

Modeling Bioenergy Supply Chains:
Feedstocks Pretreatment, Integrated System Design Under Uncertainty

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ABSTRACT

Modeling Bioenergy Supply Chains: Feedstocks Pretreatment, Integrated System Design Under Uncertainty

Biofuels have been promoted by governmental policies for reducing fossil fuel dependency and greenhouse gas emissions, as well as facilitating regional economic growth. Comprehensive model analysis is needed to assess the economic and environmental impacts of developing bioenergy production systems. For cellulosic biofuel production and supply in particular, existing studies have not accounted for the inter-dependencies between multiple participating decision makers and simultaneously incorporated uncertainties and risks associated with the linked production systems.

This dissertation presents a methodology that incorporates uncertainty element to the existing integrated modeling framework specifically designed for advanced biofuel production systems using dedicated energy crops as feedstock resources. The goal of the framework is to support the bioenergy industry for infrastructure and supply chain development. The framework is flexible to adapt to different topological network structures and decision scopes based on the modeling requirements, such as on capturing the interactions between the agricultural production system and the multi-refinery bioenergy supply chain system with regards to land allocation and crop adoption patterns, which is critical for estimating feedstock supply potentials for the bioenergy industry. The methodology is also particularly designed to incorporate system uncertainties by using stochastic programming models to improve the resilience of the optimized system design.

The framework is used to construct model analyses in two case studies. The results of the California biomass supply model estimate that feedstock pretreatment via combined torrefaction and pelletization reduces delivered and transportation cost for long-distance biomass shipment by 5% and 15% respectively. The Pacific Northwest hardwood biofuels application integrates full-scaled supply chain infrastructure optimization with agricultural economic modeling and estimates that bio-jet fuels can be produced at costs between 4 to 5 dollars per gallon, and identifies areas suitable for simultaneously deploying a set

of biorefineries using adopted poplar as the dedicated energy crop to produce biomass feedstocks. This application specifically incorporates system uncertainties in the crop market and provides an optimal system design solution with over 17% improvement in expected total profit compared to its corresponding deterministic model.

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Chapter 1

Introduction

1.1 Motivation

Identifying and evaluating the potentials of using dedicated energy crops as feedstock sources for advanced biofuel production requires a comprehensive and quantitative assessment of system decisions from economic, environmental, and social dimensions. An integrated modeling framework that is able to capture all perspectives of the bioenergy production system from agricultural land and resource allocation, energy crop adoption, feedstock procurement and transportation to biorefineries, fuel production and distribution is important to help the decision makers accurately measure the performance of specific biofuel production pathways.

One of the challenges to develop economically efficient infrastructure systems for the bioenergy industry is to model its supply potentials. Specifically, understanding how the agricultural system will respond to the bioenergy industry's efforts in promoting dedicated energy crops is a key component for estimating the feedstock supply potentials and resource constraints.

Apart from assisting decision-making for the industry, like almost every research on alternative fuels, the system analysis approach in this dissertation is also critical to answering important policy-making questions, such as the effectiveness of existing biofuels policies, and within a specific policy framework, what the optimal amount of credit or subsidy should be to achieve social optimality.

Finally, a modeling framework that is able to properly measure and incorporate the uncertainty and risk associated with the bioenergy supply chain systems is crucial to the design of reliable hedging strategies. In this dissertation, methodologies based on supply chain network optimization approaches will be proposed and implemented to address various system design problems in bioenergy production systems, with uncertainty element incorporated via stochastic programming.

1.2 Literature Review

Biofuels as an alternative energy source for transportation has attracted the attention of both academic communities and industry due to its potential of reducing fossil fuel dependency and greenhouse gas emissions as well as facilitating regional economic growth. In order to deliver competitive fuel products to the end-user market, a well designed bioenergy supply chain infrastructure system based on quantitative-oriented analysis is essential. In this section, we provide an overview of existing literature on topics related to bioenergy supply chain models and approaches to address uncertainties in the system. In Section 1.2.1, we summarise general bioenergy supply chain modeling approaches for addressing sustainability issues. Section 1.2.2 provides an overview of bioenergy supply chain modeling frameworks that incorporate uncertainties and discusses relevant computational methods for solving large-scale optimization problems in these models.

To be clear, given the large number of research works on bioenergy supply chain problems from multiple academic communities (e.g., transportation and energy, management science, chemical engineering), this literature review is by no means exhaustive. Instead, this section selects research works that are representative and most relevant to the scope of the dissertation to the best of the author’s knowledge.

1.2.1 Modeling framework and sustainability issues in bioenergy supply chain

In general, a bioenergy supply chain network consists of feedstock suppliers, conversion refineries and distribution terminals for end users. A typical bioenergy supply chain model considers the following decision making processes: long-term strategic decisions include

selecting conversion technologies, refinery locations and production capacities that cannot be reversed easily; mid-term or short-term tactical decisions include feedstock handling, transportation and logistics, and fuel product distributions. Usually, tactical decisions are made seasonally or within a short period of time to allow the decision makers to take the most possible benefit under the constraints from the long-term strategic decisions.

There are several studies that considered the system decisions in the entirety of the bioenergy supply chain. Eksioglu et al. (2009) constructed a model to determine the optimal strategic decisions like the number, size and location of biorefineries, as well as tactical decisions such as the amount of biomass shipped, processed and inventoried during a time period. Parker et al. (2010) used a mixed-integer linear optimization model to determine the optimal locations, technology types and sizes of biorefineries seeking maximum profit across biofuel supply and demand chain from feedstock sites to product fuel terminals. Tittmann et al. (2010) provided a spatial-explicit techno-economic Bioenergy Siting Model to study the bioenergy production system in California, where decisions on facility siting and size, conversion technology, feedstock profile, and feedstock supply chain configuration for the year 2015 were optimized. Lin et al. (2014) designed a model to optimize strategic and tactical decisions simultaneously for minimizing annual biomass-ethanol production costs.

By the nature of bioenergy production systems, a variety of environmental issues could arise as a result of biofuels infrastructure deployment, such as greenhouse gas emissions, water consumption and pollution, soil degradation, and the loss of biodiversities. Social impact in the bioenergy supply chain development is also an important issue that affects the overall sustainability of the system. Awudu and Zhang (2012) summarized potential social sustainability impacts of bioenergy supply chain systems, which include poverty alleviation in the rural areas, agricultural land and crop indirect impacts, and impacts on social resources such as water.

Although there are few studies focusing on sustainability issues compared to those that emphasize economic aspect of bioenergy supply chains, several modeling works have been found to integrate sustainability concepts into the supply chain optimizations, either as

environmental and social constraints or as part of the performance measures in the model objectives. Murphy and Parker (2014) used a national Geospatial Bioenergy Systems Model (GBSM) to evaluate the effect of air pollution control costs on the U.S. biofuel production. You et al. (2012) developed a multi-objective mixed-integer linear programming model to address the optimal design and planning of cellulosic ethanol supply chains under economic, environmental, and social objectives, where the environmental objective is to minimize the life cycle greenhouse gas emissions, and the social objective is to maximize the number of accrued jobs in the community. Xie and Huang (2013) also developed a multi-objective modeling framework to seek best solutions that are economically and environmentally sustainable in supplying biofuels from cellulosic biomasses.

1.2.2 Addressing system uncertainties in bioenergy supply chains: modeling and solution approaches

Biofuels are different than conventional fuel products in various ways. In terms of uncertainties and risks of the production system, bioenergy production systems especially face challenges from availability risks in feedstock supply (Yano and Lee, 1995; Richardson et al., 2011), fluctuating demand and prices (Markandya and Pemberton, 2010; Chen and Fan, 2012), and evolving policy regulations (Yeh and Sperling, 2013) .

There are different approaches to measure and incorporate uncertainties in analyses for bioenergy systems. For example, sensitivity analysis is generally used to test how variation in the output of a mathematical model can be divided and attributed to different sources of uncertainty in its input parameters. Simulation techniques are often used to obtain empirical distributions of the desired random variable when closed-form solutions for the true probabilistic distribution is hard to obtain, such as the expected total amount of biomass feedstocks available considering uncertainties in climate and agricultural conditions. In the bioenergy supply chain management area, one major approach is to extend the deterministic mathematical optimization programs into stochastic modeling frameworks. Next, we'll review such literature on addressing uncertainties and risks in bioenergy supply chain system using stochastic programming, as well as some computational methods for solving large-scale stochastic models.

Santoso et al. (2005) developed a stochastic programming model for supply chain network design problems under uncertainty. It applied the sample average approximation (SAA) strategy with accelerated Benders' decomposition algorithm to solve large-scale problems with huge number of scenarios. Empirical results were used to demonstrate the computational efficacy of the proposed method.

Sodhi and Tang (2009) presented a stochastic programming supply chain planning (SCP) model that determines the purchase of supply inputs, production decisions at conversion plants, and product inventory and selling at single warehouse under uncertain demand. It compared stochastic linear programming models with asset-liability management (ALM) and surveyed various modeling and solution techniques, including decomposition, scenario aggregation sampling methods in the literature and discussed their applicability to SCP problems.

Chen and Fan (2012) established a mixed-integer stochastic programming model for a biofuel supply chain system. The model determined refinery locations and sizes, feedstock resource allocation and logistics, ethanol production plan and transportation decisions under feedstock and product demand uncertainties. Progressive Hedging (PH) method was applied as the decomposition algorithm to solve the model for the waste-based bio-ethanol production system in California.

Awudu and Zhang (2013) proposed a stochastic linear programming model for a biofuel supply chain planning problem under product demand and price uncertainties. The probability distribution of product demand was assumed to be known and the product prices were assumed to follow Geometric Brownian Motion. Benders' decomposition with Monte Carlo simulation technique was applied to solve a representative ethanol supply chain in North Dakota.

Li and Hu (2014) formulated a two-stage stochastic program to model an advanced biofuel supply chain that comprises feedstock suppliers, distributed small-scale fast pyrolysis plants for biomass pretreatment, centralized biorefineries and fuel demand locations. Uncertainties are represented by scenarios that take biomass yield, gasoline prices, pyrolysis conversion ratio and refinery conversion ratio together. A case study based on Iowa was

implemented and showed that the stochastic model outperformed the deterministic model in the uncertain environment, especially when there was insufficient biomass.

Built on the framework of Chen and Fan (2012), Huang et al. (2014) added feedstock seasonality components and proposed a stochastic mixed-integer linear program to evaluate the economic potentiality and system efficiency of converting corn stover and forest residues to ethanol in California. Feedstock supply uncertainties due to weather condition (for corn yields) and wild fires (for forest residues) were represented by constructing ten scenarios based on historical data. The PH algorithm was applied to address computational challenges involved in the large-scale application.

So far, all the studies mentioned in this section focused on optimizing the expected cost/utility of the modeled system, which is also known as risk-neutral objective in the broader field of stochastic programming. Although risk-neutral objectives are straightforward and relatively easy to formulate, the underlying assumption that decision makers hold no risk preferences (i.e., decision makers are assumed to favor a set of strategies equally as long as they have the same outcome in expectation, regardless of how different the probabilistic distributions of their outcomes could be) may not apply to all problems of system design under uncertainty. For example, in capital-intensive production systems such as bioenergy supply chains, apart from aiming at maximizing the expected profit which could be dominated by inputs under regular environment, a decision maker may also want robust infrastructure development plans that won't lead to substantial capital losses even in the most undesirable scenarios.

Recent studies in stochastic programming and relevant applications have shown an emergence of incorporating risk measures in stochastic optimization models. Common risk measures include variance (Mulvey et al., 1995; Yu and Li, 2000), downside risk (Value at Risk) (You et al., 2009), and conditional value at risk (CVaR) (Rockafellar and Uryasev, 2000; Gebreslassie et al., 2012).¹ The selection and construction of risk measures depend on specific modeling requirements, and are often determined based on domain knowledge and constrained by computational complexity.

¹Readers can refer to Shapiro and Philpott (2007) for detailed descriptions and examples for these risk measures.

1.3 Research Questions

The main focus of this dissertation is the development and enhancement of bioenergy supply chain modeling frameworks that particularly incorporate interdependent decision makers and uncertain model environments. The methodology is designed to be spatial-explicit and flexible in its topological and modeling structure to be able to adjust to the relevant decision-making and policy questions it is used to analyze.

The modeling framework will be implemented in the dissertation to explore economic potentials of developing bioenergy infrastructure systems using lignocellulosic biomass (e.g., forestry residues and dedicated energy crops) as feedstock resources. Key decision making processes such as agricultural land management and resource allocation will be integrated to the supply chain infrastructure models as part of the system decision outputs to be optimized and estimated. System uncertainty will be incorporated and addressed using mathematical approaches from the field of operations research such as stochastic programming. Specifically, the two case studies in this dissertation seek to answer the following questions:

- Can we use biomass pretreatment technologies such as torrefaciton and pelletization to enhance the feedstock procurement and transportation system, and significantly lower the delivered cost of biomass feedstocks?
- Considering its economic and environmental impacts on the existing agricultural system, is promoting dedicated energy crops a sustainable solution for the bioenergy industry to enhance its feedstock supply for large-scale biofuel production? And if so, what is the best development strategy for a multi-refinery infrastructure system, and what will be the cost of producing and delivering biofuels from such a system?
- For a crop-based biofuel production system, how would uncertainties in the agricultural market (i.e., prices of existing crops) affect farmers' decisions in crop adoption and land displacement? And how should the bioenergy industry develop robust infrastructure planning strategies to counter the variablities in farmers' responses to feedstock purchasing prices in an uncertain environment?

There are some additional important policy and methodological research questions that can be asked but are not included due to the limited scope of this dissertation, such as follows:

- What are the trade-offs between economic performance and environmental and social benefits of biofuels produced using dedicated energy crops as feedstock resources?
- How would developing biofuel production systems from dedicated energy crops change the alternative and conventional fuels market, and what are the policy implications?
- From the computational perspective, what are some examples of recent advancement in the field of mathematical optimization and algorithm design that can be applied in the models developed in the dissertation to improve the efficiency and computational scalability of the modeling framework?

These questions go beyond the scope of the dissertation and can be used as future research directions.

1.4 Organization

The remaining parts of the dissertation is organized as follows.

Chapter 2 lays out key methodology components of the dissertation, including mathematical optimization programs for agricultural modeling, supply chain network design problems, and two-stage mixed-integer stochastic programs. Both the mathematical concepts and generic formulations are provided.

In Chapter 3 and Chapter 4, two case studies utilizing the methodologies described in Chapter 2 are provided. Specifically, Chapter 3 considers potentials of improving forestry biomass supply system in California using combined torrefaction and pelletization for feedstock pretreatment. Chapter 4 presents a full-scale application of the integrated modeling framework for the Pacific Northwest region. The framework adopts a two-stage stochastic programming approach to incorporate uncertainty elements to an integrated system consisting of farmers and the bioenergy industry as separate decision makers who

optimize their own profits. The proposed methodology is shown to be able to find robust optimal system configurations in agricultural land allocation and biorefinery siting.

Chapter 5 concludes the dissertation by summarizing the main findings from the case studies, discussing the strengths and weaknesses of the present modeling approaches, and providing recommendations for future extensions.

Chapter 2

Methodology

Summary

The main methodological goals of this dissertation include building adaptable supply chain networks to model a variety of biomass and bioenergy production system design problems, and incorporating uncertainties and risks to the deterministic decision-making framework integrating agricultural economic modeling and supply chain network optimization by applying stochastic programming approaches. In this chapter, we present the mathematical theories and formulations of major building blocks of the methodology and framework. The chapter is structured as follows: Section 2.1 presents agricultural economic models from the literature that will be utilized in this dissertation. The developed model will output agricultural production and cropland allocation decisions that maximize the landowner's profit. Section 2.2 presents the bioenergy supply chain network models, where the integration between infrastructure siting strategies and agricultural land allocation decisions will be discussed; In Section 2.3, a stochastic modeling framework built for system decisions under uncertainty, and generic two-stage stochastic programming formulations will be provided.

2.1 Agricultural Economic Models

Identifying economically feasible locations for farmland displacement and establishing dedicated energy crops is a critical component in constructing a commercially sustainable

bioenergy supply chain system. The willingness of farmland owners to adopt energy crops depends on the cost of crop production, feedstock price offered by the biorefinery developers, and the opportunity cost of replacing incumbent crops or pasture and allocating lands and resources for energy crop growth.

Howitt (1995) developed a Positive Mathematical Programming (PMP) method for calibrating economic models of agricultural production and resource allocation using nonlinear yield parameters in the cost function. PMP-based models use regional-level (e.g., county, or specifically defined cropland management zones) historical cropping patterns as inputs to capture crop-specific marginal cost information as energy crops get accessioned to the regional crop portfolio and change the incumbent crop revenues.

