Game-theoretic modeling and optimization of multi-echelon supply chain design and operation under Stackelberg game and market equilibrium

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A B S T R A C T

We propose a bilevel mixed-integer nonlinear programming (MINLP) model for the optimal design and planning of non-cooperative supply chains from the manufacturer’s perspective. Interactions among the supply chain participants are captured through a single-leader–multiple-follower Stackelberg game under the generalized Nash equilibrium assumption. Given a three-echelon superstructure, the lead manufacturer in the middle echelon first optimizes its design and operational decisions, including facility location, sizing, and technology selection, material input/output and price setting. The following suppliers and customers in the upstream and downstream then optimize their transactions with the manufacturer to maximize their individual profits. By replacing the lower level linear programs with their KKT conditions, we transform the bilevel MINLP into a single-level nonconvex MINLP, which is further globally optimized using an improved branch-and-refine algorithm. We also present two case studies, including a county-level biofuel supply chain in Illinois, to illustrate the application of the proposed modeling and solution methods.

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1. Introduction

When entering a business, a manufacturer is often encountered with questions such as where to locate the plants, what sizes the plants should be, which conversion technology to choose, how much to produce, and how to set the transfer prices (Cox, 2005). Although there is a large body of literature on the modeling and optimization of supply chain design and operations, most of these works view the supply chain from a centralized perspective and integrate the various components of the supply chain into a monolithic model (Munoz et al., 2013; Papageorgiou, 2009; Shah, 2005). Under this approach, it was implicitly assumed that the decision maker has full control over the entire supply chain so that all the strategic and operational decisions can be implemented successfully. However, the management over a supply chain is often decentralized in practice (Cachon and Netessine, 2004). In other words, different stakeholders may be in charge of different entities in the supply chain, and these stakeholders may even have conflicting interests against each other. These supply chain participants would strive to maximize their own benefits and compete with their peers, thus leading to a non-cooperative supply chain (Facchinei and Kanzow, 2007).

The goal of this work is to develop a novel game-theoretic modeling and optimization framework that addresses non-cooperative supply chain design and planning from a manufacturer’s perspective. In a non-cooperative supply chain, all of the participants act selfishly and are solely driven by their own objective. The players make decisions independently without collaboration or communication (Nash, 1951). This is different from a cooperative supply chain, where the players are willing to negotiate with each other and arrive at a unanimous agreement (Nagarajan and Sošić, 2008). Recent works on cooperative supply chains include the works by Gjerdrum et al. (2001, 2002), Zhang et al. (2013), Fernandes et al. (2013), Banaszewski et al. (2013), and Yue and You (2014). On the other hand, representative works on non-cooperative supply chains include the works by Bard et al. (2000), Ryu et al. (2004), and Zamarripa et al. (2012, 2013). To the best of our knowledge, most existing works on the optimal design and planning of non-cooperative supply chains are restricted to a rather simple supply chain structure, instead of the multi-echelon network considered in this work. Furthermore, in previous works, linearization assumptions and simplifications have been applied in order to keep the model tractable, which might lose the generality of the mathematical model. Therefore, this work aims to fill these research

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Nomenclature

Sets/indexes
- $b$: biomass types
- $i$: suppliers
- $j$: biorefineries
- $k$: customers
- $p$: biofuel types
- $q$: conversion technologies

Parameters
- $c_{ij}^r$: reference capital cost of technology $q$ at biorefinery $j$
- $c_{ij}^{(U)}$: minimum (maximum) capacity limit of biorefinery $j$ with technology $q$
- $ca_{b,i}$: harvesting cost of biomass $b$ at supplier $i$
- $cap_{j,q}$: reference capacity of technology $q$ at biorefinery $j$
- $cf_{q}$: fixed O&M cost of technology $q$ as a percentage of the capital cost
- $c_{ij,b,i,j}$: transportation cost of biomass $b$ from supplier $i$ to biorefinery $j$
- $c_{ij,b,p,j,k}$: transportation cost of biofuel $p$ from biorefinery $j$ to customer $k$
- $cp_{j,q}$: variable production cost at biorefinery $j$ with technology $q$
- $d_{p,k}^{upper}$: upper bound of the demand for biofuel $p$ at customer $k$
- $ir$: discount rate
- $lt$: lifetime of the project
- $num_{q}$: maximum number of biorefineries with technology $q$ allowed to be installed
- $p_{r,p,k}$: market price of biofuel $p$ at customer $k$
- $pr_{b}$: price of per unit of biomass $b$ offered by external market
- $pr_{p}$: price of per unit of biofuel $p$ offered by external market
- $sf$: scaling factor
- $w_{b,j,q}^{lower}$: upper bound of consumption of biomass $b$ at biorefinery $j$ via technology $q$
- $w_{p,j,q}^{upper}$: upper bound of production of biofuel $p$ at biorefinery $j$ via technology $q$

Greek parameters
- $\theta_{q}$: minimum utilization rate of biorefinery $j$ with technology $q$
- $\xi_{p}$: common functional unit corresponding to a unit of biofuel $p$
- $\chi_{b,p,j,q}$: conversion parameter between biomass $b$ and biofuel $p$ at biorefinery $j$ with technology $q$

Non-negative variables
- $Cap$: amortized capital cost
- $Com$: annual operation and maintenance cost
- $Cex-aq$: cost of biomass acquisition from the external market
- $Cex-sa$: revenue of biofuel sales to the external market
- $Cap_{j,q}$: capacity of biorefinery $j$ with technology $q$
- $F_{ij,b,i,j}$: amount of biomass $b$ shipped from supplier $i$ to biorefinery $j$
- $F_{jk,p,j,k}$: amount of biofuel $p$ shipped from biorefinery $j$ to customer $k$
- $Pa_{b,j}$: acquisition price of biomass $b$ at biorefinery $j$
- $Ps_{p,j}$: selling price of biofuel $p$ at biorefinery $j$
- $Wi_{b,j}$: acquisition target of biomass $b$ at biorefinery $j$
- $Wa_{b,j,q}$: amount of biomass $b$ to consume at biorefinery $j$ via technology $q$
- $Wo_{p,j}$: production target of biofuel $p$ at biorefinery $j$
- $Wo_{p,j,q}$: amount of biofuel $p$ to produce at biorefinery $j$ via technology $q$

Binary variables
- $X_{j,q}$: 1 if biorefinery $j$ with technology $q$ is installed; otherwise 0

Gaps by both proposing a novel single-leader–multiple-follower game-theoretic framework for general three-echelon supply chain networks and developing an effective global optimization strategy to address the resulting mathematical model.

Specifically, we consider a three-echelon supply chain superstructure, which includes a set of candidate sites for building manufacturing facilities in the middle echelon, as well as a set of given upstream suppliers and downstream customers. A single player – a manufacturer – is in charge of all the manufacturing facilities, while each supplier and customer is considered to be an independent player. The manufacturer is assumed to be the supply chain leader, who makes the decisions on supply chain design and strategic planning first. The suppliers and customers are assumed to be the followers who then maximize their own profits given the leader’s decisions. We model the leader–follower relationship as a single-leader–multiple-follower Stackelberg game. We model the competition among suppliers and customers under the assumption of generalized Nash equilibrium.

Without loss of generality, we formulate the problem above into a bilevel mixed-integer nonlinear program (MINLP). In the upper level problem, the manufacturer optimally determines the location, capacity, and technology of the manufacturing facilities, as well as the operational plans and transfer prices in order to maximize the total profit generated from all the manufacturing facilities. Discrete variables are employed to select among the candidate sites, conversion technologies, etc. Capital cost economies of scale are captured by using a nonlinear power function. To calculate the transfer payments of materials, bilinear terms are also included. Therefore, the upper level problem is nonlinear, nonconvex, and has combinatorial features. Given the manufacturer’s decisions in the upper level problem, each follower in the lower level problem optimizes its transactions with the installed manufacturing facilities to maximize its own profit. Specifically, the suppliers optimize the amount of raw materials to be sold to the manufacturing facilities and the customers optimize the amount of products to purchase from the manufacturing facilities. All of the lower level problems are formulated as linear programs (LPs).

We note that the resulting bilevel program cannot be handled directly using off-the-shelf optimization solvers. However, for the cases that all the lower level problems are LPs, we can reformulate the bilevel MINLP problem into an equivalent single-level MINLP by replacing each follower’s optimization problem with the corresponding Karush–Kuhn–Tucker (KKT) conditions (Bard, 1998). Though solvable, the resulting single-level MINLP problem can still be computationally intractable due to the presence of concave and bilinear terms as well as integer variables. To facilitate the solution process, we further propose an improved branch-and-refine algorithm which is based on a class of SOS1 (specially ordered set of type 1) piecewise linear formulations. The algorithm takes advantage of powerful mixed-integer linear programming (MILP) solvers and globally optimizes the nonconvex MINLP problem efficiently in finite iterations. To illustrate the application of the proposed
modeling and optimization framework, we also present two case studies, including a county-level case study on a potential biofuel supply chain in the state of Illinois.

