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BIOFUEL SUPPLY CHAIN RESTRUCTURING – AN ECONOMIC VIABILITY AND
ENVIRONMENTAL SUSTAINABILITY INVESTIGATION FOR ENHANCING
SECOND GENERATION BIOFUEL ADOPTION

by

RAJKAMAL KESHARWANI

A DISSERTATION

Presented to the Faculty of the Graduate School of the
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

In Partial Fulfillment of the Requirements for the Degree

DOCTOR OF PHILOSOPHY

in

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2019

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ABSTRACT

Biofuel is a promising clean alternative to fossil fuels. Currently, first generation biofuels are commercially produced by using corn grain as biomass feedstock. However, the use of edible matter of crops, may lead to a competition between food and fuel. Therefore, there is a significant push in both industry and academia to commercialize second generation biofuel manufacturing technology, which uses non-edible matter from crops. Most research focuses on individual manufacturing processes for producing second generation biofuel, but the economic and environmental impacts of a large-scale adoption of second generation biofuel manufacturing have been less widely reported.

This work investigates the optimization of first generation biofuel supply chain, and the switch to second generation biofuel supply chain, as a systems architecture optimization problem. First, first generation biofuel supply chain is modelled as a complex system of systems architecture with multiple stakeholders. After this, an initial study of critical process parameters in second generation biofuel manufacturing is conducted, and its environmental feasibility is investigated through a case study. Next, two strategies of switching from first generation to second generation supply chain architectures are explored. The mixed integer linear programming formulations of three supply chain models in two strategies are proposed to examine the performance from both economic and environmental perspectives. The models are validated through a case study based on the data extracted from the state of Missouri. The results indicate that although a large-scale adoption of second generation biofuel manufacturing is economically attractive, it will lead to higher greenhouse gas emissions.

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I thank my mother Anu Kesharwani, who through her life taught me that it is always worth adhering to the best in human nature. I thank my son Rishaan, who teaches me every day that hard work will always bear fruit. Finally, I thank the person who supported me and stood by me through this entire journey, my wife Reema. She taught me the true meaning of the saying “You can walk fast if you walk alone, but you can walk far if you walk together.”

TABLE OF CONTENTS

	Page
ABSTRACT.....	iii
ACKNOWLEDGMENTS	iv
LIST OF ILLUSTRATIONS.....	ix
LIST OF TABLES.....	xi
 SECTION	
1. INTRODUCTION.....	1
1.1. BACKGROUND AND MOTIVATION	1
1.2. AIMS AND APPROACHES.....	5
1.3. DISSERTATION SYNOPSIS	7
2. LITERATURE REVIEW.....	9
2.1. FIRST GENERATION BIOFUEL.....	9
2.1.1. Manufacturing Processes.....	9
2.1.2. Supply Chain of First Generation Biofuels	10
2.2. SECOND GENERATION BIOFUEL.....	11
2.2.1. Manufacturing Processes Specific to Second Generation Biofuels	11
2.2.2. Supply Chain of Second Generation Biofuels.....	14
2.3. SUMMARY OF LITERATURE REVIEW	19
2.3.1. Advantages and Disadvantages of First Generation Biofuels.....	19
2.3.2. Advantages of Second Generation Biofuels.....	19
2.3.3. Gaps in the Literature.....	20

3. BIOFUEL SUPPLY CHAIN OF FIRST GENERATION BIOFUELS.....	21
3.1. PROPOSED MODELS	22
3.1.1. Problem Formulation.....	26
3.1.2. An Illustrative Example.....	31
3.1.3. Solution Technique.....	34
3.2. CASE STUDY	39
3.2.1. Parameters in the Case Study	39
3.2.2. Benchmark Estimation	50
3.2.3. PSO Implementation.	51
3.3. RESULTS AND SENSITIVITY ANALYSIS	52
3.3.1. Results	52
3.3.2. Sensitivity Analysis.....	55
3.4. SUMMARY OF FIRST GENERATION BIOFUEL SUPPLY CHAIN OPTIMISATION.....	64
4. INITIAL STUDY OF SECOND GENERATION BIOFUELS	68
4.1. EFFECTS OF BIOMASS PARTICLE SIZE ON SUGAR YIELD	68
4.1.1. Experimental Configuration and Hypothesis Formulation	68
4.1.2. Experimental Results and Analysis.....	73
4.2. ENVIRONMENTAL IMPACTS OF PELLETING.....	76
4.2.1. Analysis of Benefits and Impacts of Pelletting.	76
4.2.2. Case Study.....	80
4.3. SUMMARY OF INITIAL STUDY OF SECOND GENERATION BIOFUEL SUPPLY CHAIN	88
5. ANALYTICAL MODEL OF SECOND GENERATION BIOFUEL SUPPLY CHAIN.....	90

5.1. PROPOSED MODEL.....	91
5.1.1. Corn Stover-Sourced Biofuel Supply Chain Using Distributed Preprocessing Strategy.....	96
5.1.1.1. Pathway 1: chemical pretreatment and physical densification in preprocessing center.....	96
5.1.1.2. Pathway 2: densification at preprocessing centers and AFEX at bio-refinery plants	102
5.1.2. Corn Stover-Sourced Biofuel Supply Chain Using Centralized Preprocessing Strategy.....	107
5.2. CASE STUDY	109
5.3. RESULTS AND SENSITIVITY ANALYSIS	116
5.3.1. Results.	116
5.3.2. Sensitivity Analysis.....	129
5.4. COMPARISON AMONG THREE MODELS IN TWO STRATEGIES	135
5.5. SUMMARY OF SECOND GENERATION BIOFUEL SUPPLY CHAIN OPTIMISATION.....	140
6. ECONOMIC VIABILITY AND ENVIRONMENTAL IMPACT INVESTIGATION OF CO-FERMENTATION IN BIOFUEL MANUFACTURING	144
6.1. BIOETHANOL PRODUCTION MODELS USING THREE OPTIONS	146
6.1.1. Corn-Sourced Biofuel Supply Chain.....	149
6.1.2. Corn-Stover-Sourced Biofuel Supply Chain Using Centralized Preprocessing Strategy.....	152
6.1.3. Ethanol Production through Co-Fermentation Using Corn and Corn Stover.	155
6.2. CASE STUDY	159
6.3. RESULTS	163
6.4. COMPARISON AMONG THREE MODELS.....	163

6.5. SUMMARY OF TECHNIQUE OF COFERMENTING FIRST AND SECOND GENERATION BIOFUELS	164
7. CONCLUSION AND FUTURE WORK.....	170
7.1. CONCLUSION.....	170
7.2. FUTURE WORK.....	170
BIBLIOGRAPHY	181
VITA.....	198

LIST OF ILLUSTRATIONS

	Page
Figure 1.1 First Generation Biofuel Manufacturing System	2
Figure 2.1 Corn-Sourced Bioethanol Manufacturing	9
Figure 2.2 Corn-Sourced Biofuel Supply Chain.....	10
Figure 2.3 Second Generation Biofuel Manufacturing System	12
Figure 2.4 Cellulosic Biofuel Supply Chain with Decentralized Preprocessing	15
Figure 3.1 A 4-Layer Biofuel Supply Chain Network.....	26
Figure 3.2 Three Counties in the Northern Region of Missouri	32
Figure 3.3 Eight Regions in Missouri	39
Figure 3.4 Solution Convergence	54
Figure 3.5 Effects of Variations of Biofuel and Biomass Prices	67
Figure 4.1 Knife Mill	69
Figure 4.2 Pelleting Machine	70
Figure 4.3 Pretreatment Reactor	71
Figure 4.4 ANOVA Model of Sugar Yield.....	74
Figure 4.5 Reduced ANOVA Model of Sugar Yield.....	74
Figure 4.6 Adequacy Checking Using Normal Probability Plot.....	75
Figure 4.7 Adequacy Checking Using Histogram	75
Figure 4.8 Adequacy Checking Using Residual versus Order	75
Figure 4.9 Fisher's Test Regarding Size Effects	76
Figure 4.10 Surface Plot for Corn Stover	77

Figure 4.11 Surface Plot for Wheat Straw 78

Figure 4.12 Surface Plot for Blue Bigstem 78

Figure 4.13 A Typical Supply Chain of Biomass 81

Figure 4.14 Scheduling Algorithm Example 82

Figure 4.15 Biomass Supply Chain System..... 84

Figure 5.1 Farms and Bio-Refinery Plants in Missouri 112

Figure 5.2 Average Corn Stover Transportation Amount from Farms to
Preprocessing Centers in Kilo-Tons in the Pathway 1 Supply Chain..... 120

Figure 5.3 Worth County Sourcing the Surplus Demand 121

Figure 5.4 Average Corn Stover Transportation Amount from Farms to
Preprocessing Center in Kilo-Tons in Pathway 2 Distributed Supply
Chain 126

Figure 6.1 Co-Fermentation of Corn and Corn Stover for Bioethanol Manufacturing .. 145

LIST OF TABLES

	Page
Table 3.1 Farms in the Northern Region of Missouri	31
Table 3.2 Bio-Refinery Plant in the Northern Region of Missouri.....	31
Table 3.3 Distribution Center in the Northern Region of Missouri	32
Table 3.4 Retailers Gas Stations in the Northern Region of Missouri.....	32
Table 3.5 Case Performance	33
Table 3.6 Biomass Transported from Farms to Bio-Refinery Plant in Tons	33
Table 3.7 Bioethanol Transported from Bio-Refinery Plant to Distribution Center in Gallons.....	33
Table 3.8 Biofuel Transported from Distribution Center to Retailers in Gallons	34
Table 3.9 Location Information of E85 Gas Stations in Missouri	42
Table 3.10 Information of Distribution Centers in Missouri	46
Table 3.11 Information of Location and Yearly Capacity of Bio-Refinery Plants in Missouri.....	46
Table 3.12 Information of Farms in Missouri.....	47
Table 3.13 Parameters for Calculating Transportation Emissions.....	50
Table 3.14 Capacity of Different Layers (Bioethanol Gallon Equivalent).....	51
Table 3.15 Parameters Used in PSO	53
Table 3.16 Selection of Farms in Different Regions	53
Table 3.17 Farms Selected.....	54
Table 3.18 Bioethanol Transported from Bio-Refinery Plants to Distribution Centers in Gallons	55
Table 3.19 Biomass Transported from Farms to Bio-Refinery Plants in Tons	56

Table 3.20 Biofuel Transported from Distribution Centers to Retailers in Gallons	58
Table 3.21 Performance of the Obtained Result	63
Table 3.22 Solution Performance with Different Weight Combinations	65
Table 3.23 Results Performance with Variable Demand.....	66
Table 3.24 Four Scenarios of Price Uncertainties	66
Table 3.25 Result Performance under Different Price Combinations	66
Table 4.1 Parameters Studied for Sugar Yield in Hydrolysis	71
Table 4.2 Experimental Results Regarding Sugar Yield	73
Table 4.3 Transportation and Handling Cost of Cellulosic Biomass Feedstock in Different Forms	79
Table 4.4 Transportation Distances (Miles) between Different Location Pairs	85
Table 4.5 Daily Demand at Different Biorefineries.....	85
Table 4.6 Travel Route of Transporting the Biomass with Pelleting	86
Table 4.7 Travel Route of Transporting the Biomass without Pelleting	86
Table 4.8 Emissions during Transportation with Pelleting.....	86
Table 4.9 Emissions during Transportation without Pelleting.....	87
Table 4.10 Emissions in Pelleting Process	87
Table 5.1 Conditions for Hydrolysis and Fermentation of Corn and Corn Stover	112
Table 5.2 Conditions for AFEX Pretreatment and Densification Processes	114
Table 5.3 Setup Costs and Emissions of Physical and Chemical Preprocessing.....	115
Table 5.4 Transportation Costs and Emission Related Parameters	115
Table 5.5 Performance of the Corn Sourced Supply Chain.....	116
Table 5.6 Performance of the Corn Stover Sourced Distributed Supply Chain in Pathway 1	117

Table 5.7 Optimal Average Preprocessing Center Capacities in the Pathway 1 Supply Chain	118
Table 5.8 Average Financial Performance of a 70,000 tons/year Preprocessing Center in the Distributed Supply Chain Built in Pathway 1	119
Table 5.9 Average Preprocessed Corn Stover Transported from Preprocessing Center to Bio-Refinery Plants in the Pathway 1 Supply Chain	122
Table 5.10 Optimal Preprocessing Center Capacities in Pathway 2 Distributed Supply Chain.....	123
Table 5.11 Performance of the Distributed Corn Stover Sourced Supply Chain in Pathway 2.....	123
Table 5.12 Average Financial Performance of a 52,500 Tons/Year Preprocessing Center Intended to be Built in Pathway 2 of the Distributed Supply Chain .	124
Table 5.13 Average Preprocessed Corn Stover Transported from Preprocessing Center to Biorefinery Plants in Pathway 2 Distributed Supply Chain.....	125
Table 5.14 Performance of the Corn Stover Sourced Centralized Supply Chain	127
Table 5.15 Preprocessed Corn Stover Transported from Farms to Biorefinery Plants in Centralized Supply Chain	128
Table 5.16 Performance of the Distributed Supply Chain in Pathway 1 with Different Weight Combinations	129
Table 5.17 Performance of the Supply Chain in Distributed Pathway 1 with Different Percentages of Preprocessed Biomass Sold as Animal Feed.....	130
Table 5.18 Performance of the Distributed Supply Chain in Pathway 1 with Different Prices of Secondary Product of Animal Feed and Percentages of Preprocessed Biomass Sold as Animal Feed	131
Table 5.19 Performance of the Distributed Supply Chain in Pathway 1 with Different Prices of Chemically and Physically Preprocessed Biomass Sold to the Bio-Refinery Plants.....	132
Table 5.20 Performance Comparison for Distributed Supply Chain in Pathway 1 with Different Raw Material Inventory Levels at Bio-Refinery Plants	132
Table 5.21 Performance of the Distributed Supply Chain in Pathway 2 with Different Weight Combinations	133

Table 5.22 Performance of the Distributed Pathway 2 Supply Chain with Different Prices of Physically Preprocessed Biomass Sold to the Biorefinery Plants .	134
Table 5.23 Performance Comparison for Distributed Pathway 2 Model with Different Raw Material Inventory Levels at Bio-Refinery Plants.....	134
Table 5.24 Performance of the Distributed Supply Chain in Pathway 1 with Different Weight Combinations	135
Table 5.25 Performance Comparison	136
Table 5.26 Cost Decomposition in Bio-Refinery Plants for Three Corn Stover-Sourced Supply Chain Model	137
Table 5.27 Decomposition of Emissions in the Corn Stover Supply Chain.....	138
Table 5.28 Sensitivity Analysis for Preprocessing Capacity Bounds for Distributed Pathway 1 Model	139
Table 5.29 Sensitivity Analysis for Preprocessing Capacity Bounds for Distributed Pathway 2 Model	139
Table 6.1 Operating Costs for the Processes at Biorefinery Plants	161
Table 6.2 Emission for the Processes at Biorefinery Plants	163
Table 6.3 Mass Transition Factors between the Processes at Biorefinery Plants	163
Table 6.4 Average Corn Transportation from Farms to Bio-Refinery Plants in the Corn Sourced Supply Chain	165
Table 6.5 Average Stover Transportation from Farms to Bio-Refinery Plants in the Corn-Stover-Sourced Supply Chain	166
Table 6.6 Average Corn Transportation from Farms to Bio-Refinery Plants in the Co-Fermentation Supply Chain.....	167
Table 6.7 Average Stover Transportation from Farms to Bio-Refinery Plants in the Co-Fermentation Supply Chain.....	168
Table 6.8 Performance Comparison	169
Table 7.1 Emission Comparison when Redundant Stover Handling is Considered.....	177
Table 7.2 Performance of the Pathway 1 Supply Chain with Different Stover Purchase Prices	179

Table 7.3 Performance of the Pathway 2 Supply Chain with Different Stover Purchase Prices	179
Table 7.4 Performance of the Centralized AFEX Supply Chain with Different Stover Purchase Prices.....	179

1. INTRODUCTION

1.1. BACKGROUND AND MOTIVATION

Biofuels are fuels produced directly or indirectly from organic biomass obtained from plant, animal or algae. The major advantage of using biofuels is the recycling of atmospheric carbon. Traditional fossil fuels use the carbon stock in the ground and pass it into the atmosphere in the form of gases, such as carbon dioxide, during combustion. Biofuels are produced from energy crops that consume atmospheric carbon dioxide during farming and then release it back into the atmosphere during the combustion of biofuels.

