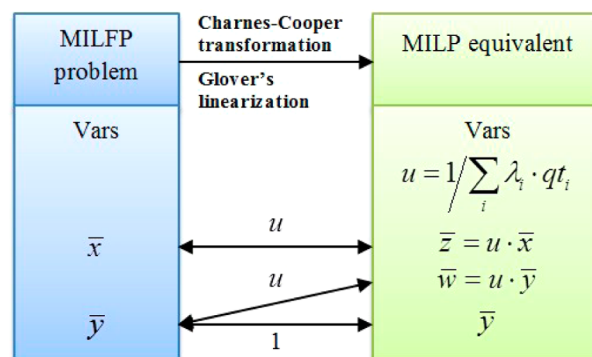


Figure 6. Illustration of the reformulation-linearization method.

Note that Uqt_i , $Ufct$, $Ucost_g$, and $Uenv_g$ are continuous variables included in \bar{z} , similar as mentioned in the previous section. The reformulated MILP problem (P1-R) would provide the same optimal objective value as the original MILFP problem (P1). Meanwhile, the optimal solution in the original feasible region can be calculated backward following the one-to-one correlation relationship.

The concern regarding the reformulation-linearization method is that the reformulated MILP problem can be computationally more expensive to be optimized due to the introduction of extra variables and constraints. However, problem (P1-R) only needs to be solved once, and the solution process of which reflects the actual gap information in real time.

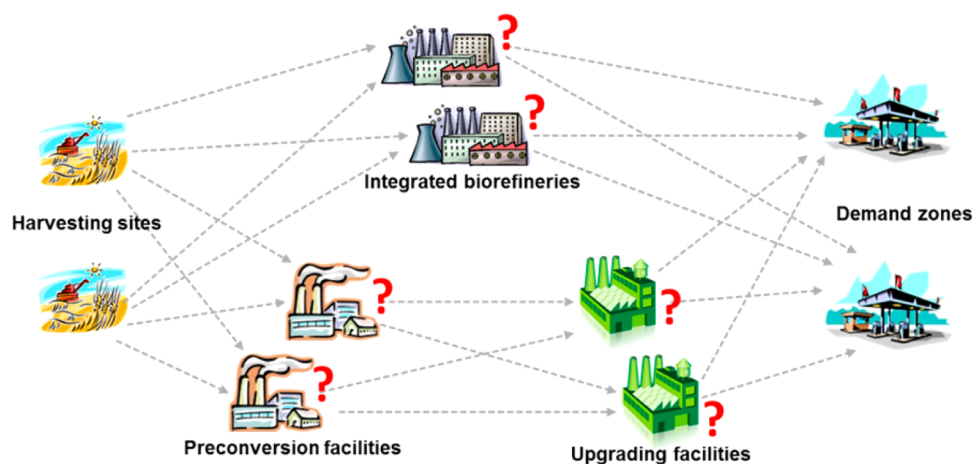


Figure 7. Supply chain network for biofuel production.

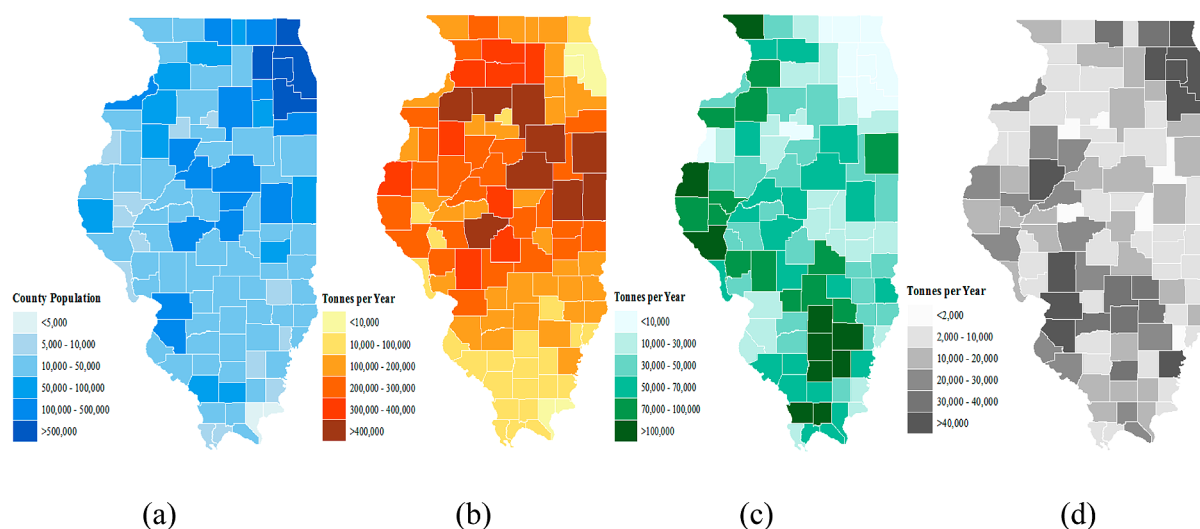


Figure 8. County-level biomass and population distribution in Illinois: (a) population distribution of Illinois; (b) spatial distribution of crop residues in Illinois; (c) spatial distribution of energy crops in Illinois; (d) spatial distribution of wood residues in Illinois.