Major novelties of this work are summarized as follows:

- A novel bilevel MINLP model is proposed for the design and strategic planning of non-cooperative supply chains;
- An extension of Stackelberg game and generalized Nash equilibrium is made to multi-echelon supply chains;
- An efficient global optimization strategy is developed for the bilevel MINLP using the KKT transformation and the improved branch-and-refine algorithm;
- A county-level case study on a potential cellulosic bioethanol supply chain in Illinois is presented.

The rest of this paper is organized as follows. We first provide a brief introduction to the concepts of Stackelberg game and generalized Nash equilibrium in Section 2. We then present a general problem statement in Section 3 and a generic model formulation in Section 4. The application on cellulosic biofuel supply chains is covered by Sections 5 and 6, followed by the solution strategies presented in Section 7. Two case studies are given in Section 8, with discussions on the results and implications.

2. Background

2.1. Stackelberg game

The first Stackelberg game was described by the German economist Heinrich Freiherr von Stackelberg in 1934, who studied the competition between two firms selling a homogeneous good (Von Stackelberg et al., 2010). The concept of Stackelberg game was then extended to a variety of research fields and applications to study the situation where a leader–follower relationship is observed (Chu and You, 2014; Chu et al., 2014). A standard Stackelberg game involves two players: a leader and a follower. The leader takes actions first and then the follower reacts to the leader’s decisions rationally. Therefore, the Stackelberg game is a sequential game. It is assumed that the leader knows in advance that the follower will observe its decisions and the leader has full knowledge of how the follower will respond to its decisions. Once the decisions have been made, the leader must commit to its decisions. In other words, once the leader has made its move, the leader cannot undo it. The leader is recognized to have certain advantages enabling it to move first (e.g., the structural advantage of manufacturer over suppliers and customers). These advantages would let the leader gain a larger profit than the follower. On the other hand, the leader must guarantee a certain degree of incentives to the follower. Otherwise the follower may refuse to participate in the supply chain and the leader’s strategic plan may become infeasible or unprofitable.

Mathematically, a single-leader–single-follower Stackelberg game can be formulated as a bilevel programming problem (Bard, 1998; Colson et al., 2007), given below

by \( y \in Y \). The leader’s objective function \( F(x, y) \), inequality constraints \( G_i(x, y) \), and equality constraints \( H_j(x, y) \) depend not only on the leader’s decisions \( x \), but also on the follower’s decisions \( y \). A bilevel program is also called a “mathematical program that contains an optimization problem in the constraints” (Bracken and McGill, 1973), because the value of \( y \) in the leader’s problem is obtained by solving the follower’s optimization problem. The follower’s objective function is denoted by \( f_i(x, y) \), the inequality constraints are denoted by \( g_i(x, y) \), and the equality constraints are denoted by \( h_j(x, y) \). Note that the leader’s decision variables \( x \) are treated as given parameters in the follower’s optimization problem, indicating that the leader’s move has already been made at the time when the follower takes actions.

2.2. Generalized Nash equilibrium

Before explaining the concept of generalized Nash equilibrium, we would like to introduce the standard Nash equilibrium problem. The Nash equilibrium was named after the American mathematician John Forbes Nash, Jr. (Nash, 1950, 1951). In game theory, the Nash equilibrium is a solution concept of a non-cooperative game involving two or more players, in which each player is assumed to know the equilibrium strategies of other players, and no player has anything to gain by changing only their own strategy (Osborne and Rubinstein, 1994). The Nash equilibrium provides a way of predicting what will happen if several players are making decisions simultaneously and if the outcome depends on the decisions of the others.

To demonstrate the mathematical expression of Nash equilibrium, let us consider a finite number of \( N \) players, which are indexed by \( v \). For each player \( v = 1, \ldots, N \), we denote its benefit function as \( f_v \), its decision variables as \( x^v \), and its strategy set as \( X_v \). Every player’s decisions are restricted to its strategy set, that is, \( x^v \in X_v \). If we define a vector

\[
\begin{align*}
    x &= (x^1, x^2, \ldots, x^N) = (x^1, \ldots, x^{v-1}, x^v, x^{v+1}, \ldots, x^N) \\
    &\in X_1 \times \cdots \times X_{v-1} \times X_v \times X_{v+1} \times \cdots \times X_N
\end{align*}
\]

then \( x^v \) is a Nash equilibrium if and only if \( x^{v-} \) solves the following maximization problem for all the players \( v = 1, \ldots, N \):

\[
\begin{align*}
    \max_{x^v} f_v(x^v, x^{v-}) \\
    \text{s.t. } x^v \in X_v
\end{align*}
\]

We can see that every player \( v \) is encountered with an optimization problem, where other players’ decisions \( x^{v-} \) are treated as given parameters. These optimization problems suggest that the set of strategy choices \( x^v \) is a Nash equilibrium if and only if no player can improve its benefit function by unilaterally changing its strategy.

In a standard Nash equilibrium problem, the strategy set of each player is considered independent of the other players’ decisions. However, in some cases, a player’s decisions might be restricted by other players’ decisions. This then leads to the concept of generalized Nash equilibrium. Assuming that there is a common strategy set \( X \), player \( v \)’s feasible set can be denoted by

\[
X_v(x^{v-}) = \{ x^v | (x^v, x^{v-}) \in X \}
\]

The generalized Nash equilibrium problems arise naturally from the standard Nash equilibrium problems if the players share some common resources or limitations. In such case, all players’ strategies might be restricted by a number of common constraints, called shared constraints (Facchinei and Kanzow, 2007). For example, when two players are competing for limited resources, the amount of resources acquired by one player would restrict the amount available to the other player. A generalized Nash equilibrium problem can have an infinite number of solutions, while not
every equilibrium solution is meaningful from a real-world standpoint (Kulkarni and Shanbhag, 2012). Therefore, the concept of normalized Nash equilibrium was proposed representing a subset of generalized Nash equilibria that is smaller, yet economically meaningful (Rosen, 1965). The normalized equilibrium is a refinement of the generalized Nash equilibrium, where the Lagrange multipliers corresponding to the shared constraints are identical for all the players. This additional property can be interpreted as equilibrium with uniform shadow prices. It is also believed that the normalized equilibria are more socially stable than other equilibria of the generalized Nash equilibrium problem (Kulkarni and Shanbhag, 2012).

3. General problem statement

We address the optimal design and planning of non-cooperative supply chains from a manufacturer’s perspective. Fig. 1 shows a three-echelon supply chain superstructure. The first echelon consists of a set of individual suppliers. The second echelon includes a set of candidate sites for building the manufacturing facilities. The third echelon consists of a set of individual customers. One decision maker, the manufacturer, is in charge of all of the manufacturing facilities belonging to one organization. In contrast, each supplier/customer is considered to be an autonomous player in the supply chain, who is responsible for its own decisions and profit.

The suppliers and customers are assumed to be established in the local market before the manufacturer arrives. At the supply chain design level, the manufacturer needs to determine the location, capacity, and technology of the manufacturing facilities. At the operational level, the manufacturer needs to determine the production plans as well as the prices for material transfers, which is treated as a single-period planning problem. As the most critical components in the supply chain, the manufacturing facilities link supply and demand by acquiring raw materials from the upstream suppliers and selling finished products to the downstream customers. Therefore, the manufacturer is considered to be the leader of the supply chain network, while the individual suppliers and customers are considered to be the followers. This corresponds to the cases where the manufacturer possesses advantages in terms of resources and technologies. This relationship between the manufacturer and the suppliers and customers is modeled as a Stackelberg game with a single leader and multiple followers. Since the suppliers and customers might compete for certain common resources or limited quotas released by the manufacturer, we adopt the assumption of normalized Nash equilibrium to model the behaviors of the followers. The following summary gives a formal statement of the key assumptions in this problem, as well as the optimization problems for the manufacturer, the suppliers, and the customers, respectively.

4. Assumptions

We consider the following assumptions in this problem:

- The cost of raw material transportation from a supplier to a manufacturing facility is covered by the supplier;
- The cost of product transportation from a manufacturing facility to a customer is covered by the customer;
- There is an external market with sufficient supply and demand but higher raw material acquisition costs and lower product selling prices;
- We consider single period planning in this work.

3.1. Manufacturer’s problem

The manufacturer’s objective is to maximize the total profit generated from all its manufacturing facilities. The given information for the manufacturer includes:

- A set of candidate locations for building manufacturing facilities;
- A set of available technology options;
- Restrictions on the number of manufacturing facilities, process capacity, etc.
- Planning horizon and project lifetime;
- Cost data on capital investment, operations and maintenance (O&M), etc.;
- Restrictions on transfer prices.

The decision variables controlled by the manufacturer include:

- Selection of location, capacity and conversion technology for manufacturing facilities;
- Strategic plans on the amount of raw materials to collect and the amount of products to produce;
- Setting of transfer prices for raw material acquisition and product sales.

3.2. Supplier’s problem

For each supplier, an optimization problem is formulated. The objective of each supplier is to maximize its own profit. The given information for each individual supplier includes:

- All of the manufacturer’s decisions;
- Available amount of raw materials that can be offered to the manufacturing facilities;
- Cost data on raw material preparation, transportation from the supplier to the manufacturing facilities, etc.