As an example, the mathematical formulation of a PMP-based agricultural model in the form of the Biomass Crop Adoption Model was presented by Jenner and Kaffka (2012) as follows:

$$\underset{X_{i,\text{land}}}{\text{maximize}} \quad \sum_{i \neq \text{Energy}} \{ [P_i(\beta_i - \omega_i X_{i,\text{land}}) - C_i] \cdot X_{i,\text{land}} \} + \quad (2.1)$$

$$[P_{\text{Energy}} Y_{\text{Energy}} - C_i] \cdot X_{\text{Energy, land}} \quad (2.2)$$

$$\text{subject to} \quad \sum_i X_{i,j} \leq \bar{R}_j \quad \forall j \in \{\text{land, water}\} \quad (2.3)$$

Subscript $i \in I$ represents the regional crop portfolio including the energy crop (i.e., $i = \text{Energy}$), and $j \in J$ represents resources (i.e., land and water) required for crop production. As model parameters, P_i is the historical price of crop i , Y_i is the expected yield of the new energy crop, and C_i is the unit cost (e.g., dollar per acre) of crop i . The decision variable $X_{i,j}$ is the amount of resource j (land or water) to be used to produce crop i . And finally, the constraint variable \bar{R}_j is the maximum amount of resource j available in the region.

The BCAM model above maximizes the total crop revenues and finds the optimal land allocation strategy when energy crops are available to displace incumbent crops that are disadvantageous in generating profit. In the first part of the model objectives (2.1), a quadratic crop production function is employed to incorporate calibrated information from

the base cropping system in coefficient β and ω .

Apart from the quadratic production functions as applied in Medellín-Azuara et al. (2010) and Jenner and Kaffka (2012), the PMP methods can also take other nonlinear curvatures to constrain the cropping patterns and preserve the core relationship information between marginal values and resource supplies within the modeled cropping system. In particular, Howitt et al. (2012) developed a PMP-based economic model that utilized exponential PMP production functions which were shown to be able to fit more desired elasticity of resource supplies without forcing unrealistic marginal cost of production at low supply values.

2.2 Bioenergy Supply Chain Network Models

A bioenergy supply chain network consists of connected and interdependent components that are involved in the feedstocks supply, facility allocation, production and shipment of fuel products to distribution service centers. In this section, topological structures of the supply chain network and mathematical formulations of supply chain optimization models will be discussed.

2.2.1 Basic bioenergy supply chain network

On an abstract level, a supply chain can be modeled as directed graphs where major system components (e.g., feedstock supplier, refinery, product distributor) are represented by a set of nodes; these nodes are connected as directed arcs which represent flow of goods. From node to node and along the directed arcs, different types of goods (feedstocks, products) are collected, transported, consumed, stored, and sold. The goal of the supply chain is to maximize the overall value (i.e., net profit) generated from the network, with system resource constraints enforced on the nodes, and flow-conservation constraints on the directed arcs (Shapiro, 2007).

Figure 2.1 illustrates the network structure of a basic biofuel supply chain system. Biomass feedstocks are collected at feedstock locations, the feedstocks are then shipped to refinery plants for conversion, the fuel products are transported from these plants to demand terminals or fuel distribution centers. Typical decision variables in a biofuel

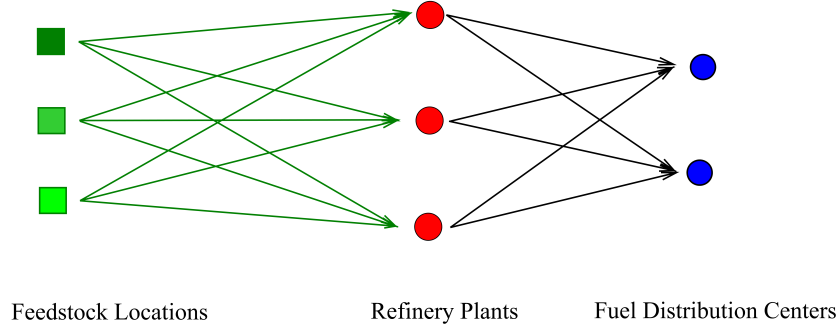


Figure 2.1: Schematic of basic bioenergy supply chain network

supply chain model include optimal refinery locations, feedstock procurement and shipment decisions, and fuel product transportation decisions. On the feedstock supply end, the basic model assumes that spatial-explicit supply curves are provided as inputs to model the procurement cost for different types of feedstocks under various supply quantities, and does not consider the competition among feedstocks, which by itself constitutes a separate decision-making problem.

This basic bioenergy supply chain network serves as a prototype and can be extended with different configurations based on the modeling requirements, which will be discussed in later sections.

2.2.2 Integrated bioenergy supply chain network incorporated with agricultural production models

The integrated modeling framework to which the stochastic programming approach will later be applied incorporates agricultural resource (i.e., land, water) allocation decisions as part of the supply chain system design, which is crucial for comprehensive evaluations of the economic and environmental performances of bioenergy production systems that are greatly influenced by cropland owners' decisions. There are several studies in the biofuel supply chain literature that have considered agricultural land allocation and feedstock market conditions using equilibrium models (Chen and Onal, 2012b,a) or game-theoretical models (Bai et al., 2012; Wang et al., 2013) to explore the behavioral interactions among decision-making agents in the system under a variety of assumptions, such of monopolistic biorefineries and cooperative games between farmers and the biofuels industry.

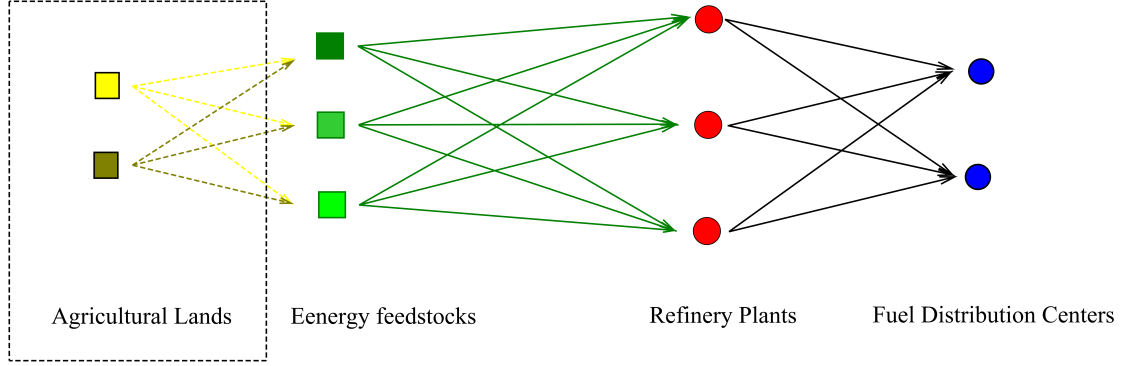


Figure 2.2: Schematic of integrated bioenergy supply chain incorporating agricultural land allocation decisions

As shown in Figure 2.2, the basic bioenergy supply chain as mentioned in Section 2.2.1 is expanded to incorporate agricultural land allocation decisions in the network. Unlike the solid-line arcs that represent shipment of physical goods (e.g., biomass and biofuel products) from feedstocks collection locations to biorefineries and to fuel distribution centers, the dash-line arcs connecting agricultural lands and energy feedstocks represent information in land allocation decisions. That is, dedicated energy feedstocks are only available when land allocation and crop adoption decisions are deemed beneficial for farmers to replace incumbent crops.

The methodology of the dissertation is an extension to previous works developed under the Advanced Hardwood Biofuels project (Parker, 2012; Bandaru et al., 2015; Li et al., 2016). The incorporation of agricultural resource allocation decisions to the bioenergy production system (Li et al., 2016; Bandaru et al., 2015) is implemented by cascading the agricultural economic model as discussed in Section 2.1 to the supply chain network model. Specifically, the agricultural model was used to generate spatial-explicit supply curves for biomass feedstocks under varying energy crop purchasing prices, and the corresponding land allocation decisions served as inputs to the supply chain network model to set up resource constraints to capture feedstocks availability. The integrated supply chain system was then optimized by maximizing the total profit of the biofuels industry while holding the assumption that farmers as individual decision makers would react to biofuels industry's pricing offers by making land allocation and crop displacement decisions to maximize their

own profit.

2.2.3 Mathematical models for bioenergy supply chains

The basic supply chain network in Figure 2.1 can be modeled by extending the canonical capacitated facility location problem (Conforti et al., 2014) by considering the cost and demand from the biofuel product distribution side, and formulated as mixed-integer programming models. Without loss of generality, here we consider the problem of minimizing the total cost of a supply chain infrastructure system in order to satisfy some fixed fuels demand at distribution terminals.

Table 2.1: Notations of the basic supply chain model

Name	Definition and Unit
Sets	
I	Index i , set of feedstock collection locations
J	Index j , set of candidate facility locations
K	Index k , set of fuel product distribution terminals
Decision Variables	
x_j	Whether to build a facility at i
y_{ij}	The amount feedstock transported from location i to facility j
z_{jk}	The amount fuel product transported from facility j to terminal k
Model Parameters	
f_j	Cost of opening a facility at j
c_{ij}	Unit feedstock transportation cost from i to j
d_{jk}	Unit fuel product transportation cost from j to k
u_j	Production capacity of facility opened at j
Continued on next page	

Table 2.1 – continued from previous page

Name	Definition and Unit
—	
v	Conversion ratio between product and resource, i.e., generating 1 unit of fuel product requires v amount of feedstocks
s_i	Maximum supply at location i
d_k	Demand at terminal k

With model indices, input parameters, and decision variables defined in Table 2.1, the mathematical formulation can be presented as follows:

$$\min_{x,y,z} \quad \sum_j f_j x_j + \sum_i \sum_j c_{ij} y_{ij} + \sum_j \sum_k d_{jk} z_{jk} \quad (2.4)$$

$$\text{s.t.} \quad \sum_j y_{ij} \leq s_i \quad \forall i \in I \quad (2.5)$$

$$\sum_j z_{jk} = d_k \quad \forall k \in K \quad (2.6)$$

$$\sum_i y_{ij} \geq v(u_j x_j) \quad \forall j \in J \quad (2.7)$$

$$\sum_k z_{jk} \leq u_j x_j \quad \forall j \in J \quad (2.8)$$

$$y_{ij} \geq 0, z_{jk} \geq 0 \quad \forall i \in I, \forall j \in J, \forall k \in K \quad (2.9)$$

$$x_j \in \{0, 1\} \quad \forall j \in J \quad (2.10)$$

The objective function (2.4) of the model is to minimize the total cost incurred in opening facilities and transporting feedstocks and fuel products. Constraint (2.5) limits the amount of feedstock collected at each location at its maximum supply. Constraint (2.6) ensures that demand at each terminal is satisfied. Constraint (2.7) guarantees fuel production at all opened facilities has sufficient feedstock provision. Constraint (2.8)

ensures that no product can be shipped from facility j unless it is open, and the total amount of fuels shipped from any facility won't exceed its capacity. Constraints (2.9) and (2.10) ensures proper supports (i.e., non-negativity and integrality) for decision variables are used.

The formulation defined by (2.5) - (2.10) for the basic supply chain network is a generic representation and can be detailed and modified to adapt to a wide variety of modeling scenarios. For instance, the case study in Chapter 3 of the dissertation uses a derivation of this formulation to model the feedstock supply part of the network. The application in Chapter 4 further extends the deterministic formulation by applying the stochastic programming approach to model system uncertainties, as will be discussed in Section 2.3.

The formulation of the integrated supply chain network as discussed in Section 2.2.2 is largely based upon the foundations of the Geo-spatial Biorefinery Siting Model (GBSM) developed by Parker (2011), which used a profit maximization approach instead of cost minimization, and was applied in multiple bioenergy system studies (Parker et al., 2010; Tittmann et al., 2010; Parker, 2012). The integration of GBSM with agricultural economic models such as BCAM (Jenner and Kaffka, 2012) was conceptualized by Bandaru et al. (2015) and formulated in detail by Li et al. (2016). From a mathematical modeling point of view, this integration was realized by adding agricultural land allocation and crop displacement decisions to the GBSM, and setting up model constraints on land resources and feedstock supplies to ensure the land use and crop displacement configurations from the GBSM result also comply with the optimal solutions obtained from the incorporated agricultural economic model. The integrated modeling framework extends the scope of the original GBSM by incorporating key system design decisions from the supply end (i.e., agriculture land allocation and energy crop adoption), which enables model users to better evaluate the economic sustainability of the overall bioenergy production system.

2.3 Stochastic Programming

Stochastic programming is an approach for modeling mathematical optimization problems that involve uncertainty (Shapiro and Philpott, 2007). In Section 2.2.3, the bioenergy

supply chain model is formulated as a deterministic optimization problem where all model parameters are known. In the real world, however, some parameters are either unknown at the time a critical decision needs to be made, or have high variance and could lie in a range of possible values. In these situations, one might formulate the problem to seek for a solution that is feasible for all possible parameter choices and optimizes a given objective function, such as to minimize the expected value of certain cost function $f(\cdot)$ as follows:

$$\min_x \mathbb{E}_{\omega \in \Omega} [f(x, \omega)] \quad (2.11)$$

Where ω represents an uncertain vector, and x represents decision variables under each uncertain scenarios. We assume that Ω follows a known probability distribution such that the expected value of $f(x, \omega)$ exist¹.

In this section, we adopt the stochastic programming approach to model the bioenergy supply chain problems to hedge against major system uncertainties such as feedstocks availability and fuel product demand. As an extension of the problem formulated in Section 2.2.3, the supply chain network model will be formulated as a stochastic mixed-integer programming problem to maximize expected total profit of the system, where optimal decisions in facility location and scale, land allocation and crop adoption, feedstock procurement and logistics, biofuel production, delivery and sales, are solved simultaneously.

2.3.1 Two-stage stochastic programming with recourse

One basic idea of two-stage programming is that decisions should be based on information available at the time they are made and not depend on future information. Based on this requirement, decisions in many biofuel supply chain management problems can be categorized as strategic (first-stage) decisions and operational (second-stage) decisions based on whether they have to be made before or after the uncertain scenarios are realized. Strategic decisions include planning decisions such as refinery locations and their sizes, and in our case, agricultural land allocation and crop adoptions. Operational decisions include feedstock procurement and shipment, biofuel production, transportation and sales.

¹In other types of stochastic programming models such as risk averse optimization, Ω also has to be defined to ensure the risk measure has certain desirable properties. Readers can refer to Shapiro and Philpott (2007) again for more details.

Strategic decisions are usually capital intensive and cannot be reverted or adjusted easily once being implemented, whereas operational decisions are more flexible and can be adjusted more easily according the realization of the uncertain scenario.

Compared to the deterministic modeling framework where the strategic and operational decisions are made concurrently, the two-stage stochastic programming framework bears the concept of recourse, where the operational decisions, which are denoted as recourse actions, are taken after uncertain scenarios or events have occurred. In other words, the first-stage decisions are made by taking the future effects of the uncertain parameters into consideration. In the second stage, the actual values of these uncertain parameters are realized and recourse actions can then be taken to obtain optimal objectives under the system setting predetermined by the first-stage decisions.

A two-stage stochastic mixed-integer linear programming model can be represented in a compact form as follows:

$$\begin{aligned}
& \max_x \quad c^T x + \mathbb{E}_{\omega \in \Omega} [Q(x, \omega)] \\
& \text{s.t.} \quad Ax = b \\
& \quad \quad x \in \mathbb{R}_+^{m_1} \times \mathbb{Z}_+^{n_1}
\end{aligned} \tag{2.12}$$

Where $\mathbb{E}(\cdot)$ is the expected value over a set of scenarios $\omega \in \Omega$. x is the vector that represents all the first-stage strategic decisions (e.g., refinery siting decisions at each potential location), $x \in \mathbb{R}_+^{m_1} \times \mathbb{Z}_+^{n_1}$ mean x contains m_1 continuous variables and n_1 integer variables. $c^T x$ is the profit (or negative cost) exclusively dependent on x (e.g., capital investment associated with infrastructure development), $\mathbb{E}_{\omega} [Q(x, \omega)]$ denotes part of the expected net profit which also depends on the second-stage variables (e.g., fuel product sales revenue less scenario-dependent costs, including operational cost of facilities, feedstock collection cost, transportation costs for feedstock and biofuel product shipment), and $\omega \in \Omega$ is the random vector that represents the uncertainty in model inputs. By

construction, the second-stage problems can be formulated as follows:

$$\begin{aligned}
Q(x, \omega) &:= \max_y q(\omega)^T y \\
\text{s.t.} \quad & W(\omega)y = h(\omega) - T(\omega)x \\
& y \in \mathbb{R}_+^{m_2}
\end{aligned} \tag{2.13}$$

Here, y is the vector that represents all the second-stage operational decisions, such as biomass and biofuel transportation, and fuel product sales. The constraints correspond to flow conservation of the supply chain network and market clearance conditions of the feedstocks and biofuels market. The generic formulation of the first-stage problem (2.12) and second-stage problem (2.13) correspond to detailed formulations described in Section 2.2.2.

