Design of Biofuel Supply Chains with Variable Regional Depot and Biorefinery Locations

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Abstract. We propose a multi-period mixed-integer linear programming (MILP) model for the design and operational planning of cellulosic biofuel supply chains. Specifically, the proposed MILP model accounts for biomass selection and allocation, technology selection and capacity planning at regional depots and biorefineries. Importantly, it considers the location of regional depots and biorefineries as continuous optimization decisions. We introduce reformulation methods for the calculation of the shipments and transportation distance in order to obtain a linear model. We illustrate the applicability of the proposed methods using a two medium-scale examples with realistic data.

Keywords: Cellulosic ethanol; biorefinery; mathematical programming; optimization; reformulation.

1 Introduction

Renewable energy can play an important role in reducing our dependence on fossil fuels, mitigating climate impacts and increasing energy security. In 2014, electricity generation from biomass accounts for 12% of all renewable energy generated in the United States [1]. In addition to heat and power generation, cellulosic biomass can be converted into biofuels (e.g., ethanol, biodiesel, “drop-in” fuels, etc.) via various technologies. Based on the REmap 2030 analysis report published by the International Renewable Energy Agency [2], the total biofuel production in the United States is expected to be 39 billion gallons.

Process systems engineering (PSE) methods have been widely applied for the design and operation planning of biofuel supply chains (SCs) [3–7], as well as the design of integrated biorefineries [8–11]. Most of the proposed SC optimization model employ economic criteria and consider a single period [12,13]. The introduction of multi-period models allows the modeling of seasonal biomass availability and biomass deterioration [14–16]. Furthermore, environmental [17,18] and social considerations [19,20] have been studied. Finally, several approaches have been proposed for the optimization of biofuel SCs under uncertainty; for example, stochastic programming [21,22], chance constraint programming [23], and robust optimization [24] methods.

Two aspects that have received limited attention are (1) the consideration of local depots for biomass densification and/or pretreatment, and (2) the selection of the location of depots and biorefineries. Specifically, most previous approaches either neglect the installation of depots or consider depots that are co-located with harvesting sites and, furthermore, are based on the assumption that biorefineries can only be installed at predefined locations that meet certain criteria (e.g., population census, transportation network, etc.) [25,26]. However, the efficiency of the biofuel SC, in terms of both cost and CO₂ emissions, can be improved by the installation of depots and the *optimization* of depot and biorefinery location (e.g., the optimal depot location can be between two harvesting sites) [27–29]. Recently, Ng and Maravelias proposed the first optimization model to account for depot installation and variable depot location [30]. However, the proposed mixed-integer non-linear programming (MINLP) model is computationally expensive and cannot be used to address medium- and large-scale problems.

Accordingly, the goal of this paper is to propose a computationally tractable multi-period mixed-integer linear programming (MILP) model that accounts for biomass selection and allocation, technology selection and capacity planning at depots and biorefineries, inventory and shipment planning, and, importantly, variable depot and biorefinery locations. The reduction of the computational requirements is achieved through a series of approximation and reformulations.

The rest of this article is structured as follows: In Section 2, we present background on biofuel SC, a formal problem statement, and the assumptions used for the formulation of the model. In Section 3, we present a basic optimization model, while in Section 4 we describe several model enhancements. In Section 5, we present two examples to illustrate the applicability of our methods. We close in Section 6 with concluding remarks. We use lowercase Greek letters for parameters; Latin letters for variable; lowercase Latin italic letters for subscripts; and uppercase U/L in superscript for upper/lower bounds.

2 Background

2.1 Cellulosic Biofuel Supply Chain

Biomass feedstocks are harvested and potentially stored at harvesting sites. Biomass can be either shipped to a biorefinery or a regional depot where it is pretreated and/or densified into a stable and dense intermediate. The primary function of the regional depot is to allow the densified biomass to be transported economically over longer distance, thus improving the overall SC economics and reducing CO₂ emissions [31]. Regional depots can be categorized as *standard* and *quality* depots [32]. The primary function of the former is to dry and densify biomass via mechanical and thermal processing technologies such as grinding, drying and pelleting. In the latter, in addition to drying and

densification, biomass is converted into intermediates that meet specific biorefinery needs. Pretreatment technologies that have low operating and capital costs, simple catalyst recovery and produce an intermediate that reduces processing intensity at the biorefinery can be considered [31]; e.g., ammonia fiber explosion (AFEX) [33], dilute acid [34], alkaline peroxide [35]. Pretreated and/or densified biomass can be stored at a depot before it is sent to the biorefinery. At the biorefinery, biomass and intermediate can be converted into biofuel via biochemical [36], thermochemical [37,38] and catalytic [39,40] platforms.

2.2 Problem Statement

In this work, we consider a one-year horizon divided into time periods $t \in \mathbf{T}$, though a multi-year horizons can also be considered. We are given biomass feedstocks (e.g., corn stover and switchgrass) at the harvesting site, intermediates produced at depots (e.g., AFEX-treated pellets), intermediates at the biorefinery, and a product (ethanol). Biomass can be converted to intermediates and ethanol through different technologies, including drying and densification with or without AFEX pretreatment at the depot. The unit production cost and conversion yield of all technologies are known. The locations of harvesting sites and biomass availability at each site and time period are given, while the locations of depots and biorefineries are optimization decisions. The unit costs associated with feedstock acquisition, inventory, and transportations are known. We are also given the regions within which potential biorefineries can be installed and the upper and lower bounds on ethanol demand.

Formally, the problem we consider is stated in terms of the following sets, subsets and parameters:

- a) Compounds $i \in \mathbf{I}$ with unit price λ_i , unit inventory costs ι_i and fixed/variable transportation unit cost κ_i^F / κ_i^V .
 - i. Biomass feedstocks $\mathbf{I}^F \subset \mathbf{I}$ at harvesting sites.
 - ii. Intermediates $\mathbf{I}^{ID} \subset \mathbf{I}$ produced at depots.
 - iii. Intermediates $\mathbf{I}^{IB} \subset \mathbf{I}$ produced at biorefineries.
 - iv. Products $\mathbf{I}^P \subset \mathbf{I}$ with minimum $\beta_{i,t}^L$ and maximum $\beta_{i,t}^U$ product demand.
 - v. By-products $\mathbf{I}^B \subset \mathbf{I}$.
- b) Harvesting sites $j \in \mathbf{J}$ with x -Cartesian coordinate x_j , y -Cartesian coordinate y_j , and biomass availability $\alpha_{i,j,t}$.
- c) Potential depots $k \in \mathbf{K}$ with variable locations.
- d) Potential biorefineries $l \in \mathbf{L}$ with variable locations within certain region.
- e) Technologies $m \in \mathbf{M}$ with unit production cost μ_m and conversion coefficient $\eta_{i,i',m}$.
 - i. Pretreatment/densification technologies at depots $\mathbf{M}^{PD} \subset \mathbf{M}$.
 - ii. Pretreatment technologies at biorefineries $\mathbf{M}^{PB} \subset \mathbf{M}$.

iii. Conversion technologies $\mathbf{M}^{\text{CB}} \subset \mathbf{M}$.

Our goal is to determine the optimal number, capacity, and location of depots and biorefineries, as well as the production, inventory, and shipment profiles of all SC nodes such that the total annual cost is minimized.

2.3 Assumptions

It is assumed that all biomass at the harvesting site will be shipped to the depots/biorefineries if the harvesting site is selected in the SC optimization model. This assumption can be easily relaxed by dividing a site into multiple *sub-sites* and thereby allowing the selection of a fraction of the availability of the site. For example, a county (a unit for which biomass availability data are typically available) can be divided into rectangular or square cells (sub-sites).