The supplier’s decision is:

- Amount of raw materials sold to each installed manufacturing facility.

3.4. Customer’s problem

An optimization problem is formulated for each customer. The objective of each customer is to maximize its own profit. Each individual customer is given the following information:

- All of the manufacturer’s decisions;
- Local demand and market price of the products;
- Cost data for transporting the products from the manufacturing facilities to the customer.
The customer's decision is:

- Amount of products to purchase from each installed manufacturing facilities.

In this single-leader–multiple-follower Stackelberg game, the manufacturer takes actions first to install the manufacturing facilities with selected technologies, release the operational plans, and set the transfer prices for raw material acquisition and product sales. After observing the manufacturer's decisions, the suppliers (customers) decide how much to sell to (purchase from) each installed manufacturing facility. A critical feature of this decentralized game-theoretic model is that the decisions of each player in the supply chain are solely driven by its own economic interest. All the players possess the choice to participate in the supply chain. From a manufacturer's perspective, the price levels for raw material acquisition and product sales must be carefully determined. If the raw material acquisition price is set too low, the suppliers might refuse to sell to the manufacturing facilities as the transaction would not be profitable. On the other hand, if the price is set too high, the manufacturer would pay unnecessary costs. The situation is similar on the customer side. If the product sales price is set too high, the customer might be reluctant to purchase from the manufacturing facilities due to the negative profit margin. On the other hand, if the price is set too low, the manufacturer is losing potential revenue. Moreover, if the manufacturer finds it unprofitable to invest in this potential supply chain, no manufacturing facilities would be built.

4. General model formulation

According to the problem statement above, this is a Stackelberg game involving a single leader and multiple followers. Assuming that the competition among the followers leads to the generalized Nash equilibria, we can integrate the mathematical model for the standard Stackelberg game (1)-(5) and the generalized Nash equilibrium model (7) and (8), thus leading to the following game-theoretic model formulation.

\[ \text{max } F(x, y) \]
\[ \text{s.t. } G_i(x, y) \leq 0, \quad i = 1, \ldots, m \]
\[ H_j(x, y) = 0, \quad j = 1, \ldots, r \]

where \( y \) solves

\[ \text{max } f(x, y^*, y^{*'}) \quad \forall y \]
\[ \text{s.t. } g_i(x, y^*, y^{*'}) \leq 0, \quad \forall y, \quad i = 1, \ldots, m' \]
\[ h_j(x, y^*, y^{*'}) = 0, \quad \forall y, \quad j = 1, \ldots, r' \]

In this general model formulation, the leading manufacturer's decisions and strategy set are denoted by vector \( x \) and \( X \), respectively. Let the followers (namely, suppliers and customers) be indexed by \( y \). The decisions and strategy set of follower \( y \) are denoted by \( y^* \) and \( Y_y \), respectively. Vector \( y^{*'} \) stands for the decisions taken by the players other than \( y \). Vector \( y \) includes the decisions of all the followers. Every follower strives to maximize its own benefit function (12) subject to constraints (13) and (14), given the leader's decisions \( x \) and other players' decisions \( y^{*'} \). Note that a subset of constraints in (13) and (14) might be shared by the followers, thus leading to a generalized Nash equilibrium problem in the lower level. We note that the leader's objective function (9), as well as constraints (10) and (11), are influenced not only by its own decisions, but also by the decisions of all the followers \( y \), where \( y \) stands for the normalized Nash equilibrium solution for the competition among the followers.

Without loss of generality, we consider the above problem as a bilevel MINLP, including nonlinear terms and discrete variables in the upper level problem, and LPs as the lower level problems. That is, functions \( F, G \) and \( H \) can be linear or nonlinear, and the leader's decision variables \( x \) can involve both discrete (e.g., those for facility location and technology selection) and continuous variables (e.g., those for production planning and transfer prices). To keep the problem tractable, the lower level functions \( f, g \) and \( h \) are all linear and \( y \) involves only continuous variables (e.g., those for material flows).

The bilevel MINLP problem formulated above is an optimization problem with a set of optimization problems in the constraint that cannot be directly handled by any off-the-shelf mathematical programming solvers. Therefore, in this section, we reformulate the bilevel problem into a single-level MINLP. This is accomplished by replacing the lower level LP problems with their KKT conditions ([Bard, 1998]). The KKT conditions of player \( i \)'s optimization problem consist of four sets of constraints, namely stationarity (15), primal feasibility (16), dual feasibility (17), and complementary slackness (18).

\[- \frac{df}{dy^i} + \sum_{i=1}^{m} \lambda_i \frac{dg_i}{dy^i} + \sum_{j=1}^{r} \mu_j \frac{gh_j}{dy^i} = 0 \tag{15} \]
\[g_i \leq 0, \quad \forall y \quad \text{and} \quad h_j = 0, \quad \forall y^i \tag{16} \]
\[\mu_i \geq 0, \quad \forall y^i \tag{17} \]
\[\mu_i \cdot g_i = 0, \quad \forall y \tag{18} \]

where \( \mu_i \) is the Lagrange multiplier corresponding to the inequality constraint \( g_i \). \(\lambda_j \) is the Lagrange multiplier corresponding to the equality constraint \( h_j \). Note that if a certain constraint is shared by multiple players, the corresponding Lagrange multiplier should be identical for all the associated players' problems under the assumption of normalized Nash equilibrium. Reformulation using the KKT conditions is a standard approach that is commonly used and computationally robust ([Bard, 1998]). The KKT conditions are sufficient and necessary, because the lower level problems are LPs. Thus, the resulting single-level MINLP problem is exactly equivalent to the original bilevel MINLP program.

In the problem setting of this work, the stationarity, primal feasibility, and dual feasibility constraints are all linear. However, bilinear terms are involved in the complementary slackness constraints, which are nonlinear and nonconvex. To improve the computational efficiency, we linearize the complementary slackness constraints (18) by introducing a set of binary variables as shown below ([Bard, 1998]).

\[\mu_i \leq M \cdot Z_i, \quad \forall y \tag{19} \]
\[-g_i \leq M (1 - Z_i), \quad \forall y \tag{20} \]

where \( Z_i \) are binary 0–1 variables which are equal to 0 if the Lagrange multiplier \( \mu_i \) is equal to zero; 1 if the inequality constraint \( g_i \) is active. In this way, we can linearize all the lower level KKT conditions.

5. Specific problem statement

We now apply the proposed game-theoretic model to study the optimal design and planning of biomass-to-ethanol supply chains. Cellulosic-biomass-derived fuel ethanol provides a promising solution to the increasing concerns on climate change, energy security, and the diminishing supply of fossil fuels. As a number of pilot-scale biorefineries have been built and have been in operation for years all over the world, there are mature technologies available in the fuel ethanol industry. Large-scale production and use of bioethanol is mainly constrained by the lack of efficient supply chains that link the biomass supply and fuel demand ([You et al., 2012]).
Different from the approaches in this work, most existing models for biofuel supply chain optimization are monolithic models, assuming that the management over the entire supply chain is centralized (Yue et al., 2014). Deterministic MILP models with spatially explicit, multi-echelon and multi-period features have been widely employed (Akgul et al., 2012; Alex Marvin et al., 2012; Andersen et al., 2013; Dunnett et al., 2008; Elia et al., 2011; Giarola et al., 2011; Yue et al., 2013). Multi-objective models have been proposed to simultaneously optimize other criteria in addition to the economic performance (El-Halwagi et al., 2013; Liu et al., 2010; Santibañez-Aguilar et al., 2011; You et al., 2012; You and Wang, 2011). Various pricing and quantity uncertainties in the biofuel supply chain have been addressed by optimization under uncertainty (Gebreslassie et al., 2012; McLean and Li, 2013; Osmani and Zhang, 2013; Tong et al., 2013, 2014a,b).

Recently, Bai et al. (2012) proposed a game-theoretic model that incorporates farmers’ decisions on land use and market choice into the biofuel manufacturer’s supply chain design problem. Yeh et al. (2014) employed a two-stage bilevel programming approach to study the bio refinery investment decision making under uncertainty in a pre-established timberlands supply chain. However, these works consider rather simple supply chain network structures, and the solutions are obtained either through model simplification or enumeration approaches. To address these limitations, we adapt the proposed game-theoretic framework to optimize the design and planning of multi-echelon biofuel supply chains, including biomass suppliers, biorefineries, and biofuel customers. Furthermore, we develop efficient solution strategies for the global optimization of the resulting bilevel MINLP problem.