Since the values of $Q(\cdot)$ in the objective function of (2.12) are determined by scenario-dependent sub-problems (2.13), it is often assumed that $\omega \in \Omega$ follows a known distribution with a finite number of realizations in order to numerically solve the two-stage problem. Without loss of generality, let's assume that Ω can be modeled as K discrete scenarios $\omega_1, \dots, \omega_K$ with probabilities p_1, \dots, p_K , then the stochastic programming problem (2.12) - (2.13) can be reformulated as its deterministic equivalent as follows:

$$\begin{aligned}
\max_{x, y_1, \dots, y_K} \quad & c^T x + \sum_{k=1}^K [p_k (q_k^T y_k)] \\
\text{s.t.} \quad & Ax = b, \quad x \in \mathbb{R}_+^{m_1} \times \mathbb{Z}_+^{n_1} \\
& W_k y_k = h_k - T_k x, \quad y_k \in \mathbb{R}_+^{m_2}, \quad k = 1, \dots, K.
\end{aligned} \tag{2.14}$$

The reformulated problem (2.14) is a standard mixed-integer program and can be solved using commercial mathematical solvers. However, as the dimension K of the scenario vector ω increases, the problem can quickly become computationally impractical due to the increased number of variables and constraints. In Section 5.2, some solution algorithms to overcome the computational challenges occurred in solving large-scale stochastic programming models in real-world applications will be discussed as one of the future research directions of the dissertation.

Chapter 3

Economic Impact of Combined Torrefaction and Pelletization Processes on Forestry Biomass Supply

Summary

In this chapter, we present an application on forestry biomass supply system design, in which feedstock pretreatment via combined torrefaction and pelletization at distributed “satellite” facilities or co-located with centralized liquid biorefineries are considered as candidates to reduce the overall biomass supply system cost. A mixed-integer linear programming model is developed to optimize the biomass supply system configurations, including feedstock logistics and pretreatment facility deployment. In addition, sensitivity analysis is conducted to investigate the uncertainties of the optimal biomass supply system under variations of key input parameters including the production scale of pretreatment facilities, road and rail transportation costs, and feedstock procurement costs.

This chapter is primarily based on the work of Li et al. (2017) with author contributions listed as follows: YL conceptualized the study, developed the methodology, conducted geospatial and mathematical model analyses, generated all the model outcomes (except for the system layout map in Figure 3.2, which was created by PT), interpreted the results, and

drafted the paper; PT provided and compiled the raw geospatial input data, participated in conceptualizing the study, collecting key model parameters from the literature, cartography, validation and interpretation of the model results; NP and BJ provided critical reviews for the analyses from input parameters, model development, interpretation of results, and construction of model scenarios for sensitivity analysis. All authors participated in paper revision, read and approved the final manuscript.

3.1 Introduction

Bioenergy has some distinct characteristics when compared to other renewables such as ancillary forest health and landfill diversion. In addition, biomass can be stored and used on demand in complement to variable solar and wind to improve the overall performance of renewable energy systems. Despite a number of favorable characteristics, reductions in the levelized cost of electricity (LCOE) from solar photovoltaics and wind turbines have made bioenergy increasingly more costly relative to other renewables (Pogson et al., 2013). The high cost of bioenergy is partly a result of the relatively high cost of feedstock acquisition in addition to escalating capital costs including emissions control. The potential for biomass to support baseload or load following electricity generating options and liquid fuel production for high value transportation and other sectors continues to motivate technical innovation for its sustainable use, however (Milbrandt et al., 2014; Jones, 2014).

Biomass feedstocks produced from forest management activities are distributed across forested landscapes in varying amounts depending upon growing conditions, management practices, and policy factors. As a result, biomass procurement and transportation costs can vary greatly and have a profound effect on the overall production cost of energy. Previous studies have extensively explored spatially-explicit supply chain designs in an attempt to optimize facility siting and scale to minimize cost or maximize profit (Parker et al., 2010; Tittmann et al., 2010; Dunnett et al., 2008). In these studies, total bioenergy production costs were derived using component costs for feedstock procurement, transportation, site-specific conversion costs, and fuel delivery costs into final demand. Sensitivity analysis in these studies showed that transportation costs have significant impact on the optimal

system configuration, highlighting the potential advantages of increasing the efficiency of biomass feedstock transport.

Combined torrefaction and pelletization (TOP process) converts heterogenous wood feedstock from forest management practices into a densified intermediate with higher energy and mass density than the original wood (Bergman, 2005; Bergman et al., 2005; Uslu et al., 2008). Dry, densified material results in reduced transport cost for feedstock delivery. Torrefaction and densification of feedstock reduce the volume of storage needed at a biorefinery, improve feedstock stability in storage, and reduce onsite handling costs, which potentially result in higher economic performance in the fuel conversion process. Torrefaction increases the friability which is advantageous for downstream size reduction (Bergman, 2005). In addition to these potential cost implications, higher efficiency in transport, storage, and processing can also reduce greenhouse gas and air pollutant emissions (Bergman, 2005; Uslu et al., 2008; International Energy Agency, 2012b).

Nonetheless, torrefaction has not been broadly commercialized and its economic benefit in the supply chain is still unclear. The purpose of this study was to evaluate the economic utility of torrefaction combined with densification in a biofuel supply chain. Specifically, we identify the size and location of TOP (torrefaction followed by pelleting) pretreatment in an optimized feedstock supply chain reflecting the specific geography of forests and transportation infrastructure in California as a model location. We use results of prior modeling work cited above as a basis for establishing the locations of biorefineries using woody biomass feedstocks. The results are used to derive the economic transport distance at which pretreatment results in net reduction in feedstock procurement costs (breakeven), and to identify variable costs in the supply chain to which the solution is particularly sensitive.

The estimates were made using a spatially-explicit supply chain optimization model based from those noted above and employing a cost-minimization objective. The model is general in approach and can be applied to other regions beyond California where sufficient data exist.

3.2 Methods

To assess the economic impact of torrefaction and pelletization on woody biomass supply chains, a mixed integer linear programming model was developed using transportation cost data from a geographic information system (GIS) analysis along with torrefaction and densification costs estimated for five pretreatment capacities or production scales . The optimization model was designed to assess whether such pretreatment could substantially reduce delivered costs of feedstock to biorefineries and if so, where and at what scale in the supply chain the pretreatment facilities should be located. The model was also employed to evaluate sensitivity of the optimal solution to the input assumptions.

3.2.1 Biomass feedstock supply chain

The optimization model was based on the previous work of Parker et al. (2010) and Tittmann et al. (2010) modified to include an additional pretreatment stage within the model framework. In this case, the biomass supply chain network consists of three layers of nodes representing (1) feedstock supply, (2) intermediate pretreatment , and (3) biorefineries. Woodchips are compared with torrefied and densified (TOP) feedstock delivered to or manufactured at the conversion facility. Wood-chips are procured at feedstock source locations, typically log landings on industrial forest operations. TOP feedstock is assumed to be generated by conversion of wood chips at the log landing, at an intermediate location, or at the biorefinery.

The two primary benefits from the use of torrefied pellets in transportation are the higher mass and energy densities compared to bulk chips. For example, torrefied biomass has a higher heating value of 21.5 GJ/ton dry basis compared with 17.5 GJ/ton for dry wood chips, both on lower heating value basis. The higher mass density increases the transportation efficiency by reducing the unit shipment cost ($\$/(\text{GJ} \cdot \text{km})$ on dry basis), especially for rail transportation. Details of the multi-modal transportation cost estimates are discussed in Section 3.3.3.5. Torrefied pellets can also offer advantages at the biorefinery for which they may fetch a higher price at plant-gate compared to green wood chips providing an additional incentive to the feedstock supplier to convert wood chips to torrefied pellets earlier in the supply chain.

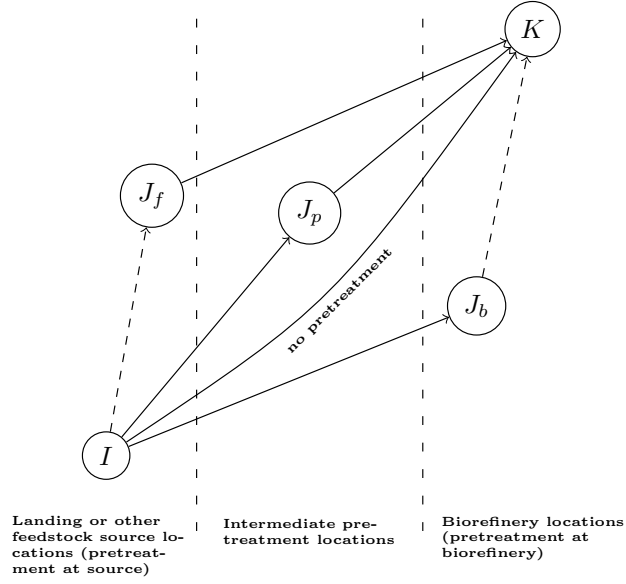


Figure 3.1: Schematic of the biomass supply chain network, dashed lines are dummy edges with zero transportation cost. J_f represents supply locations for potential distributed pretreatment facilities, J_b represents refinery locations for potential pretreatment co-located at biorefineries. See Table 3.4 for details of representative pretreatment scales.

A schematic representation of the supply chain network is shown in Figure 3.1. Note that potential pretreatment sites (J) include the biomass feedstock supply locations (J_f), intermediate potential locations (J_p) and biorefineries (J_b). Feedstock can be 1) delivered as wood chips to the biorefinery and used without pretreatment, 2) pretreated at the landing and shipped as TOP material to the biorefinery, 3) hauled as wood chip to an intermediate pretreatment facility and then shipped to the biorefinery as TOP material, or 4) hauled as wood chip to the biorefinery and pretreated there. In this way, all the feedstock shipments start from sets I , go through sets J (contains J_f , J_b and J_p) and end in sets K . We can formulate the problem as a mixed integer linear program as described in Section 3.2.2.

3.2.2 Model formulation

For convenience, all the notations used in the model are listed in Table 3.1.

Table 3.1: Model parameters and decision variables

Name	Definition and Unit
Sets	
I	Index i , set of feedstock locations
J	Index j , set of all potential pretreatment locations, including distributed, intermediate and co-located ones.
$J_f \in J$	Index j , set of dummy supply locations for potential distributed pretreatment facilities
K	Index k , set of biorefinery locations
$SC = \{d, s, m1, m2, l\}$	Index s , set of potential pretreatment facility scales (See Table 3.4 for details of representative scales)
Model input parameters	
F_s	Fixed cost (\$) of pretreatment at different scales.
TO_{ij}	unit transportation cost for shipping 1 wet ton of biomass from feedstock locations to intermediate locations, \$ · Mg wet ⁻¹
TD_{jk}	unit transportation cost for shipping 1 wet ton of (pretreated) biomass from intermediate locations to biorefineires, \$ · Mg wet ⁻¹
OD_{ik}	unit transportation cost for shipping 1 wet ton of unpretreated biomass from feedstock supply locations to biorefineires, \$ · Mg wet ⁻¹
C	unit feedstock procurement cost on wet basis, \$ · Mg wet ⁻¹
U	biorefinery cost savings from torrefied pellets, \$ · GJ ⁻¹
Continued on next page	

Table 3.1 – continued from previous page

Name	Definition and Unit
μ	LHV ratio between torrefied pellet and wood chips.
λ_w, λ_t	moisture content of green wood chips and torrefied pellets.
ν	yield of TOP from wood chips on a wet mass basis
S_i	maximum annual feedstock production for location i , Mg(wet)/year
D_k	feedstock demand of biorefinery at location k , Mg(dry)/year
Cap_s	pretreatment production capacity at different scales, Mg(wet)/year
Decision variables	
$X_{s,j} \in \{0, 1\}$	binary, build scale s facility at location j
$Y_{ij}^T \in \mathbb{R}^+$	quantity of wood chips transported from feedstock location i to pretreatment facility j , Mg wet
$Z_{jk}^T \in \mathbb{R}^+$	quantity of torrefied pellets transported from pretreatment facility j to the biorefinery k , Mg wet
$Y_{ik}^W \in \mathbb{R}^+$	quantity of wood chips shipped from feedstock location i to biorefinery k without pretreatment, Mg wet

3.2.2.1 Model objective

The model objective is to minimize the annualized total cost of supply given biomass demand and supply constraints. System costs include procurement, pretreatment, transportation, as well as the avoided refining costs, if any, from utilization of torrefied pellets instead of wood chips at the biorefinery.

$$\min. \quad Cost_{pretreatment} + Cost_{transport} + Cost_{procurement} - U \quad (3.1)$$

Pretreatment cost

$$Cost_{pretreatment} = \sum_{j \in J} \sum_{s \in SC} F_s \cdot X_{s,j} \quad (3.2)$$

represents costs to build pretreatment facilities at different scales and locations.

Transportation cost

$$Cost_{transport} = \sum_{i \in I, j \in J} TO_{ij} Y_{ij}^T + \sum_{j \in J, k \in K} TD_{jk} Z_{jk}^T + \sum_{i \in I, k \in K} OD_{ik} Y_{ik}^W \quad (3.3)$$

where TO_{ij} , TD_{jk} and OD_{ik} are unit costs for transporting one ton of material through network edges (i, j) , (j, k) and (i, k) . Note that $Cost_{transport}$ includes the transportation cost of both wood chips (TO , OD) and torrefied pellets (TD).

Procurement cost

$$Cost_{procurement} = C \cdot \left(\sum_{i \in I, j \in J} Y_{ij}^T + \sum_{i \in I, k \in K} Y_{ik}^W \right) \quad (3.4)$$

where C is the unit procurement cost. This cost reflects the assumption that wood used as feedstock for bioenergy applications would be a residual product from logging operations conducted to produce high-value solid wood products. Thus the procurement cost is assumed to be only the cost of chipping and loading logging residuals piled at the log landing and does not include a production cost associated with growing or harvesting the trees.

Utility savings from torrefied pellets

$$U = \kappa \sum_{j \in J, k \in K} \mu_t \cdot Z_{jk}^T \quad (3.5)$$

where μ_t is the LHV on a wet basis of torrefied pellets, and κ is the price premium paid ($\$ \cdot \text{GJ}^{-1}$) for dry torrefied pellet utilization by the receiving biorefineries.

3.2.2.2 Model constraints

Supply and demand constraints

$$\begin{aligned} \sum_{j \in J} Y_{ij}^T + \sum_{k \in K} Y_{ik}^W &\leq S_i, \quad \forall i \in I \\ \sum_{j \in J} \mu \cdot (1 - \lambda_t) \cdot Z_{jk}^T + \sum_{i \in I} (1 - \lambda_w) \cdot Y_{ik}^W &\geq D_k, \quad \forall k \in K \end{aligned} \quad (3.6)$$

where μ is the equivalence ratio between dry wood chips and torrefied pellets, this ratio is calculated based on their energy content (dry basis, GJ/Mg), and the net efficiency of the pretreatment process (Bergman, 2005).

Flow conservation constraints

$$\sum_{i \in I} \nu \cdot Y_{ij}^T = \sum_{k \in K} Z_{j,k}^T, \quad \forall j \in J \quad (3.7)$$

Capacity constraints

$$\sum_{i \in I} Y_{ij}^T \leq \sum_{s \in SC} Cap_s \cdot X_{s,j} \quad \forall j \in J \quad (3.8)$$

where Cap_s are the production capacity of pretreatment facilities at different scales. This forcing constraint captures the fact that if there is no facility at location j , no wood chips can be delivered there.

Other facility siting related constraints

$$\sum_{s \in SC} X_{s,j} \leq 1, \quad \forall j \in J \quad (3.9)$$

In order to maintain the network consistency, we require that at most one type of facility could be chosen at each location.

$$X_{s,j} = 0, \quad \forall j \in J_f, s \in SC \setminus \{d\} \quad (3.10)$$

At co-located supply and pretreatment locations, only distributed scale facilities are allowed to be sited.