CASE STUDY

Over the past decades, our society is making continuous efforts to search for and improve renewable sources of liquid transportation fuels. Among the various alternatives (e.g., nuclear, wind, solar cells, etc.), the biofuels is considered as the most promising candidate because of its vast domestic supply and environmental benefit.²⁰ As the fourth-generation biofuel, cellulosic drop-in fuels can be converted from the residual, nonedible parts of food crops as well as other nonfood crops thus avoiding the potential impacts on food supply.^{9,11,36} Furthermore, its “drop-in” feature enables the perfect compatibility with the current vehicle engine technology and existing fuel distribution infrastructure.²¹ Due to the Renewable Fuel Standard, which is part of the Energy Independence and Security Act of 2007,³⁷ the cellulosic biofuel industry is undergoing a rapid expansion. Hence, considering the relative maturity of biomass-to-liquid (BTL) technologies at the current stage, the study of corresponding BTL supply chain networks is significantly important and urgent.³⁸

Specific Problem Statement. In this section, we study the sustainable design of a potential hydrocarbon biofuel supply chain network in the state of Illinois. We employ a spatially explicit model, which is modified from the formulation

originally proposed by You and Wang.²¹ The underlying superstructure is given in Figure 7. We need to determine the optimal supply chain configuration (including the locations, technologies, and capacities for all the conversion facilities, as well as the amount of material flows for all the transportation links), with respect to both the economic and environmental criteria. In this problem, we define the functional unit as per gasoline-equivalent gallon (GEG) liquid transportation fuel characterized in terms of energy content. Therefore, the economic objective is minimizing the cost per GEG (including capital and operation costs) and the environmental objective is minimizing the life cycle GHG emission (in terms of CO₂ equivalent) associated with per GEG.

Considering the computation complexity of the complete problem, we study a reduced-size problem in this work. The candidate locations for harvesting sites and preconversion facilities are determined based on the total annual yields of the three biomass resources. The counties with total annual yields exceeding 280 kton are considered as potential harvesting sites, and the counties exceeding 380 ktons are considered for preconversion facility candidates. As for the integrated and upgrading facilities, the counties with population exceeding 50 000 and 100 000 are considered respectively. Every county is

considered as a demand zone. Hence, this BTL superstructure network contains 30 harvesting sites, 20 potential integrated biorefinery facilities, 20 possible locations of preconversion facilities, 21 upgrading facilities, and 102 demand zones. The potential harvesting sites and the location of candidate plants are illustrated in Figure 10a.

Three types of biomass resources are explored in this study: crop residues (including residues of corn, wheat, soybeans, etc.), energy crops (only including switchgrass), and wood residues (including forest residues and primary mills, secondary mills, urban wood residues). On the basis of the statistical data from the U.S. Department of Agriculture,³⁹ Figure 8b–d illustrates the spatial distribution of the annual yields of the three major biomass resources in 102 counties. This BTL processing network produces two types of liquid biofuel products, namely gasoline and diesel, to the demand zones. The annual demands of the entire state in 2013 are predicted based on data from U.S. Energy Information Administration,⁴⁰ which are 4535.59 and 1891.25 MM gallons/year for gasoline and diesel, respectively. We assume that the specific demand at each demand zone is proportional to the county population, which is based on the Census 2012⁴¹ data and illustrated in Figure 8a. We consider a near-term scenario to supply 5% of the fuel usage.

We assumed the moisture content of all the biomass feedstock to be 15%. The farm-to-gate acquisition costs of the feedstock are calculated from subtracting the cost of transportation and storage from the 2008 baseline price provided in the study by America's Energy Future Panel on Alternative Liquid Transportation Fuels.⁴² The acquisition costs (including pretreatment) for crop residues, energy crops, and wood residues are set to \$84.5, \$97.5, and \$50/ton, respectively.