We are given a three-echelon biofuel supply chain superstructure as shown in Fig. 2, including a set of biomass suppliers (indexed by i), a set of candidate sites for biorefineries (indexed by j), and a set of fuel ethanol customers (indexed by k). A set of conversion technology options (indexed by q) are available for building a biorefinery. A set of biomass resources (indexed by b) are offered at the biomass suppliers, and a set of biofuel products (indexed by p) are demanded at the biofuel customers. Each supplier and customer is considered to be an independent player, who already exists in the local market. A biorefinery investor is assumed to be in charge of each biorefinery. The biorefinery investor is considered to be the supply chain leader, and each supplier and customer is considered to be an independent follower, following the Stackelberg game format. When in operation, the installed biorefineries procure cellulosic biomass from the suppliers, and sell biofuel products to the customers. The upstream individual suppliers compete for the limited biomass acquisition quota released by the installed biorefineries, while the downstream individual customers compete for the limited amount of biofuel produced by the installed biorefineries. We model the competitions among these players under the assumption of generalized Nash equilibrium.

We approach this non-cooperative supply chain optimization problem from the biorefinery investor’s perspective. The objective of the biorefinery investor is to maximize the total profit generated from all the biorefineries by optimally determining the location, capacity, and conversion technology of each biorefinery, the operational plans for biomass acquisition and biofuel sales, the production level, and the setting of biomass and biofuel transfer prices at each installed biorefinery. The biorefineries generate revenue by selling biofuels to downstream customers, and they make payments to upstream suppliers for biomass acquisition. Given information to the biorefinery investor includes the supply chain structure, restrictions on process capacity and utilization, techno-economic data of different technology options, etc. Most importantly, as the supply chain leader, the biorefinery investor has the knowledge on how the suppliers and customers will react to its decisions.

A supplier generates revenue by selling biomass to installed biorefineries and covers the harvesting cost and transportation expenses. For each supplier, the objective is to maximize its profit by optimally determining the amount of biomass sold to each installed biorefinery. Given information to the suppliers includes the biomass availability, harvesting cost, transportation cost, etc. Following the assumption in Section 3.1, the biomass transportation cost from a supplier to an installed biorefinery is covered by the supplier. Therefore, the suppliers’ margins will decrease with increasing distance from the biorefinery. Each supplier must take into account the biorefinery investor’s decisions as well as the other suppliers’ decisions when making its own decisions.

A customer purchases biofuel from installed biorefineries and earns a profit by selling the purchased biofuel to satisfy local demands. For each customer, the objective is to maximize its profit by optimally determining the amount of biofuel to purchase from each installed biorefinery. Given information to the customers includes the upper bound on fuel demand, local price, transportation cost, etc. It is also assumed that the biofuel transportation cost from a biorefinery to a customer is covered by the customer. Similar to the suppliers, each customer must take into account the biorefinery investor’s decisions as well as the other customers’ decisions when making its own decisions.

In summary, the goal of this problem is to optimize the biofuel supply chain design and planning decisions from the biorefinery investor’s perspective by taking into account the autonomous behaviors of the individual suppliers and customers. As key assumptions in this problem, the biorefinery investor has knowledge on the equilibria among the followers, and each supplier and customer knows the equilibrium strategy of its competitors.

6. Specific model formulation

The problem stated above can be regarded as a Stackelberg game with the biorefinery investor as the single leader and the multiple biomass suppliers and biofuel customers as the followers, under the assumption of normalized Nash equilibrium. Therefore, a bilevel MINLP problem (P0) is proposed, with the upper level problem corresponding to the biorefinery investor’s MINLP problem, and the lower level problems corresponding to the suppliers’ and customers’ LP problems. Based on the KKT conditions of the lower-level LP problems, the bilevel MINLP problem can be reformulated into a single-level nonconvex MINLP (PS). Considering the length of the paper, the detailed mathematical model and reformulation techniques are presented in Appendix A.

7. Solution strategy

Although global optimizers for nonconvex MINLP problems are available off-the-shelf, their computational performance on
large-scale applications is somewhat lacking. To facilitate the solution of the nonconvex MINLP problem (PS), we present an improved branch-and-refine algorithm in this section. The algorithm takes advantage of the powerful MILP solvers (e.g., CPLEX) and returns the global optimal solution to the nonconvex MINLP problem by iteratively solving a sequence of MILP subproblems. Compared with the standard branch-and-refine algorithm (You and Grossmann, 2011; You et al., 2011), the proposed algorithm is improved in the following two aspects. First, a new type of piecewise linear approximations based on the SOS1 variables is employed to formulate the MILP subproblems. Second, bivariate partitioning for bilinear terms is included in the improved algorithm.

### 7.1. Piecewise linear approximation

An important step of the branch-and-refine algorithm is to iteratively construct convex relaxation problems (MILP subproblems) based on the piecewise linear approximations for the nonconvex terms. The piecewise linear approximations in this work are derived based on the SOS1 formulation (Padberg, 2000). By definition, at most one variable within an SOS1 can have a non-zero value. A number of MILP solvers allow the use of SOS1 variables (e.g., CPLEX) and have certain internal routines for solving the SOS1 formulations efficiently. It is suggested that the SOS1 formulation is more efficient compared to the other types of piecewise linear approximation formulations (Hasan and Karimi, 2010).

In the SOS1 approach, a continuous variable $X_i$ is expressed as follows (Hasan and Karimi, 2010):

$$X_i = \sum_{n=1}^{N} W_{i,n} \cdot u_{i,n}, \quad \forall i \tag{21}$$

$$\sum_{n=1}^{N} W_{i,n} = 1, \quad \forall i \tag{22}$$

$$\sum_{n=1}^{N-1} E_{i,n} = 1, \quad \forall i \tag{23}$$

$$W_{i,1} \leq E_{i,1}, \quad \forall i \tag{24}$$

$$W_{i,n} \leq E_{i,n-1} + E_{i,n}, \quad \forall i, \quad 2 \leq n \leq N - 1 \tag{25}$$

$$W_{i,N} \leq E_{i,N-1}, \quad \forall i \tag{26}$$

$$0 \leq W_{i,n} \leq 1, \quad E_{i,n} \in \text{SOS1 variables} \tag{27}$$

where the set of grid points is indexed by $n$; $N$ is the total number of grid points; $u_{i,n}$ are the values of the pre-specified grid points in the $X_i$ space; $W_{i,n}$ stands for the weighting factor corresponding to point $u_{i,n}$; $E_{i,n}$ is the position indicator which is equal to 1 if the value of $X_i$ falls in the $n$th interval and 0 otherwise. Note that $E_{i,n}$ are not binary variables. However, due to constraint (23) and the SOS1 feature, $E_{i,n}$ can only take the value of either 0 or 1.

Based on the SOS1 formulation (21)–(27), the piecewise linear approximation $RX_i$ of concave functions $X_i^\alpha$ (where $0 < \alpha < 1$) is given by (Hasan and Karimi, 2010):

$$RX_i = \sum_{n=1}^{N} W_{i,n} \cdot \text{val}_{i,n}, \quad \forall i \tag{28}$$

where $\text{val}_{i,n} = u_{i,n}^\alpha$, which is equal to the value of the power function at grid point $u_{i,n}$. A graphical illustration is shown in Fig. 3a, where the black solid line stands for the actual power function and the red solid line represents the piecewise linear approximation of the concave term. We can see that the piecewise linear function is an under-estimator of the concave function.

The piecewise linear approximation $Z_{ij}$ of a bilinear function $(X_i \cdot X_j)$ is given by (Hasan and Karimi, 2010):

$$Z_{ij} = \sum_{n=1}^{N} \sum_{n'=1}^{N} u_{i,n} \cdot u_{j,n'} \cdot K_{i,j,n,n'}, \quad \forall i,j \tag{29}$$

$$\sum_{n'=1}^{N} K_{i,j,n,n'} = W_{i,n}, \quad \forall i,j,n \tag{30}$$

$$\sum_{n=1}^{N} K_{i,j,n,n'} = W_{j,n'}, \quad \forall i,j,n' \tag{31}$$

$$K_{i,j,n,n'} \geq 0 \tag{32}$$

where $K_{i,j,n,n'}$ are auxiliary variables. Note that both $X_i$ and $X_j$ are partitioned in our approach, thus resulting in a bivariate model. A graphical illustration is shown in Fig. 3b. The black solid curve represents the contour of the bilinear function. The green solid lines represent the over-estimators of the bilinear function and the red solid lines represent the under-estimators. We can see that the piecewise linear approximations are exact at the grid points, while the approximation error increases as the distance from the grid points increases. There are also a number of univariate models, where only one variable is partitioned. Although fewer auxiliary variables are required in the univariate models, we find that the improved branch-and-refine algorithm converges much faster using the bivariate model due to smaller approximation errors in each iteration.

![Fig. 3. Piecewise linear approximations for (a) concave functions and (b) bilinear functions.](image-url)
The concave terms in (34) and (35) for calculating the capital costs can be replaced by the piecewise linear approximations in the form of (28), where \( \text{Cap}_{p,j} \) is chosen as the partitioning variable. The bilinear terms in (33) representing the transfer payments of biomass and biofuel can be replaced by the piecewise linear approximations in the form of (29), where \( P_{p,p,j,k}, F_{k,k,j,k}, \) and \( F_{j,j,k} \) are all chosen as the partitioning variables. In this way, a convex relaxation is derived and we denote this MILP subproblem as (PL). Since the original MINLP is a maximization problem, the optimal solution of the MILP subproblem would provide a valid upper bound. Additionally, any solution to the MILP subproblem (PL) is also feasible to the original MINLP problem (PS), because the constraints of both problems are the same. Therefore, a valid lower bound can be obtained by evaluating the objective function at the current solution.