Binary and non-negativity constraints

$$X_{s,j} = \begin{cases} 0 & \text{not built,} \\ 1 & \text{built.} \end{cases} \quad \forall s \in SC, \forall j \in J \quad (3.11)$$

$$Y_{ij}^T, Z_{jk}^T, Y_{ik}^W \geq 0 \quad \forall i \in I, j \in J, k \in K \quad (3.12)$$

3.3 Input Data

3.3.1 Technical characteristics of the combined torrefaction and pelletization process

Torrefaction is a thermal process performed mostly at atmospheric pressure in the absence of oxygen, at temperatures ranging between 200° and 300°C. Under these conditions water and some dry matter (mostly due to hemicellulose decomposition) are volatilized and the resulting solid product becomes more friable. The process results in improved fuel quality for combustion and gasification applications. Torrefaction has not been widely commercialized however; existing literature shows that torrefaction significantly increases energy density, hydrophobicity, friability, flowability, and combustion characteristics of biomass (Uslu et al., 2008; Tumuluru et al., 2011; Ciolkosz and Wallace, 2011; International Energy Agency, 2012b,a; Shah et al., 2012; Van der Stelt et al., 2011). On a dry basis, torrefied biomass typically contains 70% of its initial weight and 90% of its initial energy content (Bergman, 2005). Since torrefied biomass loses relatively more oxygen and hydrogen than carbon, the calorific value of the product usually increases.

Torrefied biomass prior to densification possesses some undesirable properties for transportation and storage, including increased porosity, low mass density, decreased mechanical strength and increased dust formation (Uslu et al., 2008). Densification has been widely suggested to ameliorate these issues. Pelletization densifies raw materials under pressure in order to improve uniformity and increase density. During pelletization, lignin present in wood or torrefied product typically weakens and flows, becoming a binding agent. The Energy Research Center of the Netherlands (ECN) has developed the so-called TOP process combining torrefaction and pelletization (Bergman, 2005; Bergman et al., 2005), where torrefaction is introduced between drying and size reduction steps in a traditional pelletization process. Performance data of the TOP process are as reported by ECN are listed in Table 3.2.

Table 3.2: Technical characteristics of the TOP process (Bergman, 2005; Fiala and Bacenetti, 2012)

Properties	Unit	Green wood chips	TOP pellets
Moisture content	wt%	57 %	3 %
Bulk density	kg/m ³	326	800
Bulk energy density	GJ/m ³	2.0	16.6
Heating value (LHV)	MJ/kg	6.2	20.8
LHV on dry basis	MJ/kg	17.5	21.5

^a ar = as received

Table 3.3: Economic characteristics of the TOP process (Bergman, 2005)

Item	Unit	TOP process
Feedstock type		Green wood chips
Feedstock input	1000 ton/year	170
TOP production capacity ^a	1000 ton/year	56
	MW _{th} fuel	40
Total capital investment	M\$	9.3
Total production cost ^b	\$/Mg	62.5

^a The ratio of feedstock input and TOP output will be used among all the representative scales in Table 3.4.

^b Assumptions for this economic evaluation include: 10-year depreciation period, 8000-hours load factor

3.3.2 Costs of torrefaction and pelletization process

The economy of scale is a crucial factor influencing production cost and efficiency (Jenkins, 1997). The scale effect and the existence of an optimal investment cost for capital-intensive biomass pretreatment technologies have been investigated by Uslu et al. (2008). Lacking empirical economic data on pretreatment technologies at industrial scales, the economic evaluation of the TOP process from (Bergman, 2005) is referred to in this study as the base or reference case (see Table 3.3). The formula $\frac{C}{C_0} = \left(\frac{M}{M_0}\right)^s$, where C (\$) is the installed capital cost of a facility of capacity M (MWth), and C_0 (\$) is the installed capital cost of the base plant facility of capacity M_0 (MWth), and a constant scaling factor of $s = 0.7$ is applied to model the scale effect on the TOP process, noting that a constant value may not adequately represent the economy of scale at very large sizes (Jenkins, 1997). Five representative biorefinery capacities with different capital investment costs were assumed as candidates for different locations along the supply chain network in the following scenarios (Table 3.4).

Table 3.4: Representative conversion scales for the TOP process

Scale/ID	Plant Size		Specific Investment
	kton/year(TOP pellet)	MWth-fuel(input)	Cost (\$/ton)
Distributed/Dist35	3.5	2.5	73.3
^a			
Small	28	20	39.9
Medium	56	40	31.7
1/Med56			
Medium	105	75	26.4
2/Med105			
Large/Large210	210	150	21.5

^a Distributed scale pretreatment is a mobile or portable process located at the primary collection point where wood chip van loading would take place.

3.3.3 Biomass supply chain

3.3.3.1 Transportation network

The transportation network in this study was modeled using data from the National Transportation Atlas Database (2011) of the Bureau of Transportation Statistics (Bureau of Transportation Statistics, 2011). The network includes multiple transport modes (highway, railway and marine) for bulk biomass transportation as well as inter-modal facilities and allows for unloading/loading of biomass in order to shift between transportation modes. For biomass transportation between two specific nodes (e.g., forest landing to pretreatment facility or to biorefinery), rail or marine transportation could be used on long routes for economic benefit assuming transloading is an option. The network allows for direct deliveries to biorefineries via rail or marine routes if biorefineries are proximal to rail or marine routes, otherwise biorefineries must take delivery by truck.

3.3.3.2 Feedstocks

Forest biomass feedstock data used in this analysis is derived from Sethi and Simmons (2005). The original data were generated at a 30 m spatial resolution. For the purposes of this analysis, 30m pixels were aggregated to 1.6 km harvest units to reflect the likely size of operational units. Feedstock availability is estimated based upon forest type and ownership. Supply is annualized based upon an expected rotation of 60 years on private lands and 75 years on public lands. Forest land area with administrative restrictions (wilderness areas, roadless, etc), riparian buffer zones, and slopes greater than 35% are excluded. The total feedstock resource in the original forest supply database is about 14 Tg, which is further reduced to over 12 Tg for this study by excluding feedstock points with less than 1000 Mg supply.

3.3.3.3 Biorefineries

Tittmann et al. (2010) identified optimal biorefinery locations in California based on supply chain and fuel distribution costs but without considering the pretreatment options evaluated here. In the previous analysis, biorefineries could use feedstock from a range of sources (e.g., agricultural residues). From the locations selected in the previous analysis, we identified the locations of all biorefineries using greater than 10 dry Mg/year of forest-

sourced material, resulting in 20 distinct locations, out of which we randomly selected 10 locations meeting the above criteria for this study. The baseline model considers 1.2 Tg/year to be the maximum throughput in terms of feedstock at each biorefinery.

3.3.3.4 Potential locations for biomass pretreatment facilities

We assume that the selection of potential optimal location for biomass pretreatment facilities would be significantly influenced by transportation accessibility and the geographical features of the transport network. The mean shift method (Fukunaga and Hostetler, 1975) was used to perform a clustering on all junction nodes in the road network. Junction nodes exist where two road segments intersect. Clustering is needed as in many cases multiple nodes are located in close proximity due to a freeway interchange or overpass. The clustering resulted in 90 (out of 5177) points selected as potential locations for pre-treatment facilities. For the purpose of simplicity, we did not consider any other restrictions in selecting potential locations for biomass pretreatment facilities, such as labor and land use.

3.3.3.5 Transportation cost

Biomass transportation costs are modelled by the same cost function used by Tittmann et al. (2010) for three modes: truck, rail and marine (Table 3.5).

The costs of trucking consist of two different components: a distance - dependent component and a time - dependent component. We assume that these two components do not vary by feedstock type.

Normally, trucks used for biomass transport have a 25 Mg weight limit and a volume limit of approximately 120 m³ (Idaho National Laboratory, 2010). For both wood chips and torrefied pellets, the truck load is constrained by weight rather than volume. Greater advantage would accrue to trucks of higher weight capacity, but currently regulations do not provide for this. So without any further information on truck transport, we assume that road transportation of torrefied pellets has the same unit cost (\$/ton-km) compared with shipping green wood chips.

Rail transportation cost are derived from a mileage-based rate schedule for agricultural products. According to a freight transportation & logistics organization, a common rail car has a weight limit of about 100 Mg and a volume limit of about 150 m³ (Enviromodal,

Table 3.5: Transportation cost components (on wet basis)

Mode	Cost Component	Green Wood Chips	Pelletized Biomass
Road	Loading/unloading	\$ 5 / Mg	
	Time dependent	\$ 29.21 / h per truckload ^a	
	Distance dependent	\$ 1.10 / km per truckload ^b	
	Truck payload	25 Mg	
Rail	Loading/unloading	\$ 5 / wet ton	
	Fixed cost	\$ 19.5/ Mg	\$ 9.7 / Mg
	Distance dependent	\$ 0.143 / (Mg·km)	\$ 0.008 / (Mg·km)
	Rail car capacity	50 Mg	100 Mg
Waterway	Loading/unloading	\$ 5 / Mg	
	Fixed cost	\$ 3.85 / Mg	
	Distance dependent	\$ 0.027 / (Mg·km)	
	Barge capacity	3600 Mg	

^a Including capital cost of \$ 18.80 / h and labor cost of \$ 10.41 / h

^b Including Fuel \$ 0.83 / km, Repair & Maintenance \$ 0.04 / km and Permits & Licensing \$ 0.21 / km, the truck fuel economy is assumed to be 1.42 km / L

2012). The transportation of green wood chips in rail cars is volume limited as the total weight of 150 m³ ($0.326 \text{ Mg/m}^3 \times 150 \text{ m}^3 \approx 50 \text{ Mg}$) is less than the weight limit of a rail car (100 Mg). For TOP pellets with a mass density of 0.8 ton/m³, the total weight is 120 Mg, which exceeds the 100 Mg limit, thus rail cars carrying TOP pellets are weight limited. Because rail car payloads for green wood chips and TOP pellets differ significantly, the unit transport cost for green wood chips is assumed to be twice as high as for pellets given the ratio of maximum weight per car all other costs being constant.

Similar to rail transportation, costs of marine shipment are derived from published rate schedules (Tidewater Inc., 2007). The size and capacity of barges provides that the actual payload for green wood chips and TOP pellets would both be weight limited, so no

difference in the unit transportation cost is assumed.

3.3.4 Scenarios

Sensitivity analysis was used to assess the impact of input parameters on the optimal solution. Variables evaluated were pretreatment capacity, diesel fuel price for portable and mobile equipment operation, unit transport cost of rail shipment, feedstock procurement cost and potential cost savings for torrefied pellets with biomass conversion.

As mentioned in Section 3.3.2 , the pretreatment capacity is critical to the total investment cost, and thus can significantly change the optimal supply system configuration. Besides the five representative candidate pretreatment scales selected in the baseline scenario, we set pretreatment capacity as a sensitivity variable with a range from 10×10^3 ton to 210×10^3 ton per year and a much finer increment of 5000 ton/year to examine its impact on the system.

Diesel fuel price is volatile. Between July 2008 and March 2009, for example, diesel price ranged from \$1.26/L to \$0.54/L (U.S. Energy Information Administration, 2014). To represent this fluctuation and reflect the uncertainty in diesel price, three diesel price levels - \$0.53/L, \$0.93/L and \$1.32/L were used in the sensitivity analysis.

Rail transport costs are difficult to accurately predict. Bulk rail rates depend on the volume being transported; unit trains carrying a single commodity in 100-150 cars result in substantially lower cost than mixed load trains. Previous analyses have used a published rate schedule (Union Pacific Railroad, 2007) for mixed trains. This rate is estimated to be higher than what would likely be paid Searcy et al. (2007) Sensitivity analysis was therefore conducted to reflect uncertainty regarding rail transport rates. For the fixed rail cost described in Table 3.5, we set its range from \$5.5/Mg to \$26.5/Mg with an increment of \$7/Mg on a wet basis.

The procurement cost range reflects the variability in costs associated with different harvest scenarios. Many industrial timber harvesting operations produce biomass at the landing in the form of tops and limbs. The low end procurement cost which is used in the base model makes the assumption that the limbs and tops at the landing are available at no cost and thus the only cost associated with procuring that material is incurred from

chipping and loading. The high cost estimate assumes that all the costs from harvesting, yarding, chipping and loading must be paid. Costs for high and low cases were calculated using the Fuels Reduction Cost Simulator (Fight et al., 2006).

The cost savings at biorefineries brought by the utilization of torrefied pellets arise from reductions in energy demand for drying and size reduction of biomass feedstock before final conversion. Not all conversion processes may benefit from the torrefaction of the feedstock, however. Other types of capital investment such as outside storage might also be lowered by pellet utilization due to the higher density in storage, although the need for more permanent structures to protect the quality of pellets might increase costs above more conventional outside storage of chips. Although such cost savings were widely mentioned in literature (International Energy Agency, 2012b,a; Bergman, 2005; Uslu et al., 2008), an accurate quantitative measure of such benefit is difficult. A range from 0 to \$5/GJ for the cost saving parameter is used, where \$5/GJ roughly corresponds to the point of 100% torrefied pellet utilization in our model analysis.

3.4 Results

The model was applied to California as a case study and solved using the Gurobi optimization solver (Gurobi Optimization, 2017). In Section 3.4.1 we first review the model baseline results with default assumptions specified in Section 3.3. In Section 3.4.2 we present results of the sensitivity analysis conducted on the baseline model. In Section 3.5 we present some scenario results to demonstrate the impact of integrating pre-treatment into the bioenergy supply chain. Section 3.5.1 presents general conclusions that can be drawn from this research.

3.4.1 Baseline results

In this section, we consider the baseline scenario using all 10 biorefineries and discuss pretreatment impacts on the forestry biomass supply system in California.

3.4.1.1 The feedstock supply system design

The optimal design of the baseline scenario makes use of 3 of the 5 possible pretreatment facility scales (Figure 3.2). The relatively wide range of scales is partially due to large

spatial variation in feedstock supply throughout the study region. Most of the pretreatment facilities are located close to some feedstock procurement location to take advantage of the reduced transportation cost of feedstock. For biorefineries that have abundant forest resources in the vicinity (such as the northern biorefineries in Figure 3.2), all or at least a major proportion of biomass demand is met by green wood chips, while in cases of biorefineries that are located far from forest resources such as the central part of the state, long-distance pellet shipments becomes necessary.

3.4.1.2 Delivered costs

The total delivered cost is comprised of three components: feedstock procurement cost, pretreatment cost and transportation cost.

Table 3.6 shows the average system cost breakdown for 1 GJ (dry basis) of biomass utilization at the biorefinery gate. The average total delivered cost is \$4.36/GJ, which is about \$0.24/GJ lower than a system without any pretreatment process. In the baseline scenario, 12.8 % of the final biomass energy supply to refineries is pretreated, and the procurement cost is slightly higher than the no-pretreatment-system due to the extra feedstock required to compensate for the material loss in pretreatment. The pretreatment production cost takes about 8% of the total system delivered cost. The transportation cost decreased from \$4.14/GJ to \$3.54/GJ, and shows the potential of cost saving by biomass pretreatment.