Biofuels are thus considered high potential clean energy alternatives to fossil fuels. For example, in the transportation sector, unlike some other renewable energy alternatives such as solar batteries and hydrogen cells, that require re-engineering of automobiles, biofuels can be directly substituted for petroleum fuels at gas stations. In addition, compared to other renewable sources such as wind and solar energy, bioenergy also has the advantage of serving as an energy buffer for optimizing the power grid during peak load periods.

Over the past several decades, biofuel manufacturing technologies have witnessed a rapid advancement, and four generations of biofuels have been developed or proposed. First generation biofuels use sources such as starch, sugars, animal fats, and vegetable oils. Second generation biofuels are made from the non-edible portion of crops and biological waste matter. Third generation biofuels are made from specially engineered

energy crops such as algae. Fourth generation biofuels aim to capture carbon dioxide (CO_2) at every stage of the biofuel production.

At present, first generation biofuel is in commercial production. The most popular biomass types used in first generation biofuel production mainly include corn and sugarcane, which have been widely used in the United States and Brazil, respectively. Specifically, feedstock of corn grain purchased from nearby farms is used to produce bioethanol in bio-refinery plants. A hammer milling system is typically employed in the bio-refinery plant to process corn so that milled corn can be used in the bioconversion processes of hydrolysis and fermentation to produce bioethanol as shown in Figure 1.1.

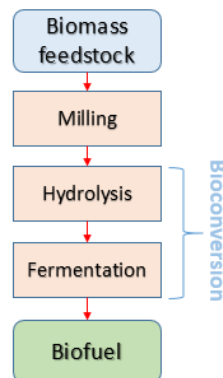


Figure 1.1 First Generation Biofuel Manufacturing System

Although proliferation of first generation biofuel manufacturing has many societal advantages such as poverty reduction potential, effects on social resources, and indirect impacts on land and crops, it is still lacking systematic research that can provide insight

about the optimal performance of first generation biofuel supply chain simultaneously on the economic, environmental, and societal fronts.

In addition, the use of edible portion of energy crops such as corn grain causes a food versus fuel competition, which can lead to a shortage of food, particularly for the lower income population that cannot afford high food prices. To address this major limitation of first generation biofuel, second generation biofuel manufacturing technology has been developed. Second generation biofuel feedstock such as cellulosic biomass typically consists of various chemical compositions such as lignin, hemicellulose, and cellulose with lower energy density; thus, preprocessing activities are needed to offer qualified feedstock of preprocessed non-edible crop matter for the bioconversion in bio-refinery plants. There is a need for a systematic research that can provide the insights regarding the relationship between some critical process parameters of the preprocessing activities and their effects on biofuel yield in bioconversion.

Furthermore, additional facilities for handling the required preprocessing activities such as chemical pretreatment to break the lignin seal around cellulose and physical densification to densify biomass needs to be deployed and operated in the supply chain. The need for such facilities requires the expansion and restructuring of the existing supply chain designed for first generation biofuel manufacturing. The transportation mode needs to be switched from the previous non-stop transportation between farms and bio-refinery plants to a one-stop mode with an intermediate stop at the preprocessing facility; the variations of the transportation emissions and costs need to be examined. There is no study that systematically quantifies the environmental and economic impacts that occur when switching first generation biofuel manufacturing to second generation

biofuel manufacturing through different preprocessing facility deployment strategies while considering the existing supply chain infrastructure.

In summary, to enable a successful switch from first generation biofuel technology to second generation biofuel technology, the following issues need to be addressed.

- There is a need for a systematic investigation of first generation biofuel supply chain to quantify its simultaneous performance on economic, environmental, and societal fronts so that a benchmark performance can be provided when studying the switch from first generation biofuel to second generation biofuel.
- There is a need for investigating the relationship between some critical parameters of preprocessing activities and their effects on biofuel yield in bioconversion when using feedstock for second generation biofuel manufacturing.
- There is a need for the clear quantification of potential economic and environmental impacts when restructuring the supply chain for second generation biofuel, considering different preprocessing facility deployment strategies

This dissertation is expected to serve decision makers in bioethanol energy, such as government agencies or policy makers. It is expected to do this through mathematical modelling which can offer insights in terms of the economic and environmental impacts of the switch of biofuel manufacturing technology from first generation to second

generation, considering both the entire supply chain's performance and the interests of individual participants in the supply chain.

1.2. AIMS AND APPROACHES

The aim of this dissertation is to offer systematic modeling and analysis of the performance of the supply chain of first generation biofuel, and the feasibility of the switch to second generation biofuel manufacturing. The number of stakeholders in the biofuel supply chain is large, the interaction of various process parameters is unclear, and restructuring of the supply chain is a complex process. Therefore such an assessment would require a clear understanding of the system boundary, holistic mathematical models that can capture the interactions of various processes, the complexities of the supply chain, and robust solving methods.

This research conducts an extensive review of first generation biofuel supply chain, various stakeholders, manufacturing processes, and process parameters. It also investigates various restructuring methodologies, additional stakeholders, manufacturing processes, and process parameters in order to convert first generation biofuel supply chain to second generation. The literature review points out a need for various system-of-systems architecture models of the supply chain, which have a well-defined boundary and right level of abstraction for individual systems; which will enable a clear understanding of interactions between the systems and the effect of such interactions on the economic and environmental performance of the supply chain.

Therefore, the focuses of this research are:

- Perform a multi-objective optimization of first generation biofuel supply chain on economic, environmental, and societal fronts, to set up a baseline to compare proposed architectures for a switch to second generation supply chain.
- Perform an investigation of the interaction of the process parameters for preprocessing that are specific to second generation biofuel manufacturing and the environmental feasibility of preprocessing.
- Perform a detailed economic and environmental investigation of restructuring strategies for a switch to second generation biofuel manufacturing.

With such a modelling approach, the system architecture alternatives for second generation biofuel supply chain can be explored, and the new restructured supply chain design can be conceptualized with realistic expectations of economic viability and environmental sustainability. Specifically, this dissertation can help industry and government bodies to make appropriate decisions in terms of the use of second generation biofuel technology through:

- Quantifying the performance of the restructured supply chain through a firm comparison with the baseline of existing first generation biofuel supply chain.
- Effectively addressing the effects between various process-parameters involved with preprocessing.

- Enabling the selection of a suitable deployment strategy for any geography depending on the goals and limitations of the decision maker.

1.3. DISSERTATION SYNOPSIS

This dissertation is organized as follow:

- Section 1, the introduction, briefly introduces the motivation of this research.
- Section 2, the literature review, reviews first generation biofuels, their manufacturing processes, the supply chain, advantages and disadvantages, and research opportunities; then it reviews second generation biofuels, advantages and challenges, their manufacturing processes, preprocessing activities, preprocessing centers, and their deployment strategies, and research opportunities.
- Section 3, the biofuel supply chain of first generation biofuels, formulates a mathematical model for the objectives of economic, environmental, and societal performance, and constraints for the supply chain consisting of farms, biorefineries, distribution centers and retailers of first generation biofuels. A heuristic algorithm of particle swarm optimization is used for multi-objective optimization. A case study using data from the state of Missouri is implemented to validate the proposed model.
- Section 4, the initial study of second generation biofuels, discusses the effects of feedstock particle size on yield after bioconversion, which is studied using design of experiments. After that, the environmental impact of physical densification is explored through a case study.

- Section 5, the analytical model of planning biofuel supply chains of second generation biofuels, proposes the restructuring and expansion of the existing first generation biofuel supply chain to switch to second generation manufacturing technology through the setup of regional preprocessing centers is proposed. Then, two strategies for the deployment of preprocessing centers are formulated through non-linear mathematical models, so that economic viability and environmental sustainability are analyzed and quantified. Next, a case study using data from the state of Missouri is implemented.
- Section 6, the analytical models of biofuel production through corn grain, corn stover and cofermentation technique. Then the three techniques are compared to find performance of the cofermentation technique in comparison to the first generation corn grain biofuel and second generation corn stover biofuel.
- Section 7, study limitation and opportunities for future work, lists contributions and limitations of the work and provides insights for future work to address limitations and expand on the work of this dissertation.

2. LITERATURE REVIEW

2.1. FIRST GENERATION BIOFUEL

First generation biofuel is typically made from starch (bioethanol) and lipids (biodiesel). At present, it is the most prevalent and commercially available technology. The feedstock for first generation biofuel is the edible portion of crops such as corn, sugarcane, and rape seed. The most popular types of biomass used by first generation bioethanol production include corn and sugar that are widely used in the United States and Brazil, respectively (Martin, 2010).

2.1.1. Manufacturing Processes. Specifically, as shown in Figure 2.1, first generation bioethanol is produced in bio-refinery plants using corn grain feedstock purchased from nearby farms. A hammer milling system is usually employed in bio-refinery plants to process corn, so that milled corn can then be used in hydrolysis and fermentation to produce bioethanol.

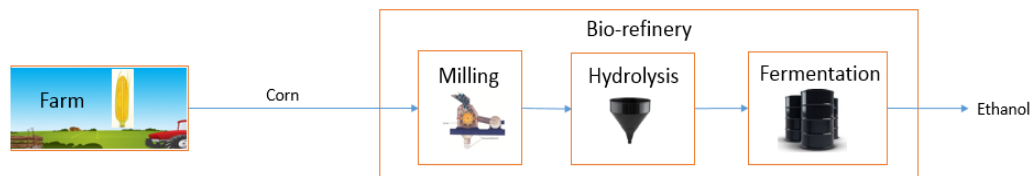


Figure 2.1 Corn-Sourced Bioethanol Manufacturing

Production of first generation biofuels has been extensively studied in the literature (Martin, 2010; Persson et al., 2009; Kim & Dale, 2005). For example, the effect

of climate variability on the net energy value of corn used for biofuel production has been investigated (Martin, 2010). Further research has been carried out on the manufacturing processes and their economic and environmental impacts, for first generation biofuels (Demirbas, 2011; Yu & Tan, 2008; Mosier & Ileleji, 2015; Vamvuka, 2011; Hettinga et al., 2009; Naik et al., 2010; De Vries et al., 2010). For example, a comparison of cost and production parameters between first generation biodiesel and bioethanol has been carried out in Demirbas's work (Demirbas, 2011).

2.1.2. Supply Chain of First Generation Biofuels. A corn-sourced biofuel supply chain includes farms, bio-refinery plants, distribution centers, and retailer gas stations as shown in Figure 2.2.

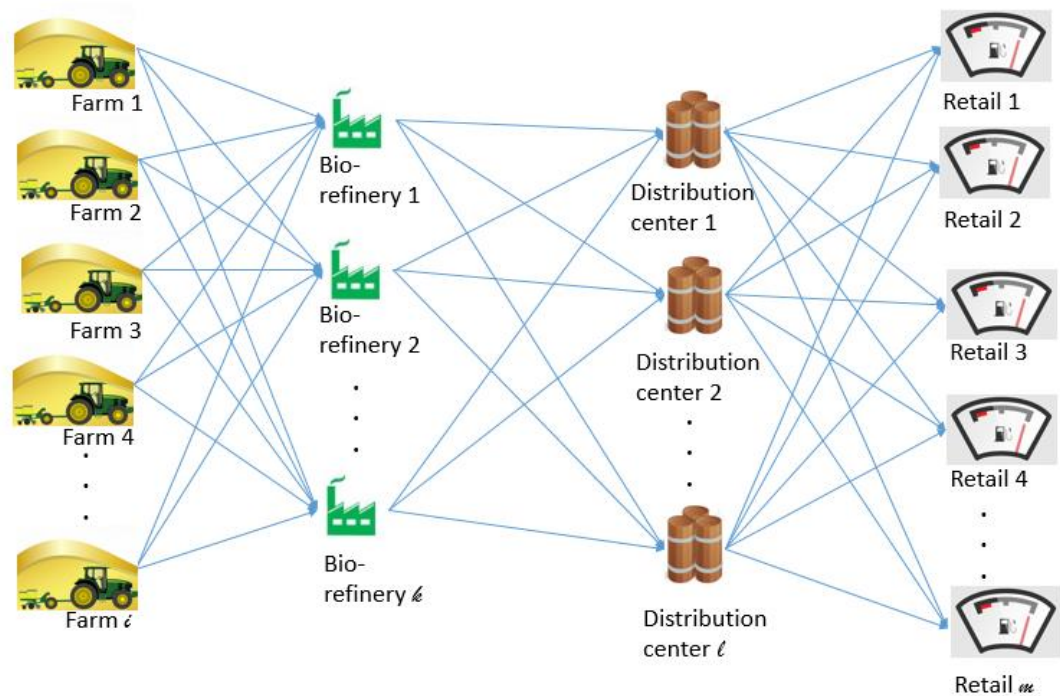


Figure 2.2 Corn-Sourced Biofuel Supply Chain

There are many works in literature regarding the supply chain of first generation biofuels (Papapostolou et al., 2011; Giarola et al., 2012a; Shi et al., 2008; Awudu et al., 2012; Tan et al., 2002; Kendall & Chang, 2009; Acquaye et al., 2011; Cherubini et al., 2009; Hussain et al., 2011; Intarapong et al., 2016). For example, Kendall et al. have conducted life cycle analysis (LCA) to estimate the greenhouse gas emissions of corn-based ethanol (Kendall & Chang, 2009). Intarapong et al. have conducted LCA of biodiesel produced from crude palm oil and waste cooking oil (Intarapong et al., 2016).

2.2. SECOND GENERATION BIOFUEL

Second generation biofuels such as cellulosic bioethanol mainly utilize the non-edible matter of crops such as corn stover, big bluestem, sorghum stalk, and wheat straw as feedstock in biofuel production (Martin, 2010). Cellulosic biomass typically consists of various chemical compositions such as lignin, hemicellulose, and cellulose with low energy density.

2.2.1. Manufacturing Processes Specific to Second Generation Biofuels. The manufacturing system of a second generation biofuel such as cellulosic ethanol consists of two major processes, i.e., feedstock preprocessing and bioconversion, as shown in Figure 2.3. Feedstock preprocessing mainly deals with physical densification and chemical pretreatment. Physical densification includes size reduction and pelleting. Size reduction converts raw cellulosic biomass into small particles through certain mechanical processes. Pelleting transforms cellulosic biomass particles into high-density pellets that can be transported and handled more efficiently. Chemical pretreatment is used to break

the lignin seal and disrupt crystalline structure of cellulose in the biomass so that the surface area that can be accessed by enzymes in the bioconversion can be increased. Bioconversion mainly deals with manufacturing processes dominated by chemical changes. It typically includes processes of hydrolysis, and fermentation. Hydrolysis can break down cellulose into fermentable sugars (e.g., glucose). Fermentation can ferment sugars into ethanol.