Furthermore, we assume that the biomass from a harvesting site is sent to only one downstream node, either a depot or a biorefinery; and, similarly, the intermediates from a depot are shipped to a single biorefinery. While better solutions can be obtained, in theory, by shipping to multiple nodes and/or continuously changing the destination of shipments coming from the same SC node, it is difficult to implement such “dynamic” operation in practice [30]. Thus, the second assumption is realistic.

It is further assumed that no biomass feedstock is stored at depots and biorefineries, and no intermediates are stored at biorefineries. Rather, biomass is stored at harvesting sites only and intermediates at depots only. This assumption has minimal effect because inventory unit costs and material deterioration coefficients are practically independent of location, which means that the solutions we obtain equivalent and representative of a family of solutions. Furthermore, in general, material storage at the origin is preferred because material losses occur before transportation and thus result in lower transportation cost.

3 Basic Model

In this section, we present a basic model for the design of biofuel SC with regional depots. We introduce the following binary variables:

- $W_j/W_k/W_l = 1$ if harvesting site j /depot k /biorefinery l is selected.
- $U_{k,m}/U_{l,m} = 1$ if technology m at depot k /biorefinery l is selected.
- $Z_{j,k}/Z_{j,l}/Z_{k,l} = 1$ if transportation along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ is selected.

and the following nonnegative continuous variables:

- $S_{i,j,t}/S_{i,k,t}/S_{i,l,t}$: inventory level of compound i at SC node $j/k/l$ at the end of period t .
- $F_{i,j,k,t}/F_{i,j,l,t}/F_{i,k,l,t}$: amount of compound i shipped along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ during period t .

- 133 • $G_{i,k,m,t}^{\text{F-PD}}$: consumption of compound $i \in \mathbf{I}^{\text{F}}$ by technology $m \in \mathbf{M}^{\text{PD}}$ at depot k during period t .
- 134 • $P_{i,k,m,t}^{\text{ID-PD}}$: production of compound $i \in \mathbf{I}^{\text{ID}}$ by technology $m \in \mathbf{M}^{\text{PD}}$ at depot k during period t .
- 135 • $G_{i,l,m,t}^{\text{F-PB}}$: consumption of compound $i \in \mathbf{I}^{\text{F}}$ by technology $m \in \mathbf{M}^{\text{PB}}$ at biorefinery l during period t .
- 136 • $G_{i,l,m,t}^{\text{IB-CB}}$: consumption of $i \in \mathbf{I}^{\text{IB}}$ by technology $m \in \mathbf{M}^{\text{CB}}$ at biorefinery l during period t .
- 137 • $G_{i,l,m,t}^{\text{ID-PB}}/G_{i,l,m,t}^{\text{ID-CB}}$: consumption of $i \in \mathbf{I}^{\text{ID}}$ by technology $m \in \mathbf{M}^{\text{PB}}/\mathbf{M}^{\text{CB}}$ at biorefinery l during
- 138 period t .
- 139 • $P_{i,l,m,t}^{\text{IB-PB}}$: production of $i \in \mathbf{I}^{\text{IB}}$ by technology $m \in \mathbf{M}^{\text{PB}}$ at biorefinery l during period t .
- 140 • $P_{i,l,m,t}^{\text{IPB-CB}}$: production of $i \in \mathbf{I}^{\text{P}}/\mathbf{I}^{\text{B}}$ by technology $m \in \mathbf{M}^{\text{CB}}$ at biorefinery l during period t .
- 141 • $L_{i,l,t}$: total sales of $i \in \mathbf{I}^{\text{P}} \cup \mathbf{I}^{\text{B}}$ from biorefinery l during period t .
- 142 • $Q_{k,m}/Q_{l,m}$: capacity of technology m at depot k /biorefinery l .
- 143 • x_k^*/x_l^* : x -Cartesian coordinate of depot k /biorefinery l .
- 144 • y_k^*/y_l^* : y -Cartesian coordinate of depot k /biorefinery l .
- 145 • $D_{j,k}/D_{j,l}/D_{k,l}$: length (distance) along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$.
- 146 • $\bar{D}_{j,k}/\bar{D}_{j,l}/\bar{D}_{k,l}$: disaggregated real variables for $D_{j,k}/D_{j,l}/D_{k,l}$.
- 147 • $\check{D}_{j,k}/\check{D}_{j,l}/\check{D}_{k,l}$: disaggregated dummy variables for $D_{j,k}/D_{j,l}/D_{k,l}$.
- 148 • $\bar{D}_{k,l-j}/\check{D}_{k,l-j}$: disaggregated real/dummy variables for $\bar{D}_{k,l}$ with respect to harvesting site j .
- 149 • $\bar{D}_{k,l-j,m}$: disaggregated real variable for $\bar{D}_{k,l}$ with respect to harvesting site j and technology m .
- 150 The constraints of the model are presented in the next subsections.

151 3.1 Material Balance

152 The material balance at a harvesting site, depot, and biorefinery is illustrated in Figure 1.

153 3.1.1 Harvesting sites

154 The biomass inventory at the harvesting site at the end of time period, $S_{i,j,t}$ is equal to the inventory
 155 at the end of the previous period after considering biomass deterioration, plus the availability of
 156 biomass, minus the shipments to other SC nodes (depots or biorefineries):

$$157 S_{i,j,t} = S_{i,j,t-1}(1 - \gamma_{i,t}) + \alpha_{i,j,t} W_j - \sum_k F_{i,j,k,t} - \sum_l F_{i,j,l,t}, \quad i \in \mathbf{I}^{\text{F}}, j, t \quad (1)$$

158 where $\gamma_{i,t}$ is material loss factor of compound i during time period t . If $W_j = 1$, harvesting site j is
 159 selected to ship compound i to depots or biorefineries (when $W_j = 0$, biomass in harvesting site j may
 160 be used for other purposes, e.g., animal feed).

161 3.1.2 Depots

162 The inventory of biomass at the depot at the end of time period, $S_{i,k,t}$ is given by:

$$163 S_{i,k,t} = S_{i,k,t-1}(1 - \gamma_{i,t}) + \sum_j F_{i,j,k,t} - \sum_{m \in \mathbf{M}^{\text{PD}}} G_{i,k,m,t}^{\text{F-PD}}, \quad i \in \mathbf{I}^{\text{F}}, k, t \quad (2)$$

164 Since, there is no biomass inventory at the depot (see assumptions in Section 2.3), $S_{i,k,t} = S_{i,k,t-1} =$
 165 0, and equation 2 can be simplified as follows:

Figure 1: Material balance.

$$\sum_j F_{i,j,k,t} = \sum_{m \in \mathbf{M}^{PD}} G_{i,k,m,t}^{F-PD}, \quad i \in \mathbf{I}^F, k, t \quad (3)$$

The production $P_{i',k,m,t}^{ID-PD}$ of intermediates $i' \in \mathbf{I}^{ID}$ is determined by:

$$P_{i',k,m,t}^{ID-PD} = \sum_{i \in \mathbf{I}^F} \eta_{i,i',m} G_{i,k,m,t}^{F-PD}, \quad i' \in \mathbf{I}^{ID}, k, m \in \mathbf{M}^{PD}, t \quad (4)$$