Table 3.6: Cost breakdown of biomass supply systems (\$/GJ)

Average cost component	With pretreatment process	No pretreatment
Total delivered cost	4.36	4.60
Procurement cost	0.47	0.46
Transportation cost	3.54	4.14
Pretreatment cost (for pellets) ^a	2.74	-

^a The percent of feedstock pretreated is 12.8 %

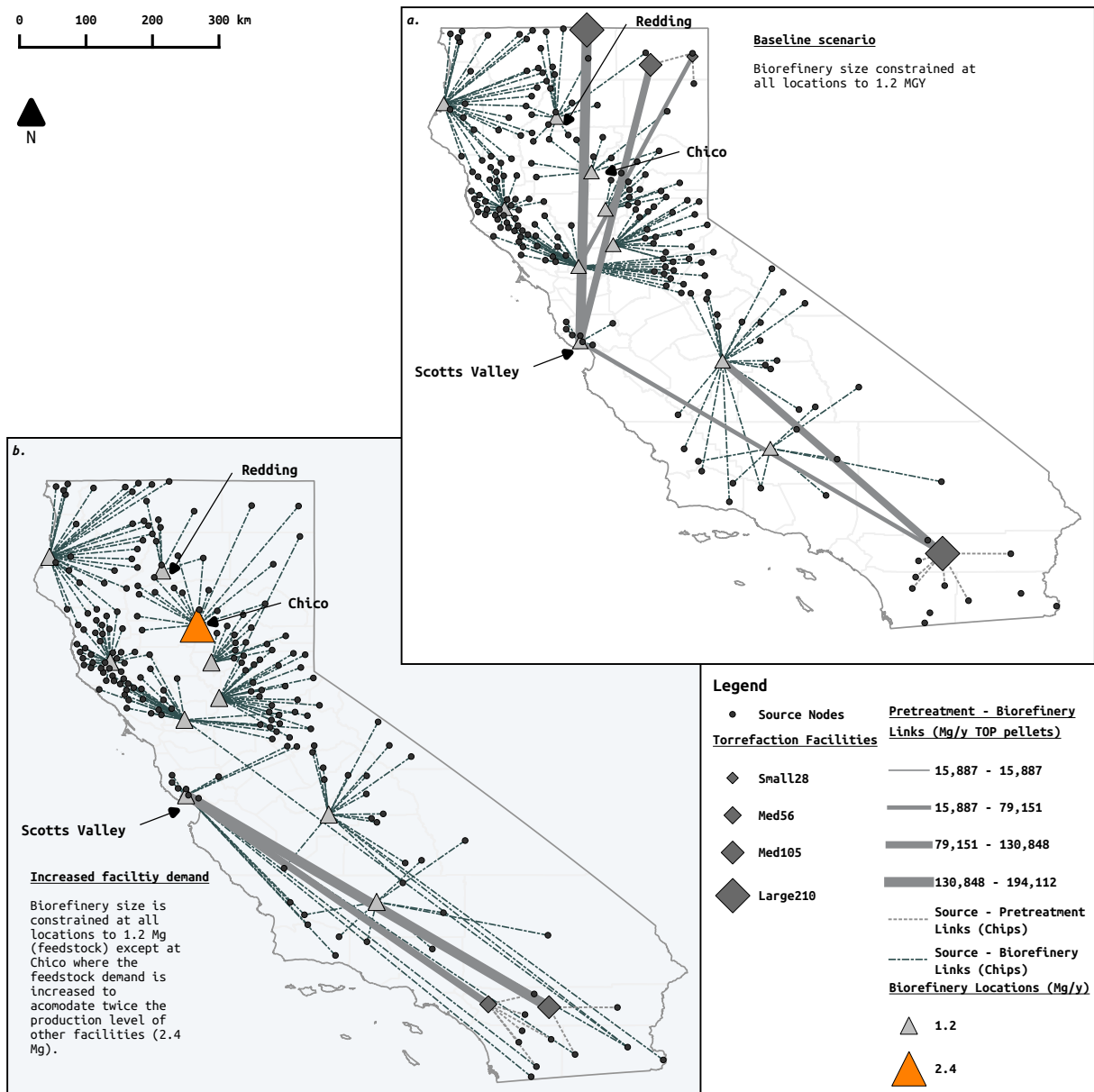


Figure 3.2: Biomass supply system layout for the base scenario (a) and for the sensitivity analysis (b) in which demand at the Chico biorefinery is doubled to accommodate production of 2.4×10^6 Mg/y. See Section 3.4.2.4 for additional detail on the increased demand scenario. Torrefaction facility size codes reference Table 3.4.

3.4.1.3 Transportation modal split

In the biomass supply system, 35% of the feedstock energy shipped is by rail transportation, and 65% is truck transportation. For the same set of input data, the corresponding no-pretreatment-system results in 25% of rail transportation usage and demonstrates the particular advantage of rail transport for high mass density material mentioned in Section 3.3.3.5 that results in a shift from volume limitation to weight limitation in transport, a feature not associated with the truck and marine transport in this analysis.

3.4.1.4 Feedstock supply curve

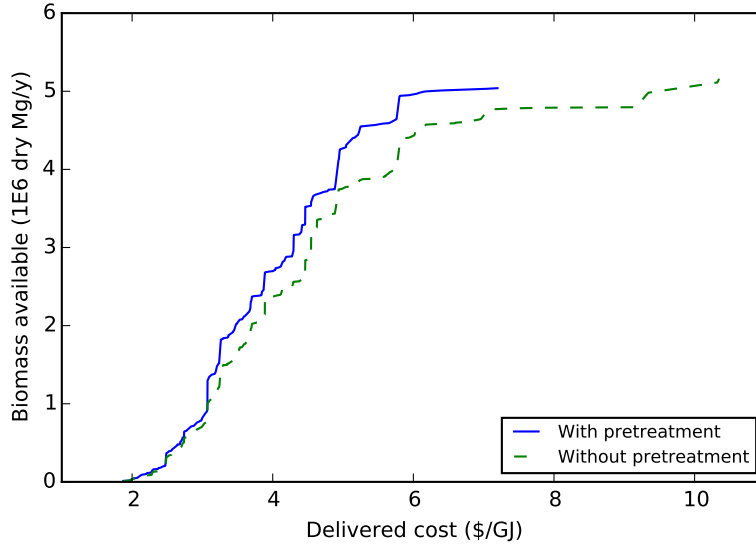


Figure 3.3: Aggregated feedstocks supply curve

To further illustrate the impact of biomass pretreatment on the feedstock supply system, we compare the aggregated biomass supply curves for two system scenarios. For the system without pretreatment, raw woodchip is the only option for biorefineries, and for the system that has pretreatment option, refineries can choose to construct pre-processing facilities when necessary. As shown at the left bottom of Figure 3.3, the average delivered costs of both systems are almost the same when the total biomass supply amount is small as only green wood chips in the vicinity of biorefineries are needed. As more biomass is required, the delivered costs of both systems start to increase, but for the system supplemented with torrefied pellets, the growth of delivered cost is not as rapid as in the system where

only untreated biomass supply is provided. The difference in delivered cost keeps growing and reaches as much as \$3/GJ when the total feedstock supply is about 5×10^6 Mg/y.

3.4.2 Sensitivity analysis of the baseline model

Iterative model runs were conducted with each changing a particular variable to evaluate the sensitivity of the results. Note that some of the input parameters directly affect the optimal solution, for example, unit feedstock procurement cost and TOP pellet utilization savings were taken as model inputs but also are part of the average delivered cost breakdown. So we only examined the total delivered cost and the transportation cost components in the sensitivity analyses, instead of all four components of the system cost.

3.4.2.1 Impact of pretreatment scale

Figure 3.4 shows how average delivered cost (\$/GJ), average transport cost (\$/GJ), the proportion of energy in pellets delivered and the fraction of rail transportation among all biomass shipments (energy basis) change with respect to changes in the pretreatment facility capacity. The total delivered cost and transport cost monotonically decrease from \$4.6 to \$4.4/GJ and from \$4.0 to \$3.5/GJ, respectively. Above approximately 100 kton/y, the transportation cost starts to fluctuate due to unstable modal shift and the cost ceases to decline substantially. The fraction of biomass supply met by pellets has an increasing trend (from 2.3% to 14.5%) as pretreatment production capacities increase. Nonetheless there are still fluctuations between 70×10^3 ton/year and 140×10^3 ton/year capacities.

Although preferred due to the economy of scale, larger facilities also require a greater amount of feedstock and will be ultimately limited by the feedstock availability and the rapid increase in delivered cost when approaching the limit of supply. There may also be technical and financial risks at very large sizes that are not represented in an assumption of constant scale factor (Jenkins, 1997).

The proportion of rail shipment also has an increasing trend from 24.5 % to 38.3%. Although rail transport exhibits a cost benefit due to higher energy and mass densities for torrefied pellets, building a pretreatment facility at an intermediate location still leads to extra biomass handling and transportation costs that depend on local network characteristics such as railway accessibility. For California, the fairly high percentage of

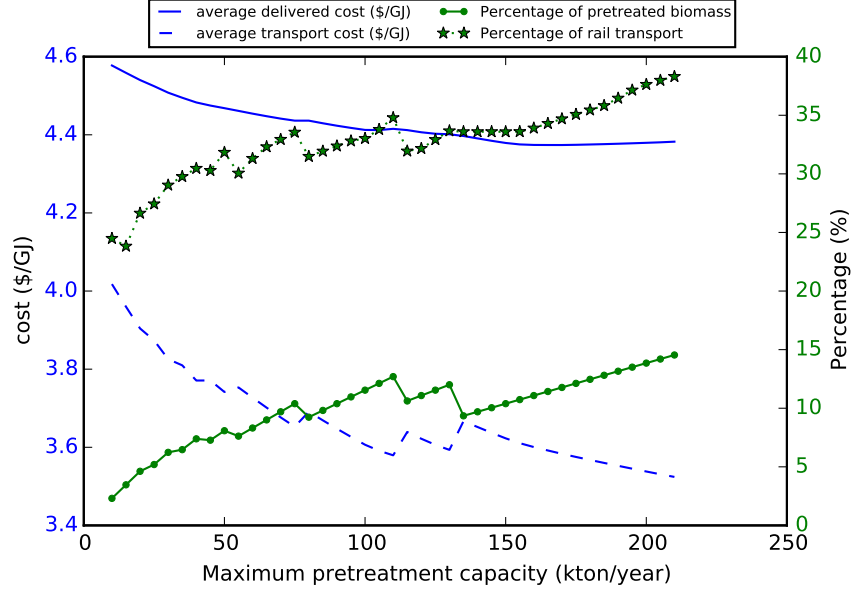


Figure 3.4: The impact of pretreatment capacities. (Average delivered and transportation costs in \$/GJ use left axis, the percentage (%) of pretreated biomass and rail transportation use right axis)

railway transportation in all pretreatment-scale scenarios shown in Figure 3.4 demonstrates how biomass pretreatment could benefit from rail transportation for long-distance shipment when a large amount of feedstock is required.

3.4.2.2 Impact of transportation cost parameters

The baseline result of the 10-biorefinery scenario from Section 3.4.1.2 indicates that transportation cost accounts for more than 80% of the total delivered cost.

In this section, we test the system with \$0.53/L, \$0.92/L and \$1.32/L diesel prices. These different prices lead to about \$0.50/GJ differences in delivered cost and about \$0.4/GJ differences in transportation cost of the system. Higher diesel prices also push for more TOP utilization and rail transport. Note that although trucking of greenwood chips and pretreated biomass had the same unit costs as both were weight limited, pellet utilization would still reduce the total tonnage of biomass transported due to the higher energy density and thus reduce the total feedstock transportation cost. The diesel price increment brings about 5%-10% increase in TOP utilization and about 10%-15% more rail transportation, measured in Mg-km.

Rail cost change has less impact on the system cost, partially due to our assumption in Section 3.3.3.5 that rail is much cheaper than trucking for biomass delivery on a \$/GJ-km basis. A \$21/Mg increase in fixed rail cost only leads to about \$0.5/GJ increase in delivered cost and about \$0.40/GJ increase in transportation cost. On the other hand, a \$21/Mg rail cost difference results in about 5%-10% decrease in TOP utilization and as much as 30% drop in the proportion of transportation by rail.

3.4.2.3 Impact of procurement cost and TOP utilization savings

Lastly, we explored the impact of procurement cost and TOP utilization savings to the system.

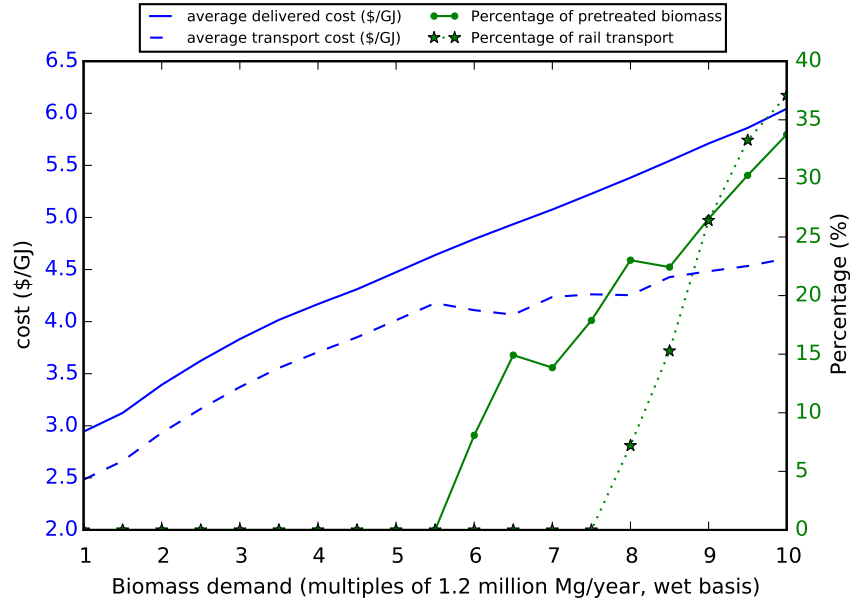
Procurement cost has a negative impact on TOP pellet utilization, as higher procurement cost of feedstocks in wet-based \$/Mg makes torrefied pellet less affordable due to the energy and material loss in the pretreatment process. In our test, the difference between a \$3.5/Mg and \$40.0/Mg procurement cost could lead to a 20% difference in TOP utilization and 10% difference in the proportion of transportation by rail.

The increase of pellet-derived savings at biorefineries, on the other hand, can lead to a significant rise in TOP utilization and rail transportation. Our investigation indicates that a \$5/GJ TOP cost saving would lead to only pellets being used and the fraction transported by rail would reach about 40%.

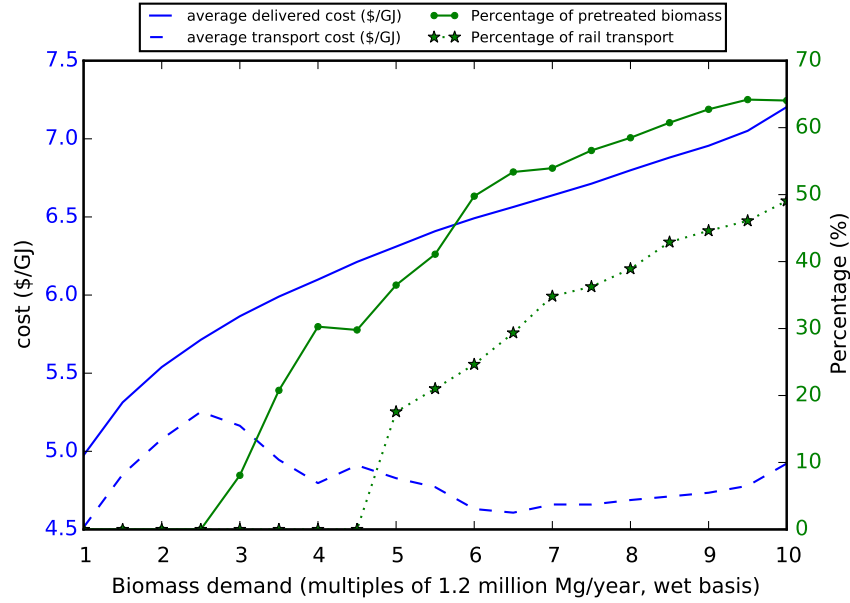
3.4.2.4 Model scenarios

Single biorefinery scenario We first studied two single-biorefinery systems, of which one has access to abundant feedstock resources within short distances (Redding biorefinery, Figure 3.2) and one that does not (Scotts Valley biorefinery, Figure 3.2). In both cases, the demand of the biorefinery was increased from 1.2 Tg/year to 12 Tg/year on a wet basis. The average delivered or transportation cost, proportion of torrefied pellet utilization and rail transport under various biomass demands for the two single biorefinery scenarios are plotted in Figure 3.5.

For the biorefinery at Redding (Figure 3.5(a)) note that before pretreatment becomes preferred, the gap between average delivered cost and transportation cost remains about the same, which means that the increase in total delivered cost is mostly due to the rise of



(a) Redding biorefinery



(b) Scotts Valley biorefinery

Figure 3.5: The impact of feedstock demand on single-refinery systems. Note that the delivered cost and transportation cost use the left vertical axis, and the percentage of TOP utilization and rail transportation use the right vertical axis.

transportation cost of biomass deliveries with longer distances. Pretreatment starts to be utilized when the demand exceeds 6.6 Tg/year, and the proportion of torrefied pellets on an energy basis grows to about 33% at the largest demand. Railway transport for biomass delivery starts at 9 Tg/year and increases to about 37% on a wet Mg-km basis.

For the biorefinery at Scotts Valley (Figure 3.5(b)) where local biomass resource is scarce, pretreatment starts at 3 Tg/year demand and reaches about 65 percent at 12 Tg/year demand. Railway transport starts to be used at 5.4 Tg/year and grows to about 50% at the largest demand. Since a major share of the feedstock is procured from longer distances compared to the Redding biorefinery, both pretreatment and rail transport become part of the solution at smaller demands and reach higher proportions. Note that the averaged transportation cost has a noticeable drop right after pretreatment becomes preferred, a trend absent from the Redding analysis. Pretreatment reduces the transportation cost more significantly on long-distance deliveries and the Scotts Valley biorefinery also receives more torrefied pellets than the Redding biorefinery.

The single-biorefinery scenario illustrates that TOP pretreatment can help in logistics by providing feedstock to a facility that needs to source feedstock from a long distance, and particularly, it takes advantage of rail transportation for long-distance feedstock shipments.

