Fair Profit Allocation in Supply Chain Optimization with Transfer Price and Revenue Sharing: MINLP Model and Algorithm for Cellulosic Biofuel Supply Chains

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A mixed-integer nonlinear programming (MINLP) formulation to simultaneously optimize operational decisions as well as profit allocation mechanisms in supply chain optimization, namely material transfer prices and revenue share policies among the supply chain participants is proposed. The case of cellulosic bioethanol supply chains is specifically considered and the game-theory Nash bargaining solution approach is employed to achieve fair allocation of profit among the collection facilities, biorefineries, and distribution centers. The structural advantages of certain supply chain participants can be taken into account by specifying different values of the negotiation-power indicators in the generalized Nash-type objective function. A solution strategy based on a logarithm transformation and a branch-and-refine algorithm for efficient global optimization of the resulting nonconvex MINLP problem is proposed. To demonstrate the application of the proposed framework, an illustrative example and a state-wide county-level case study on the optimization of a potential cellulosic bioethanol supply chain in Illinois are presented. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3211–3229, 2014
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Introduction

Supply chain optimization is an important and practical topic both for industry and academia.[1–4] Although there has been a proliferation of optimization models and methods for supply chain design and operation reported in the literature, most of these works treat the entire supply chain as a whole, without considering the conflicting interests of the divisions and participants within the supply chain system.[5,6] When the overall supply chain system is optimized in this way, there are no automatic mechanisms allowing profits to be fairly allocated among the participants, thus leading to quite uneven profit distribution and a high degree of dissatisfaction. Although a certain level of cooperation can be achieved among participants within the supply chain, efficient policies and mechanisms are needed to maximize the overall performance of the supply chain and simultaneously ensure adequate rewards for each participant, as every participant tends to seek as much value for themselves as possible. Therefore, it is the goal of this work to develop an optimization framework that simultaneously optimizes the supply chain operational decisions as well as the profit allocation mechanisms.

Game theory is a powerful tool for studying decision making under such conditions. General reviews on the applications of game theory in supply chain management are provided by Nagarajan and Sošić[7] and by Cachon and Netessine.[5] Closely related to the subject of this work is the body of literature on optimization using cooperative game theory and profit allocation mechanisms. Gjerdrum et al. first proposed a mixed-integer nonlinear programming (MINLP) mathematical formulation based on the game-theory Nash bargaining solution approach to achieve fair and optimized profit distribution in multienterprise supply chains.[8] The same authors also proposed another MINLP model for the optimal decisions on fair transfer price and inventory holding policies in two-enterprise supply chains.[9] Recently, Zhang et al. applied the game-theory Nash bargaining solution approach for fair and optimized cost distribution among participants in a general microgrid system.[10]

Instead of looking into general supply chain networks, we will focus our application on cellulosic biofuel supply chains. Cellulosic biofuels are considered as part of the solution to increasing concerns about climate change, energy security, and our heavy dependence on petroleum-derived liquid transportation fuels. A cellulosic biofuel supply chain typically consists of multiple facilities and divisions that are in charge of biomass collection, biomass-to-biofuel conversion, and biofuel distribution, respectively.[11] Therefore, an efficient optimization strategy is needed to guarantee the economic viability and sustainability of the cellulosic biofuel supply chain, not only holistically, but also by considering the payoffs of each supply chain participant. Recent works

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on biofuel supply chain optimization are reviewed as follows. Comprehensive reviews on the optimization of biofuel supply chains are presented by Yue et al. and Sharma et al.[12] Deterministic mixed-integer linear programming (MILP) models have been widely employed to investigate cost-minimizing or profit-maximizing biofuel supply chain configurations, which often incorporate spatially explicit, multiechelon, and multiperiod features.[13–21] Multiobjective optimization models have been proposed to account for other dimensions of biofuel supply chains in addition to economic performance, including environmental sustainability, social benefit, safety criteria, and so forth.[22–27] Various pricing and quantity uncertainties in the biofuel supply chain have been addressed by stochastic programming, robust approaches, fuzzy programming, and so forth.[28–33]

To the best of our knowledge, there are only a few works addressing profit allocation issues in supply chain optimization and no applications of profit allocation in biofuel supply chains have been observed. The profit allocation mechanism used in the works reviewed above is called transfer pricing policy or wholesale contract. We note that the wholesale contract is a basic side-payment contract and may not arbitrarily allocate the profit or necessarily lead to coordination of the entire supply chain.[34] Therefore, in this work, we propose using the revenue sharing policy[35,36] to allow for arbitrary allocation of the total profit and to align the interests of individual participants in the biofuel supply chain in order to maximize overall supply chain performance. Moreover, we take into account the difference in each supply chain participant's negotiation power using the generalized Nash-type objective function, thus allowing participants with structural advantages (e.g., manufacturers) to attain higher profits then other participants (e.g., suppliers and distributors). Due to the use of a Nash-type objective function, the optimization model is formulated as a nonconvex MINLP problem, of which the solution is often challenging for large-scale applications. To facilitate the solution process, we propose a global optimization strategy based on a logarithmic transformation and a branch-and-refine algorithm. We will present a small-scale case study to demonstrate the concepts and feasibility of the proposed modeling and solution framework, followed by a state-wide county-level case study on optimization of future cellulosic bioethanol supply chain in the state of Illinois to illustrate the capability of large-scale implementation and efficiency of the proposed algorithms.

Major novelties of this work are summarized as follows:

- A novel supply chain optimization framework with transfer price and revenue sharing;
- Application of game-theory generalized Nash bargaining solution approach accounting for difference in negotiation power of the participants;
- Application of revenue sharing policy for arbitrary profit allocation and coordination within the supply chain;
- A county-level case study on cellulosic bioethanol supply chain in Illinois.

The rest of this article is organized as follows. We first provide brief introductions to revenue sharing policy and generalized Nash bargaining solution, respectively. The problem statement and model formulation are presented next, followed by the reformulation and solution strategies. To demonstrate the application of the proposed modeling and solution framework, we provide a small-scale and a large-scale case study at the end, with detailed discussions of the results.

Revenue Sharing Policy

Research on supply chain optimization mainly treats the entire supply chain as a whole, assuming that there is a unique decision maker who possesses all the relevant information and has the power to implement all the decisions. However, this centralized decision making process may not be realistic in practice, where a supply chain consists of multiple divisions and participants pursuing different objectives, possibly conflicting with each other. Whang[37] indicated that these locally rational behaviors in the decentralized setting can be globally inefficient for the overall performance of the entire supply chain. Therefore, coordination mechanisms are necessary to induce individual participants to behave coherently with each other, as if the supply chain was operated under the control of a unique decision maker. The most important type of coordination mechanisms is a supply chain contract, which formally rules the transactions between supply chain participants. Using supply chain contracts in the decentralized setting, we can increase the total supply chain profit to make it equal or closer to the profit resulting from a centralized decision making process.

Different types of supply chain contracts have been developed in the literature, including but not limited to, constant wholesale price, revenue sharing, sales rebate, quantity flexibility, buyback policy, and quantity discount contract.[34] In this work, we will focus on the revenue sharing policy. Although the revenue sharing policy has not been applied in the real-world biofuel supply chains yet, it has been successfully implemented in other industries and resulted in significant improvement in the industry's total profit via supply chain coordination.[38,39] Cachon and Lariviere proposed the revenue sharing contract for a two-stage distributor-retailer supply chain.[35] Giannoccaro and Pontrandolfo extended the revenue sharing contract to a multiechelon serial supply chain.[36] Gerchak and Wang studied revenue sharing in assembly systems and provided a comparison with the wholesale price contract.[40] Pan et al. compared revenue sharing and wholesale price mechanisms in both assembly and distribution channel structures.[41] Based on the works reviewed above, we generalize the revenue sharing policy in a multiechelon multientity supply chain network addressing the pairwise relationship between adjacent supply chain participants.

For each transaction, we define the material sender as a "supplier" (indexed by s) and material receiver as a "receiver" (indexed by r). The revenue sharing contract can be described with two parameters. One is the transfer price or wholesale price the receiver pays per unit of materials transferred ω_s. The other is the share ratio of suppliers in the receiver's revenue $\phi_{s,r}$. To demonstrate the revenue sharing mechanism, we consider a simple three-echelon supply chain with a single product as shown in Figure 1. Node j is supplied by two upstream nodes $i1$ and $i2$. At the same time, node j transfers materials to two downstream nodes $k1$ and $k2$. The solid-line arrows represent material flows, and the dashed-line arrows represent monetary flows.

Under the revenue sharing policy, the profit of node $i1$ is equal to the revenue share from its downstream node j plus the transfer payment received from node j minus node $i1$'s own cost function. This cost function may involve charges

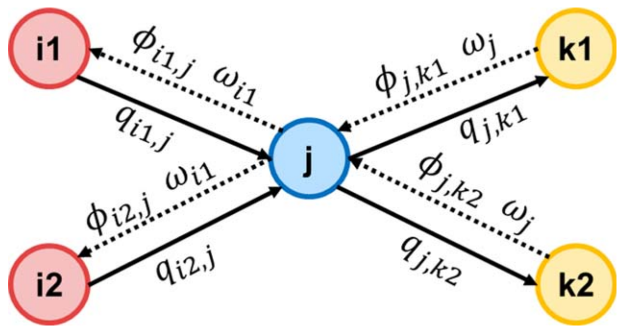

Figure 1. Demonstration of revenue sharing policy in a simplified supply chain network.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

from administration, transportation, inventory, and so forth. Similar model applies to node $i2$

$$\pi_{i1}=\phi_{i1,j}\cdot R_j+\omega_{i1}\cdot q_{i1,j}-c_{i1}\text{ and }\pi_{i2}=\phi_{i2,j}\cdot R_j+\omega_{i2}\cdot q_{i2,j}-c_{i2} \tag{1}$$

where R_r stands for the receiver's revenue; $q_{r,s}$ represents the amount of materials transferred between the supplier and receiver; c_s is the cost function of the supplier.

The profit of node j under the revenue sharing policy is given by

$$\pi_j=\left(1-\phi_{i1,j}-\phi_{i2,j}\right)\cdot R_j-c_j \tag{2}$$

The first component is the share of node j in its own revenue, excluding the revenue shared with upstream nodes $i1$ and $i2$. The second component is the cost function of node j. Note that the revenue of node j is calculated as the received transfer payment plus its shares in both downstream receivers' revenue

$$R_j=\omega_j\left(q_{j,k1}+q_{j,k2}\right)+\phi_{j,k1}R_{k1}+\phi_{j,k2}R_{k2} \tag{3}$$

As an assumption in Eq. 3, we assume that the transfer price set at the supplier is the same for all receivers,[42] thus avoiding price discrimination against small buyers. However, different transfer prices can be easily taken into account with an additional index on parameter ω.

Similarly, the profit of nodes $k1$ and $k2$ are given by

$$\pi_{k1}=\left(1-\phi_{j,k1}\right)\cdot R_{k1}-c_{k1}\text{ and }\pi_{k2}=\left(1-\phi_{j,k2}\right)\cdot R_{k2}-c_{k2} \tag{4}$$

where the revenue is equal to the sales of product if nodes $k1$ and $k2$ are directly facing external markets (indexed by m), that is

$$R_{k1}=p_{k1}\cdot q_{k1,m}\text{ and }R_{k2}=p_{k2}\cdot q_{k2,m} \tag{5}$$

where p_s stands for the selling price of the product.

The revenue sharing mechanism discussed above can be easily applied to general multiechelon supply chain structures involving multiple types of materials. Furthermore, we note that the conventional wholesale pricing policy is a special case of the revenue sharing policy where the supplier's share in the receiver's revenue is equal to 0. Due to the additional degree of freedom, the revenue sharing mechanism is more powerful than a wholesale pricing policy. The revenue sharing policy is able to arbitrarily allocate the profit and achieve channel coordination for most supply chains.

Generalized Nash Bargaining Solution Approach

Consider a group of two or more participants who are faced with a set of feasible outcomes. Any one of these outcomes will become the final result if it is unanimously agreed upon by all the participants. To reach unanimity among all the participants with possibly conflicting objectives, there is a need for bargaining and negotiation over which outcome should be agreed upon. To model this negotiation process, Nash[43] initiated a cooperative bargaining process between two players and presented an axiomatic derivation of the bargaining solution, which is a feasible outcome that satisfies a set of axioms. The axioms ensure that the solution is symmetric (indistinguishable participants should receive identical profit allocations), feasible (the sum of the allocations does not exceed the total profit), and Pareto optimal (it is impossible for any two of the participants to improve their profit over the bargaining solution at the same time). In addition, the bargaining solution should be preserved under linear transformations and be independent of irrelevant alternatives. Solutions satisfying these criteria are considered "fair" in this work.