### 7.2. Improved branch-and-refine algorithm

We know that the finer the grid partitioning we specify, the better the approximation would be. However, at the same time, as additional variables and constraints are introduced with the increase in the number of grid points, the problem size may become significantly large and computationally intractable. Therefore, we propose an improved branch-and-refine algorithm which automatically determines the grid propagation and effectively converge within finite iterations. The procedure of the improved branch-and-refine algorithm is given as follows, which is based on the work by Bergamini et al. (2008).

1. **Initialization**
   - Set iteration count \( \text{iter} = 0 \), lower bound \( LB = -\infty \), upper bound \( UB = +\infty \); Set the convergence tolerance to \( \text{tol} \); set the number of grid intervals to \( \text{nump} \) for each partitioning variable and set \( N = \text{nump} + 1 \); construct the piecewise linear approximations.

2. **Solving MILP subproblem (PL)**
   - Solve the MILP subproblem. If infeasible, stop and conclude that the original MINLP problem (PS) is infeasible. If feasible, denote the optimal objective value as \( \text{obj}^L \) and set \( UB = \min \{ UB, \text{obj}^L \} \); substitute the optimal solution into objective function (33), denote the value as \( \text{obj}^U \), and set \( LB = \max \{ LB, \text{obj}^U \} \).

3. **Convergence checking**
   - If \( |UB - LB|/LB < \text{tol} \), stop and output the current solution as the global optimal solution; Otherwise, go to the next step.

4. **Grid propagation**
   - Refine the grid partitioning to improve the approximation. If the optimal value of a partitioning variable is at the existing grid points, no update is needed for this variable; otherwise, add a grid point right at the optimal value, update \( \text{nump}, N, u, \) and \( v \) accordingly, and then go to step (2).

The branch-and-refine procedure on the concave functions is illustrated in Fig. 4. The gap between the actual function value and the under-estimator at the 1st-iteration solution is relatively large. By adding a grid point and constructing a new piecewise linear function, we can significantly reduce the gap at the 2nd iteration. The branch-and-refine procedure on bilinear functions is illustrated in Fig. 5. The gap between the actual function value and the over-estimator and under-estimator is relatively large in the 1st iteration. By simultaneously updating the grid points in the space of both variables, we replace the original convex envelope with two smaller envelopes, thus effectively reducing the approximation errors in the 2nd iteration.
The improved branch-and-refine procedure can be fully implemented using 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 (Gong and You, 2014; Yue and You, 2013). The algorithm can start with an arbitrary number of grid points. Unless otherwise stated, we employ one interval as the starting grid with two grid points at the lower and upper bounds of the partitioning variables, respectively.

8. Case studies

To illustrate the application of the proposed modeling framework and global optimization algorithm, we present two case studies on the optimal design and planning of biofuel supply chains. The small-scale illustrative example compares the differences between the centralized and decentralized design, and shows the computational efficiency of the proposed algorithm. The county-level case study on a potential biofuel supply chain in Illinois demonstrates the capability of this game-theoretic modeling and optimization framework for large-scale applications.

All the computational experiments are conducted 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 (Rosenthal, 2011). CPLEX 12 is used for solving the MILP subproblems (PL) in the improved branch-and-refine algorithm. Global optimizers, BARON 12 (Tawarmalani and Sahinidis, 2005) and SCIP 3 (Achterberg, 2009), are used for the direct solution of the single-level non-convex MINLP problem (PS).

8.1. 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 that includes 4 suppliers, 4 biofuel refinery candidate sites, and 4 customers, as shown in Fig. 5. In this problem, we consider corn stover as the sole biomass feedstock. Ethanol is the only biofuel product considered. Two types of conversion technologies are considered for biofuel production: a biochemical and thermochemical process. The biochemical conversion process is based on dilute-acid pretreatment and enzymatic hydrolysis processes, and the thermochemical process involves indirect gasification and mixed alcohol synthesis. The biomass and biofuel are assumed to be shipped exclusively by truck.

The locations and inter-site transportation distances are given in Table B1 (Supporting Information). The availability of biomass feedstock at each supplier as well as the upper bound of biofuel demand at each customer are given in Table B2 (Supporting Information). The corn stover harvesting costs and biofuel market prices at each location are also summarized in Table B2 (Supporting Information). The biomass price in the external market is set to a significantly large value (e.g., $1000/dry ton). The profit for selling surplus biofuel to the external market is set to zero. In this case, doing business with the external market becomes unprofitable for the biorefinery investor. No limit on the number of biorefineries is considered. The techno-economic data regarding the biochemical and thermo-chemical technologies are obtained from the most recent technical reports provided by the National Renewable Energy Laboratory and summarized in Table B3 (Supporting Information) (Dutta et al., 2011; Humbird et al., 2011). The capacity upper bound is set to 150 MM gallons of ethanol/year. Note that a minimum capacity requirement of 10 MM gallons/year is imposed if a biorefinery is to be built. The transportation costs are derived from the work by Searcy et al. (2007). The life time of the biofuel supply chain project is assumed to be 15 years with an annual discount rate of 10%.

The optimal supply chain design that maximizes the biorefinery investor’s profit in the non-cooperative biofuel supply chain is given in Fig. 7. The biorefinery investor decides to build a biorefinery at candidate site j4. The capacity of the biorefinery is 65 MM gallons/year and the biochemical conversion technology is selected. The biomass transfer price set at the biorefinery is $59.42/ton and the biofuel transfer price is $2.32/gallon. In the normalized Nash equilibrium, 3 suppliers are selling biomass to the biorefinery and 4 customers are purchasing biofuel from the biorefinery. The amount of biomass shipped from suppliers i2, i3, and i4 to the biorefinery is 600, 122.9, and 100 kton per year, respectively. The amount of biomass purchased by customers k1, k2, k3, and k4 from the biorefinery is 20, 30, 10, and 5 MM gallons per year, respectively. The annual profit of the biorefinery investor is $10.95 MM. The adjusted profit of suppliers i2, i3, and i4 is $1.56 MM, $0, and $0.9 MM, respectively. The adjusted profit of customers k1, k2, k3, and k4 is $0.64 MM, $1.24 MM, $1.39 MM, and $0, respectively. The total profit of the entire supply chain is $16.69 MM. As can be seen, the biorefinery investor, who is the supply chain leader, gains a much larger share in the total supply chain profit than the suppliers and customers.

It would be enlightening to compare the optimization results of the non-cooperative supply chain with that of the conventional centralized design. Therefore, we also formulate a centralized supply chain optimization model, which is an MILP problem. The objective is to maximize the total profit of the entire supply chain. Since internal transactions do not affect the total profit of the supply chain, the internal transfer prices are not considered in the monolithic model. The model formulation is standard (You et al., 2012: You and Wang, 2011), thus not provided in the paper. The optimal centralized supply chain design is shown in Fig. 8. A biorefinery is installed at candidate site j2. The capacity of the biorefinery is 65 MM gallons/year and the biochemical conversion technology is selected. The biorefinery is supplied by 3 suppliers and sells biofuel product to 4 customers. The amount of biomass shipped from suppliers i1, i2, and i4 to the biorefinery is 122.9, 600, and 100 ktons per year, respectively. The amount of biofuel shipped to customers k1, k2, k3, and k4 from the biorefinery is 20, 30, 10, and 5 MM gallons per year, respectively. The total profit of the entire supply chain is $38.21 MM.
Table 1
Model statistics and computational results of the illustrative example.

<table>
<thead>
<tr>
<th>Solution method</th>
<th># of discrete variables</th>
<th># of continuous variables</th>
<th># of constraints</th>
<th>Objective (MMS/year)</th>
<th>Relative gap</th>
<th>Solution time (CPUs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BARON 12</td>
<td>8</td>
<td>125</td>
<td>179</td>
<td>10.95</td>
<td>0</td>
<td>884</td>
</tr>
<tr>
<td>SCIP 3</td>
<td>8</td>
<td>125</td>
<td>179</td>
<td>10.95</td>
<td>0</td>
<td>168</td>
</tr>
<tr>
<td>Improved branch-and-refine</td>
<td>56 (56)</td>
<td>253 (649)</td>
<td>403 (544)</td>
<td>10.95</td>
<td>0</td>
<td>27</td>
</tr>
</tbody>
</table>

* In a num1 (num2) format: num1 corresponds to the value in the 1st iteration and num2 corresponds to the value in the last iteration.