Impact of increased feedstock demand on pretreatment location In the 10-biorefinery baseline scenario, the biorefinery at Scotts Valley (Figure 3.2) receives torrefied pellets from the pretreatment facilities in the far north of California. The long-distance shipment passes close to several biorefineries in the north. The question arises: why not ship to closer biorefineries? This model result reflects the capacity constraint imposed on all biorefinery locations of 1.2 Mg/y in the baseline scenario. Although closer locations would minimize transport cost, the total capacity constraint means that facility needs have already been met while additional feedstock is still available. To test how variability in demand at specific locations would impact the pretreatment and biomass procurement cost for more distant biorefineries, the baseline model was perturbed, increasing the capacity of the Chico refinery to 2.4 Tg/year (Figure 3.2). Due to this demand increase, biomass resources in the north no longer feed the refinery at Scotts Valley, and instead

of building two pretreatment facilities in the north as included in the baseline scenario (Figure 3.2), another pretreatment facility is deployed in the southern part of the state to ship torrefied pellets to the biorefinery at Scotts Valley in meeting the required demand there. Alternatively, the Scotts Valley biorefinery might not be constructed, or requires strategies such as contracting with biomass providers to ensure feedstock supply in a competitive and uncertain market to survive.

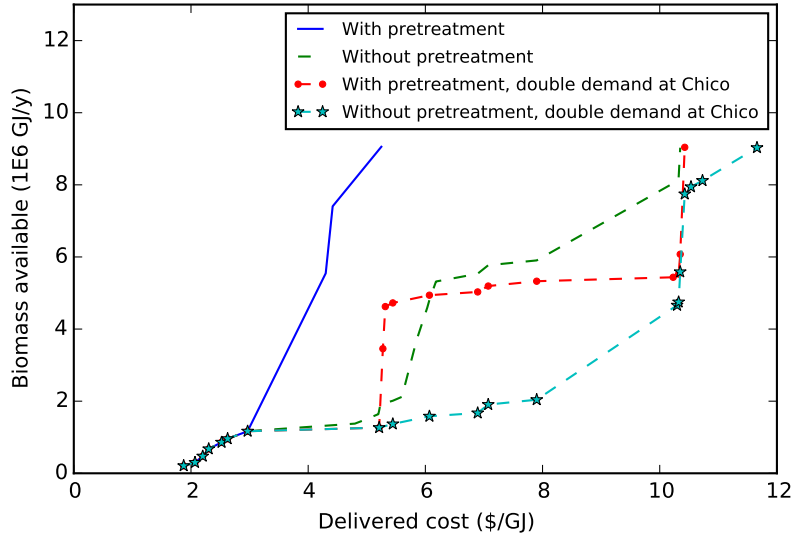


Figure 3.6: Aggregated feedstock supply curve of the Scotts Valley biorefinery

Figure 3.6 shows supply curves for feedstock delivered to the Scotts Valley biorefinery under several scenarios. For the baseline configuration with and without pretreatment, a dramatic reduction ($\approx \$5/\text{GJ}$) in the cost of procuring feedstock is achieved with the introduction of pretreatment. In addition, when the demand for feedstock is doubled at the Chico refinery, the Scotts Valley facility is in a much better position to make up for lost supply at substantially less cost with pretreatment than without, although at higher and potentially uncompetitive cost overall.

3.5 Discussion and Conclusions

The model analysis shows that torrefied pellet utilization can reduce the total cost of a biomass supply system, especially through reductions in transportation cost for long-

distance deliveries. In the baseline scenario, the total delivered feedstock and transportation costs of an optimal biomass supply system including pretreatment facilities are 5.2% (0.24 \$/GJ) and 14.5% (0.84 \$/GJ) lower than the optimal system without biomass pretreatment.

Critical factors affecting the performance of biomass pretreatment were investigated through sensitivity analysis. The deployment of a pretreatment facility is crucially dependent on the demand and the spatial characteristics of the biorefineries and the feedstock supply. Economies of scale have significant impact at smaller pretreatment sizes, but have less effect beyond about 100 kton/year. Lower feedstock procurement and higher road (truck) transportation costs both increase torrefied pellet utilization. Depending on the diesel fuel and fixed rail prices and the location of a pretreatment facility, rail transport could take up as much as 50 % of the total biomass energy or as little as 15% in the case of high fixed rail cost and low diesel price scenarios.

The model addresses the feasibility and design configuration with pretreatment included in the biomass supply system. The results provide insights into the potential for combined torrefaction and pelletization in reducing costs of bioenergy feedstocks from Californias forests. The modeling framework is flexible and could also be implemented in the investigation of other types of pretreatment and feedstocks.

The present model is limited in several ways. The additional cost savings at biorefineires brought by torrefied pellet utilization is varied from zero in the baseline scenario to as high as 5 \$/GJ in the sensitivity analysis. This effect is highly uncertain, however, and for some processes torrefied material may not represent a higher quality feedstock and hence could increase conversion costs if used. Additional information and research is needed to assess these quality implications. The model as currently implemented also ignores biomass imports, and does not consider torrefied pellets as a commodity for sale on the market, including export, which may influence the feasibility and profitability of pretreatment facilities. Impacts on the transportation network such as traffic congestion, state-wide railway capacities, and other factors were also not considered.

3.5.1 Conclusions

Feedstock pretreatment through combined torrefaction and pelletization is shown to enhance the flexibility and profitability of a biomass supply system when long-distance delivery is needed. For California's woody biomass supply, TOP process reduces the delivered cost and transportation cost by about 5% and 15%. Where transportation distances typically are less than 300 km, wood chips are, however, preferred over torrefied and pelleted material.

It is likely that initial investment in relatively small biofuels production facilities will be made in locations close to plentiful feedstock with relatively low transportation costs, making pretreatment unlikely. However, as the industry expands to meet the full supply potential or draw feedstock from outside the state, larger facilities relying on diverse sources of feedstock with longer supply chains are more likely. In this later stage of industrial development pretreatment such as evaluated here can result in lower procurement costs.

Chapter 4

Modeling Integrated Bioenergy Production System for Economic Sustainability Assessment Under Uncertainty

Summary

In this chapter, we present a full-scale application of bioenergy supply chain system model under uncertainty. The methodology and analysis in this application is an extension to the Li et al. (2016) study, which was built upon the original GBSM model developed by Parker (2011), and formulated the integrated bioenergy production system by incorporating the BCAM agricultural model by Jenner and Kaffka (2012). This chapter differentiates itself from Li et al. (2016) in two major aspects:

- **Full-scale system optimization versus single site analysis.** Li et al. (2016) built a simulation scheme to run single-site analysis by fixing the biorefinery allocation decisions in GBSM to identify a set of near-optimal biorefinery deployment options based on delivered cost of biofuel. In this study, the full model of the Pacific Northwest region involving multiple refineries and the facilitating land development is optimized to find the best system configurations in terms of biorefinery siting and land allocations. The full system optimization is primarily enabled by applying

aggregated spatial resolutions (i.e., change the feedstock procurement and land allocation decisions from $8 \times 8 \text{ km}^2$ pixel level to the county level) to gain holistic views of the modeled system for the entirety of the study region.

- **Stochastic model versus deterministic approach.** The GBSM model in Li et al. (2016) used a deterministic approach and didn't consider system uncertainties in the optimization. The methodology developed in this chapter incorporates uncertainty element in the crop market by using a two-stage stochastic programming model, which finds robust system configurations with improved economic performances in expectation.

4.1 Introduction

Biofuels has gained massive attention nowadays due to its potential for reducing greenhouse gas emissions, diversifying transportation fuels portfolio, and facilitating regional economic growth. In the U.S., biofuels has been supported by governmental policies at both federal and state level, such as the federal program of Renewable Fuel Standard (RFS2) (Environmental Protection Agency, 2013) and Californias Low Carbon Fuel Standard (LCFS) (California Air Resources Board, 2012). One of the crucial challenges for the emerging biofuel industry is to deliver economically competitive fuel products to the end-user market, which requires sophisticated biofuel production systems that integrate all components from the entire bioenergy supply chain (i.e., feedstock suppliers, conversion facilities, biomass/biofuel shipment, and fuel distribution terminals).

Most existing studies on biofuel supply chain design take a central planner's perspective and use mathematical models to determine the optimized decisions of all the agents in the system (e.g., feedstock supplier, refinery builder). Such an approach usually optimizes the system to achieve a single objective — mostly to maximize the total profit or to minimize the total cost (e.g., Eksioglu et al., 2009; Parker et al., 2010; Tittmann et al., 2010; Lin et al., 2014). Although taking the central planner's perspective is essential to study the configuration of an ideal bioenergy supply chain system, the assumption that all decisions are made by a central planner is overly crude. Instead, one of goals of this study is to build

an integrated biofuel production system that differentiates competition and coordination among various interdependent decision makers in the supply chain. In particular, this work is focused on large-scale biofuel systems using dedicated energy crops as feedstocks, where the competition between biomass feedstocks and conventional agricultural crops cannot be ignored due to the scarcity of suitable cropland. The collective decisions of cropland owners on adopting new energy crop over incumbent crops will shape the layout of the entire system.

Furthermore, this study also significantly differs from the few studies that incorporate crop land owners decisions on market choice in bioenergy supply chain (Bai et al., 2012; Wang et al., 2013), including (a) a greater focus on large-scale implementation and (b) considering a wider range of existing crops. More specifically, Bai et al. (2012) and Wang et al. (2013) developed game-theoretical models with small-scale implementations and only considered the competition between corn production for local food market versus selling to biofuel manufacturers. Yet, our study will involve an equilibrium model for agricultural land allocation decisions, and consider the competition between dedicated energy crop plantation and a large set of incumbent crops on large spatial scales. With a large-scale implementation for the Pacific Northwest US region, our study focused on providing more realistic system-level scenario analysis for relevant stakeholders (e.g., cropland owners, biofuel industry), and to support policy makers with economic and environmental analyses on both the agriculture and the fuel markets.

In addition to the inter-dependencies between different decision makers, another well-known challenge for biofuel production systems is its high degree of uncertainties due to (a) fluctuating fuel demand and prices (Markandya and Pemberton, 2010; Chen and Fan, 2012), (b) evolving policy regulations (Yeh and Sperling, 2013), and (c) in biomass feedstock supply (Yano and Lee, 1995; Richardson et al., 2011). This poses significant risks to pertinent stakeholders, especially for biofuel manufacturers where substantial investment is required to construct facilities for large-scale biofuel production (Parker, 2011; Chen and Fan, 2012), and for farmers where crop adoption and land replacement decisions are intrinsically irreversible.

Several approaches have been widely applied to deal with uncertainty issues of the biofuel supply chain system, such as sensitivity analysis (Kim et al., 2011) and simulation (Zhang et al., 2016). In the supply chain management area, however, one of the most extensively used approaches for hedging against uncertainty and risk is stochastic programming model. Such a model extends the deterministic framework by optimizing the expectation of the objective and/or minimizing certain system risk metrics across all uncertain scenarios (Santoso et al., 2005; Sodhi and Tang, 2009; Chen and Fan, 2012; Awudu and Zhang, 2013; Huang et al., 2014; Li and Hu, 2014).

In summary, the key feature of this study is the incorporation of uncertainty element to an integrated biofuel production system that considers the competitive and collaborate decision-making processes. The methodology aims at bridging previous research efforts in agricultural production models, integrated supply chain models, and robust system design approaches via stochastic programming, which simultaneously address crop competition in a multi-agent setting and the uncertainties in biofuel supply chain systems. The proposed modeling framework is applied to a case study of economic and sustainability assessment for the entire Pacific Northwest US region.

The rest of this chapter is organized as follows: The mathematical formulation of our model is provided in Section 4.2. Detailed descriptions of system components as model inputs are given in Section 4.3. The results and analyses for the study region are presented in Section 4.4. Final discussions are concluded in Section 4.5.

4.2 Methodologies

In this section, we first describe the scope of our modeling framework, including the spatial structure of the integrated biofuel supply chain, and the characteristic decision-making flow of the system. Then we present in detail the notations and mathematical formulations of our model.

4.2.1 Integrated modeling framework for bioenergy production systems

Integration of agricultural land allocation. As shown by Figure 2.2 in Section 2.2.2, the biofuel production system is modeled as an integrated supply chain network connecting agricultural landowners, bioenergy producers, and biofuel end users.

The integrated modeling framework comprises two major modeling components. The first component is an agricultural production model that determines the entering prices needed for crop displacement to occur, and the cropping patterns in agricultural land under various levels of purchasing prices offered by the biofuel industry. The second component uses a supply chain model to find optimal strategies for biofuel industry (refinery allocation, feedstock acquirement, biomass/biofuel transportation) given the feedstock supply curves and the biofuel demand functions. If biofuels could be produced and delivered to fuel distribution centers at a total cost less than the selling prices determined by the inverse demand function, then refineries will be built at proper locations, and the industry will provide feedstock purchasing prices higher enough for energy crop to be adopted by farmers and supply biofuels to meet the demand at terminals. On the other hand, if it is not profitable for the industry to produce biofuels from the energy crop, then the corresponding market share is assumed to fall into other types of fuels (e.g., conventional fuels).

To address the issue of competing crops in agricultural lands, landowners are assumed to be individual decision makers who allocate the croplands to maximize their own profit. A statewide agricultural production model developed by Howitt et al. (2012), referred to as SWAP, is incorporated to model farmers cropping behaviors. The output of SWAP as spatial-dependent biomass supply curves under a variety of feedstock purchasing prices will then serve as the input of the biofuel supply chain model.

Two-stage stochastic model. Two-stage stochastic programming (Birge and Louveaux, 2011) is a common choice for modeling uncertainties in biofuel supply chain (Chen and Fan, 2012; Huang et al., 2014; Li and Hu, 2014), and our poplar-based biofuels system model also fits naturally into this framework. Specifically, based on the magnitude of investment required and the irreversible nature, decisions in the system are catego-

rized as strategic planning decisions and operational decisions. The rationale for such a categorization is that planning decisions often require large amount capital investment, and cannot be practically reversed or adjusted once made, such as refinery locations, technology selection, and land allocation for poplar plantations. We explicitly assume that only the approximated distribution of the uncertain system parameters are known before first-stage planning decisions are made, so the main objective for such decisions is to maximize the expected profit across all possible scenarios. Operational decisions such as feedstock procurement, biomass transportation, fuel production, delivery and sales, are often more flexible and can be adjusted more easily based on the actual realizations of the system uncertainties in supply and demand. That is, we use separate operational decisions variables for each scenario and seek to optimize the operations of the system under that scenario for which the second-stage variables are specifically created. Detailed descriptions of the decision variables in each stage, and all the input parameters are listed in Table 4.1.

4.2.2 Mathematical formulation

Based on the previously stated modeling assumptions, a stochastic mixed-integer linear model is formulated in this section, with model decision variables and parameters listed in Table 4.1. The formulation is essentially a stochastic programming development of the model in Li et al. (2016), with modified spatial resolution and full set of potential locations for simultaneous biorefinery allocation and land displacement optimization in the entire study region.