The extension of the Nash bargaining solution approach to multiplayer negotiation processes is straightforward. However, the original bargaining solution treats all participants as identical players, while it is reasonable to expect that the participant with higher bargaining power (e.g., structural advantages) receives a larger share of the profit than other weaker counterparts. Therefore, relaxing the axiom of symmetry, Roth presented a generalized Nash bargaining solution in the form given by[7,44]

$$\arg\max_{\pi\in\Omega,\pi\geq d}\prod_i\left(\pi_i-d_i\right)^{\alpha_i} \tag{6}$$

where α_i is the negotiation-power indicator of participant i—the higher its value, the more advantage the participant has in profit allocation; π_i is the profit of participant i in the unanimously agreed outcome; d_i is the status quo point of participant i. The negotiation-power indicators are assumed as adjustable parameters controlled by the supply chain coordinator in this work. More sophisticated approaches to determine negotiation powers by "commitment tactics" are introduced in the work by Nagarajan and Šošić.[7] The status quo point can be interpreted as the current profit status of each participant before an unanimous agreement is achieved. Without loss of generality, we set the status quo points to zero in this work. The difference between π_i and d_i is called surplus. Equation 6 indicates that the generalized Nash bargaining solution can be obtained by maximizing the product over all the supply chain participants' surpluses. A simple illustration of the Nash bargaining solution is presented in Figure 2. The axes represent the profit of Player 1 and Player 2. The solid line indicates a linear interrelationship between the players' profit function: $\pi_1+\pi_2=4$. Assuming that the status quo points are set to zero, the profit is equal to the surplus. As can be observed, if identical negotiation powers are possessed by both players (e.g., $\alpha_1=1$ and $\alpha_2=1$), the resulting Nash bargaining solution (Point A) leads to even allocation of the profit. When the negotiation power of Player 1 is twice as large as that of Player 2 (e.g., $\alpha_1=2$ and $\alpha_2=1$), the resulting Nash bargaining solution (Point B) allocates twice the profit of Player 2 to Player 1, if no other restrictions are imposed.

In this work, the surplus of each participant in the biofuel supply chain is associated with not only the various

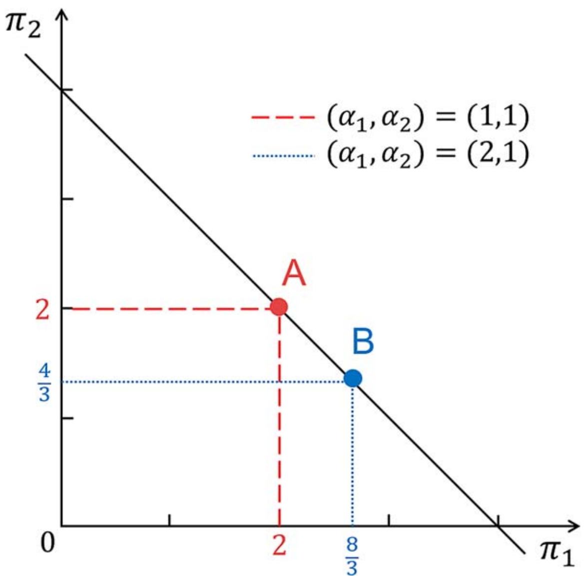

Figure 2. Illustration of the generalized bargaining solution.

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operational activities but also the parameters of the revenue sharing policy that will significantly influence the profit allocation within the biofuel supply chain. Therefore, the Nash bargaining solution should be obtained through simultaneous optimization of the operational decisions and revenue sharing mechanism so as to achieve fair profit allocation and supply chain coordination.

Problem Statement

In this section, we will formally state the addressed problem on the optimization of biofuel supply chain with transfer price and revenue sharing policy. A general three-echelon biofuel supply chain superstructure is considered (Figure 3), which includes a set of collection facilities ($i \in I$), a set of biorefineries ($j \in J$), and a set of distribution centers ($k \in K$). The green dashed-line indicates the supply chain boundary, and we will act as the supply chain coordinator in this problem. As suggested by the orange solid-lines, once the biofuel supply chain structure is given, every collection facility, biorefinery, or distribution center is considered as an individual participant in the supply chain. Cellulosic biomass ($b \in B$) is acquired at the collection facilities from suppliers. The biofuel product ($p \in P$) is produced at biorefineries and then shipped to distribution centers to fulfill the demands. The biofuel can be produced via a set of biomass conversion technologies ($q \in Q$). To account for the economies of scale on capital investment, we employ the piecewise linear cost function and specify a set of capacity levels ($r \in R$) for the biorefineries. To capture the seasonal operations in the biofuel supply chain, we consider a set of time periods ($t \in T$). We also consider a number of transfer price levels ($c \in C$) for the setting of wholesale prices.

At each collection facility, we are given the available amount of biomass as well as the acquisition price in each time period. At each biorefinery, we are given the maximum capacity and capacity levels for biorefinery construction. Construction incentives from the government are also provided. Techno-economic data are retrieved from the most up-to-date reports. Storage of both biomass feedstock and biofuel product is considered, with unit inventory holding cost specified. Specifically for biomass storage, the deterioration rate is given and accounts for the degradation and loss of biomass material. To guarantee continuous production of biofuel, a minimum utilization rate of the biorefinery capacity and a safety period for the hedging stock of biomass at biorefineries can be considered. At each distribution center, upper and lower bounds of the demand for biofuel as well as the selling price in each time period are given. The transportation distances between each pair of locations as well as the associated fixed and variable transportation costs are given. To cutoff the transportation links that are deemed unviable, we can specify a maximum distance for the shipping of biomass and biofuel.

Two key assumptions are adopted in this work. First, we assume that all information is shared among all the supply chain participants. Second, all the participants agree on the negotiation process and will accept the optimized profit allocation mechanism as their fair rewards are guaranteed. These two assumptions establish a cooperative setting among the supply chain participants and validate the Nash bargaining solution approach. These assumptions are often satisfied if all supply chain participants are divisions of one corporation, or if the different enterprises are closely related such that to the business where cooperation would improve their economic performances.

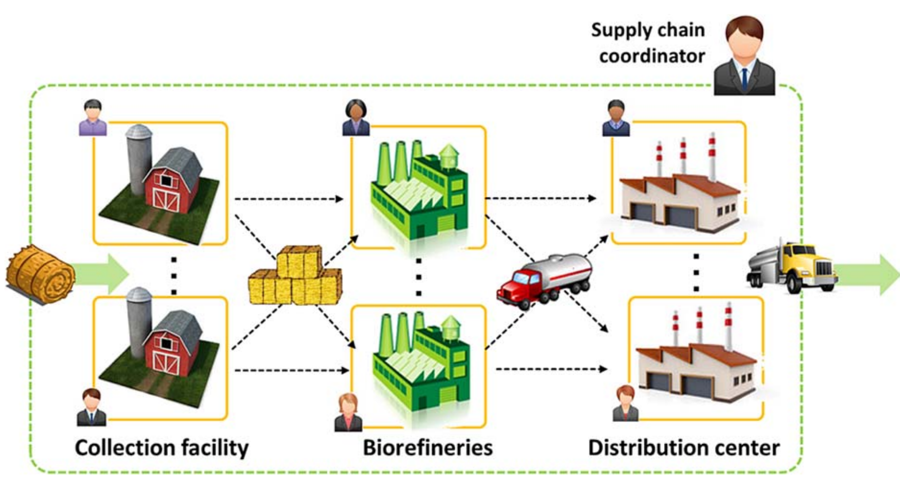

Figure 3. Superstructure of the biofuel supply chain.

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As the strategic design parameters (e.g., location, size, and/or technology of divisions) are specified, the decision variables involved in this model can be categorized as operational decisions and mechanism-related decisions. The operational decisions include:

- Timing and acquisition amount of biomass feedstock;
- Storage level and material input/output of biomass feedstock and biofuel product at biorefineries;
- Sales amount of biofuel product at distribution centers;
- Intersite transportation flows for the shipping of biomass and biofuel.
- The mechanism-related decisions include:
- Transfer price of biomass and biofuel transactions;
- Revenue sharing parameters between each pair of material supplier and receiver.

The goal of this work is to optimize the entire biomass-to-ethanol supply chain with fair profit allocation and channel coordination among the divisions and participants, which is achieved by maximizing the generalized Nash-type objective function and simultaneously optimizing the operational decisions with transfer prices and revenue sharing parameters.

Model Formulation

An MINLP formulation accounting for the transfer price and revenue sharing policy in supply chain optimization is presented in this section. Considering that the model on operational activities has been well-studied in the existing literature, we move those equations to Appendix and highlight the equations on profit allocation mechanisms in this section. A list of indices/sets, parameters, and variables is given in Notation, where all the parameters are denoted in lower-case symbols or Greek letters, and all the variables are denoted with a capitalized first letter.

Revenue conservation relationship

The revenue conservation relationship is given by the following two equations, where the revenue of biorefinery j is shared among upstream collection facilities and itself; the revenue of distribution center k is shared among upstream biorefineries and itself

$$Rvj_j = \sum_{i \in I} Rsij_{i,j} + Rsjj_j, \quad \forall j \in J \tag{7}$$

$$Rvk_k = \sum_{j \in J} Rsjk_{j,k} + Rskk_k, \quad \forall k \in K \tag{8}$$

where $Rsij_{i,j}$ is the share of collection facility i in its downstream biorefinery j's revenue; $Rsjj$ is the share of biorefinery j in its own revenue; $Rsjk_{j,k}$ is the share of biorefinery j in its downstream distribution center k's revenue; $Rskk_k$ is the share of distribution center k in its own revenue. The share ratios can be further calculated given the values of these variables. For example, the share ratio of collection facility i in biorefinery j's revenue can be calculated as $\phi_{i,j} = Rsij_{i,j}/Rvj_j$.

We introduce two auxiliary variables to indicate whether there is positive material flows in the transportation links. The binary 0–1 variable $Aij_{i,j}$ is equal to 1 if there is positive material flow from collection facility i to biorefinery j. The binary 0–1 variable $Ajk_{j,k}$ is equal to 1 if there is positive material flow from biorefinery j to distribution center k. Their relationship with transportation flow variables is given by

$$fb^L_{b,i,j,t} \cdot Aij_{i,j} \le \sum_{b \in B} \sum_{t \in T} Fbij_{b,i,j,t} \le fb^U_{b,i,j,t} \cdot Aij_{i,j}, \quad \forall i \in I, j \in J \tag{9}$$

$$fp^L_{p,j,k,t} \cdot Ajk_{j,k} \le \sum_{p \in P} \sum_{t \in T} Fpjk_{p,j,k,t} \le fp^U_{p,j,k,t} \cdot Ajk_{j,k}, \quad \forall j \in J, k \in K \tag{10}$$

where $fb^L_{b,i,j,t}$ and $fb^U_{b,i,j,t}$ are the lower and upper bounds of the transportation flow of biomass, respectively; $fp^L_{p,j,k,t}$ and $fp^U_{p,j,k,t}$ are the lower and upper bounds of the transportation flow of biofuel, respectively;$Fbij_{b,i,j,t}$ and $Fpjk_{p,j,k,t}$ represent the transportation flow between collection facilities and biorefineries and between biorefineries and distribution centers, respectively.

The revenue of biorefinery j is equal to the received transfer payment from transferring biofuels to downstream distribution centers plus its share in the downstream distribution centers' revenue. The transfer payment is equal to the amount of biofuel shipped from the biorefinery to the distribution center times the transfer price ($Tpjk_{p,j}$) set at the biorefinery. To avoid price discrimination on small buyers, we assume that the provider must offer the same price for all receivers. This relationship is modeled by

$$Rvj_j = \sum_{p \in P} \sum_{k \in K} \sum_{t \in T} Tpjk_{p,j} \cdot Fpjk_{p,j,k,t} + \sum_{k \in K} Rsjk_{j,k}, \quad \forall j \in J \tag{11}$$

The revenue of distribution center k is equal to the sales revenue from external markets, which is calculated as the sales amount ($Sld_{p,k,t}$) of all biofuels in all time periods times the biofuel prices ($ppc_{p,k}$)

$$Rvk_k = \sum_{p \in P} \sum_{t \in T} ppc_{p,k} \cdot Sld_{p,k,t}, \quad \forall k \in K \tag{12}$$

We assume that revenue can be shared between adjacent pairs of divisions and participants. However, if there is no material transfer between the pair of participants, revenue sharing between them should not be allowed. This restriction is modeled by the following two constraints

$$Rsij_{i,j} \le M \cdot Aij_{i,j}, \quad \forall i \in I, j \in J \tag{13}$$

$$Rsjk_{j,k} \le M \cdot Ajk_{j,k}, \quad \forall j \in J, k \in K \tag{14}$$

Profit and surplus

In general, the profit of a division and participant is equal to its revenue minus the expenses. The revenue of a collection facility includes the revenue shares from all its downstream biorefineries plus the transfer payments received by providing biomass to downstream biorefineries. Similar to the case of biofuel transfer, the transfer payment of biomass is equal to the amount of biomass shipped from the collection facility to the biorefinery times the transfer price of biomass ($Tpij_{b,i}$) set at the collection facility. A collection facility would offer the same transfer price for all downstream biorefineries. The expenses of a collection facility include the biomass acquisition cost. Therefore, the profit of collection facility i ($Prfi_i$) is given by

$$Prfi_i = \sum_{j \in J} Rsij_{i,j} + \sum_{b \in B} \sum_{j \in J} \sum_{t \in T} Tpij_{b,i} \cdot Fbij_{b,i,j,t} - C_i^{acquisition}, \quad \forall i \in I \tag{15}$$

The expenses of a biorefinery include the transfer payment paid to all upstream collection facilities plus the various costs on capital investment, production, transportation as well as storage. Adding the construction incentives received from the government, the profit of biorefinery j ($Prfj_j$) is given by

$$Prfj_j = Rsjj_j - \sum_{b \in B} \sum_{i \in I} \sum_{t \in T} Tpij_{b,i} \cdot Fbij_{b,i,j,t} - C_j^{capital} - C_j^{production} - C_j^{transport2J} - C_j^{storageJ} + C_j^{incentiveJ}, \quad \forall j \in J \tag{16}$$

The expenses of a distribution center include the transfer payment paid to all upstream biorefineries plus the cost of transportation. Adding the volumetric incentives, the profit of distribution center k ($Prfk_k$) is given by

$$Prfk_k = Rskk_k - \sum_{p \in P} \sum_{j \in J} \sum_{t \in T} Tpjk_{p,j} \cdot Fpjk_{p,j,k,t} - C_k^{transport2K} + C_k^{incentiveK}, \quad \forall k \in K \tag{17}$$

The surplus or payoff of collection facility i ($Supi_i$), biorefinery j ($Supj_j$), and distribution center k ($Supk_k$) is equal to their respective profit minus status quo point

$$Supi_i = Prfi_i - sqi_i, \quad \forall i \in I \tag{18}$$

$$Supj_j = Prfj_j - sqj_j, \quad \forall j \in J \tag{19}$$

$$Supk_k = Prfk_k - sqk_k, \quad \forall k \in K \tag{20}$$

where sqi_i, sqj_j, and sqk_k is the status quo point of facility i, biorefinery j, and distribution center k, respectively.