The inventory balance of intermediates at the depot is given as:

$$S_{i,k,t} = S_{i,k,t-1}(1 - \gamma_{i,t}) + \sum_{m \in \mathbf{M}^{PD}} P_{i,k,m,t}^{ID-PD} - \sum_l F_{i,k,l,t}, \quad i \in \mathbf{I}^{ID}, k, t \quad (5)$$

3.1.3 Biorefineries

Similarly, there is no biomass/intermediate inventory at the biorefinery (see assumptions in Section 2.3), which means that the mass balance of biomass and intermediate can be written as follows (see Figure 1):

$$\sum_j F_{i,j,l,t} = \sum_{m \in \mathbf{M}^{PB}} G_{i,l,m,t}^{F-PB}, \quad i \in \mathbf{I}^F, l, t \quad (6)$$

$$\sum_k F_{i,k,l,t} = \sum_{m \in \mathbf{M}^{PB}} G_{i,l,m,t}^{ID-PB} + \sum_{m \in \mathbf{M}^{CB}} G_{i,l,m,t}^{ID-CB}, \quad i \in \mathbf{I}^{ID}, l, t \quad (7)$$

where biomass, $G_{i,l,m,t}^{F-PB}$ is sent for pretreatment; and intermediates can be split into consumption level for pretreatment technologies, $G_{i,l,m,t}^{ID-PB}$, and conversion technologies, $G_{i,l,m,t}^{ID-CB}$, respectively. For example, densified biomass from the standard depot ($G_{i,l,m,t}^{ID-PB}$) need to be pretreated prior to ethanol. Pretreated densified biomass produced at the quality depot ($G_{i,l,m,t}^{ID-CB}$) on the other hand can be sent for ethanol production directly.

For pretreatment technology $m \in \mathbf{M}^{PB}$ (purple box in Figure 1), the production $P_{i',l,m,t}^{IB-PB}$ of intermediates $i' \in \mathbf{I}^{IB}$ is given by:

$$P_{i',l,m,t}^{\text{IB-PB}} = \sum_{i \in \mathbf{I}^{\text{F}}} \eta_{i,i',m} G_{i,l,m,t}^{\text{F-PB}} + \sum_{i \in \mathbf{I}^{\text{ID}}} \eta_{i,i',m} G_{i,l,m,t}^{\text{ID-PB}}, \quad i' \in \mathbf{I}^{\text{B}}, l, m \in \mathbf{M}^{\text{PB}}, t \quad (8)$$

The consumption $G_{i,l,m,t}^{\text{IB-CB}}$ of intermediates $i \in \mathbf{I}^{\text{B}}$ by technologies $m \in \mathbf{M}^{\text{CB}}$ is given by:

$$\sum_{m \in \mathbf{M}^{\text{CB}}} G_{i,l,m,t}^{\text{IB-CB}} = \sum_{m \in \mathbf{M}^{\text{PB}}} P_{i,l,m,t}^{\text{IB-PB}}, \quad i \in \mathbf{I}^{\text{B}}, l, t \quad (9)$$

For conversion technologies $m \in \mathbf{M}^{\text{CB}}$ (orange box in Figure 1), all intermediates $i \in \mathbf{I}^{\text{ID}} \cup \mathbf{I}^{\text{B}}$ are converted into products or by-products $i' \in \mathbf{I}^{\text{P}} \cup \mathbf{I}^{\text{B}}$; their production level, $P_{i',l,m,t}^{\text{IPB-CB}}$, is calculated as follows:

$$P_{i',l,m,t}^{\text{IPB-CB}} = \sum_{i \in \mathbf{I}^{\text{ID}}} \eta_{i,i',m} G_{i,l,m,t}^{\text{ID-CB}} + \sum_{i \in \mathbf{I}^{\text{B}}} \eta_{i,i',m} G_{i,l,m,t}^{\text{IB-CB}}, \quad i' \in \mathbf{I}^{\text{P}} \cup \mathbf{I}^{\text{B}}, l, m \in \mathbf{M}^{\text{CB}}, t \quad (10)$$

The mass balance of both products and by-products is given by:

$$S_{i,l,t} = S_{i,l,t-1} + \sum_{m \in \mathbf{M}^{\text{CB}}} P_{i,l,m,t}^{\text{IPB-CB}} - L_{i,l,t}, \quad i \in \mathbf{I}^{\text{P}} \cup \mathbf{I}^{\text{B}}, l, t \quad (11)$$

The total sales, $L_{i,l,t}$, are bounded within lower and upper target levels:

$$\beta_{i,t}^{\text{L}} \leq \sum_l L_{i,l,t} \leq \beta_{i,t}^{\text{U}}, \quad i \in \mathbf{I}^{\text{P}}, t \quad (12)$$

3.2 Capacity Constraints

The following constraints enforce the installation of exactly one pretreatment technology and one conversion technology at the installed depots and biorefineries, respectively:

$$\sum_{m \in \mathbf{M}^{\text{PD}}} U_{k,m} = W_k, \quad k \quad (13)$$

$$\sum_{m \in \mathbf{M}^{\text{CB}}} U_{l,m} = W_l, \quad l \quad (14)$$

where W_k/W_l are binary variables for the installation of depot k /biorefinery l , and $U_{k,m}/U_{l,m}$ indicate the selection of technology m at k/l . In addition, pretreatment technology may not be necessary at the biorefinery if all biomass is sent to quality depot.

$$\sum_{m \in \mathbf{M}^{\text{PB}}} U_{l,m} \leq W_l, \quad l \quad (15)$$

The operating capacity of technology m at depot k , $Q_{k,m}$ and biorefinery l , $Q_{l,m}$ are constrained as follows:

$$\epsilon_m^{\text{L}} U_{k,m} \leq Q_{k,m} \leq \epsilon_m^{\text{U}} U_{k,m}, \quad k, m \in \mathbf{M}^{\text{PD}} \quad (16)$$

$$\epsilon_m^{\text{L}} U_{l,m} \leq Q_{l,m} \leq \epsilon_m^{\text{U}} U_{l,m}, \quad l, m \in \mathbf{M}^{\text{PB}} \cup \mathbf{M}^{\text{CB}} \quad (17)$$

where $\epsilon_m^{\text{L}}/\epsilon_m^{\text{U}}$ are lower/upper bounds on capacity.

Consumption levels are constrained by the installed capacities, $Q_{k,m}$ and $Q_{l,m}$ as follows:

$$\sum_{i \in \mathbf{I}^{\text{F}}} G_{i,k,m,t}^{\text{F-PD}} \leq Q_{k,m}, \quad k, m \in \mathbf{M}^{\text{PD}}, t \quad (18)$$

$$\sum_{i \in \mathbf{I}^{\text{ID}}} G_{i,l,m,t}^{\text{ID-CB}} + \sum_{i \in \mathbf{I}^{\text{B}}} G_{i,l,m,t}^{\text{IB-CB}} \leq Q_{l,m}, \quad l, m \in \mathbf{M}^{\text{CB}}, t \quad (19)$$

$$\sum_{i \in \mathbf{I}^{\text{ID}}} G_{i,l,m,t}^{\text{ID-PB}} + \sum_{i \in \mathbf{I}^{\text{F}}} G_{i,l,m,t}^{\text{F-PB}} \leq Q_{l,m}, \quad l, m \in \mathbf{M}^{\text{PB}}, t \quad (20)$$

3.3 Connectivity Constraints

It is assumed that each harvesting site sends biomass feedstock to only one downstream node and each depot sends intermediates to only one biorefinery:

$$\sum_k Z_{j,k} + \sum_l Z_{j,l} = W_j, \quad j \quad (21)$$

$$\sum_l Z_{k,l} = W_k, \quad k \quad (22)$$

where $Z_{j,k}/Z_{j,l}/Z_{k,l}$ are arc selection binary variables. If an arc is selected ($Z = 1$), then the corresponding flows can be nonzero:

$$\sum_i F_{i,j,k,t} \leq \chi_{j,k}^U Z_{j,k}, \quad j, k, t \quad (23)$$

$$\sum_i F_{i,j,l,t} \leq \chi_{j,l}^U Z_{j,l}, \quad j, l, t \quad (24)$$

$$\sum_i F_{i,k,l,t} \leq \chi_{k,l}^U Z_{k,l}, \quad k, l, t \quad (25)$$

where $\chi_{j,k}^U/\chi_{j,l}^U/\chi_{k,l}^U$ are upper bounds on total shipments and can be calculated from biomass availability data.