Two types of conversion pathways are considered: centralized and distributed, respectively. The integrated pathway consists of two conversion methods, which are gasification with Fischer–Tropsch (FT) synthesis and pyrolysis followed by hydroprocessing. On the other hand, the distributed pathway first converts the feedstock to intermediate products (e.g., bio-oil and bioslurry) at preconversion facilities and then upgrades them into liquid fuel products at upgrading facilities. The two preconversion technologies considered are rotating cone reactor pyrolysis and fluidized bed reactor pyrolysis. The two upgrading technologies considered are hydroprocessing and gasification with Fisher–Tropsch (FT) synthesis. On the basis of the annual production amount for integrated biorefineries, two capacity levels are considered for both

conversion methods, which are 0–100 and 100–200 MM GEG/y. Two capacity levels for preconversion facilities with both technologies are 0–1 and 1–2 MM dry tons/y, while the capacity levels for upgrading facilities are 0–100 and 100–200 MM GEG/y. The capital cost of the conversion facilities is calculated based on literature data and a scale factor of 0.6, using the maximum and minimum of each capacity level.^{9,11,43–46} The total investment costs of the six conversion facilities in each capacity level are modeled using piecewise linear cost curve to include the economy of scale.²¹

The location of plants is set to the center of each county. Using the Google Distance Matrix API, the distance between each pair of the counties is calculated.⁴⁷ The data for truck transportation are obtained from Searcy et al.⁴⁸ and Mahmudi and Flynn.⁴⁹ The emission data regarding transportation and biomass production are based on the GREET model from Argonne national laboratory⁵⁰ and existing literature and reports.^{9,11,43–45}

All the computational experiments are carried out on a PC with Intel Core i5-2400 CPU at 3.10 GHz and 8.00 GB RAM. All models and solution procedures are coded in GAMS 23.9.⁵¹ MILP models are solved with CPLEX 12 with three processing cores under parallel mode. MINLP models are solved with SBB (simple branch-and-bound algorithm), DICOPT (outer-approximation algorithm), and the global optimizer BARON 12⁵² utilizing one processing core. The stopping tolerance for the parametric algorithm is set to 1%. The optimality tolerances for other methods are all set to 1%.

Model Formulation. The life cycle optimization model employed for this case study is a modification and simplification of the one proposed in the work by You and Wang.²¹ For the compactness of the article, detailed equations and notations are presented in the Supporting Information. The model covers the biomass feedstock supply system, integrated biorefineries, preconversion facilities, upgrading facilities, and the liquid fuel distribution system. The major properties of the BTL supply chain are described by the constraints, including biomass feedstock availability, material balance relationship, conversion facility capacity, transportation link capacity, financial constraints, etc.

As given by eq 28, the economic objective is to minimize the unit cost per GEG liquid fuel product, which is defined as the total annualized cost divided by the standard quantity of functional unit. It covers the cost of capital investment for facility establishment, biomass acquisition, production distribution, material production, transportation, and government incentives.

$$\min ftc = \frac{C_{\text{capital}} + C_{\text{acquisition}} + C_{\text{distribution}} + C_{\text{production}} + C_{\text{transportation}} - C_{\text{incentive}}}{\sum_{d \in D} \sum_{p \in P} \varphi_p \cdot \text{sold}_{d,p}} \quad (28)$$

where φ_p is the quantity of the functional unit possessed by a unit of product p ; $\text{sold}_{d,p}$ is the sales amount of product p at demand zone d .

As given by eq 29, the environmental objective is to minimize the environmental impact per GEG liquid fuel product, which is

$$\min fte = \frac{E_{\text{acquisition}} + E_{\text{distribution}} + E_{\text{production}} + E_{\text{transportation}} - E_{\text{sequestration}}}{\sum_{d \in D} \sum_{p \in P} \varphi_p \cdot \text{sold}_{d,p}} \quad (29)$$

defined as the total emissions divided by the standard quantity of functional unit. It covers the environmental impact from biomass acquisition, product distribution, material production, transportation, and sequestration credit.

Results and Discussion. The Pareto-optimal profiles for the sustainable design of the potential hydrocarbon biofuel supply chain are shown in this section. We derive the approximated Pareto curve by investigating 10 instances of the aforementioned bicriterion optimization model using the proposed solution approach. The result is presented in Figure 9. Point A corresponds to the most environmentally sustainable

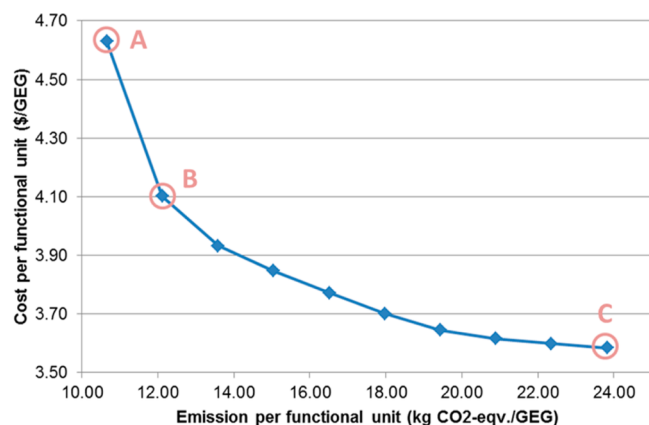


Figure 9. Pareto curve showing trade-off between economic and environmental performances.