Table 4.1: Model parameters and decision variables

Name		Definition	Unit
Sets			
Ω		Index ω , set of uncertain scenarios	
I		Index i , set of cropland areas	
Continued on next page			

Table 4.1 – continued from previous page

Name	Definition	Unit
J	Index j , set of candidate biorefinery locations	
K	Index k , set of fuel distribution terminals	
C	Index c , set of existing crop types	
PL	Index pl , set of purchasing price levels of energy crop feedstock	
S	Index s , set of biorefinery scales measured in millions of gallons per year (MGY)	
Decision Variables		
$PA_{i,pl}$	Acres of land adopted for poplar under price level pl in area i	Acres
$CD_{i,c,pl}$	Acres of land replaced for existing crop c under purchasing price pl in area i	Acres
$BD_{j,s}$	binary variable, build a biorefinery of scale s at location j if $BD_{j,s} = 1$	
$FT_{i,j}(\omega)$	Feedstock transported from supply point i to refinery at j	Dry tons per year
$PT_{j,k}(\omega)$	Fuel product transported from location j to terminal k	Gallons per year
$PS_k(\omega)$	Fuel product sales quantity at terminal k	Gallons per year
$FC_{j,s}(\omega)$	amount of feedstock that a scale s biorefinery at location j consume	
Model Parameters		
Continued on next page		

Table 4.1 – continued from previous page

Name	Definition	Unit
$Crop_less_{i,c,pl}(\omega)$	Maximum area of land at i of existing crop c to be adopted into poplar under purchasing price level pl	Acres
$Procurement_{i,pl}$	feedstock procurement cost at i under poplar price level pl	Dollars per ton
$Yield_i(\omega)$	Poplar yield in area i	Tons per acre
$TCF_{i,j}$	Feedstock transportation cost	Dollars per ton
$TCP_{j,k}$	Transportation cost for fuel products	Dollars per gallon
$Capital_{j,s}$	Annualized capital cost for building a refinery at location j	Dollars per year
$OM_{j,s}$	Biorefinery operating and management cost	dollars per year
$Var_{j,s}$	Variable cost of a scale s biorefinery in location j to produce fuel from feedstock	Dollars per ton
$M_s,$	maximum feedstock consumption capacity of a scale s biorefinery	Ton per year
η_s	conversion coefficient from poplar to bio-fuel in a scale s refinery	Gallon per ton
$Price_k(\omega)$	Biofuel sales price at terminal k	Dollar per gallon
$DE_k(\omega)$	demand for biofuel in terminal k	Gallon per year

Objective function The objective of the model is to maximize the expected total annual profit of the system, which is defined as the expected annual revenue from the sale of biofuels at fuel terminals less the expected annual cost of producing and delivering those biofuels (4.1). The expected total cost includes the procurement of poplar (4.2), the trans-

portation of feedstock to biorefineries (4.3), and of biofuel to distribution terminals (4.4), the fixed cost (4.5) and variable cost (4.6) of biofuel conversion.

$$\text{Profit} = \mathbb{E}_{\omega \in \Omega} \left[\sum_k \text{Price}_k(\omega) \cdot \text{PS}_k(\omega) \right] - \mathbb{E}_{\omega \in \Omega} [\text{Cost}] \quad (4.1)$$

$$\mathbb{E}_{\omega \in \Omega} [\text{Cost}] = \sum_{i, pl} \{ P A_{i, pl} \cdot \mathbb{E}_{\omega \in \Omega} [\text{Procurement}_{i, pl} \cdot \text{Yield}_i(\omega)] \} \quad (4.2)$$

$$+ \mathbb{E}_{\omega \in \Omega} \left[\sum_{i, j} \text{TCF}_{i, j} \cdot \text{FT}_{i, j}(\omega) \right] \quad (4.3)$$

$$+ \mathbb{E}_{\omega \in \Omega} \left[\sum_{j, k} \text{TCP}_{j, k} \cdot \text{PT}_{j, k}(\omega) \right] \quad (4.4)$$

$$+ \sum_{j, s} (\text{Capital}_{j, s} + \text{OM}_{j, k}) \cdot \text{BD}_{j, s} \quad (4.5)$$

$$+ \mathbb{E}_{\omega \in \Omega} \left[\sum_{j, s} \text{Var}_{j, s} \cdot \text{FC}_{j, s}(\omega) \right] \quad (4.6)$$

Note that the spatial-dependent land conversion decisions $PA_{i, pl}$ and facility allocation decisions $BD_{j, s}$ belong to first-stage planning decisions, thus are non-anticipative, and don't depend on uncertain scenarios ω .

Constraints on cropland allocation The optimization model has a number of constraints that represent the physical limitations and economic restrictions of the biofuel supply chain. The first set of constraints put down limits on agricultural land allocations and fix the spatial disparity between the supply chain model and the SWAP results. Specifically, given a feedstock purchasing price pl , the acres of land adopted for poplar under should be less than the total land area that various existing crops have been removed (4.7); the total acres of land got replaced from any incumbent crop should be less than what the landowners would be willing to provide under all uncertain scenarios (4.8); and all the land replacement and crop adoption decisions are made under one and the same poplar price level in each land region (4.9). Note that $PA_{i, pl}$ are mathematically redundant and only remains in the formulation for the convenience of making conceptual sense of the

model.

$$PA_{i,pl} \leq \sum_c CD_{i,c,pl} \cdot ON_{i,pl} \quad \forall i \in I, pl \in PL \quad (4.7)$$

$$CD_{i,c,pl} \leq Crop_less_{i,c,pl}(\omega) \quad \forall i \in I, c \in C, pl \in PL, \omega \in \Omega \quad (4.8)$$

$$\sum_{pl} ON_{i,pl} \leq 1, \quad \forall i \in I \quad (4.9)$$

Constraints on network flow conservation To maintain the conservation properties of the supply chain network, we require that the total amount of feedstock transported from each land region cannot exceed the total yield (4.10); the amount of feedstock consumed at each refinery location is no more than delivered (4.11); and the total amount of biofuel transported from a refinery cannot exceed the total production (4.12). Note that $FC_{j,s}(\omega)$ is also preserved in the formulation for convenience of reading the model, especially in constraints (4.10) - (4.13).

$$\sum_j FT_{i,j}(\omega) \leq \sum_{pl} Yield_i(\omega) \cdot PA_{i,pl} \quad \forall i \in I, \omega \in \Omega \quad (4.10)$$

$$\sum_s FC_{j,s}(\omega) \leq \sum_i FT_{i,j}(\omega), \quad \forall j \in J, \omega \in \Omega \quad (4.11)$$

$$\sum_k PT_{j,k}(\omega) \leq \sum_s \eta_s \cdot FC_{j,s}(\omega) \quad \forall j \in J, \omega \in \Omega \quad (4.12)$$

Forcing constraints on biorefinery siting Since biofuels could only be produced after we build the refining infrastructure, we use forcing constraints to ensure that the total amount of feedstock consumed by a scale s refinery at location j cannot exceed the maximum consumption capacity on the condition that the refinery is chosen to be constructed (4.13); and at most one scale could be selected, thus no more than one refinery could be built in each potential locations (4.14).

$$FC_{j,s}(\omega) \leq M_s \cdot BD_{j,s} \quad \forall j \in J, \forall s \in S, \omega \in \Omega \quad (4.13)$$

$$\sum_s BD_{j,s} \leq 1, \quad \forall j \in J \quad (4.14)$$

Constraints on biofuel sale Biofuel sale at each fuel distribution terminal is limited by both the total amount of fuel delivered (4.15)).

$$PS_k(\omega) \leq \sum_j PT_{j,k}(\omega) \quad \forall k \in K, \omega \in \Omega \quad (4.15)$$

$$PS_k(\omega) \leq DE_k(\omega) \quad \forall k \in K, \omega \in \Omega \quad (4.16)$$

Constraints of non-negativity and integrality All variables that represent physical quantities must take on non-negative value (4.17). The binary variables for biorefinery siting and poplar price level selection must take on a binary value of zero or one (4.18)

$$PA_{i,pl}, CD_{i,c,pl}, FT_{i,j}(\omega), PT_{j,k}(\omega), FC_{j,s}(\omega), PS_k(\omega) \geq 0 \quad (4.17)$$

$$ON_{i,pl}, BD_{j,s} \in \{0, 1\} \quad (4.18)$$

4.3 Model Inputs

The methodology described in Section 4.2 is implemented for the hardwood biofuels industry in the Pacific Northwest US region, which consists of the state of Washington, Oregon, Idaho, Northern California, and Western Montana. The model inputs for this case study are presented in this section, including characteristics of the major components in the supply chain (e.g., transportation networks, potential biorefinery locations, bio-jet fuel technology), and upstream models from other studies (Hart et al., 2015; Howitt et al., 2012) used to generate outcomes in poplar yield and cropland allocations.

4.3.1 Transportation network

The transportation cost model from previous studies (Tittmann et al., 2010; Li et al., 2017) is used to estimate the costs of delivering biomass feedstocks and biofuels in the supply chain. The transportation network data were assembled from Bureau of Transportation Statistics (Bureau of Transportation Statistics, 2011). The network includes three modes (highway, railway and marine) for bulk biomass and liquid fuel transportation with inter-modal facilities that allows for unloading/loading for biomass or fuel in order to shift between different modes. Biomass and biofuel transportation cost are modeled based on cost components listed in Table 4.2.

Table 4.2: Transportation cost components (on wet basis)

Mode	Cost component	Biomass feedstock	Liquid fuel
Road	Loading/unloading	\$5 / Mg	\$0.02/gal
	Time dependent	\$29 / h per truckload	\$32 / h per truckload
	Distance dependent	\$1.10 / km per truckload	\$1.20 / km per truckload
	Truck payload	25 Mg	8000 gallons
Rail	Loading/unloading	\$5 / Mg	\$0.015/gal
	Fixed cost	\$19.5/ Mg	\$8.8 / gal
	Distance dependent	\$0.143 / (Mg·km)	\$0.0121/ (100 gal·km)
	Rail car capacity	50 Mg	33000 gallons
Waterway	Loading/unloading	\$5 / Mg	\$0.015/gal
	Fixed cost	\$3.85 / Mg	\$1.4/gal
	Distance dependent	\$ 0.027 / (Mg·km)	\$0.024 / (100 gal·km)
	Barge capacity	3600 Mg	1.26 million gallons

The network is compiled in a GIS system and enabled for calculating the travel time and distance between any two locations in the study region. The travel information is integrated with the cost model to generate the the transportation cost for any specific routes. Least-cost routing is performed using the Network Analyst extension in ArcGIS to calculate the final transportation cost between all origin-destination pairs in the supply chain.

4.3.2 Potential poplar yield

Estimating the amount of available feedstocks for the biofuel industry based on dedicated energy crops requires robust spatial predictions of growth and yield of the crops under varying environmental conditions and across large regions (Hart et al., 2015). Headlee et al. (2013) developed a Physiological Principles in Predicting Growth (3PG) model across several states in the northern Midwest United States to predict growth and yield of hybrid poplar (*Populus spp*) based on weather, soil, site and stocking conditions, management practices and species definitions. Hart et al. (2015) modified the 3PG model by including

an additional biomass partitioning method and taking into account the impact of coppicing on post harvest regeneration.

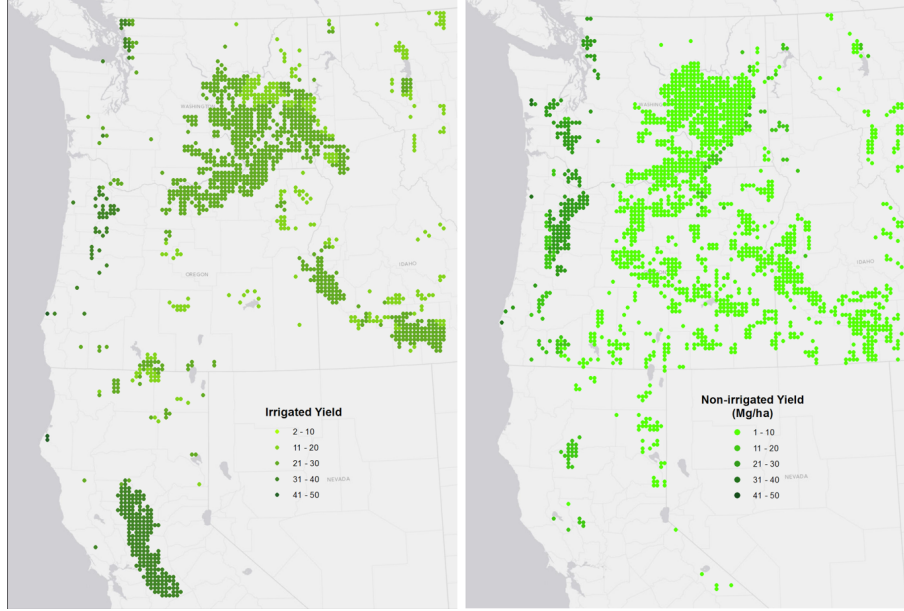


Figure 4.1: Predicted irrigated (left, for cropland) and non-irrigated (right, for rangeland) poplar yield in Mg/ha (Hart et al., 2015)

The 3PG model modified and implemented by Hart et al. (2015) was used to generate spatial-explicit poplar yield estimates for the poplar-based biofuels production system model in this study. Specifically, the 3PG model was implemented at a spatial resolution of $8 \times 8 \text{ km}^2$ throughout the entire study region of Pacific Northwest. Noted that poplar yield as biomass feedstocks was estimated for cropland and rangeland, and the cropland yields was pipelined to simultaneously feed the agricultural production model (Section 4.3.3) to create regional cropping patterns under competitions versus incumbent agricultural crops and the biofuels supply chain model as feedstock supply at adopted croplands. See Figure 4.1 created by Hart et al. (2015) for an example of the 3PG model outcomes.

4.3.3 Potential biomass feedstock resources

In the methodology Chapter (Section 2.1), we used the BCAM model developed by Jenner and Kaffka (2012) to exemplify the PMP-based approach for agricultural economic modeling. In this study, a different agricultural model called Statewide Agricultural Production

Model (SWAP) developed by Howitt et al. (2012) is incorporated with the bioenergy supply chain model described in Section 4.2 to provide inputs that estimate the price required for energy crops to enter the market and farmers' crop replacement behaviors under a range of energy crop prices. Similar to BCAM developed by Jenner and Kaffka (2012), SWAP is a mathematical optimization model that maximizes cropland owner's profit subject to land availability and water consumption constraints, and it also applies the Positive Mathematical Programming approach (Howitt, 1995) and self-calibrates its parameters to match the base dataset of incumbent crops without adopting energy crops. Nonetheless, SWAP utilized an exponential production function that is able to generate more conservative crop replacement patterns.

In this case study, SWAP is applied to the Pacific Northwest US region. Specifically, an incumbent crop mix of field, grain and other crops at each county was employed as a base dataset and the potential for growing irrigated and non-irrigated poplar was introduced as potential sources for biomass feedstocks. To incorporate the land allocation decision and feedstock availability information, the bioenergy infrastructure model takes a discrete set of potential poplar price levels for cropland decision-makers, and the price-dependent adoption patterns from the SWAP and poplar yield estimates from the 3PG model jointly provide crop-specific and spatial-explicit feedstock supply curves as inputs for the supply chain model.

4.3.4 Bio-jet fuel technology and refinery scale

The technology for producing bio-jet fuel is based on hybrid technology being developed by industry (Verser and Eggeman, 2011) that combines biochemical conversion to acetic acid and thermochemical upgrading to jet fuel. Biomass undergoes dilute acid pretreatment to hydrolyze the sugars. Sugars are fermented to acetic acid, which is sequentially converted to ethyl acetate, ethanol, ethylene, and finally a hydrocarbon end product. An unfermentable lignin stream is burned for steam and electricity production. During biofuel production, hydrogen gas is required and is obtained by steam methane reformation of natural gas. The process is an efficient use of biomass carbon, generating 334 liters of jet fuel per Mg of poplar consumed.

Techno-economic analysis of the technology at multiple scales developed by Crawford (2013) shows that the technology requires high volumes in order to approach economic viability. The 380 Ml per year (equivalent to 100 MGY) size is the most promising. The techno-economic performance of the the technology at multiple scales is shown in Table 4.3.

Table 4.3: Economic characteristics of biofuel conversion technology

Scale	Capital Cost	Fixed O&M	Variable	Natural Gas	Electricity
MLY(MGY)	(million \$)	(million \$/yr)	Cost (\$/L)	Consumed (MJ/L)	Sales (Wh/L)
95 (25)	303.5	19.6	0.26	32	53
190 (50)	477.3	29.1	0.25	31	62
380 (100)	764.3	44.5	0.24	62	62

In a previous single-site analysis work (Li et al., 2016), profitability potentials of biorefineries at multiple capacities were investigated. In this study, however, we only consider the bio-jet fuel technology at full capacity (100 million gallons per year) for the following two reasons: 1) the bio-jet technology has shown strong economies of scale as demonstrated by Li et al. (2016); 2) we are more interested in the effect of model input uncertainties on infrastructure development decisions with large capital and fixed investment, in which under-optimized decisions might show greater loss in revenues.

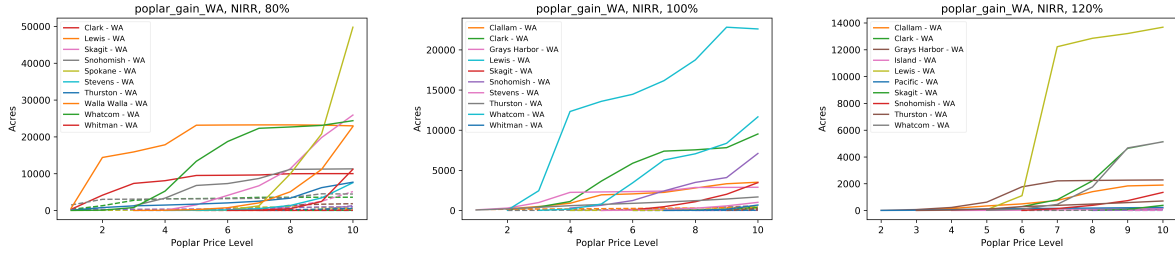
4.3.5 Potential biorefinery locations

The method for selecting potential biorefinery locations from Tittmann et al. (2010) was adopted and refined to consider land values and additional cost of rail construction to facilitate large-scale feedstock and biofuel storage and transportation. The same 668 sites as used by Li et al. (2016) are selected across the entire study region as candidate for biorefinery allocation.

4.3.6 Modeling system uncertainty

For this study, uncertainties in the agricultural market was considered. Specifically, we set up three scenarios for incumbent crop values measured in \$/acre (i.e., Default, Low - 80% of default, High - 120% of default), and use the SWAP model developed by Howitt et al. (2012) to generate results under these scenarios, which will lead to scenario-dependent

crop replacement decisions that optimize farmer's profit, and eventually change the price required for the bioenergy industry to procure sufficient biomass feedstocks for production. The incumbent crop value scenarios were constructed to represent potential crop price variations based on the USDA Monthly Farm Price Index from year 2010 to 2017 (USDA National Agricultural Statistics Service, 2019).