8.2. County-level instance in Illinois

In this section, we address a larger-scale case study on the design and strategic planning of a potential cellulosic biomass-to-ethanol supply chain in the state of Illinois, which has an abundant supply of corn stover. The state of Illinois comprises 102 counties, of which the spatial distribution of corn stover is shown in Fig. 10a and the population density is shown in Fig. 10b. We identify 10 individual suppliers, 5 candidate sites for building biorefineries, and 10 individual customers in this case study. The suppliers are located at the centers of the 10 counties with the highest biomass availability. The biorefinery candidate sites are located at the centers of the 10 counties with the highest biomass availability. The customers are located at the centers of the 10 counties with the highest population. We assume that the biofuel demand at each customer is proportional to the population of that county. The demand upper bounds are derived from the U.S. Energy Information Administration website (EIA, 2014). Due to the lack of data, the biomass harvesting cost is set to $36.78/dry ton for all the suppliers (EPA, 2007; ODOE, 2003) and the biofuel market price is assumed to be $2.50/gallon for all the customers. The transportation distances between the suppliers, biorefineries, and customers are calculated by the Haversine formula (Sinnott, 1984). This method utilizes the longitude and latitude information of the county center and takes into account the curvature of the earth and the area of the counties. Other given parameters (e.g., capacity limits, technology options, transportation costs, etc.) are the same as those of the illustrative example.

The optimal design that maximizes the biorefinery investor’s profit in the non-cooperative supply chain is presented in Fig. 10c. The optimal design decisions made by the biorefinery investor are to build two biorefineries in the Champaign County and LaSalle County, respectively. The biorefinery in Champaign County has a capacity of 130 MM gallons/year with the thermochemical technology. It receives corn stover from the suppliers in Champaign, Iroquois, McLean, and Vermilion. The biomass acquisition cost is set at $69.35/dry ton. It sells the produced fuel ethanol to the customers in Champaign, Cook, Madison, St. Clair, and Will. The biofuel sales price is set at $2.39/gallon. The biorefinery in LaSalle County has a capacity of 139 MM gallons/year with the thermochemical technology. It receives corn stover from the suppliers in Bureau, LaSalle, Lee, and Livingston. The biomass transfer price is set at $65.14/dry ton. It sells the produced fuel ethanol to the customers in Cook, Dupage, Kane, Lake, McHenry, and Winnebago. The biofuel transfer price is set at $2.42/gallon. The total profit generated from the two biorefineries is $126.68 MM. The adjusted profits of the suppliers range from $0 to $11.58 MM. The adjusted profits of the customers range from $0 to $2.04 MM. The total profit of the entire supply chain is equal to $158.00 MM. We can see that the biorefinery investor gains 80% of the supply chain profit by leveraging its leader position.

At this optimal solution, the cost for producing one gallon of fuel ethanol is $1.91. The cost breakdown is shown in Fig. 11, which shows the contributions of different supply chain activities to the biofuel cost. Capital investment accounts for the largest portion of the fuel ethanol cost, equaling 41%. The second largest component is the biomass harvesting cost, which accounts for 29% of the fuel...
ethanol cost. The fixed and variable O&M costs together share 8% of the fuel ethanol cost. The transportation of biomass also accounts for a significant portion (18%) of the fuel ethanol cost, because of the lower energy density of biomass. Since the energy density of fuel ethanol is significantly improved, the transportation cost of biofuel accounts for only 4% of the fuel ethanol cost.

The results are obtained by solving the single-level nonconvex MINLP problem with the improved branch-and-refine algorithm. Comparison of the computational performance among the different solution methods is presented in Table 2. The improved branch-and-refine algorithm converges to the global optimal solution in about 8.6 h. It takes a total of 7 iterations and the upper and lower bounds of each iteration are shown in Fig. 12. We can see that the optimal solution is obtained in the fourth iteration but the algorithm takes three more iterations to reduce the upper bound. In contrast, both global optimizers fail to converge within the 20-h limit. Specifically, BARON 12 succeeds in obtaining the optimal solution but is inefficient in reducing the upper bound, while SCIP 3 returns only a very poor suboptimal solution. Therefore, it is again shown that the improved branch-and-refine algorithm is much more efficient in solving the reformulated MINLP problem considered in this work.

9. Conclusion

A novel game-theoretic modeling and optimization framework was proposed for the design and strategic planning of non-cooperative three-echelon supply chains. As the leader, the manufacturer determined the location, capacity, and technology of manufacturing facilities, strategic plans on material input/output, as well as the transfer prices. As the follower, each supplier or customer maximized its own profit by optimizing the material transactions with the installed manufacturing facilities. We formulated a bilevel MINLP problem to model the leader–follower relationship and competition among the followers under the
assumption of the single-leader–multiple-follower Stackelberg game and the generalized Nash equilibrium. The upper level problem was a nonconvex MINLP, and the lower level problems were LPs. For efficient solution of this bilevel MINLP problem, we performed a KKT-condition-based model reformulation and developed an improved branch-and-refine algorithm. Applications of the modeling and solution framework were demonstrated via an illustrative example as well as a county-level case study on a potential biomass-to-ethanol supply chain in the state of Illinois. The results indicated that the biorefinery investor gains most of the profit of the entire supply chain by leveraging the leader position in the non-cooperative supply chain. On the other hand, the computational experiments showed that the proposed optimization approach could improve the solution efficiency by at least an order of magnitude.

This work addressed the competition within the biofuel supply chain. However, it would be also interesting to consider the competition across different types of supply chains as one of our future works. For instance, a game between biorefinery investment and its competing opponents, such as fossil fuel investment, can be considered.

Acknowledgement

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Appendix A. Specific model formulation

The bilevel MINLP problem for non-cooperative biofuel supply chains is presented in this section. A list of indices/sets, parameters and variables is given in the Nomenclature, where all parameters are denoted in lower-case symbols or Greek letters, and all variables are denoted with a capitalized first letter.

A.1. The biorefinery investor’s problem

The objective of the biorefinery investor ($Obj_{bi}$) is to maximize the total annual profit from all of the biorefineries, as given by (33). The first term represents the revenue from selling the biofuel to downstream customers, which is calculated as the product of the biofuel transfer price ($P_{b,j}$) and the total local sales amount ($\sum_{i} F_{b,j,i}$). The second term stands for the payment to upstream suppliers for biomass procurement, which is calculated as the product of the biomass transfer price ($P_{b,j}$) and the total amount of local procurement ($\sum_{i} F_{b,i}$). Following the assumptions in Section 3.1, the biomass transfer price $P_{b,j}$ is the same for all the suppliers, and the biofuel transfer price $P_{b,j}$ is the same for all suppliers at a certain biorefinery. Other components of the biorefinery investor’s objective function include the amortized capital cost ($C_{cap}$), the O&M cost ($C_{om}$), payment to external biomass acquisition ($C_{ex-acq}$), and revenue from external biofuel sales ($C_{ex-sa}$).

$$\text{max } Obj_{bi} = \sum_{p} \sum_{j} P_{p,j} \sum_{k} F_{b,p,j,k} - \sum_{b} \sum_{j} P_{b,j} \sum_{k} i F_{b,i} - C_{cap} - C_{om} - C_{ex-acq} - C_{ex-sa}$$ (33)

where $F_{b,j,i}$ stands for the amount of biomass $b$ shipped from supplier $i$ to biorefinery $j$, and $F_{b,p,j,k}$ stands for the amount of biofuel $p$ shipped from biorefinery $j$ to customer $k$. Note that both $F_{b,j,i}$ and $F_{b,p,j,k}$ are decision variables of the followers’ problems.

The amortized capital cost of the biorefineries is equal to the construction capital investment times the annuity, where the economies of scale are captured using the power function with the scaling factor denoted by $sf$.

$$C_{cap} = \frac{ir}{1 - (1 + ir)^{-n}} \sum_{j} \sum_{q} \left( \frac{Cap_{j,q}}{cap_{j,q}^0} \right)^{sf}$$ (34)

where $ir$ is the discount rate; $n$ is the lifetime of the project in terms of years; $cap_{j,q}^0$ and $Cap_{j,q}$ are the corresponding capital investment and production capacity of the reference biorefinery; $Cap_{j,q}$ is the decision variable on the capacity of biorefinery $j$ with technology $q$.

The O&M cost of the biorefineries consists of two parts. The fixed O&M cost is calculated as a certain percentage (with a factor of $c_{f}$) of the construction capital investment, which includes employee salaries, overhead, insurance, etc. The variable O&M cost is proportional to the production amount of biofuel, which accounts for the expenses on utility and consumables, as well as the credit from selling byproducts.

$$C_{om} = \sum_{j} \sum_{q} c_{q} \cdot \frac{Cap_{j,q}}{cap_{j,q}^0} \cdot \left( \frac{Cap_{j,q}}{cap_{j,q}^0} \right)^{sf} + \sum_{p} \sum_{j} \sum_{q} c_{p} \cdot \varphi_{p} \cdot Woq_{p,j,q}$$ (35)

where $c_{p,j,q}$ is the variable cost factor associated with biorefinery $j$ with technology $q$; $\varphi_{p}$ is the unit conversion factor for biofuel $p$; $Woq_{p,j,q}$ is the amount of biofuel $p$ to produce in biorefinery $j$ via technology $q$.