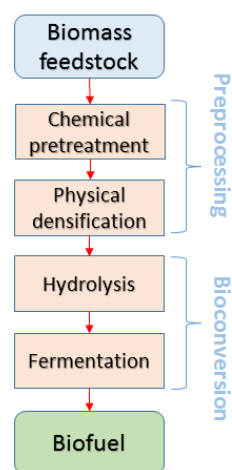


Figure 2.3 Second Generation Biofuel Manufacturing System

The manufacturing system of a second generation biofuel such as cellulosic ethanol consists of two major processes, i.e., feedstock preprocessing and bioconversion, as shown in Figure 2.3. Feedstock preprocessing mainly deals with physical densification and chemical pretreatment. Physical densification includes size reduction and pelleting. Size reduction converts raw cellulosic biomass into small particles through certain mechanical processes. Pelleting transforms cellulosic biomass particles into high-density

pellets that can be transported and handled more efficiently. Chemical pretreatment is used to break the lignin seal and disrupt crystalline structure of cellulose in the biomass so that the surface area that can be accessed by enzymes in the bioconversion can be increased. Bioconversion mainly deals with manufacturing processes dominated by chemical changes. It typically includes processes of hydrolysis, and fermentation. Hydrolysis can break down cellulose into fermentable sugars (e.g., glucose). Fermentation can ferment sugars into ethanol.

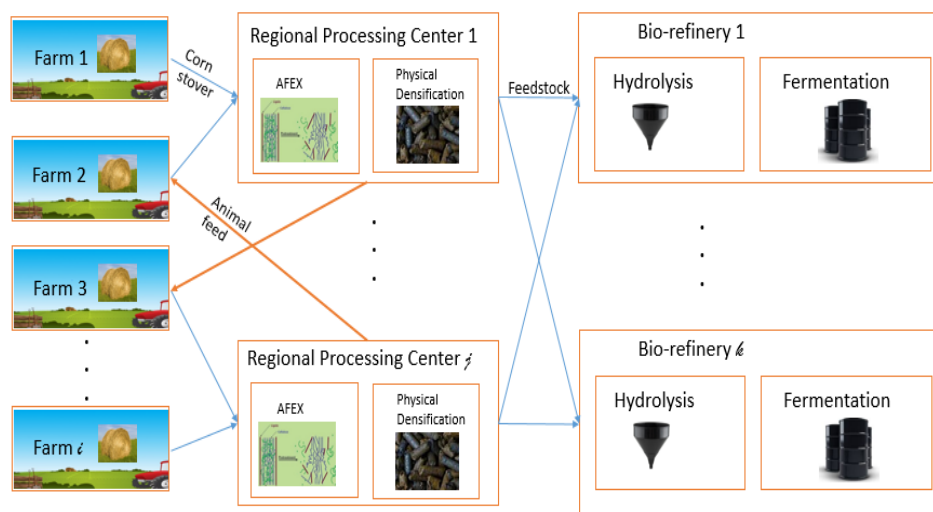
Research on manufacturing processes for second generation biofuels is mainly focused on farm related activities (land use, planting, and harvesting) (Sokhansanj et al., 2002; Melillo et al., 2009; Eliaers & De Wilde, 2013; Xu & Pang, 2008; Wang et al., 2012; Jirjis, 1995), feedstock preprocessing (size reduction, pelleting, and pretreatment) (Repellin et al., 2010; Mani et al., 2004; Bitra et al., 2009a; Bitra, 2009b; Cadoche & Lopez, 1989; Miao et al., 2011; Vidal et al., 2011; Hosseinabadi, 2014; Gislerud, 1990; Frodeson et al., 2013; Zhang, 2011; Rubin, 2008; Mansfield et al., 2006; Zhang et al., 2011; Zhang et al., 2017a; Zhang et al., 2015a; Mani et al., 2006a; Kesharwani et al., 2017b; Sun et al., 2014; Cong et al., 2011; Mani et al., 2006b; Mani et al., 2006c, Kaliyan & Morey, 2009; Song et al., 2013; Tang et al., 2015; Theerarattananoon et al., 2011; Tang et al., 2012; Tumuluru et al., 2011; Mani et al., 2003; Medic et al., 2010; Phanphanich & Mani, 2011; Humbird et al., 2011; Bals et al., 2011; Kim & Holtzapple, 2005; Yang & Wyman, 2008), and bioconversion, i.e., hydrolysis and fermentation (Carolan et al., 2007; Rijal et al., 2014; Chundawat et al., 2007; Eranki et al., 2011; Bals et al., 2014; Dale et al., 2018). For example, the size reduction of biomass has been studied by many researchers (Repellin et al., 2010; Mani et al., 2004; Bitra et al., 2009a;

Bitra et al., 2009b; Cadoche & Lopez, 1989; Miao et al., 2011; Vidal et al., 2011; Hosseinabadi, 2014; Gislerud, 1990; Frodeson et al., 2013; Zhang, 2011). Ultrasonic vibration-assisted (UVA) pelleting technologies have been proposed to reduce the particle size of biomass derived from non-edible matter of crops (Zhang, 2011; Zhang et al., 2011; Zhang et al., 2017a; Zhang et al., 2015a).

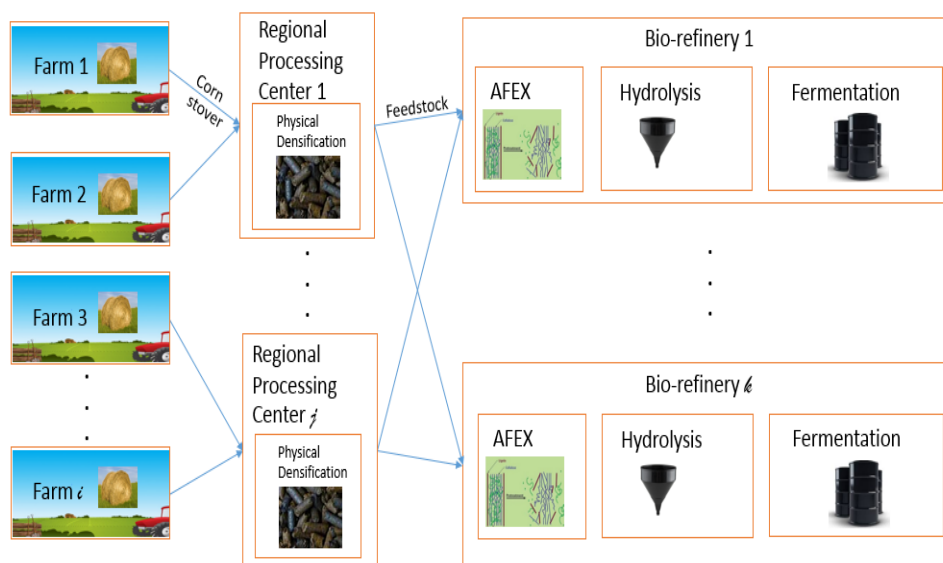
2.2.2. Supply Chain of Second Generation Biofuels. Research in second generation biofuel supply chain (BSC) design and optimization exists on both strategic and operational levels (Papapostolou et al., 2011) in present literature.

For the strategic level, the main research issue is the design and restructuring of the supply chain to integrate the preprocessing operations for the biomass. When implementing various preprocessing operations in a preprocessing facility in biofuel supply chain, generally, two different preprocessing facility deployment strategies have been considered, i.e., centralized and distributed strategies, respectively (Argo et al., 2013; Muth et al., 2014). Centralized deployment was originally proposed, which intended to integrate preprocessing of chemical pretreatment into the existing bio-refinery plant before the process of hydrolysis, while physical densification to reduce the size of biomass feedstock was not considered. Distributed preprocessing deployment was proposed later. It can be carried out by the following two pathways: 1) preprocessing activities including both chemical pretreatment and physical densification are conducted in preprocessing centers (also called quality depot (Kim & Dale, 2016) located in certain places (see Figure 2.4a); 2) physical densification is carried out in preprocessing centers (also called conventional depot (Kim & Dale, 2016), and then physically densified biomass is transported to the bio-refinery plant for further chemical preprocessing

followed by hydrolysis and fermentation (Argo et al., 2013; Muth et al., 2014) (see Figure 2.4b).



a. Pathway 1



b. Pathway 2

Figure 2.4 Cellulosic Biofuel Supply Chain with Decentralized Preprocessing

There are many works in the literature that compare centralized and distributed deployment strategies (Argo et al., 2013; Kim & Dale, 2015; Kim & Dale, 2016; Muth et al., 2014). For example, Kim et al. have discussed the effects of the size of bio-refinery plants on the minimum ethanol selling price (MESP) considering two deployment strategies, and have combined economic and environmental objectives through an eco-efficiency indicator (Kim & Dale, 2015). Later, the team proposed a supply chain model while assuming that preprocessing centers are located at grain elevators and bio-refinery plants are at coal power plants, and they have discussed the breakup of economic and environmental effects for both deployment strategies (Kim & Dale, 2016).

Generally, it has been recognized that a centralized deployment strategy is suitable for a supply chain with a relatively lower biomass handling amount in a small surrounding area, i.e., no more than 5,000 tons of biomass handled per day in a bio-refinery plant with a collection distance of 50-100 miles (Argo et al., 2013). When the processing amount is more than 5,000 tons per day and the collection distance is about 100-300 miles, the centralized strategy may lead to a significant increase in transportation cost and logistic complexity since density of cellulosic feedstocks is typically low without physical densification and biomass has to be sourced from farms far away from the bio-refinery plant (Kim & Dale, 2015).

Thus, the distributed deployment strategy is considered superior to the centralized strategy in the cellulosic supply chain, when the overall production amount is large (Argo et al., 2013, Muth et al., 2014). There exists a significant body of literature that is dedicated to the modelling of the cellulosic biofuel supply chain with distributed preprocessing centers (Kesharwani et al., 2017a; Carolan et al., 2007; Balaman et al.,

2018; Yue et al., 2013; Ng & Maravelias, 2015; Ng & Maravelias, 2017; Ng et al., 2018). For example, Ng and Maravelias have developed a mixed integer non-linear programming model for capacity and inventory planning of a biofuel supply chain including preprocessing centers, where the biomass is pretreated and/or densified (Ng & Maravelias, 2017). The model was applied in a small size numerical case considering a small region with six counties of Wisconsin to reveal the insights of supply chain performance. Carolan et al. have investigated the technical and financial feasibility of deploying regional preprocessing centers where ammonia fiber expansion (AFEX) can be implemented (Carolan et al., 2007).

In addition, at the strategic level, there also exists a large body of literature that is focused on the application of the Life Cycle Analysis (LCA) approach to study total emissions of the supply chain (Acquaye et al., 2011; Zhang et al., 2016a; Tan et al., 2002; Zhang et al., 2015b; Intarapong et al., 2016; Hussain et al., 2011; Luo et al., 2009; Kendall & Chang, 2009; Cherubini et al., 2009; Giarola et al., 2012a; Shi et al., 2008; An et al., 2011a; Gold & Seuring, 2011; Awudu & Zhang, 2012; Marland & Turhollow, 1991). For example, Tan et al. have conducted an LCA of supply chain for coconut methyl ester for producing biodiesel (Tan et al., 2002). Furthermore, there also exists a group of research studies focused on the design of BSCs to improve the competitive feedstock cost (Hess et al., 2007) and continuous feedstock supply (Sims & Venturi, 2004) to relieve impacts due to uncertainties and risks of demand and price of final biofuel products, production and yield, and transportation (Argo et al., 2013; Krishnakumar & Ileleji, 2010; Hess et al., 2009a; Giarola et al., 2012b; Kim & Dale, 2015; Kim & Dale, 2016; Muth et al., 2014).

At an operational level, there exists some literature investigating the order of physical densification and chemical pretreatment for the pathway 1 of the distributed preprocessing strategy (Li et al., 2016). Although a smaller biomass particle size can increase the effectiveness of AFEX by improving the glucan yield during hydrolysis (Rijal et al., 2014; Chundawat et al., 2007), such benefits can only be realized in certain hydrolysis conditions (Chundawat et al., 2007) and there are no clear energy savings. On the other hand, if AFEX is performed before densification, the lignin content in biomass is brought to the surface in the AFEX process, and lignin can then act like a natural binder for the formation of pellets during densification (Eranksi et al., 2011), resulting in more stable pellets for future transportation and storage at no additional cost for external binders. Furthermore, it is also mentioned in the literature that pelleting the biomass after AFEX will increase the yield by around 10% compared to AFEX treated biomass that is not pelletized (Bals et al., 2014). Therefore, when modeling the supply chain of pathway 1 in this dissertation, we follow the order of chemical pretreatment through AFEX followed by physical densification as shown in Figure 2.4a.

In addition to following the order of the two steps in preprocessing at the operational level, there also exists the research that utilizes mathematical programming to design and optimize various behaviors of the supply chain (An et al., 2011b; Zhang et al., 2016b; Ekşioğlu et al., 2009; Zhang et al., 2016c; Zhang et al., 2017b; Cambero et al., 2015; Balaman et al., 2018; You et al., 2012; Yue et al., 2013). For example, Zhang et al. proposed an integration of multimodal transport into the biofuel supply chain to minimize overall operational cost (Zhang et al., 2016b).

2.3. SUMMARY OF LITERATURE REVIEW

2.3.1. Advantages and Disadvantages of First Generation Biofuels. The main advantage of first generation biofuel supply chain network such as a corn-sourced bioethanol supply chain is that the regions with a large amount of corn production such as the states in corn-belt regions of the United States (Wikipedia, 2018), can direct surplus corn output towards bioethanol production.

The main drawback of first generation biofuel is the resultant food vs fuel competition that may be caused by their production using edible parts of the crops as the biomass feedstock, which may lead to a global food price increase and significantly influence the welfare of human beings, especially those in the lower income population who cannot afford high food prices (Demirbas, 2011).

2.3.2. Advantages of Second Generation Biofuels. Compared to first generation biofuel such as bioethanol produced from corn, second generation biofuels such as cellulosic bioethanol produced from corn stover, are particularly attractive because 1) biomass cost in the supply chain can be reduced since price of corn stover is much lower than the price of corn grain, 2) price escalation of corn can be controlled, as it will not generate a food vs fuel competition, 3) the secondary product of the pretreated biomass can be sold back to the farms as animal feed, thus in turn improving the price stability and maintaining the business relationship between the farms and the bio-refinery plants, and 4) it does not require additional wild lands planting and harvesting, which may reduce potential emissions and costs compared to first generation technology (Demirbas, 2011).

2.3.3. Gaps in the Literature. Despite a significant body of literature dedicated to supply chain modeling and techno-economic analysis for second generation biofuel manufacturing, there is no study quantifying and analyzing the environmental and economic impacts that occur when switching first generation bioethanol manufacturing using starchy feedstock to second generation bioethanol manufacturing using cellulosic feedstock considering the existing supply chain infrastructure. Many studies have focused on the techno-economic analysis for either various individual manufacturing processes or multiple manufacturing processes in the supply chain. The methods of laboratory experiments, process modeling, software simulation such as Aspen Plus (Kazi et al., 2010), and commercial databases such as ICARUS (Wooley et al., 1999) have been widely used, while integration of an analytical optimization model seeking optimal performance for techno economic analysis has been reported less. Meanwhile, there exist few mathematical models for the environmental performance in comparison to the economic concern. For example, the transportation mode may be switched from nonstop transportation between farms and bio-refinery plants in a corn sourced supply chain to a one-stop mode with an intermediate stop for proposed preprocessing centers in a distributed corn stover based supply chain. The variations of the transportation emissions and costs need to be examined.

3. BIOFUEL SUPPLY CHAIN OF FIRST GENERATION BIOFUELS

The goal of this section is to advance the research of first generation biofuel supply chain (BSC) design considering the three objectives of economic, environmental, and societal performance. System engineering principles, as indicated as a major further research direction of BSC design (Hess et al., 2007), are used to formulate a multi-layer BSC network including the layers of bio crop harvesting, bioconversion, distribution, and retail to final customers as a system of systems. The objectives of maximizing profit, minimizing transportation emissions, and maximizing market shares are targeted for optimization. The selection of the participants at each layer, and the corresponding transportation amount between each selected pair at two adjacent layers of the supply chain are modeled as decision variables. A meta-heuristic method, particle swarm optimization (PSO), is used to solve the problem to obtain a near optimal solution with a reasonable computational cost. A numerical case study employing the data from Missouri in the United States is conducted to verify the effectiveness of the proposed model. The rest of the section is organized as follows. Section 3.1 introduces the proposed multi-layer multi-objective optimization model as well as a solution technique using PSO. Section 3.2 implements the case study based on the bioethanol production in Missouri of the United States. Section 3.3 concludes the section and discusses the future work.