3.4 Cyclic Inventory

The concept of “cyclic” inventory balance is adopted to ensure the operations can be carried out in the next year and to avoid the underestimation of inventory cost. The inventory level at the beginning ($t = 0$) and end ($t = |T|$) of the horizon should be the same: $S_{i,j,t=0} = S_{i,j,t=|T|}$, $S_{i,k,t=0} = S_{i,k,t=|T|}$ and $S_{i,l,t=0} = S_{i,l,t=|T|}$.

3.5 Harvesting Site, Depot and Biorefinery Locations

Based on the Rhumb Line concept [41], the latitude and longitude of harvesting sites can be converted to the x - and y -Cartesian coordinates by projecting an oblate spheroid into a flat image. It is assumed that the coordinates for harvesting sites (x_j, y_j) are constants, whereas the coordinates for all depots (x_k^*, y_k^*) and biorefineries (x_l^*, y_l^*) are variables. The coordinates of the depot are constrained as follows:

$$x_k^* \leq x^U W_k, \quad k \quad (26)$$

$$y_k^* \leq y^U W_k, \quad k \quad (27)$$

where x^U/y^U are upper bounds of the studied region. When the depot is not selected, x_k^* and y_k^* will return to the value of 0.

The location of a biorefinery at certain city/town/village can be predetermined based on population, the available transportation network, and other factors. Most approaches in the literature, assume that potential biorefinery locations are predefined at, for example, the centroid of the selected region (gold star in Figure 2). However, a biorefinery can be installed at various points within the selected region. For example, as Figure 2 shows, it may be beneficial to be installed near the border of the

region. If the coordinates of the vertices of the region (squares in figure 2) are available, then the coordinates of the biorefinery are subject to the following convex hull constraints:

$$x_l^* = \sum_o \rho_{l,o} x_{l,o} + \epsilon(1 - W_l), \quad l \quad (28)$$

$$y_l^* = \sum_o \rho_{l,o} y_{l,o} + \epsilon(1 - W_l), \quad l \quad (29)$$

$$\sum_o \rho_{l,o} = W_l, \quad l \quad (30)$$

where $\rho_{l,o} \in [0, 1]$; $x_{l,o}/y_{l,o}$ are the coordinates of the vertices (black box). Parameter ϵ can be assumed as the midpoint of the potential biorefinery region. When the potential biorefinery is not selected, x_l^* and y_l^* will return to the value of ϵ . If the constraints defining the regions, rather than the coordinates of the vertices are available, the Quickhull Algorithm [42] can be used to calculate the coordinates of the vertices. Nonconvex regions can also be represented but at a higher computational cost.

Figure 2: Area of potential biorefinery. Orange star is the coordinate of potential biorefinery assumed in previous works. Square boxes are the coordinates of the vertices defining the convex hull of the selected region (red dashed line). White boxes are the discarded interior points.

3.6 Transportation Distance

The distance between two locations can be estimated based on flow path distance, great-circle distance, Euclidean distance, rectilinear distance, etc. The rectilinear distance is a good estimation of the transportation distance in the United States as the US interstate highway and the state roadway systems are often developed based on approximate rectilinear patterns. The rectilinear distance between two locations, $D_{j,k}$ is modeled by:

$$D_{j,k} = \Delta x_{j,k} + \Delta y_{j,k}, \quad j, k \quad (31)$$

where the absolute values of horizontal distance, $\Delta x_{j,k}$, and vertical distance, $\Delta y_{j,k}$ can be obtained by the following inequalities (two of which will become binding since the optimization tries to minimize distance):

$$\Delta x_{j,k} \geq x_j - x_k^*, \quad j, k \quad (32)$$

$$\Delta x_{j,k} \geq -(x_j - x_k^*), \quad j, k \quad (33)$$

$$\Delta y_{j,k} \geq y_j - y_k^*, \quad j, k \quad (34)$$

$$\Delta y_{j,k} \geq -(y_j - y_k^*), \quad j, k \quad (35)$$

Similar equations (Equations 31 – 35) can be applied to determine $D_{j,l}$ and $D_{k,l}$. Note that positive values of $D_{j,k}$, $D_{j,l}$, and $D_{k,l}$ are calculated even if the depot or the biorefinery are not selected.

3.7 Total Annual Cost

The total annual cost, TAC is calculated by:

$$TAC = \sum_t (C_t^{\text{FEED}} + C_t^{\text{PROD}} + C_t^{\text{INV}} + C_t^{\text{TRANS}}) + v C^{\text{CAPEX}} \quad (36)$$

where $C_t^{\text{FEED}}/C_t^{\text{PROD}}/C_t^{\text{INV}}/C_t^{\text{TRANS}}$ are feedstock/production/inventory/transportation costs during period t ; C^{CAPEX} is the total capital cost for depots and biorefinery installation; and v is a capital recovery factor.

The detailed formulations of the cost components are given as follows:

$$C_t^{\text{FEED}} = \sum_{i,j} \lambda_i \alpha_{i,j,t} W_j, \quad t \quad (37)$$

$$C_t^{\text{PROD}} = \sum_{i,k,m} \mu_m G_{i,k,m,t}^{\text{F-PD}} + \sum_{i,l,m} \mu_m (G_{i,l,m,t}^{\text{F-PB}} + G_{i,l,m,t}^{\text{ID-PB}} + G_{i,l,m,t}^{\text{ID-CB}} + G_{i,l,m,t}^{\text{IB-CB}}), \quad t \quad (38)$$

$$C_t^{\text{INV}} = \sum_i l_i (\sum_j S_{i,j,t} + \sum_k S_{i,k,t} + \sum_l S_{i,l,t}), \quad t \quad (39)$$

$$C_t^{\text{TRANS}} = \sum_{i,j,k} [(\kappa_i^{\text{F}} + \kappa_i^{\text{V}} D_{j,k}) F_{i,j,k,t}] + \sum_{i,j,l} [(\kappa_i^{\text{F}} + \kappa_i^{\text{V}} D_{j,l}) F_{i,j,l,t}] + \sum_{i,k,l} [(\kappa_i^{\text{F}} + \kappa_i^{\text{V}} D_{k,l}) F_{i,k,l,t}], \quad t \quad (40)$$

$$C^{\text{CAPEX}} = \sum_{k,m} C_{k,m}^{\text{CAPEX}} + \sum_{l,m} C_{l,m}^{\text{CAPEX}} \quad (41)$$

where $C_{k,m}^{\text{CAPEX}}/C_{l,m}^{\text{CAPEX}}$ is capital cost of technology m at depot k /biorefinery l . Note that the capital cost of each technology follows a nonlinear relationship to account for the economies of scale. A piecewise linearization is applied to obtain these capital costs (see Supplementary Material).