As mentioned in the assumptions of Section 3.1, there is an external market with sufficient biomass supply and biofuel demand. If the planned biomass acquisition amount ($W_{b,j}$) is not satisfied by the local suppliers, the biorefineries can purchase additional biomass feedstock from external markets at the unit price of $pr_{b}$, which is often much higher than those offered to the local suppliers.

$$C_{ex-acq} = \sum_{b} \sum_{j} pr_{b} \left( W_{b,j} - \sum_{i} F_{b,i} \right)$$ (36)

If the total local biofuel demand is lower than the planned biofuel production amount ($W_{p,j}$), the surplus amount of biofuel can be sold to external markets at the unit price of $pr_{p}$, which is typically lower than those to the local customers.

$$C_{ex-sa} = \sum_{p} \sum_{j} pr_{p} \left( W_{p,j} - \sum_{k} F_{p,k,j} \right)$$ (37)

The following constraint states that at most one technology can be selected at a certain biorefinery.

$$\sum_{q} X_{j,q} \leq 1, \quad \forall j$$ (38)

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

Local policies and regulations may restrict the number of biorefineries with a certain technology, which is modeled by,

$$\sum_{q} X_{j,q} \leq num_{j}, \quad \forall q$$ (39)

The biofuel production amount cannot exceed the installed capacity. On the other hand, the conversion processes in a biorefinery should not be kept idle for a long period of time. These relationships are given by:

$$\varphi_{p,j} \cdot Cap_{j,q} \leq \sum_{p} \varphi_{p} \cdot Woq_{p,j,q} \leq Cap_{j,q}, \quad \forall j, q$$ (40)
where \(\theta_{b,j,q}\) is the minimum utilization rate of the biorefinery capacity.

If biorefinery \(j\) with technology \(q\) is built, its capacity must lie between the specified lower \((c_{L,j,q}^l)\) and upper \((c_{L,j,q}^u)\) bounds. If the biorefinery is not installed, its capacity should be zero.

\[
\begin{align*}
    c_{L,j,q}^l \cdot X_{j,q} \leq \text{Cap}_{j,q} \leq c_{L,j,q}^u \cdot X_{j,q}, & \quad \forall j, q
\end{align*}
\]

To facilitate the presentation of the model, we employ two auxiliary variables \(W_{iqb,j,q}\) and \(W_{opq,j,q}\). The former stands for the consumption amount of biomass \(b\) at biorefinery \(j\) via technology \(q\), and the latter stands for the production amount of biofuel \(p\) at biorefinery \(j\) via technology \(q\). Constraints (42) and (43) indicate that if the biorefinery is not installed, the corresponding \(W_{iqb,j,q}\) and \(W_{opq,j,q}\) should be zero.

\[
\begin{align*}
    W_{iqb,j,q} \leq w_{U,j,q}^b \cdot X_{j,q}, & \quad \forall b, j, q
\end{align*}
\]  
\[
\begin{align*}
    W_{opq,j,q} \leq w_{U,j,q}^p \cdot X_{j,q}, & \quad \forall p, j, q
\end{align*}
\]

where \(w_{U,j,q}^b\) and \(w_{U,j,q}^p\) are the upper bounds for biomass consumption and biofuel production, respectively.

The total amount of biomass \(b\) procured by biorefinery \(j\) is equal to the sum of biomass consumption via all technology options. Similarly, the total amount of biofuel \(p\) sold by biorefinery \(j\) is equal to the sum of biofuel production via all technology options. These mass balance relationships are given by constraints (44) and (45), respectively.

\[
\begin{align*}
    \sum_{q} W_{iqb,j,q} = W_{ib,j}, & \quad \forall b, j
\end{align*}
\]  
\[
\begin{align*}
    \sum_{q} W_{opq,j,q} = W_{op,j}, & \quad \forall p, j
\end{align*}
\]

A linear model is assumed for the conversion from biomass to biofuel at the biorefineries, as given by:

\[
\begin{align*}
    W_{iqb,j,q} = x_{b,p,j,q} \cdot W_{opq,j,q}, & \quad \forall b, p, j, q
\end{align*}
\]

where \(x_{b,p,j,q}\) is the conversion factor regarding the conversion from biomass \(b\) to biofuel \(p\) at biorefinery \(j\) via technology \(q\).

The variables in the biorefinery investor’s problem are summarized below, where both nonnegative continuous variables and binary 0-1 variables are involved.

\[
\begin{align*}
    P_{b,j}, P_{p,j}, C_{p,j,q}, W_{ib,j}, W_{op,j}, W_{iqb,j,q}, W_{opq,j,q} \geq 0; & \quad X_{j,q} \in (0, 1)
\end{align*}
\]  
\[\text{(47)}\]

A3. The biofuel customer’s problem

We also formulate an optimization problem for each customer, since every individual customer in the supply chain is considered to be an independent player. Given the locations, biomass price offers, and procurement plans of the biorefineries determined in the leader’s problem, each supplier maximizes its own profit \((\text{Obj}_{b,i}^{\text{sup}})\) after anticipating the decisions of other competing suppliers, as given by (48).

\[
\text{max} \quad \text{Obj}_{b,i}^{\text{sup}} = \sum_{b} \sum_{j} (P_{b,j} - c_{b,i} - c_{ijb,i,j})F_{ib,j,i}, & \quad \forall i
\]

where the profit margin for selling a unit of biomass \(b\) to biorefinery \(j\) is equal to the difference between the biomass acquisition price \((P_{b,j})\) and the costs of harvesting \((c_{b,i})\) and transportation \((c_{ijb,i,j})\). If the profit margin is nonnegative, the transaction is considered profitable for supplier \(i\).

The total amount shipped to all the biorefineries cannot exceed the biomass availability at supplier \(i\). This relationship is given by:

\[
\sum_{j} F_{ib,j,i} \leq a_{b,i}, & \quad \forall b, i
\]

where \(a_{b,i}\) stands for the amount of biomass \(b\) available at supplier \(i\).

The following constraint (50) is shared by all suppliers. It states that the total amount of biomass \(b\) shipped from all suppliers to a biorefinery \(j\) should not exceed the planned amount of procurement at biorefinery \(j\). From supplier \(i\)'s perspective, the decisions of other suppliers \((F_{ib,j,i} \text{ for } i' \neq i)\) are exogenous to its optimization problem. Therefore, \(F_{ib,j,i}\) are treated as parameters in supplier \(i\)'s problem.

\[
\sum_{i} F_{ib,j,i} + \sum_{i' \neq i} F_{ib,j,i'} \leq W_{ib,j}, & \quad \forall b, i, j
\]

The only variable in supplier \(i\)'s problem is \(F_{ib,j,i}\) which should be nonnegative.

\[
F_{ib,j,i} \geq 0
\]

The leader’s decision variables \((P_{b,j} \text{ and } W_{ib,j})\) are considered to be given parameters in the suppliers’ optimization problems in the Stackelberg leader–follower game format. The decisions of other suppliers \((F_{ib,j,i} \text{ for } i' \neq i)\) are treated as constants from supplier \(i\)'s perspective under the assumption of generalized Nash equilibrium. Therefore, supplier \(i\)'s optimization problem is formulated as an LP.
The only variable in customer $k$’s problem is $F_{jkp,j,k}$, which should be non-negative.

$$F_{jkp,j,k} \geq 0 \quad (55)$$

The leader’s decision variables ($p_{p,j}$ and $W_{op,j}$) are similarly considered to be given parameters in the customers’ optimization problems in the Stackelberg leader–follower game format. The decisions of the other customers $F_{jkp,j,k}$ are viewed as constants from customer $k$’s perspective under the assumption of generalized Nash equilibrium. Therefore, we formulate customer $k$’s optimization problem into an LP as well.

### 4.4. MINLP formulation

To summarize, the biorefinery investor’s problem is considered to be the upper level problem, and the suppliers’ and customers’ problems are considered to be the lower level problems. The biorefinery investor’s problem includes the objective function (33) and constraints (34)–(47). Specifically, discrete variables are used to model the selection of biorefinery locations and conversion technologies. Power functions are used to capture the economies of scale in the capital cost. Bilinear terms are used to calculate the transfer payments between the biorefiners and the suppliers and customers. Therefore, the upper level problem is a nonconvex MINLP. The supplier’s problem includes the objective function (48) and constraints (49)–(51), while the customer’s problem includes the objective function (52) and constraints (53)–(55). Both the suppliers’ and the customers’ problems are formulated as LPs. We denote the above bilevel MINLP problem as (P0).

As mentioned in Section 4, since the lower level problems of (P0) are all LPs, one can replace these optimization problems with their corresponding KKT conditions. Let $\lambda_{b,i}$, $\lambda_{b,j}$, and $\lambda_{b,k}$ be the Lagrange multipliers for constraint (49)–(51), respectively. The KKT conditions corresponding to supplier $i$’s optimization problem are presented below.

$$c_{ijb,i} + c_{ib,i} - p_{ib,j} + \lambda_{b,i} + \lambda_{b,j} + \lambda_{b,k} = 0, \quad \forall b, i, j \quad (56)$$

$$\lambda_{b,i} (a_{ib,i} - \sum_{j} F_{ib,j}) = 0, \quad \forall b, i \quad (57)$$

$$\lambda_{b,j} (W_{ib,j} - \sum_{i} F_{ib,j}) = 0, \quad \forall b, j \quad (58)$$

$$\lambda_{b,k} F_{ib,j} = 0, \quad \forall b, i, j \quad (59)$$

$$\lambda_{b,i} \lambda_{b,j} \lambda_{b,k} \geq 0 \quad (60)$$

Constraint (56) is the stationarity constraint. Constraints (57)–(59) are the complementarity slackness constraints. Constraint (60) indicates the dual feasibility constraints. The primal feasibility constraints are the same as (49)–(51), thus not repeated here. We note that the Lagrange multiplier of the shared constraint $\lambda_{b,j}$ is identical for all the suppliers under the assumption of the normalized Nash equilibrium.