Nash-type objective function

To find the Nash bargaining solution, we maximize the generalized Nash-type objective function as given by the following equation

$$\max \prod_{i \in I} Supi_i^{\alpha} \prod_{j \in J} Supj_j^{\beta} \prod_{k \in K} Supk_k^{\gamma} \tag{21}$$

where α, β, and γ represent the negotiation power of collection facilities, biorefineries, and distribution centers, respectively.

In summary, constraints (7)–(14) model the revenue conservation relationship among participants in the biofuel supply chain; constraints (15)–(20) calculate the profit and surplus for each collection facility, biorefinery, and distribution center. In addition, the problem includes constraints (A1)–(A8), (A13), (A18)–(A20), (A22)–(A26), and (A28), which model the various operational activities, for example, acquisition, production, transportation, storage, and sales. The objective is given by Eq. 21, which maximizes the generalized Nash-type objective function. We denote the proposed problem as (P), which is formulated as a nonconvex MINLP, where bilinear terms are present in constraints (11) and (15)–(17) for calculation of the transfer payments, and the Nash-type objective function (21) is highly nonlinear and nonconvex. As this nonconvex MINLP formulation can be computationally expensive for large-scale implementations, we propose an efficient solution strategy that will be presented in the next section.

Reformulation and Solution Strategy

Discrete transfer price levels

Following the approach in the work by Gjerdrum et al.,[8,9] instead of treating the transfer price as a continuous variable, we consider a set of discrete transfer price levels ($c \in C$). This is reasonable as the setting of transfer prices is usually restricted due to administrative and policy issues in practice.

Therefore, the transfer price can be expressed by

$$Tpij_{b,i} = \sum_{c \in C} prci_{b,i,c} \cdot Dbi_{b,i,c} \forall b \in B, i \in I \tag{22}$$

$$\sum_{c \in C} Dbi_{b,i,c} = 1, \quad \forall b \in B, i \in I \tag{23}$$

where $prci_{b,i,c}$ is the prespecified transfer price level for biomass b at collection facility i at level c; $Dbi_{b,i,c}$ is the binary 0–1 variable which is equal to 1 if transfer price level c for biomass b at collection facility i is chosen. Equation 23 indicates that only one transfer price level can be chosen and Eq. 22 shows that the transfer price variable is equal to the active transfer price level.

Substituting Eq. 22 into Eqs. 15 and 16 leads to the bilinear terms ($Dbi_{b,i,c} \cdot Fbij_{b,i,j,t}$) expressed as products of a binary variable and a continuous variable. We can apply Glover's linearization scheme and introduce an auxiliary variable $Vbij_{b,i,j,t,c}$ to replace the bilinear term as shown below[45]

$$Vbij_{b,i,j,t,c} \le Fbij_{b,i,j,t}, \quad \forall b \in B, i \in I, j \in J, t \in T, c \in C \tag{24}$$

$$Vbij_{b,i,j,t,c} \le fb_{b,i,j,t}^{U} \cdot Dbi_{b,i,c}, \quad \forall b \in B, i \in I, j \in J, t \in T, c \in C \tag{25}$$

$$Vbij_{b,i,j,t,c} \ge Fbij_{b,i,j,t} - M\left(1 - Dbi_{b,i,c}\right), \quad \forall b \in B, i \in I, j \in J, t \in T, c \in C \tag{26}$$

After introducing the constraints above, Eqs. 15 and 16 can now be reformulated as

$$Prfi_i = \sum_{j \in J} Rsij_{i,j} + \sum_{b \in B} \sum_{j \in J} \sum_{t \in T} \sum_{c \in C} prci_{b,i,c} \cdot Vbij_{b,i,j,t,c} - C_i^{acquisition}, \quad \forall i \in I \tag{27}$$

$$Prfj_j = Rsjj_j - \sum_{b \in B} \sum_{i \in I} \sum_{t \in T} \sum_{c \in C} prci_{b,i,c} \cdot Vbij_{b,i,j,t,c} - C_j^{capital} - C_j^{production} - C_j^{transport2J} - C_j^{storageJ} + C_j^{incentiveJ}, \quad \forall j \in J \tag{28}$$

In this way, we have linearized the bilinear terms corresponding to the transfer payment of biomass between collection facilities and biorefineries. Similarly, we can also linearize the bilinear terms regarding the transfer payment of biofuel between biorefineries and distribution centers by introducing the following constraints

$$Tpjk_{p,j} = \sum_{c \in C} prcj_{p,j,c} \cdot Dpj_{p,j,c}, \quad \forall p \in P, j \in J \tag{29}$$

$$\sum_{c \in C} Dpj_{p,j,c} = 1, \quad \forall p \in P, j \in J \tag{30}$$

$$Vpjk_{p,j,k,t,c} \le Fpjk_{p,j,k,t}, \quad \forall p \in P, j \in J, k \in K, t \in T, c \in C \tag{31}$$

$$Vpjk_{p,j,k,t,c} \le fp_{p,j,k,t}^{U} \cdot Dpj_{p,j,c}, \quad \forall p \in P, j \in J, k \in K, t \in T, c \in C \tag{32}$$

$$Vpjk_{p,j,k,t,c} \ge Fpjk_{p,j,k,t} - M\left(1 - Dpj_{p,j,c}\right), \quad \forall p \in P, j \in J, k \in K, t \in T, c \in C \tag{33}$$

Therefore, Eqs. 11 and 17 can be reformulated as

$$Rvj_j = \sum_{p\in P}\sum_{k\in K}\sum_{t\in T}\sum_{c\in C} prcj_{p,j,c} \cdot Vpjk_{p,j,k,t,c} + \sum_{k\in K} Rsjk_{j,k}, \quad \forall j \in J \tag{34}$$

$$Prfk_k = Rskk_k - \sum_{p\in P}\sum_{j\in J}\sum_{t\in T}\sum_{c\in C} prcj_{p,j,c} \cdot Vpjk_{p,j,k,t,c} - C_k^{transport2K} + C_k^{incentiveK}, \quad \forall k \in K \tag{35}$$

Using discrete transfer price levels, the bilinear terms regarding the material transfer payment are linearized. Now, the only nonlinear term present in problem (P) is the generalized Nash-type objective function (21).

Logarithm transformation

The objective function (21) is nonlinear and nonconvex, which can make the solution of the proposed problem computationally expensive. However, as the objective function is expressed as the product of multiple exponential terms, performing the logarithm transformation on the objective function can be very helpful, as given by

$$\max \sum_{i\in I} \alpha \ln Supi_i + \sum_{j\in J} \beta \ln Supj_j + \sum_{k\in K} \gamma \ln Supk_k \tag{36}$$

We note that the natural logarithm function is monotonically increasing and the surpluses of the participants in the biofuel supply chain are strictly positive. Therefore, replacing Eq. 21 with (36) will not affect the feasible region and optimal solution of the problem. The major advantage of this logarithm transformation is that, because the natural logarithm function is concave, the objective function (36) expressed as the sum of a series of independent natural logarithm functions is also concave. After linearization of the bilinear terms on the material transfer payment, the constraints become linear, and after the logarithm transformation, the objective becomes the maximization of a concave function. Therefore, the reformulated problem becomes a convex MINLP problem where the global optimal solution can be obtained using convex MINLP solvers, which is often more efficient than solving the original nonconvex problem directly with global optimizers.

In summary, the constraints of the reformulated problem include Eqs. 7–10, 12–14, 18–20, and 22–35 regarding the revenue sharing policy and reformulation constraints as well as Eqs. A1–A8, A13, A18–A20, A22–A26, and A28 related to the various operational activities. The objective of the reformulated problem is given by Eq. 36. We denote this reformulated problem as (PR).

Branch-and-refine algorithm

In this section, we present a branch-and-refine algorithm to efficiently solve the reformulated MINLP problem (PR), which is based on the iterative solution of a series of MILP subproblems. The MILP subproblem is derived using the linear outer-approximation of the concave natural logarithm terms in objective function (36). Denote Sup_{lc} as a generic representation of the surplus of participant lc (namely, $Supi_i$, $Supj_j$ and $Supk_k$) and let $N_{lc}=\{1,2,3,...,n\}$ denote the set of grid intervals. Then, the linear outer-approximation of natural logarithm function $\ln(Sup_{lc})$ is formulated as follows

$$rSup_{lc} \le val_{lc,n} + grad_{lc,n}\left(Sup_{lc} - u_{lc,n}\right), \quad \forall lc \in \{i,j,k\}, n \in N_{lc} \tag{37}$$

where $rSup_{lc}$ is introduced as an auxiliary variable which is equal to the upper bound of the value of function $\ln(Sup_{lc})$; $u_{lc,n}$ is the grid point in the space of Sup_{lc}; $val_{lc,n}$ is the function value at grid point $u_{lc,n}$: $val_{lc,n} = \ln u_{lc,n}$; and $grad_{lc,n}$ is the gradient at grid point $u_{lc,n}$: $grad_{lc,n} = \frac{1}{u_{lc,n}}$. A graphical illustration of the outer-approximation is given in Figure 4a. We note that linear outer-approximation $rSup_{lc}$ is equal to $\ln(Sup_{lc})$ only at the grid points, while $rSup_{lc}$ is greater than $\ln(Sup_{lc})$ in the rest of the space of Sup_{lc}.

Replacing $\ln(Sup_{lc})$ with $rSup_{lc}$, the objective of the MILP subproblem is given by

$$\max \sum_{i\in I} \alpha \cdot rSupi_i + \sum_{j\in J} \beta \cdot rSupj_j + \sum_{k\in K} \gamma \cdot rSupk_k \tag{38}$$

The constraints of the MILP subproblem include all the constraints in (PR) and an additional constraint (37) for the outer-approximation. We denote this MILP subproblem as (PRL). The feasible region of (PRL) is identical to that of (PR). The optimal value of objective function (38) provides an upper bound of objective function (36). The optimal solution to (PRL) is always a feasible solution of (PR), so substituting the optimal solution of (PRL) into function (36) leads to a lower bound of the objective function (36) in (PR). We note that the finer the grid resolution is, the closer the outer-approximation is to the nonlinear objective function, but at the same time the larger the problem size is.[46–48] Based on the aforementioned lower and upper bounds, we propose a branch-and-refine algorithm that will automatically determine the propagation of grids and effectively converge in a limited number of iterations.

The procedure of the proposed branch-and-refine algorithm is given as follows and a dynamic graphical illustration is shown in Figures 4b, c.