4 Model Reformulation

4.1 Approximation of Feedstock Shipment

The basic formulation (Equations 1 – 35) and cost equations (Equations 36 – 39, 41) in the proposed models are linear, except the bilinearities ($D_{j,k} F_{i,j,k,t}$, $D_{j,l} F_{i,j,l,t}$, and $D_{k,l} F_{i,k,l,t}$) in the calculation of transportation cost (Equation 40). In this work, we have to consider the optimal depot and biorefinery locations which means that the depot and biorefinery locations, and therefore the distances, are variables. Nonetheless, based on the assumptions discussed in Section 2.3, we can develop an approximation and reformulation that will allow us to replace variables F with constants. Specifically, since all biomass of type $i \in \mathbf{I}^{\text{F}}$ from selected harvesting site j is eventually shipped to a depot or biorefinery, we can replace the sum $\sum_{k,t} F_{i,j,k,t} + \sum_{l,t} F_{i,j,l,t}$ with $\sum_t \alpha_{i,j,t}$. The timing of the shipment can be ignored since all biomass will always be shipped. Thus, at the harvesting site, $\alpha \times D$

can be used to replace the terms of $F \times D$. A small error though is introduced because the actual shipments will be slightly lower than $\sum_t \alpha_{i,j,t}$ due to biomass deterioration during storage. An approximation of this error can be calculated prior to optimization based on some extreme inventory profiles. Specifically, for arc $j \rightarrow k / j \rightarrow l$, $F_{i,j,k,t}$ and $F_{i,j,l,t}$ can be replaced by the availability $\alpha_{i,j,t}$ of biomass feedstock $i \in \mathbf{I}^F$ multiplied by correction factor δ_i (see Figure 3), which represents the ratio of output (biomass shipment to the depot/biorefinery) over input (total availability of biomass).

Figure 3: Approximation of amount of feedstock shipment

Figure 4: Harvested biomass and shipment. Positive bar indicates biomass availability; negative bar indicates biomass shipment. Inventory levels at the end of each period shown as black boxes. The ratios for biomass shipment and availability for Figure 4a, b, and c are 1, 0.875, and 0.944, respectively.

For example, consider the one-year harvesting, shipment and resulting inventory profiles at the harvesting site shown in Figure 4. We assume that 100 kt of biomass is available annually, 60% of it is harvested during period 1 and the remaining is harvested during period 2. We further assume that biomass deteriorates at a 5% rate per period. If biomass is directly shipped to the depot (Figure 4a), the inventory levels are zero and therefore the ratio (correction) is equal to 1 ($\delta_i = 1$). In the other extreme, all biomass is stored at the harvesting site and shipped at the end of the year ($t = 4$) as shown

in Figure 4b. The highest inventory level, obtained at the end of period 2, is 92.5 kt instead of 100 kt due to biomass losses and the total shipment is 87.5 kt. In this case, the total losses are 12.5 kt (100 – 87.5), and therefore $\delta_i = 0.875$. If biomass is shipped at a constant rate throughout the year (Figure 4c), then $\delta_i = 0.944$. As we will see in Section 5, the loss rate is significantly smaller, leading to correction factors larger than 0.95. Based on these calculations, we can choose the average value or a correction factor that corresponds to what we think is a reasonable inventory profile.

The flow, $F_{i',k,l,t}$, of intermediate $i' \in \mathbf{I}^{\text{ID}}$ from depot k to biorefinery l can be calculated based on the flow from the harvesting site, $F_{i,j,k,t} \approx \delta_i \alpha_{i,j,t}$ according to our approximation, multiplied by the conversion factor $\eta_{i,i',m}$ (see Equations 3 and 4). Thus, after deterioration due to storage at the depot, the shipment of intermediate to the biorefinery can be approximated by $\zeta_{i'} \eta_{i,i',m} \delta_i \alpha_{i,j,t}$ where $\zeta_{i'}$ is the correction factor for intermediate storage losses at the depot. Similarly, $\zeta_{i'}$ can be precalculated based on the ratio of intermediate shipment to the biorefinery and biomass consumption at the depot. The accuracy of the correction factors we use can be checked post optimization using the exact biomass/intermediate shipments obtained.

4.2 Transportation Distance

Based on the reformulation described in the previous subsection, the approximate shipments of biomass/intermediates is always non-zero ($\delta_i \alpha_{i,j,t}$ or $\zeta_{i'} \eta_{i,i',m} \delta_i \alpha_{i,j,t}$). Therefore, to correctly calculate transportation cost, these values should be multiplied by zero distance if the corresponding arcs ($Z_{j,k}/Z_{j,l}/Z_{k,l}$) are not selected. To address this, we disaggregate all distance components into actual, $\bar{D}_{j,k}/\bar{D}_{j,l}/\bar{D}_{k,l}$, and dummy, $\check{D}_{j,k}/\check{D}_{j,l}/\check{D}_{k,l}$, distance variables:

$$D_{j,k} = \bar{D}_{j,k} + \check{D}_{j,k}, \quad j, k \quad (42)$$

$$D_{j,l} = \bar{D}_{j,l} + \check{D}_{j,l}, \quad j, l \quad (43)$$

$$D_{k,l} = \bar{D}_{k,l} + \check{D}_{k,l}, \quad k, l \quad (44)$$

subject to the following variable upper bound constraints:

$$\bar{D}_{j,k} \leq \tau_{j,k}^U Z_{j,k}, \quad j, k \quad (45)$$

$$\check{D}_{j,k} \leq \tau_{j,k}^U (1 - Z_{j,k}), \quad j, k \quad (46)$$

$$\bar{D}_{j,l} \leq \tau_{j,l}^U Z_{j,l}, \quad j, l \quad (47)$$

$$\check{D}_{j,l} \leq \tau_{j,l}^U (1 - Z_{j,l}), \quad j, l \quad (48)$$

$$\bar{D}_{k,l} \leq \tau_{k,l}^U Z_{k,l}, \quad k, l \quad (49)$$

$$\check{D}_{k,l} \leq \tau_{k,l}^U (1 - Z_{k,l}), \quad k, l \quad (50)$$

where $\tau_{j,k}^U/\tau_{j,l}^U/\tau_{k,l}^U$ are upper bounds on distance. When an arc is selected ($Z = 1$) the dummy variables become zero via Equations. (46), (48), and (50). Therefore, the real distance equals to

calculated distance ($\bar{D}_{j,k} = D_{j,k}$). In contrast, $\bar{D}_{j,k} = 0$ if the arc is not selected. For example, HS1 in Figure 5a is selected to provide biomass to the depot. $\bar{D}_{\text{HS1},\text{D1}}$ (red line) is equal to $D_{\text{HS1},\text{D1}}$ as $\check{D}_{\text{HS1},\text{D1}}$ is forced to be zero (Equation 46). When $Z = 0$, $\bar{D} = 0$, and D will equal to $\check{D}$. For instance, HS2 is not selected to provide biomass to the depot, $\bar{D}_{\text{HS2},\text{D1}} = 0$ and $\check{D}_{\text{HS2},\text{D1}} = D_{\text{HS2},\text{D1}}$ (gray line). Note that only real variables, $\bar{D}_{j,k}$, $\bar{D}_{j,l}$, and $\bar{D}_{k,l}$ (color lines) will be considered in the cost calculation.

Figure 5: (a) Disaggregated real distances. Color/white boxes represent the SC node is selected and not selected, respectively. Real distances are shown in red and blue lines whereas dummy distances are shown in gray lines. (b) Disaggregated variables for $\bar{D}_{k,l}$.