solution, with the lowest GHG emission of 10.66 kg CO₂ equiv/GEG but the highest unit cost of \$4.63/GEG. On the other hand, point C corresponds to the most economical solution, with the highest GHG emission of 23.82 kg CO₂ equiv/GEG but the lowest unit cost of \$3.58/GEG. Considering the trade-offs between the economic and environmental criteria, we identify a “good choice” solution (point B) with the GHG emission of 12.12 kg CO₂ equiv/GEG and the unit cost of \$4.10/GEG, which significantly reduces the cost with a small sacrifice in the GHG emission. However, note that all the solutions on the Pareto curve are considered Pareto-optimal, among which one can choose for the supply chain design according to the preference. Solutions on the left emphasize more on reducing the environmental impact and green manufacturing, while the solutions on the right tend to pursue a more cost-effective product system.

The Pareto-optimal supply chain profile corresponding to the most environmentally sustainable solution (point A) is illustrated in Figure 10b. Only the centralized pathway is observed with 10 integrated biorefineries established mainly in the northern Illinois. The installed production capacities of these integrated biorefineries range from 21.5 to 72.1 MM GEG per year. The technology of fast pyrolysis plus hydroprocessing is selected by all the integrated biorefineries, which is consistent with our previous work.²¹ This suggests that the technology of fast pyrolysis followed by hydroprocessing yields biofuel products in a more environmentally friendly way, though can be more cost-intensive compared to the technology of gasification plus FT synthesis. The results also indicate that reduction of GHG emissions can be achieved by employing the centralized pathway to avoid the additional emissions from transportation and distributed production.

The Pareto-optimal supply chain profile corresponding to the good choice solution (point B) is illustrated in Figure 10c. We observe 10 integrated biorefineries, 5 preconversion facilities, and 1 intermediate upgrading facility. The installed capacities of the integrated biorefineries range from 20.0 to 34.1 MM GEG/

y. The technology of pyrolysis plus hydroprocessing is selected by all the integrated biorefineries. The installed capacities of the preconversion facilities range from 200.0 to 465.0 kton/y. The technology of the rotating cone process which produces bio-oil is selected by all the preconversion facilities. The installed capacity of the upgrading facility is 106.4 MM GEG/y, and the technology of hydroprocessing is selected. Compared with the most environmentally sustainable solution, the total capacity of the integrated biorefineries has decreased. Instead, part of the demand is supplied through the distributed pathway, which helps to achieve a lower cost per functional unit with a slight increase in the product carbon footprint. The distributed pathway is first introduced in northeastern Illinois, because there is higher demand as well as higher biomass resource supply in that area. Also, we note that the upgrading facility in Dupage County is located so that the transportation distances from the five preconversion facilities and to the demand zones in high population densities are optimized.

The Pareto-optimal supply chain profile corresponding to the most economical solution (point C) is illustrated in Figure 10d. As can be seen, 10 integrated biorefineries, 9 preconversion facilities, and 2 upgrading facilities are established. The installed capacities of the integrated biorefineries range from 20.0 to 195.0 MM GEG/y. The technology of gasification plus FT synthesis is selected by all the integrated biorefineries. The installed capacities of the preconversion facilities range from 200.0 to 725.5 kton/y. The rotating cone process is selected by preconversion facilities with smaller (<400 kton/y) capacities, while the fluidized bed process is selected for relatively large-size preconversion facilities. The smaller upgrading facility in Madison County with installed capacity of 50 MM GEG/y selects the technology of hydroprocessing and receives intermediate products from south Illinois. The larger upgrading facility in Dupage County with installed capacity of 200 MM GEG/y selects the technology of gasification plus FT synthesis and mainly supplies northeastern Illinois. This solution profile reveals the trend that the more distributed the biofuel supply chain configuration, the more cost-effective the product system. Also, we note the optimal selection of conversion technologies is influenced by the capacity levels of the facilities. In Figure 11, we present the cost breakdown for the most cost-effective solution. As can be observed, the acquisition cost for biomass feedstock constitutes the most expensive part, which suggests that biomass price has a significant influence on the economic sustainability of the product system. Not as significant as in usual processes, the investment cost in this biofuel supply chain accounts for 22% of the total cost. The ratio of fixed operation and maintenance (O&M) cost to the variable production cost is largely dependent on the selected conversion technologies. Finally, the transportation cost contributes 14% to the total cost.