3.1. PROPOSED MODELS

Notations:

List of indexes of the model

Index	Description
J	index of farms in supply chain
K	index of bio-refinery plants in supply chain
L	index of distribution centers in supply chain
M	index of retail gas stations in supply chain

List of variables of the model

Variable	Description
----------	-------------

Binary decision variables

s_j	binary decision variable. It takes the value of one if farm j is selected, and zero otherwise
s_k	binary decision variable. It takes the value of one if bio-refinery plant k is selected, and zero otherwise
s_l	binary decision variable. It takes the value of one if distribution center l is selected, and zero otherwise
s_m	binary decision variable. It takes the value of one if retail gas station m is selected, and zero otherwise

Continuous nonnegative decision variables

b_k^j	biomass feedstock transported in mass from farm j to bio-refinery plant k
b_l^k	bioethanol transported in volume from bio-refinery plant k to distribution center l
b_m^l	biofuel transported in volume from distribution center l to retail gas station m

List of parameters of the model

Parameter	Description
<u>Cost related parameters</u>	
$C_{l,m}$	price of biofuel per gallon that retail gas station m pays to distribution center l to purchase biofuel
$C_{j,k}$	price of biomass per ton that bio-refinery plant k pays to farm j to purchase biomass
O_k	operating cost (\$ per gallon bioethanol produced) of bio-refinery plant k
O_l	operating cost (\$ per gallon biofuel blended) of distribution center l
T_k^j	transportation cost of biomass per unit mass per unit distance from farm j to bio-refinery k
T_l^k	transportation cost of bioethanol per unit volume per unit distance from bio-refinery plant k to distribution center l

T_m^l transportation cost of biofuel per unit volume per unit distance from distribution center l to retailer m

Emission related parameters

e_1^0 CO₂ emissions of the truck used in the transportation of biomass per unit distance without load

e_2^0 CO₂ emissions of the truck used in the transportation of bioethanol/biofuel per unit distance without load

α_1 rate of increase of emissions per unit distance when unit biomass load (in mass) is added to the truck in biomass transportation

α_2 rate of increase of emissions per unit distance when unit bioethanol/biofuel load (in volume) is added to the truck in bioethanol/biofuel transportation

Transportation related parameters

D_k^j distance from farm j to bio-refinery plant k

D_l^k distance from bio-refinery plant k to distribution center l

D_m^l distance from distribution center l to retail gas station m

Capacity related parameters

K_m^{\max} capacity in volume of biofuel sale by retail gas station m

M_k^j mass capacity of truck that transports biomass from farm j to bio-refinery plant k

M_l^k volume capacity of truck that transports bioethanol from bio-refinery plant k to distribution center l

M_m^l volume capacity of truck that transports biofuel from distribution center l to retailer m

Process related parameters

β volume percentage of bioethanol when mixed with gasoline to generate biofuel in distribution center

γ_{1k} lower bound of the ratio between the outflow materials from a bio-refinery plant k and inward materials to the bio-refinery plant k

γ_{2k} upper bound of the ratio between the outflow materials from a bio-refinery plant k and inward materials to the bio-refinery plant k

γ_{1l} lower bound of the ratio between the outflow materials from distribution center l and inward materials to the distribution center l

γ_{2l} upper bound of the ratio between the outflow materials from distribution center l and inward materials to the distribution center l

ς_k bioethanol conversion coefficient of bio-refinery plant k (gallon bioethanol per ton biomass feedstock)

ζ_l process efficiency of distribution center l

Miscellaneous parameters

A the total gasoline (including biofuel) consumption

B the biofuel demand

3.1.1. Problem Formulation. This section describes the formulation of the multi-objective optimization model for a four-layer BSC network that includes farms, bio-refinery plants, distribution centers, and retail gas stations as shown in Figure 3.1. The farm is the source for the biomass. The biomass (such as corn) is harvested so that it can be used as feedstock at the bio-refinery plant. The bio-refinery plant converts the biomass to bioethanol and then transports the bioethanol to the distribution center. The distribution center blends the bioethanol with gasoline with a given mixing ratio to generate biofuel as per the demand from the retail gas station. Finally, the biofuel is transported to the retail gas station so that it can be purchased by the final customers.

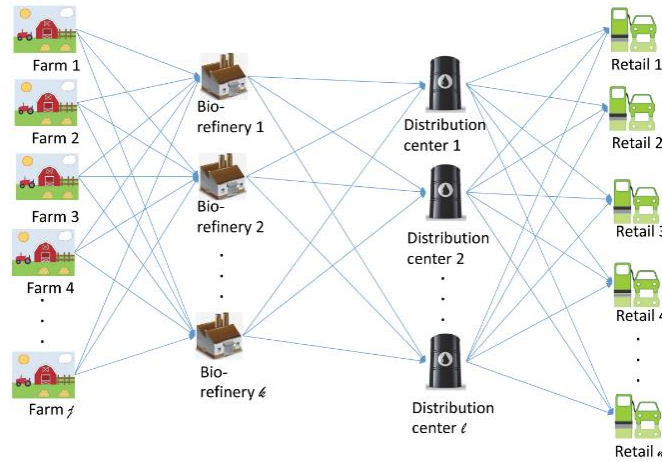


Figure 3.1 A 4-Layer Biofuel Supply Chain Network

There are multiple participators existing in each layer with various capacities, efficiencies, locations, and costs. The objective is to select participators from each layer and identify their corresponding supply amount to the downstream participators to

minimize the emissions in transportation, maximize the profit, and maximize the market share of the biofuel supplied with respect to the total gasoline consumption. These three objectives are concerned about the environmental, economic, and societal benefits of substituting biofuel for traditional gasoline.

The tradeoff exists between the objective of maximizing the market share of the biofuel supplied and the objective of minimizing the transportation emissions. The increase of the market share implies an increase of the biofuel production, which will lead to the increase of the transportation in the supply chain; thus, the emission will also be increased. A balance between these two concerns needs to be identified.

As for the relationship between the market share and profit, the variation of one objective due to the change of the other is uncertain. There exists the possibility that the increases of the market share and the profit of the supply chain can be achieved simultaneously. However, such a synchronized variation is not guaranteed. Increasing (or decreasing) the market share does not necessarily increase (or decrease) the profit of the supply chain. Similar insights can be obtained in terms of the relationship between transportation emission and the profit of the supply chain.

Such tradeoffs and uncertain variation relationships between different pairs of the objectives imply the necessity of a joint optimization model considering three objectives and the possibility of simultaneously achieving the system optimality from three aspects.

Thus, the three aforementioned objectives are formulated as follows:

$$\min \sum_j \sum_k s_j s_k E_k^j + \sum_k \sum_l s_k s_l E_l^k + \sum_l \sum_m s_l s_m E_m^l \quad (1)$$

$$\max R - C_P - C_T - C_O \quad (2)$$

$$\max \frac{\sum_l \sum_m s_l s_m b_m^l}{A} \quad (3)$$

In equation (1), E_k^j represents the emissions incurred in biomass transportation from farm j to bio-refinery plant k . E_l^k represents the emissions incurred in bioethanol transportation from bio-refinery plant k to distribution center l , and E_m^l represents the emissions incurred in biofuel transportation from distribution center l to retailer m . They can be calculated as follows:

$$E_k^j = ((e_1^0 + \alpha_1 M_k^j)(D_k^j) + e_1^0 D_k^j) \lceil b_k^j / M_k^j \rceil \quad (4)$$

$$E_l^k = ((e_2^0 + \alpha_2 M_l^k)(D_l^k) + e_2^0 D_l^k) \lceil b_l^k / M_l^k \rceil \quad (5)$$

$$E_m^l = ((e_2^0 + \alpha_2 M_m^l)(D_m^l) + e_2^0 D_m^l) \lceil b_m^l / M_m^l \rceil \quad (6)$$

where $\lceil \cdot \rceil$ denotes ceiling function. Equations (4), (5), and (6) assume that the truck used for transportation will be empty on its return trip.

Equation (2) reflects the objective of maximizing the profit. In equation (2), R , C_P , C_T , and C_O are the revenue of selling biofuel to retail gas stations, the cost of biomass purchased from farms, the transportation cost, and the operation cost of bio-refinery plant and distribution center, respectively. They can be formulated as follows:

$$R = \sum_l \sum_m s_l s_m b_m^l C_{l,m} \quad (7)$$

$$C_P = \sum_j \sum_k s_j s_k b_k^j C_{j,k} \quad (8)$$

$$C_T = \sum_j \sum_k s_j s_k T_k^j D_k^j b_k^j + \sum_k \sum_l s_k s_l T_l^k D_l^k b_l^k + \sum_l \sum_m s_l s_m T_m^l D_m^l b_m^l \quad (9)$$

$$C_O = \sum_k \sum_j s_j s_k O_k b_k^j \zeta_k + \sum_l \sum_k s_k s_l O_l \zeta_l b_l^k / \beta \quad (10)$$

Note that the scope of calculating the profit of the BSC is bounded from the bio-refinery plant to the distribution center. Thus, the operation costs of farm and retail stations are not included in equation (10).

In equation (3), A is the total demand or consumption of gasoline (including biofuel) in the market, and it reflects the objective of maximizing the market share of biofuel supply to accelerate the substitution for traditional fossil fuels.

The constraints are formulated as follows:

$$\sum_k s_j s_k b_k^j \leq R_j^{\max}, \forall j \quad (11)$$

$$\sum_j s_j s_k b_k^j \zeta_k \leq Q_k^{\max}, \forall k \quad (12)$$

$$\sum_k s_k s_l b_l^k \zeta_l \leq \beta W_l^{\max}, \forall l \quad (13)$$

$$\sum_l s_l s_m b_m^l \leq K_m^{\max}, \forall m \quad (14)$$

$$\gamma_{1k} (\zeta_k \sum_j s_j s_k b_k^j) \leq \sum_l s_k s_l b_l^k \leq \gamma_{2k} (\zeta_k \sum_j s_j s_k b_k^j), \forall k \quad (15)$$

$$\gamma_{1l}(\zeta_l \sum_k s_k s_l b_l^k) \leq \sum_m s_l s_m b_m^l \beta \leq \gamma_{2l}(\zeta_l \sum_k s_k s_l b_l^k), \forall l \quad (16)$$

$$\sum_l \sum_m s_l s_m b_m^l \geq B \quad (17)$$

$$s_k = 1, \forall k \quad (18)$$

Equation (11) illustrates that the total supply from farm j cannot exceed its capacity. Equation (12) shows that the total biomass transported from different farms to each bio-refinery plant cannot exceed the capacity of the bio-refinery plant. Equation (13) demonstrates that the total amount of bioethanol transported from different bio-refinery plants to each distribution center cannot exceed the capacity of the distribution center. Equation (14) requires that the total amount of biofuel transported from different distribution centers to each retail gas station cannot exceed the capacity of the retail gas station. Equations (15) and (16) constrain that the outward materials from a certain node of either the bio-refinery plant or the distribution center need to be controlled within a given range based on the total input materials received by that node. It implies that the inventory variation of the bio-refinery plant and the distribution center should be controlled within an acceptable range. It is assumed that the inventory of the raw materials of each selected bio-refinery plant and distribution center varies such that the sum of the outward materials is bounded between γ_{1k} and γ_{2k} , and between γ_{1l} and γ_{2l} of the total inward materials, respectively. Here, it is assumed that γ_{1k} and γ_{1l} are less than 100%, while γ_{2k} and γ_{2l} are larger than 100%. Equation (17) requires that the supply of biofuel should meet the market demand. Equation (18) ensures that all the bio-refinery plants in the supply chain are selected, as bio-refinery plants are set up through

long-term strategic investments by the government, especially for the bioconversion process in biofuel manufacturing.

3.1.2. An Illustrative Example. To illustrate the effectiveness of the proposed model in Section 2.1, a small-size example is introduced considering the biofuel supply chain in a small region including three counties (Macon, Marion, and Shelby) of northern Missouri in the United States as shown in Figure 3.2. The example includes two farms, one bio-refinery plant, one distribution center, and three gas stations. The relevant parameters of the farms, bio-refinery plant, distribution center, and gas stations are given in Tables 3.1 to 3.4, respectively. Note that the detailed explanations of such parameters are given in Section 3.3. Some other parameters required for calculation like the travel distance, emission rate, and transportation cost rate, are also given in Section 3.3.

Table 3.1 Farms in the Northern Region of Missouri

Farm	County	Latitude	Longitude	Production (corn) (tons)	Selling Price (corn) (\$/ton)
1	Marion	39.85	-91.64	168,639	184
2	Shelby	39.84	-92.11	155,882	174

Table 3.2 Bio-Refinery Plant in the Northern Region of Missouri

PLANT	COUNTY	Region	Latitude	Longitude	CAPACITY
POET Bio-refining	Macon	Northern	39.75	-92.383	46 MG/yr. of ethanol

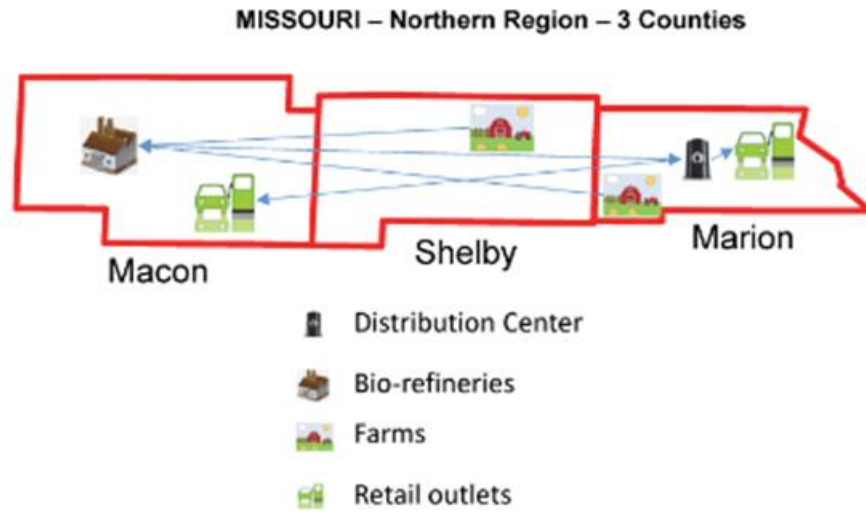


Figure 3.2 Three Counties in the Northern Region of Missouri

Table 3.3 Distribution Center in the Northern Region of Missouri

Distribution Center	County	Latitude	Longitude	Region	Capacity (gallon/yr.)	Price (\$/gallon)
Magellan Pipeline Company, L.P.	Marion	39.881	-91.555	Northern	22,926,288	1.89

Table 3.4 Retailers Gas Stations in the Northern Region of Missouri

Gas Station Name	Longitude	Latitude	Region	demand	County
MFA Oil Petro-Card 24	-92.037978	39.703897	Northern	3,184,188	Shelby
MFA Oil Petro-Card 24	-92.469474	39.755182	Northern	3,184,188	Macon
Fastlane #63	-91.529231	39.917639	Northern	3,184,188	Marion

Three objectives are normalized and then combined using a conventional weighted aggregation method with an equal weight setting (see details of the normalization strategy in Section 3.3). The constraints are integrated into the combined objective as penalty terms. The decision variables of the transportation amounts are

discretized into 20 discrete values. All the combinations of the possible solutions are compared using MATLAB R2014a (x64) by a desktop with Intel®Core™ i5-2400 CPU@3.10GHz with 4GB ram and a 64-bit operating system. The computational time is 49 seconds. The bio-refinery plant, distribution center, and all the retailers are selected. The farm in Shelby is selected, while the one in Marion is not selected. The performance of the small case is shown in Table 3.5. The optimal transportation amounts are shown in Tables 3.6-3.8.