As mentioned earlier, $F_{i',k,l,t}$ can be approximated by $\zeta_{i'}\eta_{i',m}\delta_i\alpha_{i,j,t}$. In order to calculate transportation cost from k to l accurately, $\bar{D}_{k,l}$ is further disaggregated into $\bar{D}_{k,l-j,m}$ to trace the amount of biomass shipped from site j and densified through technology m :

$$\bar{D}_{k,l} = \bar{D}_{k,l-j} + \check{D}_{k,l-j}, \quad j, k, l \quad (51)$$

$$\bar{D}_{k,l-j} = \sum_{m \in \mathbf{M}^{\text{PD}}} \bar{D}_{k,l-j,m}, \quad j, k, l \quad (52)$$

where disaggregated variables are subject to:

$$\bar{D}_{k,l-j} \leq \tau_{k,l}^U Z_{j,k}, \quad j, k, l \quad (53)$$

$$\check{D}_{k,l-j} \leq \tau_{k,l}^U (1 - Z_{j,k}), \quad j, k, l \quad (54)$$

$$\bar{D}_{k,l-j,m} \leq \tau_{k,l}^U U_{k,m}, \quad j, k, l, m \in \mathbf{M}^{\text{PD}} \quad (55)$$

In the example shown in Figure 5b, technology of PD2 is selected at the depot. For biomass shipped from HS1, $\bar{D}_{\text{D1},\text{B1}-\text{HS1},\text{PD2}} = \bar{D}_{\text{D1},\text{B1}-\text{HS1}} = \bar{D}_{\text{D1},\text{B1}}$. Note that $\bar{D}_{\text{D1},\text{B1}-\text{HS1},\text{PD1}} = 0$ since only one technology is selected at the depot. On the other hand, for HS2, $\bar{D}_{\text{D1},\text{B1}-\text{HS2}}$ is equal to zero as no biomass from HS2 is shipped to D1.

4.3 Revised Transportation Cost

Based on the reformulations introduced in the previous subsections, transportation cost can be calculated based on the total shipments, and the latter can be treated as parameters, thereby resulting in a linear transportation cost estimation:

$$C_t^{\text{TRANS}} = \sum_{i,j,k} [\kappa_i^F F_{i,j,k,t} + \kappa_i^V (\delta_i \alpha_{i,j,t}) \bar{D}_{j,k}] + \sum_{i,j,l} [\kappa_i^F F_{i,j,l,t} + \kappa_i^V (\delta_i \alpha_{i,j,t}) \bar{D}_{j,l}] + \sum_{i,k,l} \kappa_i^F F_{i,k,l,t} + \sum_{i,i',j,k,l,m} \kappa_{i'}^V (\zeta_{i'} \eta_{i',m} \delta_i \alpha_{i,j,t}) \bar{D}_{k,l-j,m}, t \quad (56)$$

4.4 Tightening Constraints

The total amount of biomass shipped from a harvesting site to a depot is bounded by multiples of the total availability of biomass and the selection binary for arc $j \rightarrow k$.

$$\sum_{i,t} \pi_i \alpha_{i,j,t} Z_{j,k} \leq \sum_{i,t} F_{i,j,k,t} \leq \sum_{i,t} \alpha_{i,j,t} Z_{j,k}, \quad j, k \quad (57)$$

where π_i is the correction factor based on the worst case scenario. For example, in Figure 4, the upper bound is set to 100 kt. The worst case scenario is when all biomass is stored at the harvesting site and shipped at the end of the year (Figure 4b). Therefore, $\pi_i = 0.875$ resulting in a lower bound of 87.5 kt.

Similarly, we can write variable lower/upper bounding constraints for the total amount of biomass shipped to a biorefinery:

$$\sum_{i,t} \pi_i \alpha_{i,j,t} Z_{j,l} \leq \sum_{i,t} F_{i,j,l,t} \leq \sum_{i \in I^F,t} \alpha_{i,j,t} Z_{j,l}, \quad j, l \quad (58)$$

The total shipments out of a harvesting site can also be variable lower/upper bounded as follows:

$$\sum_{i,t} \pi_i \alpha_{i,j,t} W_j \leq \sum_{i,k,t} F_{i,j,k,t} + \sum_{i,l,t} F_{i,j,l,t} \leq \sum_{i,t} \alpha_{i,j,t} W_j, \quad j \quad (59)$$

Finally, the lower bounds of transportation distance are added into the model and given by:

$$\tau_{j,l}^L \leq D_{j,l}, \quad j, l \quad (60)$$

$$\tau_{j,l}^L Z_{j,l} \leq \bar{D}_{j,l}, \quad j, l \quad (61)$$

where $\tau_{j,l}^L$ is minimum distance between arc j and l , and it can be predetermined from the minimum distance between harvesting site and the vertices of the potential biorefinery location.

4.5 Relative Error Calculation

Based on the biomass shipments obtained from the optimal/best solution, we can post-calculate the “real” TAC and then the relative error:

$$\%error = \frac{TAC^{\text{real}} - TAC^{\text{approx}}}{TAC^{\text{real}}} \times 100\% \quad (62)$$

where TAC^{approx} is the approximate value and TAC^{real} is the real value.

5 Applications

We present two examples based on the same region, Southern Wisconsin. We consider two types of biomass: corn stover (CS) and switchgrass (SG), both of which are abundant in the selected region. The availability of biomass is extracted from the US Department of Agriculture [43] and the Energy Biosciences Institute [44]. Candidate biorefinery locations were restricted to cities with populations between 3,000 and 10,000 in 2014 for a maximum of one biorefinery per county [45] and total biomass availability more than 120,000 ton per year. The latitude and longitude of harvesting sites and potential biorefineries are converted to Cartesian coordinates based on the Rhumb Line concept [41]. *Infeasible* areas due to geographical impediment (e.g., lakes, reserved forests) are excluded from the studied region during preprocessing. The rectilinear distance measurement method is used to estimate the distance. Both CS and SG are harvested at the site during summer and fall. We consider four time periods (spring, summer, fall and winter).

Collected CS and SG are sent for cutting and shredding, windrowing and baling prior to transporting to the depot/biorefinery. The capacity of the depot is set between 100 and 200 dry t/d. Economics of larger depot may not improve as it costs more to transport the biomass at a larger distance. We consider two technologies at the depot. In the first technology (DD), CS and SG are dried, densified, and pelletized directly without any chemical or physiochemical pretreatment. CS pellets (CSP) and SG pellets (SGP) are the intermediates produced by the technology DD. In the second technology (AFEXDD), CS and SG are pretreated via ammonia fiber explosion prior to densification. CS AFEX pellet (CSAP) and SG AFEX pellet (SGAP) are produced by the technology AFEXDD. At the biorefinery, we consider one pretreatment technology, AFEX; and two conversion technologies, simultaneous saccharification and fermentation (SSCF) and separate hydrolysis and fermentation (SHCF). Untreated biomass and intermediates (CS, SG, CSP and SGP) are pretreated via AFEX. The pretreated biomass and intermediate (CSA and SGA) produced at the biorefinery, CSAP, and SGAP are further processed in either SSCF or SHCF for ethanol production.