To illustrate the effectiveness of the proposed solution strategy, we also present the computational results in this section to compare the proposed tailored MILFP algorithms with the general-purposed MINLP ones. The original MILFP model consists of 244 discrete variables, 131 351 continuous variables, and 30 826 constraints. We have applied the tailored MILFP methods (parametric algorithm and reformulation-linearization method) and general-purpose MINLP solvers (DICOPT, SBB, and BARON 12⁵²) to optimize 10 instances of the ϵ -constraint method. The solution reports for the three selected instances are summarized in Table 3. As can be observed, the parametric algorithm is demonstrated to be the

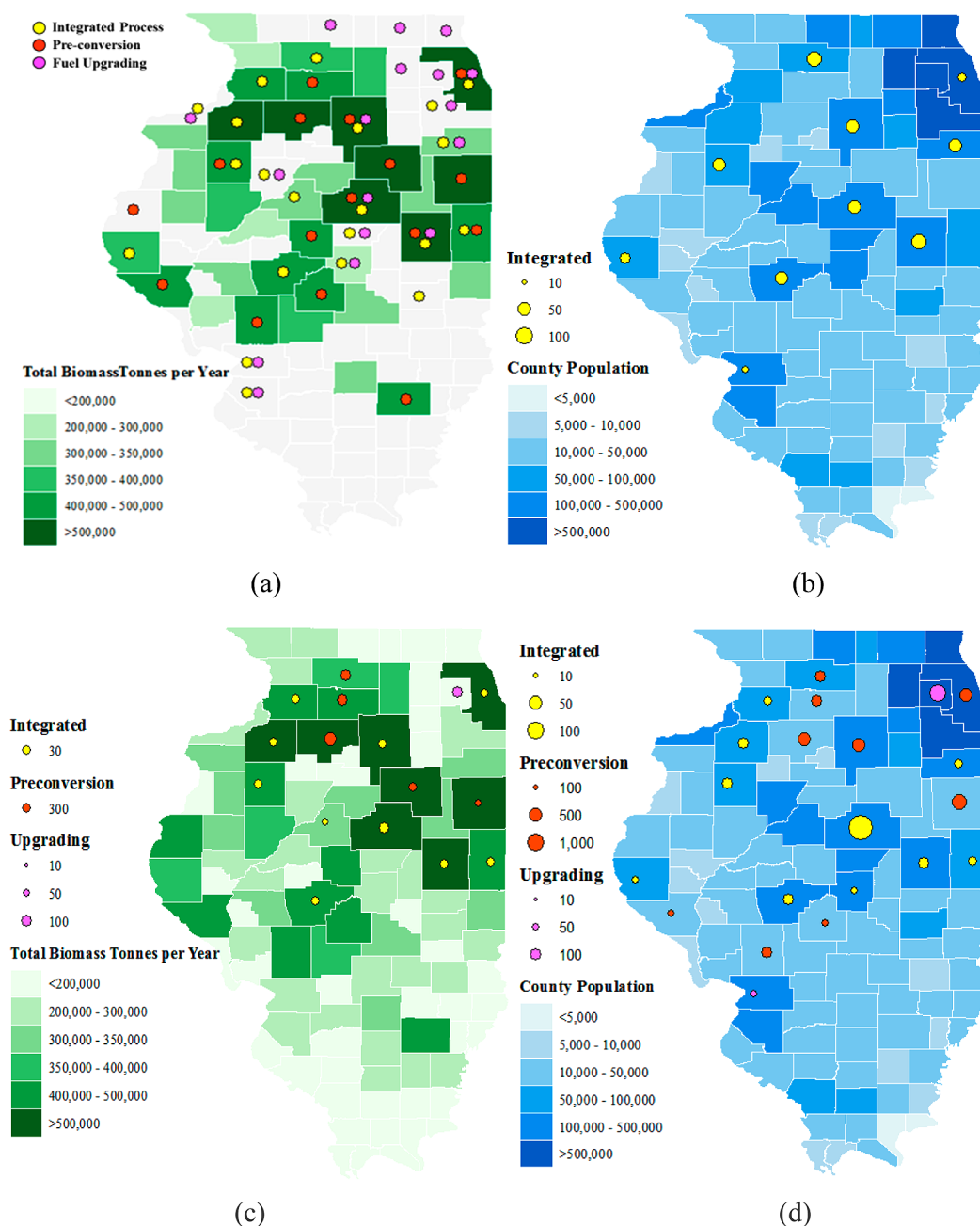


Figure 10. Optimal design for minimized cost per GEG with population density background. (a) Candidate plants with potential harvesting sites as background. (b) Most environmentally sustainable biofuel supply chain profile with population distribution as background. (c) Good choice solution with biomass resources distribution as background. (d) Most economical biofuel supply chain profile with population distribution as background.