1. Initialization
   Set iteration count $iter = 0$, lower bound $LB = -\infty$, upper bound $UB = +\infty$; set optimality tolerance to ε, and convergence tolerance to tol; set the number of grid intervals to $pnum_{lc}$ and set $N_{lc} = \{1, 2, ..., pnum_{lc}+1\}$; construct outer-approximation by setting $u_{lc,n}$, $val_{lc,n}$, and $grad_{lc,n}$.
2. Solving (PRL)
   Set $iter = iter + 1$. Solve MILP problem (PRL) to the optimality gap of ε. If infeasible, stop and conclude that problem (PR) is infeasible. If feasible, denote the optimal objective value as obj^{U} and set $UB = \min[UB, obj^{U}]$; substitute the optimal solution into objective function (36), denote the value as obj^{L}, and set $LB = \max[LB, obj^{L}]$.
3. Convergence checking
   If $gap = (UB - LB)/LB < tol$, stop and output the current solution as the optimal solution to (PR); Otherwise, go to the next step.
4. Grid propagation
   Refine the grid to improve the approximation, locate the grid interval that the optimal solution is at: $[u_{lc,\bar{n}}, u_{lc,\bar{n}+1}]$. Here are three grid propagation strategies[49]:
   a. Add a grid point right at the optimal value of Sup_{lc}: $u_{lc}^{sol} = Sup_{lc}^{*}$.
   b. Add a grid point at the middle (bisection) point $u_{lc}^{bis} = \left(u_{lc,\bar{n}} + u_{lc,\bar{n}+1}\right)/2$.
   c. Add a grid point at $u_{lc}^{wt} = w \cdot u_{lc}^{sol} + (1-w)u_{lc}^{bis}$, where parameter w can be adjusted by the user and satisfies $0 \le w \le 1$.

we employ two intervals as the starting grid with three evenly distributed grid points. Three grid propagation strategies are presented above, of which the bisection method is found to be the most efficient with the least number of iterations for this specific problem.

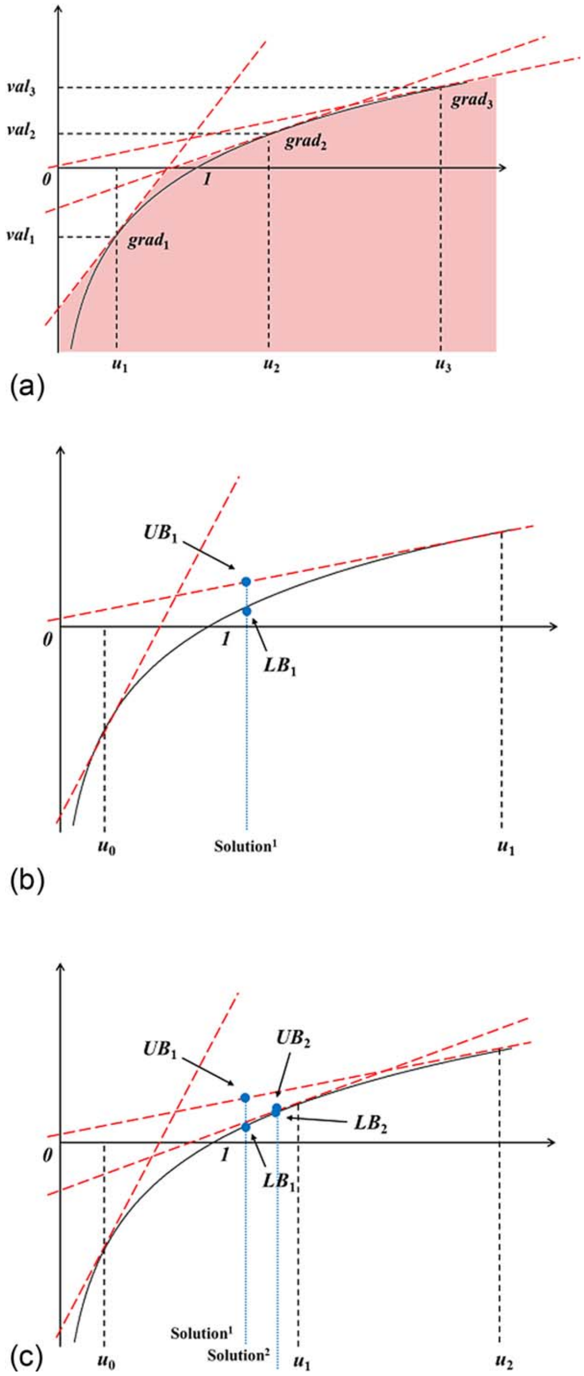

Figure 4. Illustration of the branch-and-refine algorithm.

(a) Outer-approximation; (b) solution to iteration 1; (c) solution to Iteration 2 using the bisection method. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Update $pnum_{lc}$, N_{lc}, $u_{lc,n}$, $val_{lc,n}$, and $grad_{lc,n}$. Go to step (2).

We note that the entire branch-and-refine procedure requires only an MILP solver (e.g., CPLEX). Although a nonlinear programming (NLP) solver can be used to solve the lower bounding problem in the reduced variable space, it is generally not necessary and not included in the proposed algorithm framework.[50–52] The algorithm can start with an arbitrary number of grid intervals. Unless otherwise stated, we employ two intervals as the starting grid with three evenly distributed grid points.

Illustrative Example

To demonstrate the application of the proposed modeling and solution framework, we first present a small-scale case study, which is based on a biofuel supply chain superstructure of three collection facilities, three biorefineries, and three distribution centers as shown in Figure 5a. In this work, we consider corn stover as the sole biomass feedstock. Ethanol is considered as the only biofuel product. Two types of conversion technologies are considered for biofuel production. The first one is the biochemical conversion based on dilute-acid pretreatment and enzymatic hydrolysis processes. The other one is the thermochemical pathway by indirect gasification and mixed alcohol synthesis. One year is divided into four time periods, each representing a quarter. Truck transportation is assumed as the only shipping mode. However, different transportation modes can be easily accounted for by adding an additional index to the transportation flow variables.[24]

The locations and intersite transportation distances are given in Table 1. The maximum transportation distances for biomass feedstock and biofuel product are set as 100 and 300 km, respectively. The corn stover biomass is only available in the fourth quarter. The availability of biomass

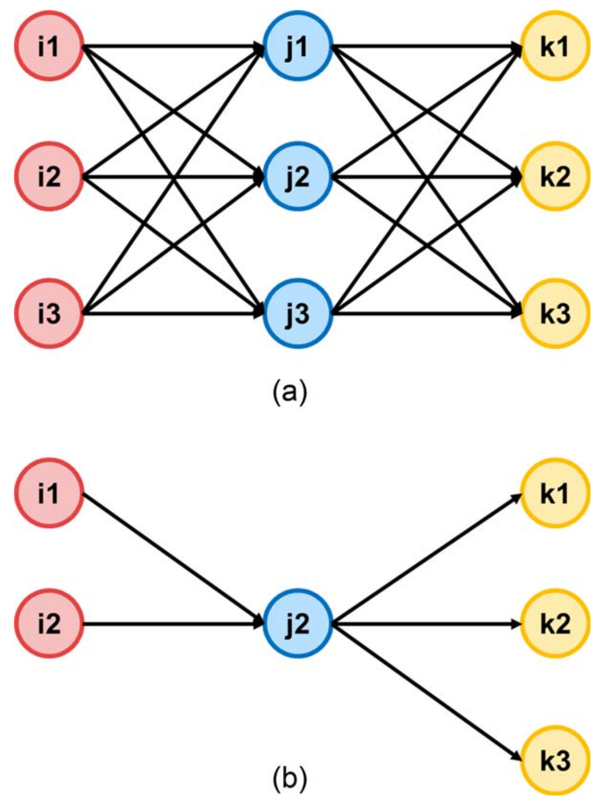

Figure 5. Biofuel supply chain network of the illustrative example.

(a) Superstructure of the supply chain; (b) optimized supply chain network. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 1. Intersite Transportation Distances (km)

	Location 1	Location 2	Location 3
Location 1	20	60	180
Location 2	60	20	80
Location 3	180	80	15

feedstock at each collection facility as well as the lower and upper bounds of biofuel demand at each distribution center are given in Table 2. The techno-economic data regarding the biochemical and thermochemical technologies are derived from the most recent technical reports provided by National Renewable Energy Laboratory and summarized in Table 3.[53,54] We consider three capacity levels for the biorefineries, namely 5–50, 50–100, and 100–150 MM gallons of ethanol/year. Note that a minimum capacity requirement of 5 MM gallons/year is imposed if a biorefinery is to be built. The effective operation time is assumed to be 24 h per day and 350 days per year. The moisture content of biomass is assumed to be 20% in weight and the deterioration rate is set to 0.5%. We set the safety period to 7 days and allow for zero utilization rates. The corn stover acquisition cost is assumed to be \$36.78 per dry ton and the same for all locations. The ethanol selling price is assumed to be \$2.2 per gallon. Both the fixed and variable transportation costs are derived from the work by Searcy et al.[55] We set the unit inventory holding cost of biomass feedstock to \$0.10/(ton·day) and ignore the inventory holding cost for ethanol. The lifetime of the biofuel supply chain project is assumed to be 15 years and an annual discount rate of 10% is considered. Incentives are not considered in this case study.

Superstructure optimization

We first perform a superstructure optimization to identify the max-profit design and the number of supply chain participants to provide input data for the profit allocation problem. We note that negotiation and profit allocation are only meaningful after the supply chain participants are determined, so we limit the scope of this work to a supply chain operations problem. The superstructure optimization problem is formulated as an MILP model (P0) involving Eqs. A1–A29, as shown in Appendix. The MILP was solved using CPLEX 12 on a PC with Intel® Core™ i5–2400 CPU @ 3.10 GHz and 8.00 GB RAM. All models and solution procedures are coded in GAMS 24.2.1. The optimality tolerance was set to 0. This MILP model consists of 18 binary variables, 226 continuous variables, and 293 constraints. As the problem size is rather small, the problem was solved within 1 CPUs.

The optimal biofuel supply chain network is shown in Figure 5b. As can be seen, the collection facilities in Location 1 and Location 2 are selected, and only one biorefinery is built in Location 2. Biochemical conversion technology is employed by the biorefinery. The annual ethanol production capacity of the biorefinery is 88.75 MM gallon. The maximum profit of the entire supply chain is \$3.58 MM per year.

Profit allocation

Case 1. Based on the optimal solution obtained above, we know that the negotiation process will involve the following supply chain participants: two collection facilities at Locations 1 and 2; one biorefinery at Location 2; and three distribution centers at Locations 1, 2, and 3. Before solving the problem (PR), we need to specify the transfer price levels for each material transaction and the negotiation-power indicator of each participant. We consider five transfer price levels evenly distributed between \$18.39 and \$73.56 per dry ton for the transaction of corn stover. The lower and upper bounds correspond to half and two times of the biomass acquisition cost, respectively. We also consider five transfer price levels evenly distributed between \$1.1 and \$2.2 per gallon for the transaction of ethanol. The lower bound corresponds to half of the biofuel selling price and the upper bound equals the selling price. In the first case, we assume all the collection facilities, biorefineries, and distribution centers have the same negotiation power, thus α, β, and γ are all set to 1.

Considering the relatively small size of the problem, DICOPT is used to directly solve the convex MINLP problem (PR) with 20 binary variables, 212 continuous variables, and 455 constraints. The optimality gap was set to 0 and the global optimal solution was returned within 1 CPUs. The optimal value of the reformulated objective, given by Eq. 36, is 38.352.

Under the revenue sharing policy, the optimized profit allocation among the supply chain participants is shown in Figure 6, indicating that the participants each would obtain a surplus of \$597 K every year. It is important to note that the overall profit of the entire supply chain in this Nash bargaining solution is also \$3.58 MM per year, which is no less than the maximum profit calculated in the superstructure optimization problem without considering the profit allocation within the supply chain. This suggests that the optimized revenue sharing policy allows the participants to achieve a unanimous agreement on profit allocation, while at the same time guaranteeing maximum economic performance of the entire supply chain. In other words, the revenue sharing policy coordinates the biofuel supply chain. The transfer prices of corn stover at both the collection facility in Locations 1 and 2 are equal to \$18.39 per dry ton, and the transfer price of ethanol at the biorefinery in Location 2 is equal to \$1.65 per gallon. The optimized revenue sharing parameters are shown in Table 4. The second column indicates the transfer prices. Starting from the third column, each cell (*row*, *col*) indicates the share of participant *row* in the revenue of participant *col*. Note that the sum of each column may not be strictly equal to 1 due to rounding errors. It is interesting to observe that the collection facilities can

Table 2. Biomass Availability and Biofuel Demand

	Biomass Availability (dry kton)				Biofuel Demand Upper Bound (MM gallon)				Biofuel Demand Lower Bound (MM gallon)			
Quarters	First	Second	Third	Fourth	First	Second	Third	Fourth	First	Second	Third	Fourth
Location 1	0	0	0	200	12.5	16.25	13.75	15	10	13	11	12
Location 2	0	0	0	1000	6.25	7.5	6.25	6.25	5	6	5	5
Location 3	0	0	0	700	1.25	1.25	1.25	1.25	1	1	1	1

Table 3. Techno-Economic Data of the Reference Biorefineries

Facility Type	Capacity (MM gallon/year)	Capital Cost (MM $)	Fixed O&M Percentage	Variable O&M Cost ($/gallon)	Yield (gallon/dry ton)
Biochemical	61.0	422.5	2.5%	0.340	79.0
Thermochemical	64.7	515.8	4.5%	−0.115[a]	67.0

[a]Negative due to co-product credits.

quote a transfer price of corn stover that is even lower than the biomass acquisition price to the biorefinery, in return for revenue share from the biorefinery, thus coordinating the supply chain.