It is assumed that the material loss factors of CS/SG, CSP/SGP, and CSAP/SGAP for on-site storage are 1.5%, 0.7% and 0.2% every three months, respectively. Based on the availability of biomass at each period, the correction factors δ_i and ζ_i are precalculated. The ranges of correction factor for compounds are $\delta_{CS}/\delta_{SG} \in [0.961, 1]$, $\zeta_{CSP}/\zeta_{SGP} \in [0.982, 1]$, and $\zeta_{CSAP}/\zeta_{SGAP} \in [0.995, 1]$. In this study, it is assumed that the correction factors are the average values: $\delta_{CS}/\delta_{SG} = 0.981$, $\zeta_{CSP}/\zeta_{SGP} = 0.991$, and $\zeta_{CSAP}/\zeta_{SGAP} = 0.997$. We further assume that depots and biorefineries operate 85 days during every period. An annual discount rate of 10% and a project lifetime of 25 years are considered for the calculation of the annualized capital cost. The detailed descriptions of the cost and conversion data are provided in the Supplementary Material [29,32,46–51]. Note that all costs are indexed to 2014 dollars and calculated based on dry mass basis. We present two examples in next sub-sections.

5.1 Example 1

We consider a biofuel SC in South Central Wisconsin (215 km × 120 km) that includes Columbia, Dane, Dodge, Grant, Green, Iowa, Jefferson, Lafayette, Richland, Rock, and Sauk counties. Based on the preliminary screening, four potential biorefinery locations (Oregon Village, Columbus, Mayville and Beloit) are identified. For this example, we identify only two biorefineries which are located near to the center of studied region: Oregon Village and Columbus. At most three depots can be installed in the studied region. We discretize these 11 counties into 64 cells (Figure 6). The minimum ethanol demand is assumed to be 340 million L/y. Our objective is to minimize *TAC*. The resulting MILP model, which consists of 431 binary variables and 8,030 continuous variables, was implemented in GAMS [52] and solved using CPLEX.

The best solution was found after 3,405 CPU seconds with an optimality gap equal to 0.43%. The minimum total annual cost obtained is \$ 251.44 million. Figure 6 illustrates the optimal locations of the depots and the biorefinery. As shown, for the harvesting sites (light red regions) which are located near the biorefinery, direct biomass shipments are chosen. As the distance between the harvesting sites and the biorefinery increases (e.g., sites located at light blue regions), the transportation cost of direct biomass shipment increases and at some point becomes larger than the depot cost (capital and operating) plus the intermediate transportation cost. Thus, depots at the light blue regions are selected to convert biomass to a higher bulk density pellet. Two depots employing DD technologies are selected in Grant and Dodge counties. Specifically, the depots are installed at Far East Wyalusing and North East Iron Ridge with the capacities of 113 and 109 t/d, respectively. The biorefinery with AFEX and SHCF is installed at West Oregon village. Note that only half of the available biomass in Richland County is utilized.

The total biomass losses at the harvesting sites before shipped to the depots and the biorefinery are 1,387 t/y and 19,837 t/y, respectively which yield a total shipments:availability ratio equal to 0.982 and 0.983, respectively. At the depot, the overall loss is 785.3 t/y which leads to a ratio equal to 0.990. Note that the ratios calculated based on the actual shipment (0.982, 0.983, and 0.990) are very similar to the correction factors that were used (0.981, 0.991, 0.997). As a result, the transportation cost based on the calculated flows (USD 30.08 million) is less than 0.1% higher than the linearly approximated transportation cost (USD 30.06 million). Therefore, the “real” *TAC* is \$ 251.46 million, which is only 0.01% higher than the *TAC* obtained by the proposed model.

Figure 6: Best SC configuration for Example 1

For comparison purposes, we extended the MINLP model [30] to account for variable biorefinery locations and solved Example 1 using a resource limit of 15,000 CPU seconds. The best solution obtained using the extended MINLP model had a TAC of \$ 251.91 million (relative gap of 1.8%) which is worse than the solution obtained by the proposed model. The higher TAC was primarily due to the selection of three depots instead of two.

5.2 Example 2

We consider a biofuel SC in South Wisconsin (300 km × 200 km) that includes 32 counties (Adams, Calumet, Columbia, Crawford, Dane, Dodge, Fond du Lac, Grant, Green, Green Lake, Iowa, Jefferson, Juneau, Kenosha, La Crosse, Lafayette, Manitowoc, Marquette, Milwaukee, Monroe, Ozaukee, Racine, Richland, Rock, Sauk, Sheboygan, Vernon, Walworth, Washington, Waukesha, Waushara, and Winnebago). We divide the area into 194 cells and each cell has 9,500 to 13,000 t/y of CS and SG except for the counties with small biomass availability (e.g., Milwaukee and Ozaukee). The minimum ethanol demand is assumed to be 560 million L/y. Based on the preliminary screening, four potential biorefinery locations (Oregon Village, Columbus, Mayville and Beloit) are identified. In this example, Beloit is not included as a potential biorefinery location as it would lead to large transportation cost since it is near the state line between Wisconsin and Illinois. Our objective is to minimize *TAC*. To reduce the computational requirements, we partition the original problem into subproblems with fixed number of SC nodes. Each subproblem can be represented by a duplet, D.B, where D is the number of depots, and B denotes the selected biorefineries. For example, in instance D3.B0 we minimize the

TAC of a SC that consists of three depots and a biorefinery at Oregon Village. We combine nine options for depots: zero to nine depots (D0 to D9); and three options for biorefineries: Oregon Village (BO), Columbus (BC), and Mayville (BM). A total of 30 configurations is generated based on these options.

The best solution was found with eight depots and a biorefinery installed in Columbus (D8.BC). The relative gap is 1.06%. The minimum *TAC* is \$ 403.29 million. Figure 7 illustrates the optimal locations of the depots and the biorefinery. As shown, there are two depots to be installed in Grant County and one depot in six other counties (La Crosse, Monroe, Vernon, Lafayette, Calumet, and Manitowoc). For all depots, DDs with different capacities are installed. The area of biomass shipped to the depot is bounded by a red line. Part of biomass in La Crosse, Monroe and Grant counties are not selected for ethanol production. The biorefinery is located at South West Columbus. At the biorefinery, both AFEX and SSCF are selected for bioethanol production. Similar to Example 1, the *TAC* is recalculated (USD 403.48 million) based on the flow obtained in the best solution. The calculated *TAC* is only 0.05% higher than the approximate value obtained using the proposed model.

Figure 8 shows biomass availability, shipment, and inventory profiles at two different harvesting sites (Dodge and Lafayette counties). The distance between the harvesting sites and the biorefinery are 17 and 155 km, respectively. When the destination is close (Figure 8a), both CS and SG are shipped immediately. As the distance increases (Figure 8b), CS is stored (red dashed line) and only shipped during period 1. This is because as the distance increases, transportation cost increases, which means that it is more profitable to store for longer periods of time the biomass that was harvested further away because this will lead to lower total transportation cost. Please note that SG is sent for ethanol production directly during periods 2 and 3 in order to achieve minimum ethanol demand for each period.

Figure 9a shows biomass consumption (positive red bar) and production of pellets (blue bar) at the depot located at Layette County. We observe that production consumption is constant the year. This production profile leads to the smallest capital investment (for the same total production). Pellets are stored (blue dashed line) and shipped to the biorefinery during period 1 (50,000 t).

The consumption and production levels at the biorefinery are shown in Figure 9b. At the biorefinery, biomass and pellets are converted to ethanol at $t = 1$ whereas only biomass is used for ethanol production during the remaining periods. Note that no ethanol is stored (i.e., production = sales) which means that the biorefinery operates at full capacity during the entire year to maximize the utilization of expensive assets.