(a) Low crop value scenario (b) Default scenario (c) High crop value scenario

Figure 4.2: Example of SWAP model outcomes in different incumbent crop value scenarios (from left to right: 80%/100%/120% of default crop values). The X-axis represents poplar price levels in \$/ton, and Y-axis represents the area of adopted cropland in acres. Each colored line represents a single county. Legends only show top 10 counties in highest possible poplar adoption.

Using the SWAP outcomes for the Washington state as an example, Figure 4.2 shows the acres of non-irrigated cropland replaced by poplar growth at county-level under the three scenarios as defined above. With lower (80%) incumbent crop values (Figure 4.2(a)), poplar adoption starts to incur at a poplar price of $< \$2/\text{ton}$ in some counties, and goes up to $> 20,000$ acres in Spokane, Skagit, Whatcom, Lewis, and Walla Walla county. Under default (100%) incumbent crop value scenario (Figure 4.2(b)), starting price for poplar adoption is about $\$2/\text{ton}$, and total adopted lands can only go to $< 10,000$ acres in most counties apart from Lewis. Under the high (120%) crop value scenario, starting biomass purchasing prices for significant amount of poplar adoption is about $> \$4/\text{ton}$, and highest potential adopted lands are below 6,000 for most counties, with the exception of Lewis county that can potentially adopt 12,000 to 14,000 acres of poplar under $\$7/\text{ton}$ to $\$10/\text{ton}$ purchasing prices.

In this case study, uncertainties in the crop market are considered as the main risk component that drives the variation of spatial displacement in poplar adoption patterns. A

variety of SWAP model results will then be incorporated by the supply chain infrastructure model as land allocation and feedstock availability constraints under the corresponding incumbent crop value scenarios.

4.4 Results and Discussion

Table 4.4: Comparison of model results (total land conversion, fuel production, profit)

	Deterministic (1)	Semi-Stochastic (2)	Stochastic (3)
Scenarios	Default scenario	Uncertainty scenarios incorporated	Uncertainty scenarios incorporated
Model Setup	Deterministic supply chain model	Biorefineries sited by the deterministic model, land conversion decisions and operational decisions under each scenarios optimized using stochastic supply chain model	Two-stage stochastic supply chain model
Total land conversion (Acres)	490,872	484,299	452,389
Converted crop-lands (Acres)	30,735	17,594	95,305
Converted marginal lands (Acres)	460,137	466,705	357,084
Total fuel production (MGY)	500	489 (expected)	489 (expected)
Total Profit (M \$)	314.09	228.82 (expected)	268.16 (expected)

(A \$5/gal fuel price and revenue from co-produced electricity are assumed in all the models)

In this case study, three models were developed to investigate the impact of modeling strategies on the profitability and spatial layout of the optimized systems (see Table 4.4). Specifically, we built and compared the following models:

- (1) a deterministic model to demonstrate the system configuration in an idealized environment without uncertainty.
- (2) a semi-stochastic model where the biorefinery allocation decisions were adopted from the deterministic model, while the rest of the decisions were optimized using a two-stage stochastic supply chain model with land conversions treated as first-stage variables, and other decisions (i.e., feedstock procurement, fuel product transportation and consumption, etc.) treated as second-stage variables. Uncertain scenarios as discussed in Section 4.3.6 were incorporated. The aims of building model 2 are twofold: 1) to examine the changes in land conversion strategies in order to serve the same set of biorefineries as determined in model 1 when uncertainties were considered; 2) to compare the impact of uncertainties on economic performances of the system.
- (3) A two-stage stochastic supply chain model that simultaneously optimizes the strategic decisions (i.e., biorefinery allocation and land conversions) and operational decisions with uncertain scenarios incorporated. The goal of model 3 is to illustrate the optimal system configurations developed to hedge against risks in feedstock supplies and crop market prices, and to compare strategies optimized by all three models to measure the benefit of a full-fledged two-stage stochastic supply chain model.

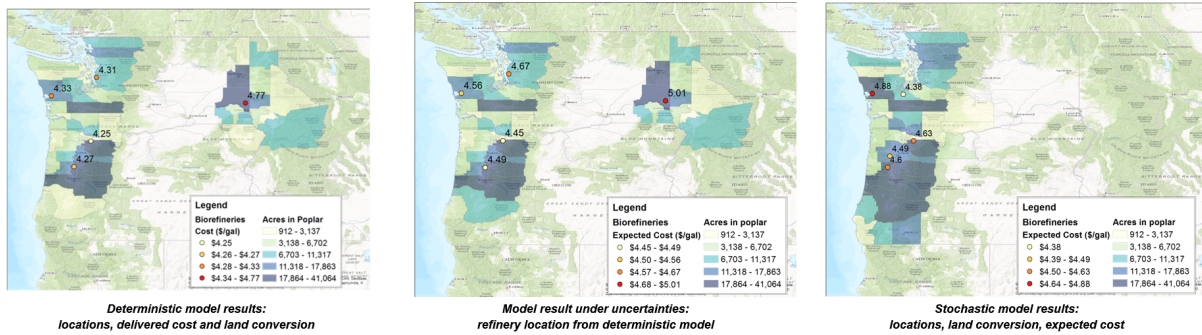


Figure 4.3: Comparison of spatial model outputs: refinery locations and bio-jet fuel delivered cost

As shown in Table 4.4, the deterministic model has the highest total converted lands, total fuel production, and a profit significantly higher than the expected profits from the (semi-) stochastic models. As the deterministic model was only designed for decision-making

under the default scenario, the results only represents the highest achievable performance under that scenario when crop price and feedstock supply uncertainties are not considered. The disadvantages of the deterministic modeling approach are demonstrated by a 27% lower total profit in expectation and under-utilization of biorefinery capacities when undesirable SWAP scenarios (defined in Section 4.3.6) are incorporated, as shown in the semi-stochastic model results. Notice that under crop price uncertainties, the economically available croplands dropped from 30,735 acres to 17,594 acres ($> 42\%$), and with the fixed biorefinery allocation decisions, the semi-stochastic model has to convert more marginal lands at higher costs (Figure 4.3) to compensate the lack of feedstocks from converted croplands, thus lead to lower expected fuel production, and significantly lower expected profit.

With the full-fledged stochastic model, however, the crop price uncertainties are hedged mainly by taking them into consideration of the biorefinery siting decisions, and only choose to allocate the plants to potential locations with sufficient amount of suitable croplands under all SWAP scenarios. This interpretation is supported by the distantly highest croplands conversion in the stochastic model results (3.1x compared to the deterministic model, and 5.4x compared to the semi-stochastic model), and the reallocated biorefineries shown in Figure 4.3, where all five refineries are located in the west coast. Specifically, the refinery previously located near Lewiston, ID by the deterministic model is removed, as it is especially unfit for tough supply scenarios with an expected delivered cost over \$5/gal in the semi-stochastic model results.

It's worth noting that the stochastic programming model in this study as defined by (4.1) - (4.18) is computed by converting the two-stage formulation into its deterministic equivalent, and directly optimizing the reformulated¹ mixed-integer program using the Gurobi optimization solver (Gurobi Optimization, 2017). Simple and straightforward as it seems, one major limitations of this approach is that it is computationally inefficient or even incapable of handling the increased model dimension if complicated probabilistic distributions of the uncertain scenarios ω need to be incorporated per modeling requirements.

¹Details of the reformulation are described in Section 2.3.1.

Potential enhancement to the present numeric approach in this study via decomposition and simulation will be discussed in the final chapter (Section 5.2) of the dissertation as one of the future research directions.

4.5 Conclusion

In this study, we show that uncertainties in the crop market could raise the estimates of jet fuel delivered cost by 2 to 8% depending on refinery location and whether the uncertainties are accounted for in the system planning. The benefit of building refineries at coastal areas of the Washington and Oregon state with poplar growth is amplified under uncertain crop pricing scenarios.

The robustness of the designed biofuel production system to hedge against cost and supply risks can be significantly improved by using stochastic supply chain models with a two-stage decision setting. Specifically, in this case study, the improvement in expected total profit is $> 17\%$.

Chapter 5

Conclusions

Summary

This chapter highlights the main conclusions of the dissertation and outlines potential directions for future research.

5.1 Conclusions

In this dissertation, I developed bioenergy supply chain models that are able to incorporate system uncertainties and integrate multiple decision-making agents to make spatial-explicit system design decisions. These decisions include agricultural land allocation and energy crop adoptions, biomass feedstock collection and transportation, siting locations and scales of biofuel conversion facilities, and distribution and sales for fuel products. The integration of agricultural economics is implemented by linking the supply chain infrastructure model to an agricultural production model, which optimizes the profits of farmers by allocating farmlands and making adjustments to existing crop portfolios to facilitate bioenergy production using energy crops as feedstocks. The integrated modeling approach enables the bioenergy industry to take into account farmer's responses and natural resource constraints when calculating the potential volumes of biomass feedstocks to support large-scale bioenergy production, and can help policy makers better evaluate the impact of bioenergy infrastructure development on the crop market and local environment. The flexibility and scalability of the methodology also allow modelers to specify the topological

structures of the supply chain networks and integrate system uncertainties via stochastic programming.

The methodology was demonstrated by two real-world applications with different modeling scopes and geospatial scales. Specifically, the California biomass feedstock supply case study showed that biomass pretreatment via combined torrefaction and pelletization is able to enhance the profitability of the feedstock supply system by reducing the overall delivered cost and transportation cost for long-distance biomass shipment. The Pacific Northwest bioenergy system study presented an enhanced supply chain model that incorporated uncertainty element to an existing integrated modeling framework (Bandaru et al., 2015; Li et al., 2016) to estimate the economic feasibility and seek optimal design decisions for the combined system under uncertainty. The reformulated stochastic optimization program was designed to cope with uncertainties in the crop market, and was able to find optimal solutions that improve the expected total profit by over 17% compared to the configured system where major strategic decisions were optimized by the deterministic model. The model results found that the system can produce jet fuel at costs between 4.4 to 4.9 dollars per gallon in expectation.

5.2 Future Research Directions

There are several limitations to the present modeling framework which can be addressed with future research effort.

5.2.1 System dynamics

The modeling framework as currently set out only applies to static optimization problems and is designed to determine long-term optimal system planning strategies. However, building a completely new alternative fuel production system may involve multiple planning stages with evolving technological and market conditions. One of the candidate approaches for incorporating system dynamics to the current modeling framework is called multi-stage optimization, in which model variables are created to capture decisions within each stage of a specified planning horizon, as well as transitional dependencies between multiple stages. The decision variables are required to simultaneously satisfy evolving

resource, supply, demand, and technological constraints from both within and between stages. From the computational perspective, however, expanding the dimension along which system design decisions are made will significantly increase the dimension of the formulated mathematical optimization problem, which is similar to the challenge brought by incorporating uncertainty to the supply chain models via stochastic programming.

5.2.2 Solution algorithms

The current implementation of the integrated framework doesn't integrate algorithmic techniques tailored for efficiently solving the formulated mathematical models (e.g., two-stage stochastic mixed-integer programs), thus will have difficulties handling problems of very large scales. Specifically, the stochastic programming model in Chapter 4 were optimized by converting the two-stage stochastic formulation into its deterministic equivalent and directly solving the resulting mixed-integer programming model using a commercial mathematical optimization solver (Gurobi Optimization, 2017). This naive implementation will become computationally inefficient or even infeasible when a significantly large number of scenarios are needed to represent the uncertainties in the input data. There are a few well established decomposition and simulation methods to handle computational challenges in large-scale stochastic programming (SP) models. For example, the Progressive Hedging (PH) algorithm (Rockafellar and Wets, 1991) partitions a SP model incorporating multiple scenarios by relaxing the non-anticipativity constraints and iteratively solve sub-problems that penalize non-anticipative solutions for all scenarios until a sufficient convergence is reached. Alternatively, Monte Carlo simulation methods such as Sample Average Approximation (SAA) can be used to estimate the expected value of recourse function $\mathbb{E}_\omega[Q(x, \omega)]$ in the model objective (2.12) by the sample average function $\frac{1}{N} \sum_{n=1}^N [Q(x, \omega)]$ and the resulting heuristic solution is shown to have statistically guaranteed optimality gaps (Mak et al., 1999; Ahmed et al., 2002). Exploring and encapsulating effective numeric algorithms to efficiently solve the formulated stochastic models will further enable the methodology and integrated framework to scale up for more demanding modeling requirements and complex bioenergy systems.

5.2.3 Risk-averse preference

The stochastic modeling approach in the dissertation employed risk-neutral objective functions, that is, to optimize only the expected value of a certain system objective without considering risk-averse preferences of the decision makers. Under the risk-neutral assumption, alternative solutions with similar expected values but potentially better distributions (e.g., smaller variance in total system profit, lower capital loss in undesirable extreme events) in the model outcome are not particularly favored. In reality, however, risk-averse preferences of different agents can be diverse. For example, while policy makers or a central planner may care more about the overall system profitability in expectation, an individual infrastructure developer or a cropland owner may also want to ensure that the total net revenues led by their key resource allocation decisions are beyond acceptable levels even under the worst possible scenarios.

Risk averse optimization is a branch of stochastic optimization that focuses on modeling decision maker's risk-aversion behaviors, and has been widely applied in almost all areas where stochastic models are involved, such as finance, medicine, and engineering. Based on Shapiro and Philpott (2007) and Shapiro et al. (2014), typical risk averse optimization approaches include the following:

Chance constraints. Chance constraints in the form of $G(x, \omega) > \tau$ (x represents the decision variables and ω is the scenario vector) can be added to a stochastic programming model formulated as (2.12) to control the probability of certain undesirable events so the corresponding objectives can be satisfied (e.g., production rate of allocated biorefineries be above X% at a pre-determined high confidence level for profitability reason) for all possible realization of the modeled scenarios $\omega \in \Omega$;

Mean-risk models. Mean-risk models add a risk/dispersion measure to the objective function in (2.11) to characterize the model outcome along with its expected value, the resulting objective function is to minimize the weighted sum of mean cost and the risk measure:

$$\min_x \mathbb{E}_{\omega \in \Omega}[f(x, \omega)] + \lambda R_{\omega \in \Omega}(X, \omega) \quad (5.1)$$

Typical risk measures $R_{\omega \in \Omega}(X, \omega)$ include the following:

- Variance
- Value at Risk (VaR), defined as the threshold value such that the probability of the outcome being greater than this value is under a predetermined confidence level $1 - \alpha$):

$$\text{VaR}_{1-\alpha}(X) = \sup\{t : \Pr(X \geq t) \geq 1 - \alpha\} \quad (5.2)$$

- Conditional Value at Risk (CVaR, defined as the expectation of the outcome conditional on the outcome being lower than the VaR, which measures the expected outcome in the $1 - \alpha$ worst possible scenarios):

$$\text{CVaR}_{1-\alpha}(X) = E[X|X \leq \text{VaR}_{1-\alpha}] \quad (5.3)$$

From a point of view of multi-objective optimization, a well-defined mean-risk model can provide decision makers a set of efficient solutions in the sense that it minimizes system risk for a given value of the mean outcome, and for a given value of risk it maximizes the mean outcome in (2.12).

Adopting risk averse optimization approaches in the integrated bioenergy system models requires higher levels of modeling and computational efforts, which makes it more important to integrate efficient solution algorithms as previously discussed into the present methodology framework.

5.2.4 Policy analysis

The implications drawn from the case studies in this dissertation are limited due to a lack of comprehensive and comparative policy analysis. Future research can focus on utilizing the model analyses to improve policy-making processes for biofuels. For example, a variety of policies that are potentially suitable for biofuel production can be hypothesized and included in the modeling framework to identify the most effective policy instruments to balance between system profitability and environmental restrictions or social impacts, or to inspect the economic feasibility for the bioenergy industry to develop systems required to achieve certain policy goals.

In the context of bioenergy production system modeling, an exemplary policy-related enhancement to the model developed in Chapter 4 is to include the carbon credits (e.g., Renewable Identification Numbers from RFS2) generated by biofuel production as reduced system cost to the refineries, and calculate the RIN-calibrated delivered cost for bio-jet fuels so we can better evaluate its competitiveness in the fuel market. From the uncertainty and risk analysis perspective, considering how the uncertainty in the valuation of carbon credits as a result of credit trading activities in the market would impact the demand for the modeled biofuel product, thus change the best infrastructure development and production strategies for bioenergy industry is also a potential policy question that can be answered by constructing and incorporating new scenarios in the stochastic modeling framework.

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