Similarly, let $\mu_{p,k}$, $\mu_{p,j}$, and $\mu_{p,k}$ be the Lagrange multipliers of constraint (53)–(55), respectively. The KKT conditions corresponding to customer $k$’s optimization problem are presented below.

$$p_{p,j} + c_{jkp,j,k} - p_{p,k} + \mu_{p,k} + \mu_{p,j} - \mu_{p,k} = 0, \quad \forall p, j, k \quad (61)$$

$$\mu_{p,k} (d_{p,k} - \sum_{j} F_{jkp,j,k}) = 0, \quad \forall p, k \quad (62)$$

Constraint (61) is the stationarity constraint. Constraints (62)–(64) are the complementarity slackness constraints. Constraint (65) indicates the dual feasibility constraints. The primal feasibility constraints are the same as (53)–(55). Similar to the suppliers’ problems, the Lagrange multiplier of the shared constraint $\mu_{p,j}$ is identical for all the customers under the assumption of the normalized Nash equilibrium.

Therefore, by replacing the followers’ problems with their corresponding KKT conditions, we can transform the original bilevel MINLP problem into a single-level MINLP problem. We denote this single-level MINLP problem as (PS), which includes the objective function given in (33) subject to the constraints (34)–(47), (49)–(51), and (53)–(65). We note that, although the bilinear terms in the complementary slackness constraints (57)–(59) and (62)–(64) can be linearized by introducing a set of binary variables (see Section 4), the problem still includes non-convex nonlinear terms, including the bilinear terms in (33) and the power function in (34) and (35). The resulting single-level nonconvex MINLP might still be computationally intractable for large-scale applications.

### Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compchemeng.2014.08.010.

### References


Andersen FE, Diaz MS, Grossmann IE. Multiscale strategic planning model for the design of integrated ethanol and gasoline supply chain. AIChE J 2013;59:4655–72.


Dutta A, Talmadge M, Hensley J, Worley M, Dudgen D, Barton D, et al. Process design and economics for the conversion of lignocellulosic biomass to ethanol: thermo-
chemical pathway by indirect gasification and mixed alcohol synthesis. National

EIA. Fuel ethanol consumption estimates, 2012. U.S. Energy Information Admin-
istration. 2014.

El-Halwagi AM, Rosas C, Ponce-Ortega JM, Jiménez-Gutiérrez A, Manna MS,
El-Halwagi MM. Multibjective optimization of biorefineries with economic and

Elia JA, Baliban RC, Xiao X, Floudas CA. Optimal energy supply network determina-
tion and life cycle analysis for hybrid coal, biomass, and natural gas to liquid
(CBCTL) plants using carbon-based hydrogen production. Comput Chem Eng 2011;
35:1259–69.

EPA. Biomass combined heat and power catalog of technologies. U.S. Environmental

Facchinei F, Kanzow C. Generalized Nash equilibrium problems. 4OR

Fernandes Lj, Velas S, Barbosa-Póvoa AP. Strategic network design of downstream
petroleum supply chains: single versus multi-entity participation. Chem Eng Res

Gebreslassie BH, Yao Y, You F. Design under uncertainty of hydrocarbon biorefinery
supply chains: multibjective stochastic programming models, decomposi-
tion algorithm, and a comparison between CVaR and downside risk. AIChE J
2012;58:2155–79.

Giarola S, Zamboni A, Bezzo F. Spatially explicit multi-objective optimisation for
design and planning of hybrid first and second generation biorefineries. Comput

Gjerdum J, Shah N, Papageorgiou LG. Transfer prices for multiprertice supply

Gjerdum J, Shah N, Papageorgiou LG. Fair transfer price and inventory holding

Gong J, You F. Optimal design and synthesis of algal biorefinery processes for bio-
logical carbon sequestration and utilization with zero direct greenhouse gas
emissions: MINLP model and global optimization algorithm. Ind Eng Chem Res
2014;53:1563–79.

Grossmann IE. Enterprise-wide optimization: a new frontier in process systems engi-

Hasan M, Karimi I. Piecewise linear relaxation of bilinear programs using bivariate

economics for biochemical conversion of lignocellulosic biomass to ethanol:
dilute-acid pretreatment and enzymatic hydrolysis of corn stover. National

Kulkarni AA, Shanbhag UV. On the variational equilibrium as a refinement of the

Liu P, Georgiadis MC, Pistikopoulos EN. Advances in energy systems engineering.

McLean K, Li X. Robust scenario formulations for strategic supply chain optimization

Muñoz E, Capón-García E, Lainez JM, Espuña A, Puigjaner L. Integration of enterprise

Nagarajan M, Sościł G. Game-theoretic analysis of cooperation among supply chain


ODDIE. Biomass resource assessment and utilization options for three counties in

Osborne MJ, Rubinstein A. A course in game theory. Cambridge, Massachusetts: MIT

Osmanı A, Zhang J. Stochastic optimization of a multi-feedstock
lignocellulosic-based bioethanol supply chain under multiple uncertainties.

Padberg M. Approximating separable nonlinear functions via mixed zero-one pro-

Papageorgiou LG. Supply chain optimisation for the process industries: advances

Rosen JB. Existence and uniqueness of equilibrium points for concave n-person

Rosenthal RE. GAMS – a user’s guide. Washington, DC: CAMS Development Corp;
2011.

Ryu J-H, Dua V, Pistikopoulos EN. A bilevel programming framework for enterprise-

Santibañez-Aguilar JE, González-Campos JB, Ponce-Ortega JMA, Serna-González M,
El-Halwagi MM. Optimal planning of a biomass conversion system consid-
ering economic and environmental aspects. Ind Eng Chem Res 2011;50:
8558–70.

Searcy E, Flynn P, Ghafoori E, Kumar A. The relative cost of biomass energy transport.
Biofuels Bioprod Biorefining 2007;137–140.


Tawalalami M, Sahinidis NV. A polyhedral cutting-plane-and-cut approach to global opti-

Tong K, Gleeson MJ, Rong G, You F. Optimal design of advanced drop-in hydrocar-
bon biofuel supply chain integrating with existing petroleum refineries under

Tong K, Gong J, Yue D, You F. Stochastic programming approach to optimal design
and operations of integrated hydrocarbon biofuel and petroleum supply chains.

Tong K, You F, Rong G. Robust design and operations of hydrocarbon biofuel sup-
ply chain integrating with existing petroleum refineries considering unit cost

New York: Springer; 2010.

Yeh K, Lee JH, Whittaker C, Reafff MJ. Two stage bilevel programming approach
for representation of biorefinery investment decision making in a pre-established
timberland supply chain. In: Eden M, Sirola JD, Towler GP, editors. 8th
international conference on foundations of computer-aided process design.
Washington, USA: Cie Elm; 2014.

You F, Grossmann IE. Stochastic inventory management for tactical process planning

You F, Pinto JM, Grossmann IE, Megan L. Optimal distribution-inventory planning of
industrial gases. II. MINLP models and algorithms for stochastic cases. Ind Eng

You F, Tao L, Grazianno DJ, Snyder SW. Optimal design of sustainable cellulosic bio-
fuel supply chains: multibjective optimization coupled with life cycle assessment

You F, Wang B. Life cycle optimization of biomass to liquid supply chains with
distributed – centralized processing networks. Ind Eng Chem Res 2011;50:
10102–27.

Yue D, Kim MA, You F. Design of sustainable product systems and supply chains with
life cycle optimization based on functional unit: general modeling framework,
mixed-integer nonlinear programming algorithms and case study on hydrocar-

Yue D, You F. Planning and scheduling of flexible process networks under uncertainty
with stochastic inventory: MINLP models and algorithms. AIChE J 2013;
59:1511–32.

Yue D, You F. Fair profit allocation in supply chain optimization with transfer price
and revenue sharing: MINLP model and algorithm for cellulosic biofuel supply

Yue D, You F, Snyder SW. Biomass-to-bioenergy and biofuel supply chain optimiza-

Zamarripa MA, Aguirre AM, Méndez CA, Espuña A. Improving supply chain planning

Zamarripa MA, Aguirre AM, Méndez CA, Espuña A. Mathematical programming and
game theory optimization-based tool for supply chain planning in coopera-

Zhang D, Samsatli NJ, Hawkes AD, Brett DJL, Shah N, Papageorgiou LC. Fair elec-
tricity transfer price and unit capacity selection for microgrids. Energy Econ