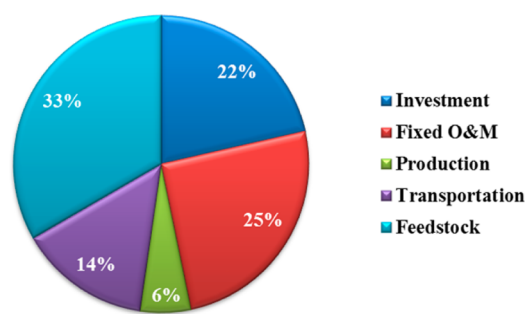


Figure 11. Cost breakdown for most economical solution.

most efficient among the five algorithms, of which the solution time for all 10 instances ranges from 1.5 to 373.5 CPUs. The reformulation-linearization method tends to be slower for this problem, of which the solution time for all 10 instances ranges from 59.2 to 2853.7 CPUs. Though it is a local optimizer, DICOPT appears to be a good solver for this problem, which also converges fast for this problem. SBB and BARON 12 exceed the preset computation time limit (2 h) in most instances, and the current best solutions are recorded. Overall, the parametric algorithm exhibits the best computation performance among all the investigated solution methods and, thus, is recommended for the global optimization of MILFP models encountered in the life cycle optimization for sustainable design of product system.

Table 3. Solution Reports for the Case Study

| instances | ϵ | unit cost (\$/GEG) | unit impact (kg CO ₂ equiv/GEG) | time (CPUs) | gap | solver |
|-----------|------------|--------------------|--|-------------|-------|-----------------------------|
| A | 10.66 | 4.63 | 10.66 | 1.5 | 1% | parametric algorithm |
| | | 4.63 | 10.66 | 80.8 | 1% | reformulation-linearization |
| | | 4.63 | 10.66 | 3.7 | 1% | DICOPT |
| | | | | 7200 | | SBB |
| | | 4.63 | 10.66 | 5276.3 | 1% | BARON 12 |
| B | 12.12 | 4.10 | 12.12 | 20.0 | 1% | parametric algorithm |
| | | 4.10 | 12.12 | 125.1 | 1% | reformulation-linearization |
| | | 4.10 | 12.12 | 31.8 | 1% | DICOPT |
| | | 4.12 | 12.12 | 7200 | 4.7% | SBB |
| | | 4.15 | 12.12 | 7200 | 4.5% | BARON 12 |
| C | 23.83 | 3.58 | 23.83 | 244.3 | 1% | parametric algorithm |
| | | 3.58 | 23.83 | 215.4 | 1% | reformulation-linearization |
| | | 3.58 | 23.83 | 406.3 | 1% | DICOPT |
| | | 3.62 | 22.44 | 7200 | 8.3% | SBB |
| | | 4.15 | 23.83 | 7200 | 20.7% | BARON 12 |

CONCLUSIONS

In this paper, we proposed a life cycle optimization framework for sustainable design of product system and supply chain network under economic and environmental concerns. This general modeling framework coupled the classic LCA methodology with multiobjective optimization, which could provide environmental impact evaluation from a life cycle perspective while generate and optimize solution alternatives automatically. Because the economic and environmental performances of a product system would be measured eventually through the provision of function from the finished products, we proposed using two functional-unit-based economic and environmental objectives, respectively, to achieve a more sustainable system design. We also proposed effective solution strategies for the resulting bicriterion optimization problems. For illustration, we applied the proposed life cycle optimization framework to the sustainable design of a hydrocarbon biofuel supply chain in Illinois. A Pareto curve was obtained which clearly revealed the trade-off between economic and environmental concerns in decision making. The results indicated that the most environmentally sustainable design can be achieved with a unit cost of \$4.63/GEG and GHG emission of 10.66 CO₂ equiv/GEG for the biomass-derived gasoline and diesel, while the most economical design leads to a unit cost of \$4.10/GEG and GHG emission of 12.12 CO₂ equiv/GEG.

ASSOCIATED CONTENT

Supporting Information

Detailed mathematical model formulation and notations for the case study. This material is available free of charge via the Internet at <http://pubs.acs.org>.

AUTHOR INFORMATION

Corresponding Author

*E-mail: you@northwestern.edu.

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

We gratefully acknowledge the financial support from the Initiative for Sustainability and Energy at Northwestern University (ISEN).