Table 3.5 Case Performance

Biofuel supply (gallons)	11.34 x 10 ⁶
Operating cost (\$)	2.52M
Raw material cost (\$)	3.78M
Transportation cost (\$)	0.84M
Revenue (\$)	21.84M
Profit (\$)	14.7M
Emission (lbs. of CO2 equivalent)	1.26 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO2 equivalent per gallon)	0.09

Table 3.6 Biomass Transported from Farms to Bio-Refinery Plant in Tons

	Bio-refinery node #
Farm Node #	1
1	0.00
2	60,651.36

Table 3.7 Bioethanol Transported from Bio-Refinery Plant to Distribution Center in Gallons

	Distribution Center #
Bio-refinery node #	1
1	8,597,307.6

Table 3.8 Biofuel Transported from Distribution Center to Retailers in Gallons

Distribution Center #	Retailer #		
	1	2	3
1	3,821,025.6	3,821,025.6	3,821,025.6

3.1.3. Solution Technique. The problem formulated in Section 3.2.1 is a mixed integer nonlinear programming (MINLP) that involves highly non-linear calculations as well as both binary and continuous variables. Exhaustive search can only be used for the cases with a very limited size as illustrated in Section 3.2.2. As for the large size problem, the calculation towards the optimal solution is a huge challenge. There are various calculus-based algorithms for solving MINLP in literature and commercial software packages with the assumption of convexity so that the convergence to the global optimum can be guaranteed; however, they cannot be used to address the problem with non-convex and non-differentiable search space.

Thus to solve the problem formulated in Section 3.2.1, particle swarm optimization (PSO) is employed. PSO is a typical population-based meta-heuristic algorithm inspired and characterized by the foraging behaviors of animal swarms (Poli et al., 2007) to solve this high-dimension optimization problem for a near optimal solution. In PSO, the population dynamics simulate the behavior of a bird flock, where social sharing of information happens and individuals profit from the discoveries and previous experience of all other companions during the search for food. Each particle in the swarm is assumed to “fly” over the search space looking for promising regions (optimal solutions) on the landscape. PSO does not require continuity and differentiability on the search space of the optimization problem (Chou et al., 2013); thus, it has been widely

used in solving many different scheduling problems for finding near-optimal solutions of complex combinatorial problems (Moslehi & Mahnam, 2011; Pongchairerks & Kachitvichyanukul, 2009; Parsopoulos & Vrahatis, 2002).

By implementing PSO, each candidate solution is encoded as a particle in the swarm. Each particle consisted of the information that the nodes selected in each layer, and the materials that are transported between the nodes. Let $x_i = [s_j, s_k, s_l, s_m, b_{jk}, b_{kl}, b_{lm}]$ denote a certain particle i . The fitness of each particle is quantified by combining the three objectives using the conventional weighted aggregation (CWA) method (Parsopoulos & Vrahatis, 2002; Jin et al., 2001) and integrating the constraints in equations (11) - (18) as the penalty terms as shown in equation (19), where w_1 , w_2 , and w_3 are the weights used for the three objectives; M is a large real number; and E_n , P_n , and B_n are the normalized results of transportation emissions, profit, and market share, respectively. They can be formulated as shown in (20) – (22).

$$\begin{aligned}
Fitness = & w_1 E_n - w_2 P_n - w_3 B_n + M \left[\sum_j \min(1 - (\sum_k s_j s_k b_k^j / R_j^{\max}), 0)^2 \right. \\
& + \sum_k \min(1 - (\sum_j s_j s_k b_k^j \varsigma_k / Q_k^{\max}), 0)^2 + \sum_l \min(1 - (\sum_k s_k s_l b_l^k \zeta_l / \beta W_l^{\max}), 0)^2 \\
& + \sum_m \min(1 - (\sum_l s_l s_m b_m^l / K_m^{\max}), 0)^2 + \sum_k \min(s_k - 1, 0)^2 \\
& + \sum_k \min(\gamma_{2k} \varsigma_k \sum_j s_j s_k b_k^j / \sum_l s_k s_l b_l^k - 1, 0)^2 \\
& + \sum_k \min(\sum_l s_k s_l b_l^k / \gamma_{1k} \varsigma_k \sum_j s_j s_k b_k^j - 1, 0)^2 \\
& + \sum_l \min(\gamma_{2l} \zeta_l \sum_k s_k s_l b_l^k / \sum_m s_l s_m b_m^l \beta - 1, 0)^2 \\
& + \sum_l \min(\sum_m s_l s_m b_m^l \beta / \gamma_{1l} \zeta_l \sum_k s_k s_l b_l^k - 1, 0)^2 \\
& \left. + \min(\sum_l \sum_m s_l s_m b_m^l - B, 0)^2 \right]
\end{aligned} \tag{19}$$

$$E_n = \frac{\sum_j \sum_k s_j s_k E_k^j + \sum_k \sum_l s_k s_l E_l^k + \sum_l \sum_m s_l s_m E_m^l}{E_U} \quad (20)$$

$$P_n = \frac{R - C_P - C_T - C_O}{P_U} \quad (21)$$

$$B_n = \frac{\sum_l \sum_m s_l s_m b_m^l / A}{B_U} \quad (22)$$

Normalization is used in the fitness value due to the concern of various scales of the numerical values of the results from three objectives. In equations (20), (21), and (22), E_U , P_U , and B_U are the benchmark values of emission, profit, and market share, respectively. The value of B_U can be obtained using the existing or current market share as the benchmark. The values of E_U and P_U can be estimated based on a certain good solution obtained using a certain heuristic method so that the current biofuel demand can be satisfied while the capacity constraints are not violated (see details in Section 3.3).

The particles change their positions (i.e., update their fitness value) based on equation (23) in PSO:

$$\begin{aligned} v_i^{s+1} &= z v_i^s + c_1 r_1 (p b_i^s - x_i^s) + c_2 r_2 (g b^s - x_i^s) \\ x_i^{s+1} &= x_i^s + \chi v_i^{s+1} \end{aligned} \quad (23)$$

where $p b_i^s$ is the best position (i.e., the position with the lowest fitness value) of particle i up to iteration s , $g b^s$ is the best position of the entire swarm up to iteration s , v_i^s is the velocity of particle i up to iteration s , χ is the constriction factor which controls and constricts the velocity's magnitude, z is the inertia weight that determines the effect of the

previous velocity on the current velocity of the particle, c_1 and c_2 are two positive constants, and r_1 and r_2 are two random numbers between zero and one.

To improve search space exploration during the beginning of the algorithm and its convergence towards the end, the inertial weight is adjusted per iteration according to equation (24):

$$z = z_{\max} - \frac{z_{\max} - z_{\min}}{s_{\max}} \times s \quad (24)$$

where z_{\max} and z_{\min} are the largest and smallest inertia weights, respectively, and s_{\max} is the target iteration number.

Conventionally, the initial position of each particle in the swarm can be initialized by randomly assigning the values to the elements in x_i^1 . However, considering the complexity of this model, the feasibility of the initial solution may influence the quality of the final solution. A fully random initiation may lead to a significant reduction of the number of feasible solutions in the swarm, which may incur additional iterations for the final convergence. Therefore, instead of employing random initiation, this section proposes to initialize the positions for all the particles considering the feasibility (i.e., the initial solutions could be generated using a certain heuristic method considering the constraints) (see details in Section 3.3). Meanwhile, the initial velocity is initialized as zero for all the particles.

In addition, equation (25) is used to limit the part regarding node selection in the updated position to be either zero or one:

$$x_{s_{j,k,l,m}} = \begin{cases} 0, & \text{if } x_{s_{j,k,l,m}} + \chi v_{s_{j,k,l,m}} < 0.5 \\ 1, & \text{if } x_{s_{j,k,l,m}} + \chi v_{s_{j,k,l,m}} \geq 0.5 \end{cases} \quad (25)$$

The subscript $s_{j,k,l,m}$ in equation (26) is used to denote the part of the particle that is related to the decision of node selection.

Similarly, equation (26) is used to limit the part of material transportation in the updated position to be a non-negative value:

$$x_b = \begin{cases} 0, & \text{if } x_b + \chi v_b < 0 \\ x_b + \chi v_b, & \text{otherwise} \end{cases} \quad (26)$$

The subscript b in equation (26) is used to denote the part of the particle that is related to transportation amount.

In summary, when implementing the PSO, a swarm of particles considering the feasibility with respect to the constraints will be generated and the velocity for each particle will be initiated. The fitness of each particle will be evaluated using equation (19). The position with the best fitness of each particle so far will be identified and stored. The global best of the entire swarm will be updated if necessary. The velocity and position of each particle will then be updated using equation (23). Such a procedure will be repeated until the maximum iteration number is reached.

3.2. CASE STUDY

In this section, the proposed BSC design and optimization model is implemented using the relevant data of corn supply and bioethanol production in Missouri, United States. Missouri is located on the “corn belt” in the Midwest of the United States. Approximately 1.7 million tons of corn are produced in the state each year (USDA, 2012). It ranks 13th in bioethanol production in the United States (Eia.gov, 2015). Most of the energy generated from renewable energy resources is from conventional hydroelectric power, solar, and wind (Eia.gov, 2015), which implies the possible necessity of improving the performance of the entire supply chain of biofuel in the state.

3.2.1. Parameters in the Case Study. The detailed data of the facilities at each layer of the BSC located in eight different regions of Missouri as shown in Figure 3.3 are introduced in this section.

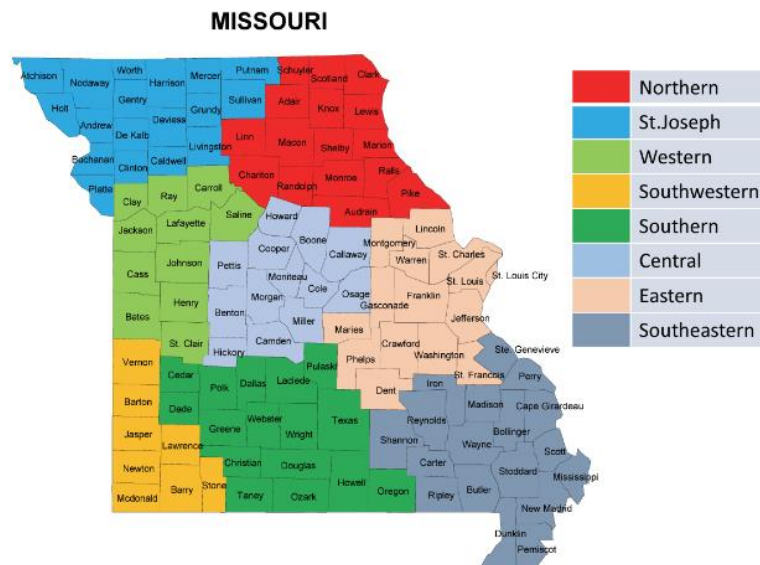


Figure 3.3 Eight Regions in Missouri

Biofuel Demand at Retailer Gas Station

The typical types of biofuel that are reported in the market include E10, E15, and E85, or mixtures of 10%, 15%, and 85% bioethanol and 90%, 85%, and 15% gasoline, respectively.

As of 2013, there are only 24 fueling stations selling E15 out of 180,000 gas stations in the United States (Maps.nrel.gov, 2017). This small percentage makes it an unattractive candidate for analysis. There are gas stations in Missouri selling the E10 variant along with regular gasoline. However, our survey with quite a few gas stations reveals that they have stopped selling E10 due to its unpopular demand. Thus, E10 is also excluded for the analysis in this case. Consequently, E85 stations are assumed to be the main facilities to meet the biofuel demand in Missouri. There are 97 E85 gas stations in Missouri (Maps.nrel.gov, 2017). The price of E85 is derieved from E85prices.com (E85prices.com, 2018). The longitude and latitude values of each station are shown in Table 3.9 so that the distance between these stations and their upstream distribution centers can be calculated. In this case, a straight-line distance between the two locations is used to approximate the transportation distance.

The total biofuel demand in Missouri was 308.87 million gallons in 2015, which is roughly 20% of the total gasoline demand (Eia.gov, 2015). The amount sold from each gas station is obtained by equally dividing the total biofuel demand by the number of E85 gas stations which is, 3,184,188 gallon per year for each station. It is assumed that the selling capacity of each gas station (K_m^{\max}) is 120% of the selling amount from each station.

Distribution Center

There are 20 distribution centers in Missouri, as shown in Table 3.10. There is limited data on the capacity of the distribution centers. The distribution centers are operated as petroleum terminals with a marginal capacity dedicated to bioethanol. It is assumed that the capacity of each distribution center is equal to the 120% of the combined capacity of the E85 gas stations operating in the region where the distribution center is located (Moed.uscourts.gov, 2018a; Moed.uscourts.gov, 2018b). The operating cost for the distribution center is set to be \$0.50/barrel (or \$0.119/gallon) of biofuel produced (Quora.com, 2017a). The process efficiency of each distribution center is assumed to be 0.98 due to the small loss in the transportation and storage of bioethanol.

The historical E85 selling price by the distribution centers in Missouri is examined (Eia.gov, 2018a). The historical data set can be fitted into a uniform distribution with a p-value that is larger than 0.05, which means at the significance level of 0.05, the null hypothesis that the price fluctuation follows a uniform distribution cannot be rejected. In addition, the lower bound and upper bound of the historical data set are \$1.55 per gallon and \$2.15 per gallon, respectively. Therefore, we assume that the fluctuation of the E85 selling price by the distribution centers follows a uniform distribution with lower and upper bounds of \$1.55 per gallon and \$2.15 per gallon, respectively. Thus, the price that each gas station pays to the distribution center is randomly selected from such a uniform distribution as shown in Table 3.10.

Table 3.9 Location Information of E85 Gas Stations in Missouri

Station Name	Longitude	Latitude	Station Name	Longitude	Latitude	Station Name	Longitude	Latitude
Conoco Convenient Food Mart	-92.256	38.588	Fastlane #34	-90.653	38.76	Rhodes 101 Stop	-89.528	37.296
Conoco Convenient Mart	-92.149	38.55	MFA Oil Petro-Card 24	-92.192	40.439	Kum & Go #578	-92.144	37.823
Break Time Convenience Store #3023	-92.334	38.954	Murphy USA #7416	-90.992	38.54	St Louis Veterans Affairs Medical Center - Jefferson Barracks Division	-90.289	38.509
Break Time Convenience Store #3061	-93.213	39.108	Fastlane Muegge	-90.54	38.761	Break Time Convenience Store #3133	-89.653	37.183
Mobil On the Run	-90.481	38.794	Break Time Convenience Store #3032	-91.944	38.861	Energy Express	-90.488	38.596
Fort Leonard Wood	-92.128	37.741	Mobil on the Run #607	-90.363	38.687	Kansas City Veterans Affairs Medical Center	-94.528	39.067
Break Time Convenience Store #3090	-94.797	39.77	Kum & Go #551	-93.296	37.175	West Gate Express - Conoco	-92.224	37.807
MFA Oil Petro-Card 24	-89.35	36.922	Kum & Go #558	-93.262	37.197	Signal Food	-93.223	37.07
Break Time Convenience Store #3111	-94.856	40.345	Ray Carroll Fuels	-93.429	39.365	Grand Slam Phillips 66 - Conoco	-94.58	39.106
MFA Oil Petro-Card 24	-92.454	39.432	MFA Oil Petro-Card 24	-92.797	39.431	Kum & Go #472	-93.276	37.226
MFA Oil Petro-Card 24	-89.967	36.684	MFA Oil Petro-Card 24	-92.038	39.704	Break Time Convenience Store #3138	-92.296	38.932

Table 3.9 Location Information of E85 Gas Stations in Missouri (cont.)