For comparison, we have also considered several solution methods other than DICOPT for the convex MINLP problem (PR), namely BARON 12, SBB, and the proposed branch-and-refine algorithm. We use the default initialization scheme of all the solvers. The optimality gaps for solving MINLP with SBB and BARON 12 (using CONOPT 3 as NLP solver) are set to 0. The optimality gap for solving MILP subproblem (PRL) in the branch-and-refine algorithm is set to 0, and the convergence tolerance is set to 10^{-6}. The computational results are summarized in Table 5. The upper and lower bounds of each iteration in the branch-and-refine algorithm are shown in Figure 7. We can see that all the solution methods are able to solve this small-scale convex MINLP problem effectively. BARON 12 is relatively slower because it is developed as a global optimizer and involves additional routines for global considerations that are absent in local solvers such as DICOPT and SBB. The branch-and-refine algorithm solves the problem in 1 CPUs and 11 iterations, while the gap between upper and lower bounds decreases within 1% in the first three iterations. We note that due to the small size of the problem, the relative efficiency of the branch-and-refine algorithm has not been fully revealed yet.

Case 2. To explore more possibilities with the proposed modeling framework, we consider the difference in the participants' negotiation power in the second case. All the given information is the same as that in Case 1, except for the negotiation-power indicators. To account for the structural advantage of production facility, we assume that the negotiation power of the biorefinery is higher than that of the collection facilities and distribution centers. Therefore, we set $\alpha=1$, $\beta=2$, and $\gamma=1$. Again, we solved this problem directly using DICOPT. The optimal profit allocation profile among the biofuel supply chain participants is presented in Figure 8 and the corresponding revenue sharing policy is summarized in Table 6. As can be seen, because of its higher negotiation power, the biorefinery obtains double the portion ($1.02 MM per year) of the revenue in the Nash bargaining solution compared to the other biofuel supply chain participants ($512 K per year). Comparing with the revenue sharing policy in Case 1, we can observe the following major changes. First, the share of the biorefinery in Location 2 in its own revenue has increased by 1% from 88.4 to 89.5%. Second, the transfer price of corn stover at the collection facility in Location 1 becomes $32.18 per dry ton instead of $18.39 per dry ton.

Case 3. In the third case, we compare the performance of revenue sharing policy with that of a wholesale price contract. Problem (PR) can be easily modified to model the wholesale pricing mechanism, by fixing the suppliers' share of the receivers' revenue (namely, $Rsij_{i,j}$ and $Rsjk_{j,k}$) to zero. In this case, profit allocation can be achieved only by transferring payment and prohibiting revenue sharing. When only five transfer price levels are given, problem (PR) is infeasible indicating that some division will have negative surplus in this condition. Therefore, we consider more transfer price levels for the wholesale pricing mechanism. We also note that the optimal profit allocation profile is very sensitive to the specified number of transfer price levels, thus we present the results of three instances in Figure 9, with 20, 100, and 500 transfer price levels, respectively. The models were solved with the proposed branch-and-refine algorithm. The overall solution times of the three instances are 7, 30, and 2227 CPUs, respectively.

From Figure 9, we can see that the optimized profit allocation profile under wholesale contract can be very different depending on the number of transfer price levels specified. When only 20 transfer price levels are specified, the collection facility in Location 2 turns out to be the most profitable division. However, as the specified number of transfer price levels increases, the profit allocation profile evolves into that as shown in Figure 9c. In the case of 500 transfer price levels, the two collection facilities and the biorefinery have the same surplus, while the distribution centers differ in surplus due to the different level of biofuel demand.

The profit allocation profile of the instance where the transfer prices are discretized into 500 levels is considered very close to that where the transfer prices are treated as continuous variables. Comparing with the profit allocation profile under revenue sharing policy in Figure 6, we can see that the wholesale pricing contract does not evenly allocate the profit among the participants in this biofuel supply chain network, which reveals the limitation of the wholesale

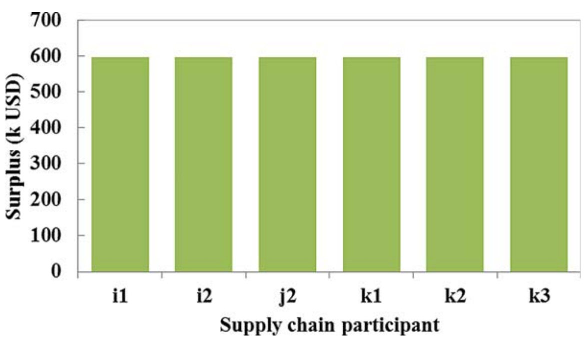

Figure 6. Profit allocation profile for Case 1.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 4. Optimized Revenue Sharing Policy for Case 1

	Transfer Price	$j2$	$k1$	$k2$	$k3$
$i1$	$18.39 per dry ton	1.6%			
$i2$	$18.39 per dry ton	10.0%			
$j2$	$1.65 per gallon	88.4%	22.4%	22.4%	17.1%
$k1$			77.6%		
$k2$				77.6%	
$k3$					82.9%

Table 5. Computational Performances of Different Solution Methods

	DICOPT	SBB	BARON 12	Branch-and-Refine
Objective value	38.352	38.352	38.352	38.352
Solution time (CPUs)	<1	<1	4	<1

pricing contract. Although the throughput of the distribution center in Location 3 is smaller compared to the other participants, the significant difference in surplus as shown in Figure 9c would still cause a certain level of dissatisfaction if a fairer profit allocation is possible. Furthermore, the revenue sharing policy is less sensitive to the specified number of transfer prices. The reason is that the revenue sharing policy possesses an additional degree of freedom to arbitrarily share the revenue among the biofuel supply chain participants.

County-Level Case Study in Illinois

In this section, we address a large-scale case study on the design and operation of a potential cellulosic biomass-to-ethanol supply chain in the state of Illinois, which has an abundant supply of corn stover. The state comprises 102 counties, of which the spatial distribution of corn stover is shown in Figure 10a. Similar to the approach in the illustrative example, we first consider a supply chain superstructure consisting of 102 potential collection facilities, 102 potential biorefineries, and 102 distribution centers. The centroid of each county is considered as the location of the facility. The transportation distances between each pair of counties are calculated using the Haversine formula.[56] It utilizes the longitude and latitude information of the centroids and takes into account the curvature of the earth and the area of the counties. Similar to that in the work by You et al.,[25] the lower bound of biofuel demand in each county in each quarter is assumed to correspond to the scenario for year 2022. According to the Renewable Fuels Standard, at least 16 billion gallons of cellulosic ethanol must be produced/consumed in the United States every year by that time.[57] Since about 5.6% of the cellulosic biomass available in the United States is in Illinois, we assume that the same portion of the 16 billion gallons will be produced/consumed in Illinois, that is, approximately 895 MM gallons per year state-wide. The

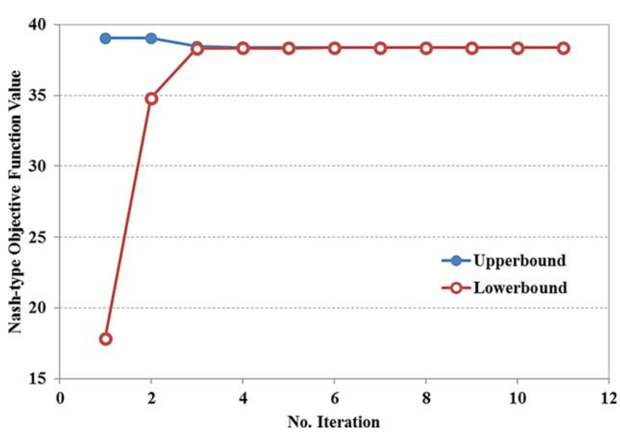

Figure 7. Iterations of the branch-and-refine algorithm.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

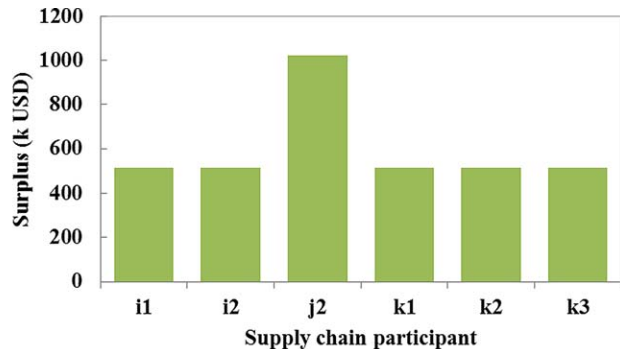

Figure 8. Optimized profit allocation profile for Case 2.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

lower bound of biofuel demand in each county is assumed to be proportional to its population (Figure 10b), based on the data from the United States Census Bureau.[58] The lower bound of biofuel demand in each quarter is assumed based on historical data from the United States Energy Information Administration database.[59] The demand upper bound is assumed to be 10% higher than the corresponding lower bound. The other input data are the same as those given in the previous illustrative example. All the computational experiments are performed on the same machine as that used in the illustrative example.

Superstructure optimization

We are given a biofuel supply chain superstructure involving 102 potential collection facilities, 102 potential biorefineries, and 102 distribution centers. To provide input data for the profit allocation problem, we first identify the optimal strategic design decisions that would maximize the overall profit of the entire supply chain. We employ the MILP model (P0) presented in Appendix for superstructure optimization, which is modified from the existing models.[21,24,25] The formulated MILP contains 612 binary variables, 37,344 continuous variables, and 10,107 constraints. Considering the large scale of the relevant MILP, the optimality tolerance is set to 0.1%.

It took 36,904 CPUs (around 10 h) for CPLEX to retrieve the optimal solution, which has a profit of $129.88 MM per year for the entire supply chain. A total of 47 collection facilities are selected, mostly located in central Illinois where the supply of corn stover is the most abundant. A total of seven biorefineries are installed as shown in Figure 10c. Six out of the seven biorefineries are built at the maximum capacity of 150 MM gallons/year to lower the unit cost, taking advantage of economies of scale. The thermochemical conversion technology option is selected by these six biorefineries. In contrast, the biorefinery in Iroquois county has an installed capacity of 86.4 MGY, where the biochemical conversion technology is chosen. This indicates that the thermochemical technology is more suitable for large-scale

Table 6. Optimized Revenue Sharing Policy for Case 2

	Transfer Price	*j*2	*k*1	*k*2	*k*3
*i*1	$32.18 per dry ton	0.6%			
*i*2	$18.39 per dry ton	10.0%			
*j*2	$1.65 per gallon	89.5%	22.4%	22.6%	17.9%
*k*1			77.5%		
*k*2				77.4%	
*k*3					82.1%

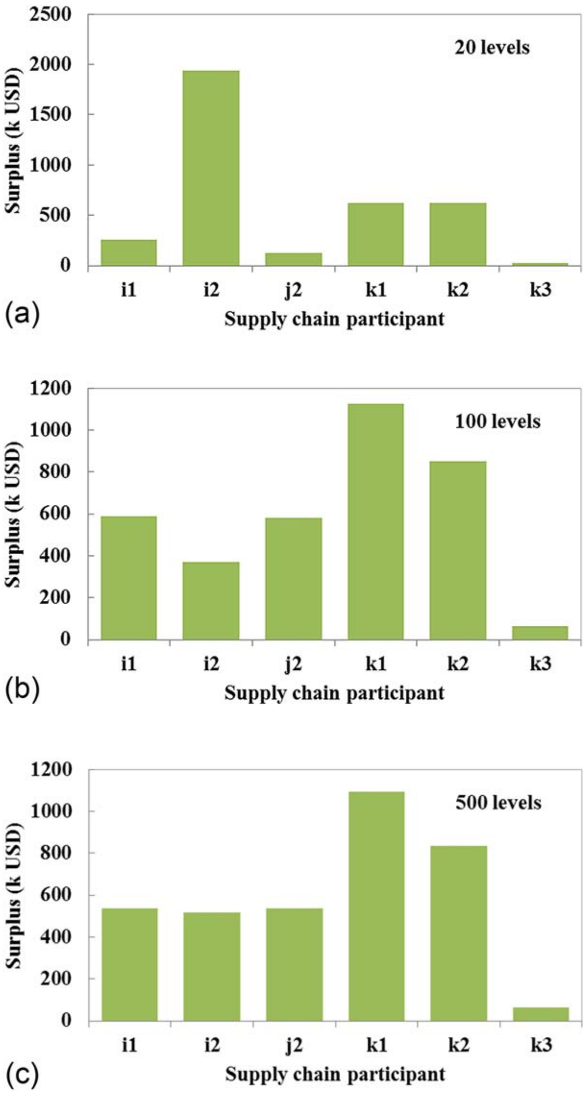

Figure 9. Optimized profit allocation profile under wholesale pricing contract with (a) 20 transfer price levels; (b) 100 transfer price levels; (c) 500 transfer price levels.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

biorefineries, whereas the biochemical technology is more suitable for small- and medium-scale biorefineries.