REFERENCES

- Mejia, G.; Velasco, N. *Production Systems and Supply Chain Management in Emerging Countries: Best Practices*; Springer: Heidelberg, 2012.
- Grossmann, I. E.; Guillén-Gosálbez, G. Scope for the application of mathematical programming techniques in the synthesis and planning of sustainable processes. *Comput. Chem. Eng.* **2010**, *34* (9), 1365–1376.
- Shah, N. Process industry supply chains: Advances and challenges. *Comput. Chem. Eng.* **2005**, *29* (6), 1225–1235.
- Grossmann, I. E. Enterprise-wide optimization: A new frontier in process systems engineering. *AIChE J.* **2005**, *51* (7), 1846–1857.
- Varma, V. A.; Reklaitis, G. V.; Blau, G. E.; Pekny, J. F. Enterprise-wide modeling & optimization - An overview of emerging research challenges and opportunities. *Comput. Chem. Eng.* **2007**, *31* (5–6), 692–711.
- Othman, M. R.; Repke, J. U.; Wozny, G.; Huang, YL. A Modular Approach to Sustainability Assessment and Decision Support in Chemical Process Design. *Ind. Eng. Chem. Res.* **2010**, *49* (17), 7870–7881.
- Nikolopoulou, A.; Ierapetritou, M. G. Optimal design of sustainable chemical processes and supply chains: A review. *Comput. Chem. Eng.* **2012**, *44*, 94–103.
- Srivastava, S. K. Green supply-chain management: A state-of-the-art literature review. *Int. J. Manage. Rev.* **2007**, *9* (1), 53–80.
- Wang, B.; Gebreslassie, B. H.; You, F. Sustainable design and synthesis of hydrocarbon biorefinery via gasification pathway: Integrated life cycle assessment and technoeconomic analysis with multiobjective superstructure optimization. *Comput. Chem. Eng.* **2013**, *52* (0), 55–76.
- Cano-Ruiz, J. A.; McRae, G. J. Environmentally conscious chemical process design. *Annu. Rev. Energy Environ.* **1998**, *23*, 499–536.
- Gebreslassie, B. H.; Slivinsky, M.; Wang, B.; You, F. Life cycle optimization for sustainable design and operations of hydrocarbon biorefinery via fast pyrolysis, hydrotreating and hydrocracking. *Comput. Chem. Eng.* **2013**, *50* (0), 71–91.
- Fava, J. A. *A Technical Framework for Life-Cycle Assessment*; SETAC Foundation: Pensacola, 1994.
- Azapagic, A. Life cycle assessment and its application to process selection, design and optimization. *Chem. Eng. J.* **1999**, *73* (1), 1–21.
- Azapagic, A.; Clift, R. The application of life cycle assessment to process optimization. *Comput. Chem. Eng.* **1999**, *23* (10), 1509–1526.
- Seuring, S.; Müller, M. From a literature review to a conceptual framework for sustainable supply chain management. *J. Cleaner Prod.* **2008**, *16* (15), 1699–1710.