Station Name	Longitude	Latitude	Station Name	Longitude	Latitude	Station Name	Longitude	Latitude
Express Fuel Center	-89.533	37.086	MFA Oil Petro-Card 24	-92.469	39.755	Platte-Clay Fuels	-94.77	39.36
Break Time Convenience Store #3028	-92.338	38.909	Kum & Go #497	-93.43	37.146	Mobil On The Run	-90.28	38.816
Break Time Convenience Store #3001	-92.293	38.96	Mobil On the Run	-90.348	38.622	Kum & Go #779	-94.016	40.266
MFA Oil Petro-Card 24	-92.82	38.445	Ray Carroll Fuels C-Store	-93.987	39.279	Mobil on the Run #613	-90.347	38.522
Break Time Convenience Store #3095	-93.736	38.756	MFA Oil Petro-Card 24	-93.496	39.348	Kum & Go #453	-94.478	37.073
Break Time Convenience Store #3151	-89.583	36.859	Kum & Go #488	-93.311	37.252	Kum & Go #468	-93.286	37.206
MFA Oil Petro-Card 24	-93.598	40.074	Kum & Go #489	-93.363	37.16	Kum & Go #465	-93.296	37.117
MFA Oil Petro-Card 24	-92.899	39.76	Kum & Go #566	-93.313	37.255	Kum & Go #480	-93.291	37.16
MFA Oil Petro-Card 24	-92.144	39.222	Platte-Clay Fuels	-94.381	39.37	Break Time Convenience Store #3150	-92.671	37.686
Break Time Convenience Store #3024	-92.338	38.965	Fastlane #47	-90.929	38.949	Temp Stop	-93.252	38.673

Table 3.9 Location Information of E85 Gas Stations in Missouri (cont.)

Station Name	Longitude	Latitude	Station Name	Longitude	Latitude	Station Name	Longitude	Latitude
MFA Oil Petro-Card 24	-89.957	36.794	Temp Stop	-94.34	38.916	Break Time Convenience Store #3016	-92.371	38.978
Break Time Convenience Store #3036	-93.734	39.069	Break Time Convenience Store #3124	-91.886	39.173	Mobil on the Run	-90.415	38.599
MFA Oil Petro-Card 24	-89.875	37.745	Kum & Go #449	-94.41	36.84	Temp Stop #115	-94.631	39.247
Break Time Convenience Store #3049	-92.19	38.578	Break Time Convenience Store #3147	-89.529	36.894	Break Time Convenience Store #3160	-92.319	38.913
MFA Oil Petro-Card 24	-91.858	39.163	Fastlane #63	-91.529	39.918	Kum & Go #454	-94.478	37.051
MFA Oil Petro-Card 24	-92.583	40.232	Midwest Petroleum - Phillips	-92.338	38.91	Kum & Go #1463	-93.347	37.212
MFA Oil Petro-Card 24	-91.716	39.657	Express Mart - Phillips 66	-90.413	38.213	Kum & Go #1484	-93.308	37.183
MFA Oil Petro-Card 24	-94.341	37.841	Ray Carroll Fuels	-93.672	39.295	Kum & Go #706	-93.212	37.026
East Gate Express	-92.627	37.668	Kum & Go #571	-93.809	37.095	Kum & Go #1458	-93.469	37.119
MFA Oil Petro-Card 24	-90.985	38.407	Conoco Phillips - Crossroads General Store	-91.195	39.333	Kum & Go #464	-93.295	37.166
I-55 Motor Plaza	-90.406	38.287	Break Time Convenience Store #3125	-90.434	36.791			
Break Time Convenience Store #3123	-93.276	37.197	Woods Express	-93.219	38.704			

Bio-refinery Plant

There are six bio-refinery plants in Missouri with capacities from 20 to 60 million gallon of bioethanol per year (Renewable Fuels Association, 2017). The average yearly operating cost is estimated to be \$0.1410 per gallon bioethanol produced (Shapouri & Gallagher, 2002). The information of location and capacity of each plant is given in Table 3.11. The conversion efficiency from corn to bioethanol is 105 gallon of bioethanol produced per ton of corn (Articles.extension.org, 2017).

Corn Supply at Farm

The data of the corn supply in Missouri is obtained from the National Agricultural Statistics Service (NASS) provided by the U.S. Department of Agriculture (2012) (USDA, 2012). Sixty-three out of 115 counties in Missouri plant corn. In this case study, each of these 63 counties is modeled as a pseudo “farm” providing corn to the supply chain. The latitude and longitude of the center of each county are used to approximately represent the location of each pseudo “farm” so that the distance between the farm and its downstream bio-refinery plant could be calculated. The yearly corn supply (unit: ton) of each farm is illustrated in Table 3.12. The average price of corn is around \$180/ton (Balaman et al., 2018) over the last five years. We assume that the price fluctuates around \$180/ton with a bandwidth of 5% in both directions, *i.e.*, \$171-\$189/ton.

In summary, sixty-three farms provide corn throughout the eight regions of Missouri in this case study. In addition, there are 97 E85 gas stations, twenty distribution centers, and six bio-refinery plants throughout eight, eight, and three regions, respectively.

Table 3.10 Information of Distribution Centers in Missouri

Distribution Center	County	Latitude	Longitude	Region	Capacity (gallon/yr.)	Price (\$/gallon)
J D Street - St. Louis	St. Louis	38.583	-90.218	Eastern	9,552,606	1.88
Ayers Oil Company – Canton	Lewis	40.135	-91.519	Northern	22,926,288	1.99
TransMontaigne - Cape Girardeau	Cape Girardeau	37.285	-89.528	Southeastern	12,736,836	2
ERPCO Cape Girardeau	Scott	37.285	-89.528	Southeastern	12,736,836	1.9
Magellan Pipeline Company, L.P.	Jasper	37.322	-94.303	Southwestern	6,368,418	1.81
Magellan Pipeline Company, L.P.	Boone	38.886	-92.266	Central	30,568,398	2
Phillips 66 PL - Jefferson City	Cole	38.547	-92.216	Central	30,568,398	1.81
Phillips 66 PL - Mount Vernon	Lawrence	37.104	-93.819	Southwestern	6,368,418	1.98
American River Trans. Co., North	St. Louis	38.583	-90.219	Eastern	9,552,606	1.87
Magellan Pipeline Company, L.P.	Marion	39.881	-91.555	Northern	22,926,288	1.89
Magellan Pipeline Company, L.P.	Greene	37.159	-93.424	Southern	84,063,042	1.97
Buckeye Tank Terminals LLC - Sugar Creek	Jackson	39.12	-94.445	Western	21,015,750	1.8
Magellan Terminals Holdings LP	St. Charles	38.799	-90.613	Eastern	9,552,606	1.94
Swiss-port SA Fuel Services	St. Louis	38.731	-90.348	Eastern	9,552,606	2.04
Allied Aviation Service of Kansas City	Platte	39.312	-94.716	St. Joseph	22,926,288	1.86
Buckeye Terminals, LLC - St. Louis North	St. Louis	38.68	-90.201	Eastern	9,552,606	1.77
Kinder Morgan Trans-mix Co., LLC	St. Louis	38.579	-90.224	Eastern	9,552,606	1.82
TransMontaigne - Mt Vernon	Lawrence	37.189	-93.78	Southwestern	6,368,418	1.86
Sinclair Transport.- East Carrollton, MO	Carroll	39.358	-93.496	Western	21,015,750	1.84
Oak-mar Terminal	Pemiscot	36.299	-89.781	Southeastern	12,736,836	1.79

Table 3.11 Information of Location and Yearly Capacity of Bio-Refinery Plants in Missouri

PLANT	COUNTY	Latitude	Longitude	CAPACITY
POET Bio-refining	Macon	39.750	-92.383	46 MG/yr. of ethanol
Golden Triangle Energy Cooperative	Holt	40.194	-95.441	20 MG/yr. of ethanol
Mid Missouri Energy	Saline	39.196	-93.382	50 MG/yr. of ethanol
POET Bio-refining	Audrain	39.247	-91.645	50 MG/yr. of ethanol
Life-Line Foods	Buchanan	39.740	-94.845	50 MG/yr. of ethanol
Show Me Ethanol, LLC	Carroll	39.364	-93.451	60 MG/yr. of ethanol

Table 3.12 Information of Farms in Missouri

County code #	County	Latitude	Longitude	Corn supply capacity (ton)	Corn selling price (\$/ton)	Corn stover supply capacity (ton)	Corn stover selling price (\$/ton)
1	Andrew	39.96	-94.81	150,397	173	150,397	56
2	Atchison	40.42	-95.48	385,424	186	385,424	61
3	Caldwell	39.67	-93.99	49,548	179	49,548	62
4	Clay	39.32	-94.48	37,325	184	37,325	59
5	Clinton	39.65	-94.48	123,678	177	123,678	61
6	Daviess	40	-93.99	103,530	187	103,530	56
7	Holt	40.07	-95.19	315,805	188	315,805	64
8	Nodaway	40.29	-94.81	379,055	172	379,055	58
9	Ray	39.34	-93.99	119,855	185	119,855	56
10	Worth	40.47	-94.32	40,632	174	40,632	64
11	Adair	40.2	-92.54	46,500	183	46,500	60
12	Chariton	39.53	-93.02	227,774	180	227,774	62
13	Randolph	39.42	-92.5	45,858	180	45,858	61
14	Sullivan	40.18	-93.18	44,137	174	44,137	62
15	Audrain	39.22	-91.91	278,525	173	278,525	61
16	Knox	40.21	-92.22	157,408	182	157,408	63
17	Lewis	40.05	-91.75	178,195	175	178,195	55
18	Marion	39.85	-91.64	168,639	184	168,639	58
19	Monroe	39.55	-92.07	168,593	175	168,593	61
20	Pike	39.4	-91.29	186,120	177	186,120	61
21	Scotland	40.49	-92.18	126,194	182	126,194	62
22	Shelby	39.84	-92.11	155,882	174	155,882	61
23	Cass	38.66	-94.32	83,520	174	83,520	57
24	Henry	38.34	-93.83	46,195	177	46,195	57
25	Johnson	38.67	-93.83	114,185	174	114,185	56
26	Lafayette	39	-93.99	323,181	172	323,181	64
27	St Clair	38	-93.83	35,511	183	35,511	60
28	Boone	39.05	-92.38	64,117	188	64,117	58
29	Callaway	38.89	-91.91	88,578	178	88,578	59

Table 3.12 Information of Farms in Missouri (cont.)

County code #	County	Latitude	Longitude	Corn supply capacity (ton)	Corn selling price (\$/ton)	Corn stover supply capacity (ton)	Corn stover selling price (\$/ton)
30	Cole	38.51	-92.26	12,771	185	12,771	58
31	Dallas	37.69	-93.02	1326,9231	175	1326,9231	59
32	Hickory	37.98	-93.3	6,630	179	6,630	56
33	Laclede	37.7	-92.54	5,213	187	5,213	57
34	Maries	38.17	-91.95	4,055	179	4,055	58
35	Miller	38.21	-92.38	3,475	178	3,475	56
36	Morgan	38.37	-92.86	13,244	176	13,244	65
37	Osage	38.39	-91.91	28,927	188	28,927	61
38	Pettis	38.69	-93.34	163,747	180	163,747	59
39	Polk	37.68	-93.34	5,882	185	5,882	58
40	Saline	39.19	-93.18	447,882	185	447,882	57
41	Franklin	38.4	-91.14	52,733	174	52,733	56
42	Gasconade	38.43	-91.48	15,819	186	15,819	55
43	Jefferson	38.23	-90.53	5,412	177	5,412	65
44	Perry	37.72	-89.78	76,066	176	76,066	60
45	St Charles	38.73	-90.83	120,510	188	120,510	65
46	Ste Genevieve	37.89	-90.22	39,397	186	39,397	60
47	St Francois	37.77	-90.49	3,764	179	3,764	59
48	St Louis	38.61	-90.41	10,638	188	10,638	58
49	Warren	38.73	-91.14	50,598	173	50,598	55
50	Barry	36.64	-93.83	15,531	183	15,531	60
51	Barton	37.48	-94.32	170,393	176	170,393	62
52	Christian	37	-93.18	2,956	182	2,956	65
53	Dade	37.49	-93.99	41,303	176	41,303	59
54	Greene	37.33	-93.5	4,648	174	4,648	62
55	Lawrence	37.15	-93.83	25,117	187	25,117	64
56	Howell	36.85	-91.91	2,866	173	2,866	65
57	Webster	37.35	-92.86	4,283	172	4,283	57
58	Butler	36.7	-90.38	69,833	185	69,833	56
59	Cape Girardeau	37.38	-89.63	83,322	173	83,322	60
60	Mississippi	36.87	-89.32	199,075	186	199,075	56
61	New Madrid	36.52	-89.78	206,268	176	206,268	55
62	Pemiscot	36.22	-89.81	66,923	179	66,923	63
63	Stoddard	36.87	-89.93	233,093	176	233,093	60

Transportation Cost

The transportation between farms and bio-refinery plants is conducted by carrying solid biomass (i.e., corn), while the transportation between bio-refinery plants and distribution centers as well as between distribution centers and retailer gas stations is conducted by carrying fluid (i.e., bioethanol and biofuel). The cost of transportation between the farm and bio-refinery plant is set as \$0.195 per mile per ton if the travel distance is less than 25 miles, \$0.143 if the travel distance is between 25 and 100 miles, and \$0.078 if the travel distance is more than 100 miles (Ekşioğlu et al., 2009). The cost of bioethanol and biofuel transportation from a bio-refinery plant to a distribution center and from a distribution center to a retail gas station is \$0.001 per mile per gallon (Ekşioğlu et al., 2009).

Transportation Emission

The fuel efficiency of the truck is set to be 5 miles per gallon (MPG) with no load and 3 MPG with a full load (Carbonfund.org, 2018). An average emission factor of 22.2 pounds per gallon (PPG) of CO₂ of diesel consumed is used to count the fleet emission for delivery trucks (Carbonfund.org, 2018). From these values, the truck would emit 4.44 pounds of CO₂ per mile with no load (22.2 PPG/5 MPG), and 7.4 pounds of CO₂ per mile with a full load (22.2 PPG/3 MPG). It is assumed that semi-trailer trucks are used to carry biomass with a capacity of 40 tons (Thetruckersreport.com, 2017), and fuel-carrying trucks are used to carry bioethanol and biofuel with a volume capacity of 11000 gallon (Quora.com, 2017b). The values of α_1 and α_2 can also be obtained. The parameters that are used in calculating the transportation emission are summarized in Table 3.13.

Table 3.13 Parameters for Calculating Transportation Emissions

Parameter	Value
e_1^0	4.44 lbs./mile
α_1	0.074/mile/ton
e_2^0	4.44 lbs./mile
α_2	0.00027/mile/gallon

3.2.2. Benchmark Estimation. The biofuel's market share in 2015 (i.e., 20%) is used as the benchmark of B_U . The values of E_U and P_U are estimated based on a feasible solution that can satisfy the current demand at gas stations without violating the constraints of the capacity of each node. For convenience, it is called the benchmark solution. The benchmark solution is identified using a certain heuristic method so that it could specify certain selections of the nodes at different layers as well as the corresponding transportation amounts between all the pairs of selected suppliers and consumers for the calculation of E_U and P_U .

To facilitate such a heuristic method, the capacity of each layer in the supply chain as shown in Table 3.14 should be first examined. It can be seen that the supply of corn has the largest capacity. The capacity of the bio-refinery plants ranks second, the distribution center ranks third, and the gas station ranks last. Considering such a situation and constraint (18), this study selected all the nodes of the bio-refinery layer, distribution layer, and the retailer layer, while randomly selecting part of the nodes at the farm layer to initiate the benchmark solution.

Table 3.14 Capacity of Different Layers (Bioethanol Gallon Equivalent)

	Farm	Bio-refinery Plant	Distribution Center	Gas Station/Distribution center
Capacity	591,392,200	276,000,000	370,641,600	262,532,844

The biofuel demand of each retailer station is assigned to various distribution centers according to the capacity proportions of different distribution centers so that the transportation amount from distribution centers to retailer gas stations can be built for the benchmark solution.