Profit allocation

Based on the optimal solution obtained above, we solve problem (PR) in this section to simultaneously optimize the operational decisions and revenue sharing policy in the biofuel supply chain network involving 47 collection facilities, 7 biorefineries, and 102 distribution centers. The same as in Case 1 of the illustrative example, we consider five transfer price levels for the transfer payments of biomass and biofuel. We do not differentiate the negotiation power of participants, thus setting α, β, and γ all equal to 1. The relevant MINLP model (PR) includes 1313 binary variables, 26,013 continuous variables, and 68,598 constraints. The optimal results presented below are obtained using the proposed branch-and-refine algorithm.

The optimal profit allocation profile of the state-wide biofuel supply chain in Illinois is shown by the polar area chart in Figure 11, where the red, blue, and orange bars stand for the surplus of collection facilities, biorefineries, and distribution centers, respectively. The lowest profit among the participants is \$328.44 K per year at the distribution center in Hardin County, of which the biofuel demand is also the lowest among all the counties. The highest profit is \$934.79 K per year at the collection facilities in Christian County, Fayette County, Macon County, and Peoria County, as well as the distribution centers in Greene County, Macoupin County, and Shelby County. In the Nash bargaining solution, the profit is allocated as fairly as possible. However, as the demands at some distribution centers are lower than the others by orders of magnitude (e.g., a maximum of 0.33 MM gallons/year in Stark County versus 398.64 MM gallons/year in Cook County), it is understandable to have different levels of profit among the distributors. As we move toward upstream of the supply chain, we can see that the profit allocation among collection facilities and biorefineries is relatively more even, because these divisions can receive revenue shares from their downstream divisions. The sum of the profits of all the supply chain participants is equal to \$129.88 MM per year. Thus, the supply chain is coordinated under the revenue sharing policy.

The tables of revenue sharing parameters are very large, so they are not provided in the article but are available in Supporting Information. To present the revenue sharing

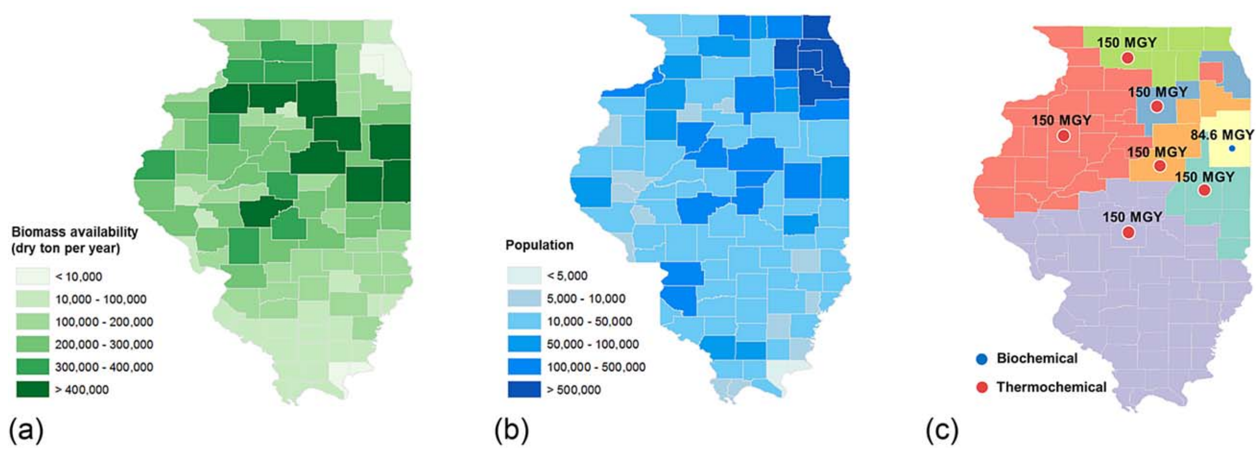

Figure 10. County-level geographical information: (a) spatial distribution of corn stover availability; (b) population density in Illinois; (c) optimal supply chain network with serving zones as the background.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

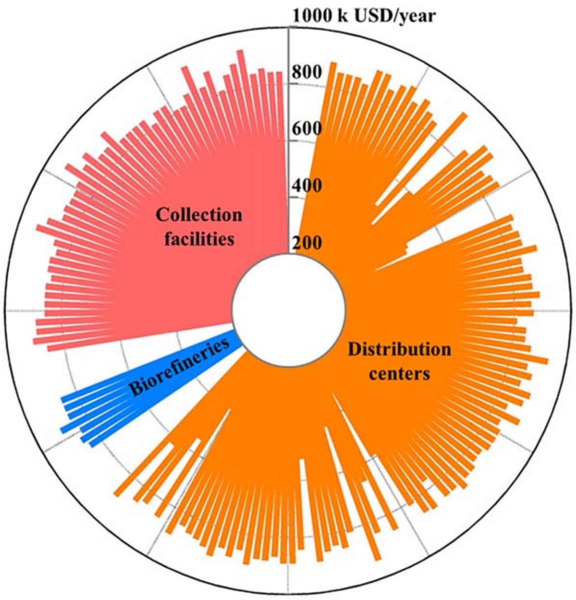

Figure 11. Profit allocation profile among the statewide biofuel supply chain participants.

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relationship among the supply chain participants, we employ the Circos plot[60] which has been successfully used and referenced in many scientific publications to visualize large datasets.[61] The revenue sharing relationships between the collection facilities and biorefineries are presented in Figure 12a, and those between the biorefineries and distribution centers are presented in Figure 12b. In general, a Circos plot visualizes the rectangular tables in a circular layout. Each band in the Circos plot represents a cell in the table, of which the two ends correspond to the relevant row and column, and the width indicates the value in the cell. Figure 12a indicates that most revenue of the seven biorefineries is kept to themselves to offset the costs and only about 10% is shared with their upstream collection facilities. The band connections show that one biorefinery is supplied by multiple collection facilities. From Figure 12b, we can see that the revenue of different distribution centers vary significantly due to the very different level of biofuel demand in the counties across Illinois. The large distribution centers keep slightly more than 50% of the revenue to themselves and share the rest with upstream biorefineries. Whereas, for those distribution centers that have less revenue, they tend to keep a larger portion of the revenue to themselves or even choose not to share their revenue.

The service zones of each biorefinery are presented in Figure 10c. In cases that a distribution center is supplied by multiple biorefineries, it is considered in the service zone of its major supplier. As can be seen, the southern region is supplied by the biorefinery in Christian County, and the northwestern region is supplied by the biorefinery in Knox County. The remaining five biorefineries are installed to serve the northeastern region, as that is the most densely populated area in Illinois. It is interesting to see that DuPage County in the Chicago area is primarily supplied by the biorefinery in Knox County in the northwest. The major reason for this biorefinery to serve such a remote distribution center might be to collect the high sales revenue in DuPage County in order to offset its costs and maintain a fair amount of profit. We present the inventory levels of biomass feedstock and biofuel product at each biorefinery in each quarter, respectively, in Figures 13a, b. As can be seen, the inventory level of corn stover coincides with the seasonal availability of biomass supply. The inventory of corn stover reaches its peak in the fourth quarter, when the harvesting time window for corn is open in the Midwest. The corn stover is then stored for ethanol production throughout the rest of the year. The inventory at the biorefinery in Iroquois County is lower than the others because of its smaller process capacity. In contrast, there seems no pattern for the inventory level of bioethanol. However, we note that the optimal tactics tend to convert as much biomass as possible in each quarter (e.g., operating at full capacity), as the transportation and storage costs of ethanol are much lower than that of corn stover. Therefore, if the production level exceeds the demand in a certain quarter, surplus of ethanol can be observed in the

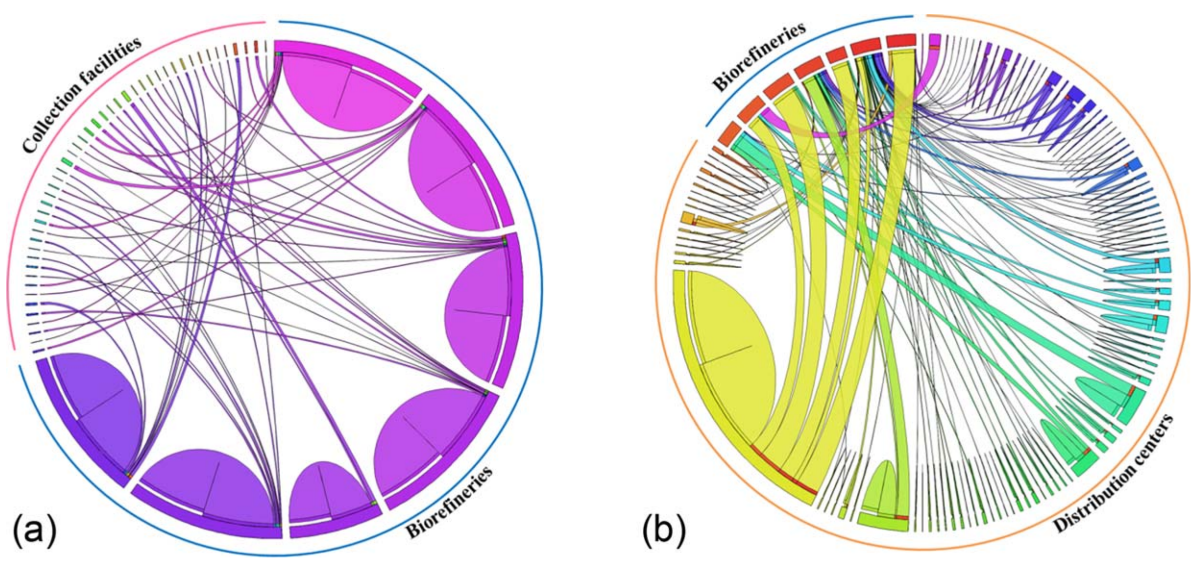

Figure 12. Revenue sharing relationship between (a) the collection facilities and biorefineries; (b) the biorefineries and the distribution centers.

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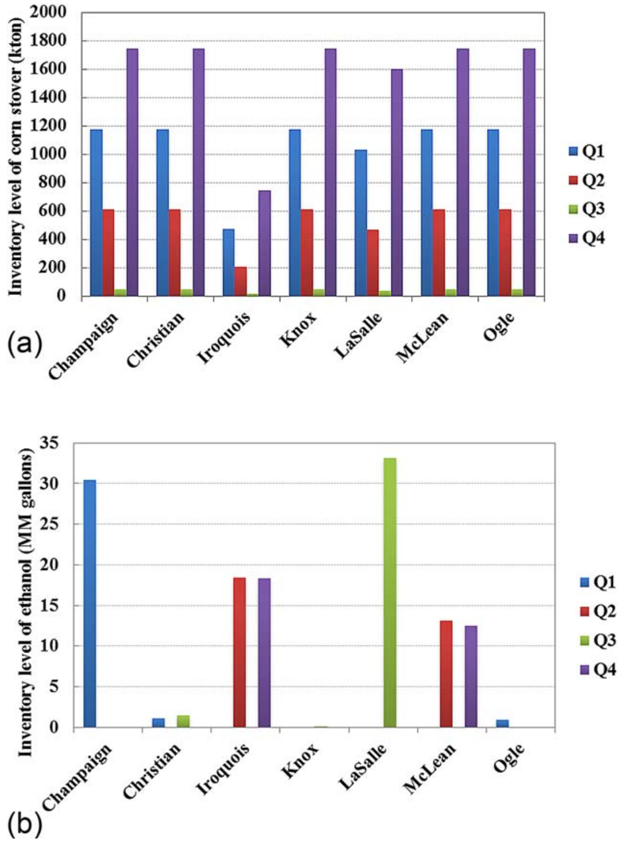

Figure 13. Inventory profile of (a) biomass feedstock and (b) biofuel product.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

inventory profile, which can be stored to compensate the deficit in demand in other quarters.

The cost breakdown is shown in Figure 14, which demonstrates the contributions of different supply chain activities and operations to the biofuel cost. Capital investment accounts for the largest portion of the biofuel cost, equaling 36%. The second largest component is the biomass acquisition cost, which accounts for slightly more than one quarter of the biofuel cost. The fixed and variable O&M costs together share 8% of the biofuel cost. The transportation cost accounts for a significant portion (19%) of the biofuel cost, mainly due to the low energy density of biomass feedstock. Storage accounts for 10% of the biofuel cost. Dividing the total supply chain cost by the total quantity of ethanol sold to the markets, we obtain an average unit cost for biofuel product at $2.07 per gallon, which indicates a margin of $0.13 per gallon at the selling price of $2.20 per gallon.

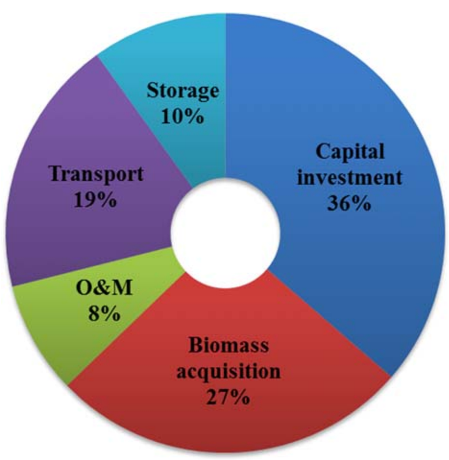

Figure 14. Cost breakdown of the optimal biofuel supply chain.