- (16) Hugo, A.; Pistikopoulos, E. N. Environmentally conscious long-range planning and design of supply chain networks. *J. Cleaner Prod.* **2005**, *13* (15), 1471–1491.
- (17) Liu, P.; Georgiadis, M. C.; Pistikopoulos, E. N. Advances in Energy Systems Engineering. *Ind. Eng. Chem. Res.* **2010**, *50* (9), 4915–4926.
- (18) Elia, J. A.; Baliban, R. C.; Xiao, X.; Floudas, C. A. Optimal energy supply network determination and life cycle analysis for hybrid coal, biomass, and natural gas to liquid (CBGTL) plants using carbon-based hydrogen production. *Comput. Chem. Eng.* **2011**, *35* (8), 1399–1430.
- (19) Santibañez-Aguilar, J. E.; González-Campos, J. B.; Ponce-Ortega, J. M.; Serna-González, M.; El-Halwagi, M. M. Optimal Planning of a Biomass Conversion System Considering Economic and Environmental Aspects. *Ind. Eng. Chem. Res.* **2011**, *50* (14), 8558–8570.
- (20) You, F. Q.; Tao, L.; Graziano, D. J.; Snyder, S. W. Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input-output analysis. *AIChE J.* **2012**, *58* (4), 1157–1180.
- (21) You, F. Q.; Wang, B. Life Cycle Optimization of Biomass-to-Liquid Supply Chains with Distributed-Centralized Processing Networks. *Ind. Eng. Chem. Res.* **2011**, *50* (17), 10102–10127.
- (22) Giarola, S.; Zamboni, A.; Bezzo, F. Spatially explicit multi-objective optimization for design and planning of hybrid first and second generation biorefineries. *Comput. Chem. Eng.* **2011**, *35* (9), 1782–1797.
- (23) Akgul, O.; Shah, N.; Papageorgiou, L. G. An optimization framework for a hybrid first/second generation bioethanol supply chain. *Comput. Chem. Eng.* **2012**, *42*, 101–114.
- (24) Cucek, L.; Varbanov, P. S.; Klemes, J. J.; Kravanja, Z. Total footprints-based multi-criteria optimization of regional biomass energy supply chains. *Energy* **2012**, *44* (1), 135–145.
- (25) Santibañez-Aguilar, J. E.; Ponce-Ortega, J. M.; González-Campos, J. B.; Serna-González, M.; El-Halwagi, M. M. Synthesis of Distributed Biorefining Networks for the Value-Added Processing of Water Hyacinth. *ACS Sustain. Chem. Eng.* **2013**, *1* (2), 284–305.
- (26) Gebreslassie, B. H.; Waymire, R.; You, F. Sustainable design and synthesis of algae-based biorefinery for simultaneous hydrocarbon biofuel production and carbon sequestration. *AIChE J.* **2013**, *59* (5), 1599–1621.
- (27) Hwang, G. L.; Masud, A. S. M. *Multiple objective decision making - Methods and Applications*; Springer: Berlin, 1979.
- (28) Bajalinov, E. B. *Linear-fractional programming: theory, method, applications and software*; Kluwer Academic Publishers: Boston, 2003.
- (29) Bazaraa, M. S.; Sherali, H. D.; Shetty, C. M. *Nonlinear programming: theory and algorithms*; Wiley: New York, 2004.
- (30) Floudas, C. A. *Deterministic global optimization: theory, methods and applications*; Kluwer Academic Publishers: Boston, 1999.
- (31) You, F. Q.; Castro, P. M.; Grossmann, I. E. Dinkelbach's Algorithm as An Efficient Method to Solve A Class of MINLP Models for Large-Scale Cyclic Scheduling Problems. *Comput. Chem. Eng.* **2009**, *33* (11), 1879–1889.
- (32) Goedkoop, M.; Spriensma, R. *Eco-indicator 99: A Damage Oriented Method for Life Cycle Impact Assessment ; Methodology Report*; PRé, Product Ecology consultants: Washington, D.C., 2001.
- (33) You, F.; Pinto, J. M.; Grossmann, I. E.; Megan, L. Optimal Distribution-Inventory Planning of Industrial Gases. II. MINLP Models and Algorithms for Stochastic Cases. *Ind. Eng. Chem. Res.* **2011**, *50* (5), 2928–2945.
- (34) You, F.; Wassick, J. M.; Grossmann, I. E. Risk management for a global supply chain planning under uncertainty: Models and algorithms. *AIChE J.* **2009**, *55* (4), 931–946.
- (35) Chu, Y. F.; You, F. Q. Integration of scheduling and control with online closed-loop implementation: Fast computational strategy and large-scale global optimization algorithm. *Comput. Chem. Eng.* **2012**, *47*, 248–268.
- (36) An, H.; Wilhelm, W. E.; Searcy, S. W. Biofuel and petroleum-based fuel supply chain research: A literature review. *Biomass Bioenergy* **2011**, *35* (9), 3763–3774.
- (37) Energy Independence and Security Act of 2007. Public Law 110-140; United States Government: Washington, D.C., 2007; Vol In: RL34294.
- (38) Gebreslassie, B. H.; Yao, Y.; You, F. Design under uncertainty of hydrocarbon biorefinery supply chains: Multiobjective stochastic programming models, decomposition algorithm, and a Comparison between CVaR and downside risk. *AIChE J.* **2012**, *58* (7), 2155–2179.
- (39) NASS. National Agricultural Statistics Service. 2012.
- (40) U.S. Energy Information Administration. www.eia.doe.gov (accessed Oct 2012).
- (41) U.S. Census Bureau. <http://www.census.gov> (accessed Oct 2012).
- (42) *Liquid Transportation Fuels from Coal and Biomass: Technological Status, Costs, and Environmental Impacts*; The National Academies Press: Washington, D.C., 2009.
- (43) Swanson, R. M.; Platon, A.; Satrio, J. A.; Brown, R. C. Techno-economic analysis of biomass-to-liquids production based on gasification. *Fuel* **2010**, *89*, S2–S10.
- (44) Wright, M. M.; Daugaard, D. E.; Satrio, J. A.; Brown, R. C. Techno-economic analysis of biomass fast pyrolysis to transportation fuels. *Fuel* **2010**, *89*, S11–S19.
- (45) Anex, R. P.; Aden, A.; Kazi, F. K.; et al. Techno-economic comparison of biomass-to-transportation fuels via pyrolysis, gasification, and biochemical pathways. *Fuel* **2010**, *89*, S29–S35.
- (46) Wright, M. M.; Brown, R. C.; Boateng, A. A. Distributed processing of biomass to bio-oil for subsequent production of Fischer–Tropsch liquids. *Biofuels, Bioprod. Biorefin.* **2008**, *2* (3), 229–238.
- (47) Google Distances Matrix API. <https://developers.google.com/maps/documentation/distancematrix/> (accessed Nov 2012).
- (48) Searcy, E.; Flynn, P.; Ghafoori, E.; Kumar, A. The relative cost of biomass energy transport. *Appl. Biochem. Biotechnol.* **2007**, *137*, 639–652.
- (49) Mahmudi, H.; Flynn, P. C. Rail vs truck transport of biomass. *Appl. Biochem. Biotechnol.* **2006**, *129* (1–3), 88–103.
- (50) Argonne GREET Model. <http://greet.es.anl.gov/> (accessed Oct 2010).
- (51) Rosenthal, R. E. *GAMS - A User's Guide.*: GAMS Development Corp.: Washington, D.C., 2011.
- (52) Tawarmalani, M.; Sahinidis, N. V. A polyhedral branch-and-cut approach to global optimization. *Math. Program.* **2005**, *103* (2), 225–249.