The transportation between bio-refinery plants and distribution centers is estimated as follows. The total biofuel demand from all retailer stations is transferred to the total bioethanol by the given percentage mixing rate β . After that, it is equally assigned to each bio-refinery plant to obtain bioethanol production. Then, the obtained bioethanol production at each bio-refinery plant is allocated to each of the distribution centers according the proportion of their respective capacities so that the transportation of each bio-refinery plant and distribution center pair could be obtained.

The transportation between farm and bio-refinery plant is estimated as follows. The bioethanol production in each bio-refinery plant is transferred to the biomass requirement. After that, the biomass requirement is equally assigned to the farms that are randomly selected so that the transportation of each farm and bio-refinery plant pair could be obtained. Using such estimated transportation amounts as well as node selections, E_U , and P_U can be estimated accordingly.

3.2.3. PSO Implementation. The node selection part of the solution is initiated using the same strategy for the benchmark solution as introduced in Section 3.3.2. The

various transportation amounts between distribution centers and retailer gas stations as well as between bio-refinery plants and distribution centers are generated by randomly varying the corresponding transportation amount in the benchmark solution within the range of 80% and 120%. The range between 80% and 120% is tuned by trial and error so that the tradeoff between the diversity of the initial solutions in PSO and the violation of the capacity constraints could be balanced. Further, based on the randomly selected farms, the total output from the bio-refinery plant is converted into the biomass requirement and then this requirement is divided equally to all the selected farms to find the transportation amount between each selected farm and each bio-refinery plant pair.

The PSO algorithm is encoded using the parameters shown in Table 3.15 based on MATLAB R2014a (x64). The software is run on a desktop with Intel®Core™ i5-2400 CPU@3.10GHz with 4GB RAM and a 64-bit operating system. The swarm size and iteration number in PSO are tuned to balance the trade-off between computational cost and solution quality. In this case, it is found that 2000 and 1000 are reasonable parameters regarding the swarm size and iteration number.

3.3. RESULTS AND SENSITIVITY ANALYSIS

3.3.1. Results. First, the situation of equal weights for all three objectives is examined (i.e., w_1 , w_2 , and w_3 are set as $1/3$). Using the aforementioned parameters to run the PSO for the case study, it took 2,070 seconds to complete the computation with the evolution of the fitness value, as shown in Figure 3.4. In the solution, the farms are partially selected, while the bio-refinery plants, distribution centers, and retail gas stations are fully selected to build the supply chain. This matches the fact that the corn stover

supply in Missouri is much larger than the existing demand of biofuel as well as the capacities of bioconversion and distribution facilities.

Table 3.15 Parameters Used in PSO

Parameter	Value
χ	1
z_{\max}	0.9
z_{\min}	0.25
c_1	1.7
c_2	1.7

Table 3.16 shows the selection of the farms located in each region. Table 3.17 illustrates the selection of the farms.

Table 3.16 Selection of Farms in Different Regions

Regions	Eastern	Northern	Southeastern	Central	Southern	Southwestern	St. Joseph	Western
# selected	7	9	3	5	6	3	8	7
# total	8	11	8	8	8	3	9	8

The transportation amounts between bio-refinery plants and distribution centers, farms and bio-refinery plants, and distribution centers and retailer stations are illustrated in Tables 3.18, 3.19, and 3.20, respectively.

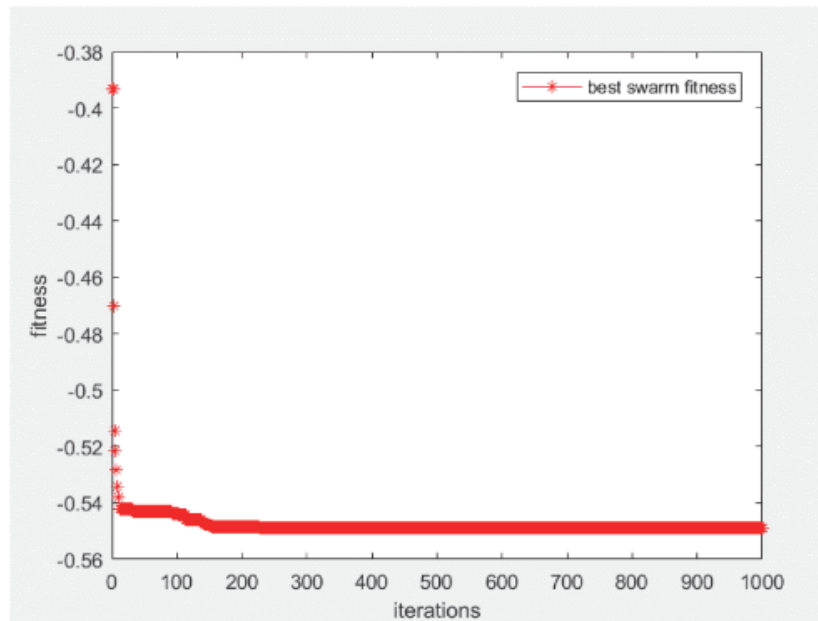


Figure 3.4 Solution Convergence

Table 3.17 Farms Selected

Farm Node #	County	Region	Selected	Farm Node #	County	Region	Selected	Farm Node #	County	Region	Selected
1	Andrew	St. Joseph	0	22	Shelby	Northern	1	43	Jefferson	Eastern	1
2	Atchison	St. Joseph	1	23	Cass	Western	1	44	Perry	Southeastern	0
3	Caldwell	St. Joseph	1	24	Henry	Western	1	45	St Charles	Eastern	1
4	Clay	Western	1	25	Johnson	Western	0	46	Ste Genevieve	Southeastern	0
5	Clinton	St. Joseph	1	26	Lafayette	Western	1	47	St Francois	Eastern	1
6	Daviess	St. Joseph	1	27	St Clair	Western	1	48	St Louis	Eastern	0
7	Holt	St. Joseph	1	28	Boone	Central	0	49	Warren	Eastern	1
8	Nodaway	St. Joseph	1	29	Callaway	Central	1	50	Barry	Southwestern	1
9	Ray	Western	1	30	Cole	Central	1	51	Barton	Southwestern	1
10	Worth	St. Joseph	1	31	Dallas	Southern	1	52	Christian	Southern	1
11	Adair	Northern	1	32	Hickory	Central	1	53	Dade	Southern	0
12	Chariton	Northern	1	33	Laclede	Southern	1	54	Greene	Southern	1
13	Randolph	Northern	1	34	Maries	Eastern	1	55	Lawrence	Southwestern	1
14	Sullivan	St. Joseph	1	35	Miller	Central	1	56	Howell	Southern	0
15	Audrain	Northern	1	36	Morgan	Central	0	57	Webster	Southern	1
16	Knox	Northern	0	37	Osage	Central	1	58	Butler	Southeastern	0
17	Lewis	Northern	1	38	Pettis	Central	1	59	Cape Girardeau	Southeastern	1
18	Marion	Northern	1	39	Polk	Southern	1	60	Mississippi	Southeastern	0
19	Monroe	Northern	0	40	Saline	Western	1	61	New Madrid	Southeastern	1
20	Pike	Northern	1	41	Franklin	Eastern	1	62	Pemiscot	Southeastern	1
21	Scotland	Northern	1	42	Gasconade	Eastern	1	63	Stoddard	Southeastern	0

Table 3.18 Bioethanol Transported from Bio-Refinery Plants to Distribution Centers in Gallons

Distribution center node #										
Bio-refinery node #	1	2	3	4	5	6	7	8	9	10
1	1,057,408	2,537,779	1,409,877	1,409,877	704,939	3,383,705	3,383,705	704,939	1,057,408	2,537,779
2	459,743	1,103,382	612,990	612,990	306,495	1,471,176	1,471,176	306,495	459,743	1,103,382
3	1,149,356	2,758,455	1,532,475	1,532,475	766,238	3,677,940	3,677,940	766,238	1,149,356	2,758,455
4	1,149,356	2,758,455	1,532,475	1,532,475	766,238	3,677,940	3,677,940	766,238	1,149,356	2,758,455
5	1,149,356	2,758,455	1,532,475	1,532,475	766,238	3,677,940	3,677,940	766,238	1,149,356	2,758,455
6	1,379,228	3,310,146	1,838,970	1,838,970	919,485	4,413,529	4,413,529	919,485	1,379,228	3,310,146
Distribution center node #										
Bio-refinery node #	11	12	13	14	15	16	17	18	19	20
1	9,305,189	2,326,297	1,057,408	1,057,408	2,537,779	1,057,408	1,057,408	704,939	2,326,297	1,409,877
2	4,045,735	1,011,434	459,743	459,743	1,103,382	459,743	459,743	306,495	1,011,434	612,990
3	10,114,336	2,528,584	1,149,356	1,149,356	2,758,455	1,149,356	1,149,356	766,238	2,528,584	1,532,475
4	10,114,336	2,528,584	1,149,356	1,149,356	2,758,455	1,149,356	1,149,356	766,238	2,528,584	1,532,475
5	10,114,336	2,528,584	1,149,356	1,149,356	2,758,455	1,149,356	1,149,356	766,238	2,528,584	1,532,475
6	12,137,204	3,034,301	1,379,228	1,379,228	3,310,146	1,379,228	1,379,228	919,485	3,034,301	1,838,970

3.3.2. Sensitivity Analysis. In addition, the results of the model using different weight combinations are examined, as shown in Table 3.22. The best fitness is obtained by combination 7 with more production and profit as well as less emissions than the equal weight case (combination 10).

It seems that a larger weight for a certain objective cannot necessarily guarantee a more desirable result of the objective. For example, the combination with a higher weight of market share (combination 9) led to a result of less biofuel supplied compared to combinations 1, 3, 5, and 8; this implies that the three objectives are mutually

interdependent. The biofuel supplied also plays a critical role in total transportation emissions and total profit of the supply chain.

Table 3.19 Biomass Transported from Farms to Bio-Refinery Plants in Tons

Farm Node #	Bio-refinery node #					
	1	2	3	4	5	6
1	0	0	0	0	0	0
2	24,869	10,813	27,031	27,031	27,031	32,437
3	3,197	1,390	3,475	3,475	3,475	4,170
4	2,409	1,048	2,618	2,618	2,618	3,142
5	7,980	3,470	8,674	8,674	8,674	10,409
6	6,680	2,905	7,261	7,261	7,261	8,714
7	20,377	8,860	22,149	22,149	22,149	26,578
8	24,458	10,634	26,584	26,584	26,584	31,901
9	7,734	3,363	8,406	8,406	8,406	10,087
10	2,622	1,140	2,850	2,850	2,850	3,420
11	3,001	1,305	3,262	3,262	3,262	3,914
12	14,697	6,390	15,975	15,975	15,975	19,170
13	2,959	1,287	3,217	3,217	3,217	3,860
14	2,848	1,239	3,096	3,096	3,096	3,715
15	17,971	7,814	19,534	19,534	19,534	23,441
16	0	0	0	0	0	0
17	11,498	4,999	12,498	12,498	12,498	14,997
18	10,881	4,731	11,828	11,828	11,828	14,193
19	0	0	0	0	0	0
20	12,009	5,222	13,054	13,054	13,054	15,664
21	8,143	3,541	8,851	8,851	8,851	10,621
22	10,058	4,373	10,933	10,933	10,933	13,119
23	5,389	2,343	5,858	5,858	5,858	7,029
24	2,981	1,296	3,240	3,240	3,240	3,888
25	0	0	0	0	0	0
26	20,853	9,067	22,666	22,666	22,666	27,199
27	2,292	997	2,491	2,491	2,491	2,989
28	0	0	0	0	0	0
29	5,716	2,485	6,213	6,213	6,213	7,455
30	825	359	896	896	896	1,075
31	86	38	93	93	93	112
32	428	186	465	465	465	558

Table 3.19 Biomass Transported from Farms to Bio-Refinery Plants in Tons (cont.)

Farm Node #	Bio-refinery node #					
	1	2	3	4	5	6
33	337	147	366	366	366	439
34	262	114	285	285	285	342
35	225	98	244	244	244	293
36	0	0	0	0	0	0
37	1,867	812	2,029	2,029	2,029	2,435
38	10,566	4,594	11,484	11,484	11,484	13,781
39	380	166	413	413	413	496
40	28,899	12,565	31,411	31,411	31,411	37,694
41	3,403	1,480	3,699	3,699	3,699	4,438
42	1,021	444	1,110	1,110	1,110	1,332
43	350	152	380	380	380	456
44	0	0	0	0	0	0
45	7,776	3,381	8,452	8,452	8,452	10,142
46	0	0	0	0	0	0
47	243	106	265	265	265	317
48	0	0	0	0	0	0
49	3,265	1,420	3,549	3,549	3,549	4,259
50	1,003	436	1,090	1,090	1,090	1,308
51	10,994	4,780	11,950	11,950	11,950	14,340
52	191	83	208	208	208	249
53	0	0	0	0	0	0
54	300	131	327	327	327	392
55	1,621	705	1,762	1,762	1,762	2,114
56	0	0	0	0	0	0
57	277	121	301	301	301	361
58	0	0	0	0	0	0
59	5,377	2,338	5,844	5,844	5,844	7,013
60	0	0	0	0	0	0
61	13,309	5,787	14,467	14,467	14,467	17,360
62	4,318	1,878	4,694	4,694	4,694	5,633
63	0	0	0	0	0	0

Table 3.20 Biofuel Transported from Distribution Centers to Retailers in Gallons

Distribution center node #	Retailer Node #									
	1	2	3	4	5	6	7	8	9	10
1	0	0	0	0	585,182	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	1,755,542
3	0	0	0	0	0	0	0	1,170,360	0	0
4	0	0	0	0	0	0	0	1,170,360	0	0
5	0	0	0	0	0	0	0	0	0	0
6	1,755,546	1,755,546	1,755,546	0	0	0	0	0	0	0
7	1,755,546	1,755,546	1,755,546	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	585,182	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	1,755,542
11	0	0	0	0	0	3,511,092	0	0	0	0
12	0	0	0	1,755,541	0	0	0	0	0	0
13	0	0	0	0	585,182	0	0	0	0	0
14	0	0	0	0	585,182	0	0	0	0	0
15	0	0	0	0	0	0	3,511,073	0	3,511,073	0
16	0	0	0	0	585,182	0	0	0	0	0
17	0	0	0	0	585,182	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0
19	0	0	0	1,755,541	0	0	0	0	0	0
20	0	0	0	0	0	0	0	1,170,360	0	0

Distribution center node #	Retailer Node #									
	11	12	13	14	15	16	17	18	19	20
1	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	1,755,542	0
3	1,170,360	1,170,360	0	0	0	0	1,170,360	0	0	0
4	1,170,360	1,170,360	0	0	0	0	1,170,360	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	1,755,546	1,755,546	1,755,546	0	0	0	0	1,755,546
7	0	0	1,755,546	1,755,546	1,755,546	0	0	0	0	1,755,546
8	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	1,755,542	0
11	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	1,755,541	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	3,511,073	0	0
16	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0
19	0	0	0	0	0	1,755,541	0	0	0	0
20	1,170,360	1,170,360	0	0	0	0	1,170,360	0	0	0

[illegible]

Table 3.20 Biofuel Transported from Distribution Centers to Retailers in Gallons
(cont.)