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Table 7. Computational Performances of Different Solution Methods

	DICOPT	SBB	BARON 12	Branch-and-Refine
Objective value	1031.9	–	–	1046.9
Solution time (CPUs)	36,000[a]	2066[b]	36,000[c]	11,788

[a]Exceeding specified time limit 36,000 seconds (10 hours) and suboptimal solution returned.
[b]Solver failure encountered.
[c]No feasible solution returned within 36,000 seconds (10 hours).

To compare the performances of different solution methods on this large-scale MINLP problem, we present in Table 7 the computational results of DICOPT, SBB, BARON 12, and the proposed branch-and-refine algorithm. The optimality gap for all the solvers, including CPLEX for the branch-and-refine algorithm, is set as 0.1%. The convergence tolerance for the branch-and-refine algorithm is set to 10^{-4}. The computation time limit is set as 36,000 s, that is, 10 h.

From Table 7, we can see that only the proposed branch-and-refine algorithm successfully returned the optimal solution within the computation time limit. It took a total of seven iterations and 11,788 CPUs (~3.3 h) to converge to the specified optimality tolerance, and the upper bound and lower bounds of each iteration are shown in Figure 15. The gap between upper and lower bounds decreases within 1% in the first three iterations. DICOPT returned a suboptimal solution within the 10-hour limit. We note that although DICOPT also employs outer-approximation, it is less efficient than the proposed branch-and-refine algorithm because NLP problems need to be solved during the solution process of DICOPT. SBB terminated during the solution process due to solver failure. BARON 12 failed to obtain a feasible solution within the computation time limit. Therefore, the proposed branch-and-refine algorithm is more efficient than

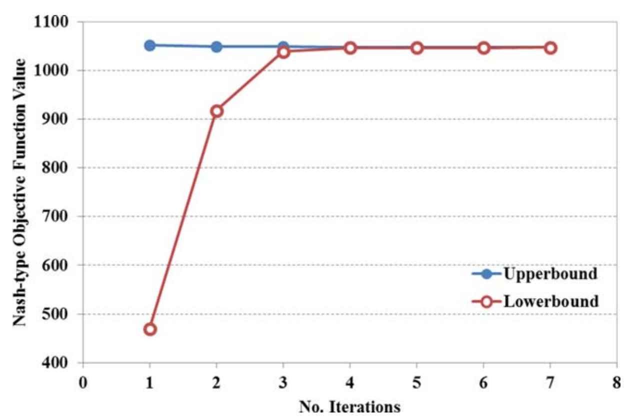

Figure 15. Iterations of the branch-and-refine algorithm.

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DICOPT, SBB, and Baron 12 for solving this class of large-scale problems.

Conclusions

A novel MINLP model was proposed for the optimization of biofuel supply chains considering the issue of fair profit allocation. We employed the revenue sharing policy, which is able to arbitrarily distribute the profit and coordinate the supply chain. The generalized Nash-type objective function was proposed to address the difference in negotiation power among supply chain participants. The operational decisions and revenue sharing contract parameters were simultaneously optimized. The proposed problem was formulated as a nonconvex MINLP model, which were efficiently solved using the logarithm transformation and branch-and-refine algorithm based on the piecewise linear outer-approximation. Applications were illustrated by a small-scale illustrative example and a large-scale state-wide county-level case study for a potential biomass-to-ethanol supply chain in Illinois. Specifically for the latter case study, results showed that a maximum profit of the entire supply chain of \$129.88 MM per year can be achieved under the coordination of the revenue sharing policy, corresponding to an average ethanol production cost of \$2.07 per gallon. The proposed branch-and-refine algorithm was shown to be much more efficient in solving the large-scale profit allocation problems compared to the general-purpose MINLP solvers.

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Notation

Sets/Indices

B = set of biomass indexed by b
C = set of transfer price levels indexed by c
I = set of collection facilities indexed by i
J = set of potential biorefineries indexed by j
K = set of distribution centers indexed by k
P = set of biofuel products indexed by p
Q = set of conversion technologies indexed by q
R = set of capacity levels of biorefineries indexed by r
T = set of time periods

Parameters

$av_{b,i,t}$ = available amount of biomass b at collection facility i in time period t
$cac_{b,i,t}$ = acquisition cost of biomass b at collection facility i in time period t
$cfj_{j,q}$ = fixed O&M cost of biorefinery j as a percentage of the capital investment
$cld_{k,p,t}$ = distribution cost of product p at distribution center k in time period t
$cpj_{j,q}$ = variable production cost at biorefinery j with technology q
$crj_{q,r}$ = reference capital cost corresponding to technology q and capacity level r
$dfcb_b$ = fixed transportation cost of biomass b
$dfcp_p$ = fixed transportation cost of biofuel p
$dm^{L(U)}_{p,k,t}$ = lower (upper) bound of demand for biofuel p at distribution center k in time period t
$dsij_{i,j}$ = transportation distance from collection facility i to biorefinery j
$dsjk_{j,k}$ = transportation distance from biorefinery j to distribution center k
$dvcb_b$ = variable transportation cost of biomass b
$dvcp_p$ = variable transportation cost of product p
$fb^{L(U)}_{b,i,j,t}$ = lower (upper) bound of transportation flow of biomass b from collection facility i to biorefinery j in time period t
$fp^{L(U)}_{p,j,k,t}$ = lower (upper) bound of transportation flow of biofuel p from biorefinery j to distribution center k in time period t
h_t = duration of time period t
$hbj_{b,j,t}$ = unit inventory holding cost of biomass b at biorefinery j in time period t
$hpj_{p,j,t}$ = unit inventory holding cost of biofuel p at biorefinery j in time period t
$incm$ = maximum amount of incentive allowed for construction of a biorefinery
$incp$ = maximum incentive allowed as a percentage of the construction investment
$incv_p$ = volumetric incentive for sales of biofuel p
ir = discount rate
lt = lifetime of the project
mc_b = moisture content of biomass b
$mdb_{b,t}$ = maximum transportation distance allowed for biomass b in time period t
$mdp_{p,t}$ = maximum transportation distance allowed for biofuel p in time period t
nj = maximum number of biorefineries allowed to be built
$ppc_{p,k}$ = market price of product p at distribution center k
$prci_{b,i,c}$ = transfer price level c of biomass b at collection facility i
$prcj_{p,j,c}$ = transfer price level c of biofuel p at biorefinery j
$prj_{q,r}$ = reference capacity corresponding to technology q and capacity level r
rt = effective operating time during a year
$sfb_{j,t}$ = safety period of biomass storage at biorefinery j in time period t
sqi_i = status quo point of collection facility i
sqj_j = status quo point of biorefinery j
sqk_k = status quo point of distribution center k
$wcij_{i,j,t}$ = flow capacity of transportation link from collection facility i to biorefinery j in time period t

Greek parameters

α = negotiation-power indicator of collection facilities
β = negotiation-power indicator of biorefineries
γ = negotiation-power indicator of distribution centers
$\delta_{b,t}$ = deterioration rate of biomass b in time period t
$\theta_{j,q}$ = minimum utilization rate of biorefinery j with technology q
φ_p = capacity factor of biofuel product p
$\chi_{b,p,q}$ = conversion parameter from biomass b to product p using technology q

Binary variables

$Aij_{i,j}$ = 1 if there is positive flow from collection facility i to biorefinery j; 0 otherwise
$Ajk_{j,k}$ = 1 if there is positive flow from biorefinery j to distribution center k; 0 otherwise
$Dbi_{b,i,c}$ = 1 if transfer price level c for biomass b is chosen at collection facility i; 0 otherwise
$Dpj_{p,j,c}$ = 1 if transfer price level c for product p is chosen at biorefinery j; 0 otherwise
$X_{j,q,r}$ = 1 if biorefinery j with technology q and capacity level r is installed; 0 otherwise

Nonnegative continuous variables

$Bmp_{b,i,t}$ = amount of biomass b purchased at collection facility i in time period t
$C^{(cat)}_{(fac)}$ = cost or incentive at facility (fac) in category (cat)
$Capj_{j,q}$ = capacity of biorefinery j with technology q
$Clvj_{j,q,r}$ = auxiliary variable for capacity of biorefinery j with technology q and capacity level r
$Fbij_{b,i,j,t}$ = amount of biomass b shipped from collection facility i to biorefinery j in time period t
$Fpjk_{p,j,k,t}$ = amount of biofuel p shipped from biorefinery j to distribution center k in time period t
Inc_j = incentives received for the construction of biorefinery j
Inv_j = capital investment for building biorefinery j
Opr_j = fixed O&M cost of biorefinery j
$Prfi_i$ = profit of collection facility i
$Prfj_j$ = profit of biorefinery j

$Prfk_k$ = profit of distribution center k
$Rsij_{i,j}$ = share of collection facility i in the revenue of biorefinery j
$Rsjj_j$ = share of biorefinery j in its own revenue
$Rsjk_{j,k}$ = share of biorefinery j in the revenue of distribution center k
$Rskk_k$ = share of distribution center k in its own revenue
Rvj_j = revenue of biorefinery j
Rvk_k = revenue of distribution center k
$Sbj_{b,j,t}$ = inventory of biomass b at biorefinery j at the end of time period t
$Sld_{p,k,t}$ = sales amount of product p at distribution center k in time period t
$Spj_{p,j,t}$ = inventory of product p at biorefinery j at the end of time period t
$Supi_i$ = surplus of collection facility i
$Supj$ = surplus of biorefinery j
$Supk_k$ = surplus of distribution center k
$Tpij_{b,i}$ = transfer price of biomass b at collection facility i
$Tpjk_{p,j}$ = transfer price of product p at biorefinery j
$Vbij_{b,i,j,t,c}$ = auxiliary variable for transfer payment between collection facility i and biorefinery j
$Vpjk_{p,j,k,t,c}$ = auxiliary variable for transfer payment between biorefinery j and distribution center k
$Wbj_{b,j,q,t}$ = amount of biomass b consumed at biorefinery j via technology q in time period t
$Wpj_{p,j,q,t}$ = amount of product p produced at biorefinery j via technology q in time period t

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Appendix

Superstructure optimization problem

We present the superstructure optimization problem (P0) in this section. The solution of problem (P0) is considered as a preprocessing step, which provides input data (e.g., supply chain design and number of participants) for the profit allocation problem (P) or (PR). If a supply chain design is prespecified, the step of superstructure optimization can be skipped.

Constraints (A1) and (A2) model the biomass feedstock supply system, which accounts for the seasonal nature in biomass availability. Constraints (A3)–(A17) model the construction and operation of the biorefineries as well as the conversion from biomass feedstock to biofuel product. Constraint (A18)–(A20) model the product distribution system and sales of biofuel. Equations A21–A28 calculate the various costs and incentives associated with each collection facility, biorefinery, and distribution center. The objective of this superstructure optimization problem is given by Eq. A29, which maximizes the overall profit of the entire supply chain.

Biomass Feedstock Supply System. The total amount of biomass b purchased at collection facility i in time period t ($Bmp_{b,i,t}$) cannot exceed its available amount ($av_{b,i,t}$). We note that different values of parameter $av_{b,i,t}$ can reflect factors such as seasonality, harvesting windows, and geographical availability. Unless otherwise specified, all the weight-related biomass quantities are in terms of dry weight

$$Bmp_{b,i,t} \le av_{b,i,t}, \quad \forall b \in B, i \in I, t \in T \tag{A1}$$

The total purchased amount of biomass b at collection facility i in time period t is all shipped to downstream biorefineries for further processing

$$Bmp_{b,i,t} = \sum_{j \in J} Fbij_{b,i,j,t}, \quad \forall b \in B, i \in I, t \in T \tag{A2}$$

where $Fbij_{b,i,j,t}$ is the amount of biomass b shipped from collection facility i to biorefinery j in time period t.

Biomass-to-Ethanol Refining System. The amount of biomass shipped between collection facilities and biorefineries is limited by the capacity of the transportation link ($wcij_{i,j,t}$). Because biomass feedstocks have not been dried during transportation, we should take the moisture content (mc_b) into account. Thus, the shipping capacity constraint is given by

$$\sum_{b \in B} \frac{Fbij_{b,i,j,t}}{1-mc_b} \le wcij_{i,j,t}, \quad \forall i \in I, j \in J, t \in T \tag{A3}$$

We consider a maximum transportation distance for the shipping of biomass feedstocks, because long-distance transportation of biomass feedstocks is not economically feasible due to their low energy density. The relationship is given by

$$Fbij_{b,i,j,t} = 0, \quad \forall b \in B, i \in I, j \in J, t \in T | dsij_{i,j} > mdb_{b,t} \tag{A4}$$

where $dsij_{i,j}$ is the transportation distance from collection facility i to biorefinery j; $mdb_{b,t}$ is the maximum transportation distance allowed for the shipping of biomass b in time period t.