Figure 7: Best SC configuration for Example 2

Figure 8: Consumption, production, shipment, and inventory levels at the harvesting sites. Inventory of biomass is shown with red dashed line. Net biomass accumulation (availability – shipments) at the harvesting site (red bar).

Figure 9: Consumption and production levels at (a) the depot and (b) the biorefinery. Inventory of pellet is shown with blue dashed line. Biomass (red bar), net pellet accumulation (production – shipments) (blue bar), and ethanol (green bar) are shown.

6 Conclusions

The goal of this paper was to propose an MILP model that allows us to address larger-scale SC problems that are common in real-world applications. The proposed MILP model treats the locations of depots and biorefineries as optimization decisions. We proposed an approximation method for approximating the amount of biomass and intermediates of shipment. The correction factors can be precalculated based on the availability of biomass at certain period and its deterioration factor. We also reformulated the transportation distance and added tightening constraints in the proposed model. Furthermore, the proposed model can be revised to handle different features and practical considerations.

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546 Nomenclature

547 Sets

548	$i \in \mathbf{I}$	Compounds
549	$j \in \mathbf{J}$	Harvesting sites
550	$k \in \mathbf{K}$	Depots
551	$l \in \mathbf{L}$	Biorefineries
552	$m \in \mathbf{M}$	Technologies
553	$o \in \mathbf{O}$	Vertices
554	$t \in \mathbf{T}$	Time periods

555 Subsets

556	$\mathbf{I}^{\text{F/ID/IB/P/B}}$	Biomass feedstocks; intermediates produced at depots; intermediates produced at biorefineries; products; by-products
558	$\mathbf{M}^{\text{PD/PB/CB}}$	Pretreatment and/or densification technologies at depot; pretreatment technologies at biorefinery; conversion technologies at biorefinery

560 Parameters

561	$\alpha_{i,j,t}$	Availability of compound i at harvesting site j during period t (t)
562	$\beta_{i,t}^{\text{L}}/\beta_{i,t}^{\text{U}}$	Lower/upper bound on product demand during period t (t)
563	$\gamma_{i,t}$	Material loss factor of compound i during period t
564	δ_i/ζ_i	Correction factor for compound i
565	$\eta_{i,i',m}$	Conversion coefficient of compound i to compound i' by technology m
566	ι_i	Unit inventory cost of compound i (\$/t)
567	$\kappa_i^{\text{F}}/\kappa_i^{\text{V}}$	Fixed/variable unit transportation cost of compound i (\$/t or \$/t-km)
568	λ_i	Unit cost of compound i (\$/t)
569	μ_m	Unit production cost of technology m (\$/t)
570	ν	Capital recovery factor
571	x_j/y_j	Predefined x-/y-Cartesian coordinate of harvesting site j (km)
572	$x_{l,o}/y_{l,o}$	Coordinates of the vertices of a potential biorefinery l (km) location

573 Binary Variables

574	$U_{k,m}/U_{l,m}$	=1 if technology m at depot k /biorefinery l is selected
575	$W_j/W_k/W_l$	=1 if harvesting site j /depot k /biorefinery l is selected
576	$Z_{j,k}/Z_{j,l}/Z_{k,l}$	=1 if transportation along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ is selected

577 Continuous Nonnegative Variables

578	$\check{D}_{j,k}/\check{D}_{j,l}/\check{D}_{k,l}$	Disaggregated dummy variables for $D_{j,k}/D_{j,l}/D_{k,l}$ (km)
579	$\bar{D}_{j,k}/\bar{D}_{j,l}/\bar{D}_{k,l}$	Disaggregated real variables for $D_{j,k}/D_{j,l}/D_{k,l}$ (km)

580	$\bar{D}_{k,l-j,m}$	Disaggregated real variable for $\bar{D}_{k,l}$ with respect to harvesting site j and
581		technology m (km)
582	$\bar{D}_{k,l-j}/\check{D}_{k,l-j}$	Disaggregated real/dummy variables for $\bar{D}_{k,l}$ with respect to harvesting
583		site j (km)
584	$C^{\text{CAPEX}}/C_{k,m}^{\text{CAPEX}}/C_{l,m}^{\text{CAPEX}}$	Total capital cost; capital cost of technology m at depot k /biorefinery l (\$)
585	$C_t^{\text{FEED}/\text{INV}/\text{PROD}/\text{TRANS}}$	Feedstock/inventory/production/transportation costs during period t (\$)
586	$D_{j,k}/D_{j,l}/D_{k,l}$	Distance along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ (km)
587	$F_{i,j,k,t}/F_{i,j,l,t}/F_{i,k,l,t}$	Amount of compound i shipped along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ during period t
588		(t)
589	$G_{i,k,m,t}^{\text{F-PD}}$	Consumption level of compound $i \in \mathbf{I}^{\text{F}}$ by technology $m \in \mathbf{M}^{\text{PD}}$ at depot k
590		during period t . (t)
591	$G_{i,l,m,t}^{\text{F-PB}}$	Consumption level of compound $i \in \mathbf{I}^{\text{F}}$ by technology $m \in \mathbf{M}^{\text{PB}}$ at
592		biorefinery l during period t (t)
593	$G_{i,l,m,t}^{\text{IB-CB}}$	Consumption level of compound $i \in \mathbf{I}^{\text{IB}}$ by technology $m \in \mathbf{M}^{\text{CB}}$ at
594		biorefinery l during period t (t)
595	$G_{i,l,m,t}^{\text{ID-PB}}/G_{i,l,m,t}^{\text{ID-CB}}$	Consumption level of compound $i \in \mathbf{I}^{\text{ID}}$ by technology $m \in \mathbf{M}^{\text{PB}}/\mathbf{M}^{\text{CB}}$ at
596		biorefinery l during period t (t)
597	$L_{i,l,t}$	Total sales of compound $i \in \mathbf{I}^{\text{P}} \cup \mathbf{I}^{\text{B}}$ from biorefinery l during period t (t)
598	$P_{i,k,m,t}^{\text{ID-PD}}$	Production level of compound $i \in \mathbf{I}^{\text{ID}}$ by technology $m \in \mathbf{M}^{\text{PD}}$ at depot k
599		during period t (t)
600	$P_{i,l,m,t}^{\text{IB-PB}}$	Production level of compound $i \in \mathbf{I}^{\text{IB}}$ by technology $m \in \mathbf{M}^{\text{PB}}$ at
601		biorefinery l during period t (t)
602	$P_{i,l,m,t}^{\text{IPB-CB}}$	Production level of compound $i \in \mathbf{I}^{\text{P}}/\mathbf{I}^{\text{B}}$ by technology $m \in \mathbf{M}^{\text{CB}}$ at
603		biorefinery l during period t (t)
604	$Q_{k,m}/Q_{l,m}$	Capacity level of technology m at depot k /biorefinery l (t)
605	$S_{i,j,t}/S_{i,k,t}/S_{i,l,t}$	Inventory level of compound i at SC node $j/k/l$ at the end of time period t
606		(t)
607	x_k^*/x_l^*	x -Cartesian coordinate of depot k /biorefinery l (km)
608	y_k^*/y_l^*	y -Cartesian coordinate of depot k /biorefinery l (km)
609	$\Delta x_{j,k}/\Delta x_{j,l}/\Delta x_{k,l}$	Horizontal distance along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ (km)
610	$\Delta y_{j,k}/\Delta y_{j,l}/\Delta y_{k,l}$	Vertical distance along arc $j \rightarrow k/j \rightarrow l/k \rightarrow l$ (km)
611	TAC	Total annual cost (\$/y)

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