The mass balance relationship for biomass feedstocks at biorefineries is given by the following equation. The inventory level of biomass b at biorefinery j at the end of time period t ($Sbj_{b,j,t}$) is equal to the inventory level at the end of the previous time period after accounting for the deterioration of biomass plus the total amount of biomass b shipped to biorefinery j from upstream collection facilities in time period t minus the total amount of biomass consumed for biofuel production in time period t.

$$\begin{aligned} Sbj_{b,j,t} = (1-\delta_{b,t}) Sbj_{b,j,t--1} + \sum_{i \in I} Fbij_{b,i,j,t} \\ - \sum_{q \in Q} Wbj_{b,j,q,t}, \quad \forall b \in B, j \in J, t \in T \end{aligned} \tag{A5}$$

where $\delta_{b,t}$ is the deterioration rate of biomass b in time period t; $Wbj_{b,j,q,t}$ is the amount of biomass b consumed at biorefinery j using conversion technology q in time period t. Note that we assume cyclic planning in this model. For instance, if t is the fourth quarter then $t--1$ is the third quarter, while if t is the first quarter then $t--1$ is the fourth quarter.

To guarantee continuous biofuel production, we assume that a certain amount of safety inventory of biomass feedstocks should be kept at biorefineries to hedge against potential supply disruptions. The level of safety stock can be empirically determined by the safety period ($sfb_{j,t}$) and material consumption rate. This relationship is modeled by the following constraint

$$Sbj_{b,j,t} \geq \frac{sfb_{j,t}}{h_t} \sum_{q \in Q} Wbj_{b,j,q,t}, \quad \forall b \in B, j \in J, t \in T \qquad \text{(A6)}$$

where h_t is the duration of time period t.

The mass balance relationship for biofuel product p at biorefinery j in time period t is given by the equation below. The inventory level of biofuel p at biorefinery j at the end of time period t ($Spj_{p,j,t}$) is equal to the inventory level at the end of the previous time period plus the total amount of biofuel produced at biorefinery j in time period t minus the total amount of biofuel shipped to downstream distribution centers

$$Spj_{p,j,t} = Spj_{p,j,t--1} + \sum_{q \in Q} Wpj_{p,j,q,t} - \sum_{k \in K} Fpjk_{p,j,k,t}, \quad \forall p \in P, j \in J, t \in T \qquad \text{(A7)}$$

where $Wpj_{p,j,q,t}$ is the amount of biofuel p produced via technology q at biorefinery j in time period t; $Fpjk_{p,j,k,t}$ is the amount of biofuel p shipped from biorefinery j to distribution center k in time period t. Here, we ignore the loss of biofuel during storage.

The relationship between the amount of ethanol produced at each biorefinery in each time period and the amount of biomass feedstock consumed is given by the following equation

$$Wpj_{p,j,q,t} = \sum_{b \in B} \chi_{b,p,q} \cdot Wbj_{b,j,q,t}, \quad \forall p \in P, j \in J, q \in Q, t \in T \qquad \text{(A8)}$$

where $\chi_{b,p,q}$ is a linear conversion factor, regarding the conversion from biomass b to biofuel p using technology q.

The following constraint states that at most one technology and one capacity level can be chosen at a certain biorefinery

$$\sum_{q \in Q} \sum_{r \in R} X_{j,q,r} \leq 1, \quad \forall j \in J \qquad \text{(A9)}$$

where $X_{j,q,r}$ is a binary 0–1 variable which is equal to 1 if biorefinery j with technology q and capacity level r is built; 0 otherwise.

Due to policy and budget considerations, there may be restrictions on the total number of biorefineries to be installed. This relationship is modeled by

$$\sum_{j \in J} \sum_{q \in Q} \sum_{r \in R} X_{j,q,r} \leq nj \qquad \text{(A10)}$$

where nj is the maximum number of biorefineries allowed to be built.

The annual capacity of biorefinery, in terms of the total amount of ethanol produced in a year, is defined according to the upper and lower bounds for each capacity level

$$prj_{q,r-1} \cdot X_{j,q,r} \leq Clvj_{j,q,r} \leq prj_{q,r} \cdot X_{j,q,r}, \quad \forall j \in J, q \in Q, r \in R \qquad \text{(A11)}$$

where $prj_{q,r}$ is the upper bound of the biofuel production capacity with capacity level r; $Clvj_{j,q,r}$ is an auxiliary variable for the capacity of biorefinery j with technology q and capacity level r.

The installed capacity of biorefinery j with technology q ($Capj_{j,q}$) is equal to the summation of auxiliary capacity variables over all the capacity levels, as given by the following equation

$$Capj_{j,q} = \sum_{r \in R} Clvj_{j,q,r}, \quad \forall j \in J, q \in Q \qquad \text{(A12)}$$

The biofuel production amount in biorefinery j with conversion technology q in time period t cannot exceed the annual production capacity multiplies the duration of the time period divided by the effective production time of a year (rt). Conversely, there is a minimum utilization rate ($\theta_{j,q}$) of the biorefinery, which bounds the biofuel production from below

$$\theta_{j,q} \frac{h_t}{rt} Capj_{j,q} \leq \sum_{p \in P} \varphi_p \cdot Wpj_{p,j,q,t} \leq \frac{h_t}{rt} Capj_{j,q}, \quad \forall j \in J, q \in Q, t \in T \qquad \text{(A13)}$$

where φ_p is the capacity factor of biofuel p, which is useful when multiple products are involved.

We capture the economies of scale in capital investment of installing biorefinery j (Inv_j) using the interpolated piecewise linear function given by

$$Inv_j = \sum_{q \in Q} \sum_{r \in R} \left[crj_{q,r-1} \cdot X_{j,q,r} + \left(Clvj_{j,q,r} - prj_{q,r-1} \cdot X_{j,q,r} \right) \left(\frac{crj_{q,r} - crj_{q,r-1}}{prj_{q,r} - prj_{q,r-1}} \right) \right], \quad \forall j \in J \qquad \text{(A14)}$$

where $crj_{q,r}$ is the reference capital investment for building biorefinery with technology q at the capacity of $prj_{q,r}$.

The fixed O&M cost at biorefinery j (Opr_j) as a certain percentage ($cfj_{j,q}$) of the construction investment is given by

$$Opr_j = \sum_{q \in Q} cfj_{j,q} \sum_{r \in R} \left[crj_{q,r-1} \cdot X_{j,q,r} + \left(Clvj_{q,r} - prj_{q,r-1} \cdot X_{j,q,r} \right) \left(\frac{crj_{q,r} - crj_{q,r-1}}{prj_{q,r} - prj_{q,r-1}} \right) \right], \quad \forall j \in J \qquad \text{(A15)}$$

The total incentives received for the construction of biorefinery j (Inc_j) cannot exceed the maximum allowable amount ($incm$) and cannot be greater than a certain percentage of the construction investment ($incp$). This relationship is modeled by the following two constraints

$$Inc_j \leq incm \sum_{q \in Q} \sum_{r \in R} X_{j,q,r}, \quad \forall j \in J \qquad \text{(A16)}$$

$$Inc_j \leq incp \cdot Inv_j, \quad \forall j \in J \qquad \text{(A17)}$$

Biofuel Distribution System. All the biofuel p received at distribution center k in time period t from upstream biorefineries is distributed and sold in the same region and time period

$$\sum_{j \in J} Fpjk_{p,j,k,t} = Sld_{p,k,t}, \quad \forall p \in P, k \in K, t \in T \qquad \text{(A18)}$$

where $Sld_{p,k,t}$ is the amount of biofuel p sold in distribution center k in time period t.

Similar to that of biomass transportation, we also consider a maximum transportation distance for the shipping of biofuel ($mdp_{p,t}$). However, the maximum transportation distance of biofuel products is often much larger than that of biomass feedstock, due to the improved energy density and stability

$$Fpjk_{p,j,k,t}=0, \quad \forall p \in P, j \in J, k \in K, t \in T | dsjk_{j,k} > mdp_{p,t} \tag{A19}$$

The amount of biofuel p sold in distribution center k in time period t should be within the demand upper bound ($dm^U_{p,k,t}$) and lower bound ($dm^L_{p,k,t}$)

$$dm^L_{p,k,t} \le Sld_{p,k,t} \le dm^U_{p,k,t}, \quad \forall p \in P, k \in K, t \in T \tag{A20}$$

Costs and Incentives. The annualized capital cost of biorefinery j ($C_j^{capital}$) is equal to the construction capital investment times the annuity

$$C_j^{capital} = \frac{ir}{1-(1+ir)^{-lt}} Inv_j, \quad \forall j \in J \tag{A21}$$

where ir is the discount rate; lt is the lifetime of the project in terms of years.

The biomass acquisition cost at collection facility i ($C_i^{acquisition}$) is equal to the biomass purchasing amount times the acquisition prices ($cac_{b,i,t}$), which covers the farmer premium as well as the machine and labor expenses for biomass collection

$$C_i^{acquisition} = \sum_{b \in B} \sum_{t \in T} cac_{b,i,t} \cdot Bmp_{b,i,t}, \quad \forall i \in I \tag{A22}$$

The production cost at biorefinery j consists of two components, namely fixed O&M cost and variable O&M cost. The fixed O&M cost is calculated in Eq. A15, while the variable O&M cost is proportional to production amount of biofuel, which accounts for expenses of utility, consumables, and so forth

$$C_j^{production} = Opr_j + \sum_{p \in P} \sum_{q \in Q} \sum_{t \in T} cpj_{j,q} \cdot \varphi_p \cdot Wpj_{p,j,q,t}, \quad \forall j \in J \tag{A23}$$

where $cpj_{j,q}$ is the cost factor regarding biorefinery j with technology q.

We assume that the transportation cost is afforded by the receiver of materials. Therefore, biorefinery j is responsible for the biomass shipping cost from all upstream collection facilities to itself ($C_j^{transport2J}$); and distribution center k is responsible for the biofuel shipping cost from all upstream biorefineries to itself ($C_k^{transport2K}$). We consider two types of transportation cost. The fixed transportation cost is independent of the shipping distance (e.g., loading, unloading). The variable transportation cost is proportional to the shipping distance (e.g., fuel usage). This relationship is modeled by the following two equations

$$C_j^{transport2J} = \sum_{b \in B} \sum_{i \in I} \sum_{t \in T} \left(dfcb_b + dvcb_b \cdot dsij_{i,j} \right) Fbij_{b,i,j,t}, \quad \forall j \in J \tag{A24}$$

$$C_k^{transport2K} = \sum_{p \in P} \sum_{j \in J} \sum_{t \in T} \left(dfcp_p + dvcp_p \cdot dsjk_{j,k} \right) Fpjk_{p,j,k,t}, \quad \forall k \in K \tag{A25}$$

where $dfcb_b$ and $dvcb_b$ is the fixed and variable transportation cost for biomass b, respectively; $dfcp_p$ and $dvcp_p$ is the fixed and variable transportation cost for biofuel p, respectively.

The storage cost at biorefinery j ($C_j^{storageJ}$) includes the inventory holding cost for both biomass feedstocks and biofuel products as shown below

$$\begin{aligned} C_j^{storageJ} = & \sum_{b \in B} \sum_{t \in T} h_t \cdot hbj_{b,j,t} \cdot Sbj_{b,j,t} \\ & + \sum_{p \in P} \sum_{t \in T} h_t \cdot hpj_{p,j,t} \cdot Spj_{p,j,t}, \quad \forall j \in J \end{aligned} \tag{A26}$$

where $hbj_{b,j,t}$ and $hpj_{p,j,t}$ is the unit inventory holding cost at biorefinery j in time period t for biomass b and biofuel p, respectively.

The annualized construction incentive for building biorefinery j ($C_j^{incentiveJ}$) is equal to the total amount of construction incentive received times the annuity

$$C_j^{incentiveJ} = \frac{ir}{1-(1+ir)^{-lt}} Inc_j, \quad \forall j \in J \tag{A27}$$

The volumetric incentive for selling biofuels at distribution center k ($C_k^{incentiveK}$) is equal to the sales amount of all biofuels times their respective volumetric incentive ($incv_p$)

$$C_k^{incentiveK} = \sum_{p \in P} \sum_{t \in T} incv_p \cdot Sld_{p,k,t}, \quad \forall k \in K \tag{A28}$$

Objective Function of Superstructure Optimization Problem. The total profit of the entire biofuel supply chain is equal to the biofuel sales revenue at all the distribution centers and in all the time periods minus the various costs associated with activities at collection facilities, biorefineries, and distribution centers

$$\begin{aligned} \max & \sum_{k \in K} \sum_{p \in P} \sum_{t \in T} ppc_{p,k} \cdot Sld_{p,k,t} - \sum_{i \in I} C_i^{acquisition} \\ & - \sum_{k \in K} \left(C_k^{transport2K} - C_k^{incentiveK} \right) \\ & - \sum_{j \in J} \left(C_j^{capital} + C_j^{production} + C_j^{transport2J} + C_j^{storageJ} - C_j^{incentiveJ} \right) \end{aligned} \tag{A29}$$

As can be seen, the superstructure optimization problem is formulated as an MILP model, where the constraints and objective function are all linear. Binary 0–1 variables are included to determine the location, technology, and capacity level of biorefineries. By solving problem (P0), we can obtain the optimal supply chain structure and number of participants in the negotiation process, which serve as the basis for the profit allocation problem (P) or (PR).

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