	Retailer Node #									
Distribution center node #	41	42	43	44	45	46	47	48	49	50
1	0	0	0	0	0	0	585,182	0	0	0
2	0	0	1,755,542	1,755,542	1,755,542	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	585,182	0	0	0
10	0	0	1,755,542	1,755,542	1,755,542	0	0	0	0	0
11	3,511,092	0	0	0	0	3,511,092	0	0	0	3,511,092
12	0	1,755,541	0	0	0	0	0	1,755,541	1,755,541	0
13	0	0	0	0	0	0	585,182	0	0	0
14	0	0	0	0	0	0	585,182	0	0	0
15	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	585,182	0	0	0
17	0	0	0	0	0	0	585,182	0	0	0
18	0	0	0	0	0	0	0	0	0	0
19	0	1,755,541	0	0	0	0	0	1,755,541	1,755,541	0
20	0	0	0	0	0	0	0	0	0	0

	Retailer Node #									
Distribution center node #	51	52	53	54	55	56	57	58	59	60
1	0	0	0	585,182	0	0	0	0	0	0
2	0	0	0	0	0	1,755,542	0	0	1,755,542	0
3	0	0	0	0	0	0	0	1,170,360	0	0
4	0	0	0	0	0	0	0	1,170,360	0	0
5	0	0	0	0	0	0	1,170,357	0	0	0
6	0	0	0	0	0	0	0	0	0	1,755,546
7	0	0	0	0	0	0	0	0	0	1,755,546
8	0	0	0	0	0	0	1,170,357	0	0	0
9	0	0	0	585,182	0	0	0	0	0	0
10	0	0	0	0	0	1,755,542	0	0	1,755,542	0
11	3,511,092	3,511,092	0	0	0	0	0	0	0	0
12	0	0	1,755,541	0	1,755,541	0	0	0	0	0
13	0	0	0	585,182	0	0	0	0	0	0
14	0	0	0	585,182	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0
16	0	0	0	585,182	0	0	0	0	0	0
17	0	0	0	585,182	0	0	0	0	0	0
18	0	0	0	0	0	0	1,170,357	0	0	0
19	0	0	1,755,541	0	1,755,541	0	0	0	0	0
20	0	0	0	0	0	0	0	1,170,360	0	0

[illegible]

[illegible]

The performance of the obtained solution is shown in Table 3.21.

Table 3.21 Performance of the Obtained Result

Biofuel supply (gallons)	340.59 x 10 ⁶
Operating cost (\$)	70.29M
Raw material cost (\$)	118.23M
Transportation cost (\$)	67.28M
Revenue (\$)	649.42M
Profit (\$)	393.62M
Emission (lbs. of CO ₂ equivalent)	124.50 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO ₂ equivalent per gallon)	0.36

Furthermore, the results of the equal weight combination case with the variations of demand are examined (i.e., a 15% lower and a 15% higher biofuel demand in Missouri). The comparison between these two demand variations and the current demand is shown in Table 3.23. Even for a higher market demand of biofuel, the model still can find the solution to build the supply chain. This matches the fact that the raw material of corn provision at the upstream of the supply chain is fairly abundant so that the supply chain with current available facility options at different layers is flexible to meet a higher market demand.

Finally, the performance of the model is tested with respect to variable biomass purchase prices and biofuel selling prices to the retailer gas station using the current biofuel demand level as well as equal weight combination. Unlike traditional fossil fuel whose feedstock price is correlated to final product price, biomass product (i.e., biofuel) is correlated to petroleum fuels, while the biomass feedstock price is highly correlated to

climate and weather. Four scenarios of price combinations are examined in Table 3.24.

The comparison results among the four scenarios are given in Table 3.25 and Figure 3.5.

As seen in Figure 3.5a and 3.5b, regarding the total biofuel produced, two input factors of biofuel price and corn price have strong interactions. The increase of the corn price leads to different directions of the variation of biofuel supplied at different levels of biofuel selling price (Figure 3.5a). A higher selling price leads to an increase of biofuel supply if the corn price increased, while a lower biofuel selling price results in a slight decrease of biofuel supplied if the corn price increased. A similar explanation can be given to the variations of biofuel supplied when increasing the biofuel selling price given different levels of corn prices (Figure 3.5b). The decrease of the biofuel supplied at a lower level of corn price is much larger than a higher level of corn price. However, as for the profit variation, there is no indication of such strong interactions between the two prices. As illustrated in Figure 3.5c and 3.5d, the variation lines depending on different levels of biofuel prices (Figure 3.5c) and corn prices (Figure 3.5d) are more parallel. The increase or decrease of a certain price given different levels of the other price will lead to a close variation of the total profit.

3.4. SUMMARY OF FIRST GENERATION BIOFUEL SUPPLY CHAIN OPTIMISATION

This section proposes a multi-objective BSC model that considered the objectives of profit, transportation emission, and biofuel supply towards sustainability. Particle swarm optimization is used to solve the problem to obtain a near optimal solution with a reasonable computational cost. A numerical case study based on the state of Missouri in the United States is used to illustrate the effectiveness of the proposed model. The

proposed model enables a strategic selection of around 77% of the total corn planting counties as the source to supply corn stover to the biofuel supply chain in Missouri. Compared to the benchmark scenario, a 21% transportation emission reduction, a 33% profit improvement, and a 2% market share augmentation can be achieved. In addition, the proposed model is generic and scalable which can be applied to various sizes of the supply chain for either optimizing an existing BSC or designing a new BSC network considering multiple objectives from economic, environmental, and societal aspects towards sustainability.

Table 3.22 Solution Performance with Different Weight Combinations

Combination	Combination 1	Combination 2	Combination 3	Combination 4	Combination 5
Weights (w_1, w_2, w_3)	(0.6,0.2,0.2)	(0.2,0.6,0.2)	(0.2,0.2,0.6)	(0.4,0.4,0.2)	(0.2,0.4,0.4)
Biofuel supply (gallons)	368.57 x 10 ⁶	342.25 x 10 ⁶	346.49 x 10 ⁶	333.39 x 10 ⁶	370.64 x 10 ⁶
Operating cost (\$)	76.22M	70.63M	71.15M	68.47M	78.24M
Raw material cost (\$)	127.70M	118.03M	118.51M	114.07M	130.82M
Transportation cost (\$)	74.37M	70.05M	107.04M	66.46M	75.90M
Revenue (\$)	702.84M	652.62M	660.68M	635.73M	706.75M
Profit (\$)	424.55M	393.91M	363.98M	386.74M	421.79M
Emission (lbs. of CO ₂ equivalent)	130.99 x 10 ⁶	124.60 x 10 ⁶	163.27 x 10 ⁶	115.79 x 10 ⁶	132.53 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO ₂ equivalent per gallon)	0.36	0.36	0.47	0.35	0.36
Combination	Combination 6	Combination 7	Combination 8	Combination 9	Combination 10
Weights (w_1, w_2, w_3)	(0.4,0.2,0.4)	(0.8,0.1,0.1)	(0.1,0.8,0.1)	(0.1,0.1,0.8)	(0.33,0.33,0.33)
Biofuel supply (gallons)	337.34 x 10 ⁶	348.96 x 10 ⁶	335.99 x 10 ⁶	343.34 x 10 ⁶	340.59 x 10 ⁶
Operating cost (\$)	69.43M	71.68M	70.05M	70.05M	70.29M
Raw material cost (\$)	115.18M	119.30M	117.24M	117.88M	118.23M
Transportation cost (\$)	67.60M	70.42M	67.90M	104.71M	67.28M
Revenue (\$)	643.29M	665.43M	640.75M	654.66M	649.42M
Profit (\$)	391.09M	404.04M	385.57M	361.57M	393.62M
Emission (lbs. of CO ₂ equivalent)	117.67 x 10 ⁶	115.38 x 10 ⁶	118.11 x 10 ⁶	154.87 x 10 ⁶	124.50 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO ₂ equivalent per gallon)	0.35	0.34	0.35	0.45	0.36

Table 3.23 Results Performance with Variable Demand

Combination	Lower demand	Current demand	Higher demand
Weights (w_1, w_2, w_3)	(.33,.33,.33)	(.33,.33,.33)	(.33,.33,.33)
Biofuel supply (gallons)	358.87 x 10 ⁶	340.59 x 10 ⁶	368.90 x 10 ⁶
Operating cost (\$)	70.96M	70.29M	78.15M
Raw material cost (\$)	127.97M	118.23M	130.85M
Transportation cost (\$)	73.15M	67.28M	115.30M
Revenue (\$)	684.69M	649.42M	703.46M
Profit (\$)	412.61M	393.62M	379.18M
Emission (lbs. of CO ₂ equivalent)	124.50 x 10 ⁶	124.50 x 10 ⁶	178.68 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO ₂ equivalent per gallon)	0.34	0.36	0.50

Table 3.24 Four Scenarios of Price Uncertainties

	Corn purchase price	Biofuel selling price
Scenario 1	High: \$190 - \$200	Low: \$1.45 - \$1.55
Scenario 2	Low: \$160 - \$170	High: \$2.15 - \$2.27
Scenario 3	High: \$190 - \$200	High: \$2.15 - \$2.25
Scenario 4	Low: \$160 - \$170	Low: \$1.45 - \$1.55

Table 3.25 Result Performance under Different Price Combinations

Combination	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Weights (w_1, w_2, w_3)	(.33,.33,.33)	(.33,.33,.33)	(.33,.33,.33)	(.33,.33,.33)
Biofuel supply (gallons)	353.78 x 10 ⁶	338.89 x 10 ⁶	370.61 x 10 ⁶	365.14 x 10 ⁶
Operating cost (\$)	70.96M \$	75.81M \$	77.1M \$	75.63M \$
Raw material cost (\$)	145.09M \$	142.43M \$	102.8M \$	100.83M \$
Transportation cost (\$)	68.84M \$	75.51M \$	108.53M \$	74.14M \$
Revenue (\$)	516.96M \$	848.02M \$	809.52M \$	557.1M \$
Profit (\$)	232.06M \$	554.26M \$	521.08M \$	306.49M \$
Emission (lbs. of CO ₂ equivalent)	121.87 x 10 ⁶	138.88 x 10 ⁶	129.73 x 10 ⁶	131.27 x 10 ⁶
Emission per unit bioethanol supply (lbs. of CO ₂ equivalent per gallon)	0.35	0.4	0.35	0.36

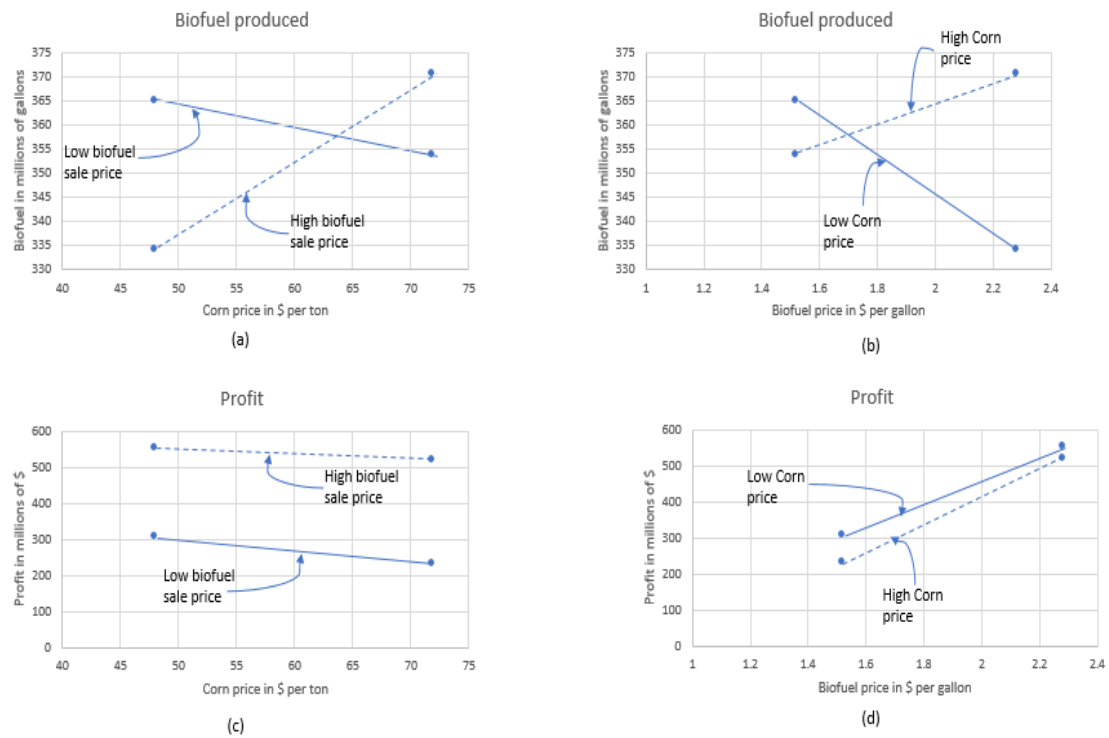


Figure 3.5 Effects of Variations of Biofuel and Biomass Prices

For future work, the analysis of the allocation of the total profit of the entire BSC into different players at various layers can be further studied. In addition, the integration of the pre-processing units that can densify the biomass and reduce the transportation cost in the BSC can be investigated. The net benefits with respect to emission reduction and transportation cost reduction need to be verified.

4. INITIAL STUDY OF SECOND GENERATION BIOFUELS

In this section, we investigate the effects of critical parameters on the sugar yield in second generation biofuel production. Experiments considering different particle sizes obtained in size reduction for three different types of biomass are designed and conducted and the experimental results of the sugar yield in hydrolysis are analyzed. In this section, both positive and negative impacts of pelleting in biofuel manufacturing regarding GHG emissions will be analyzed. A numerical case study focusing on the transportation of biomass is conducted to examine the net impacts or benefits of such concerns through comparison between the scenarios with and without pelleting process.

The rest of the section is organized as follows. In Section 4.1, the effects on sugar yield of the particle size are examined through design of experiments. In Section 4.2, the environmental impacts of pelleting are analyzed through a numerical case study. The conclusions are drawn and the future work is proposed in Section 4.3.

4.1. EFFECTS OF BIOMASS PARTICLE SIZE ON SUGAR YIELD

4.1.1. Experimental Configuration and Hypothesis Formulation. Four individual processes (i.e. size reduction, pelleting, pretreatment, and hydrolysis) are included in the experiments for three different biomass types (i.e. corn stover, wheat straw, and big bluestem).

For size reduction, we use a knife mill (Model No. SM 2000, Retsch GmbH, Haan, Germany), and its milling chamber is shown in Figure 4.1. It is equipped with a three-phase 1.5 kW electric motor. The rotation speed of the motor is 1720 rpm. At the

beginning of each test, the knife mill is run for 10 s before loading any biomass to avoid the current spike. Then, 25 g of biomass is loaded into the knife mill. This amount is enough to keep the milling chamber approximately full (in volume). During knife milling, more biomass is loaded into the milling chamber by the mill operator at a rate that would keep the milling chamber approximately full (in volume) but without causing overloading. Three different sieve sizes, i.e., 1mm, 2mm, and 4mm are tested. In each test, the total amount of biomass loaded into the milling chamber is 100 g. The milling time varies under different conditions. When a smaller sieve size is used, it takes a longer time to mill the same amount of biomass. Six experimental runs are tested for each sieve size for each biomass type. The energy consumption (electric power consumption) and weight of the obtained size-reduced biomass are recorded.

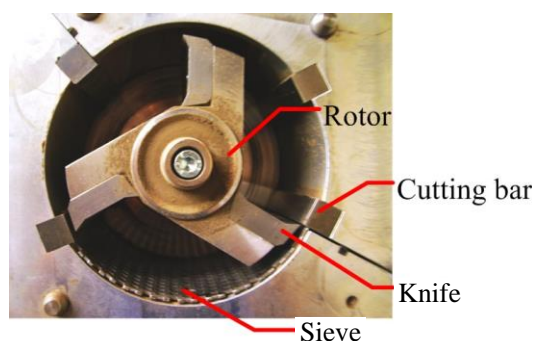


Figure 4.1 Knife Mill

For pelleting, we use a modified ultrasonic machine (Model No. AP-1000, SonicMill, Albuquerque, NM, USA) as shown in Figure 4.2. One gram of size-reduced

biomass with different size distributions from the size reduction step is used as the input. The energy consumption (electric power consumption) is recorded.

For the pretreatment, 5 g of biomass and 150 mL of 1.5% sulfuric acid are loaded in the 600 mL vessel of a Parr pressure reactor (Model No. 4760A, Parr Instrument Co., Moline, IL, USA) as shown in Figure 4.3. Pretreatment time is 30 min, and pretreatment temperature is 140 °C. After pretreatment, biomass particles are washed with 50-60 °C distilled water using a suction filtration system with P4 grade filter paper to conduct solid-liquid separation.

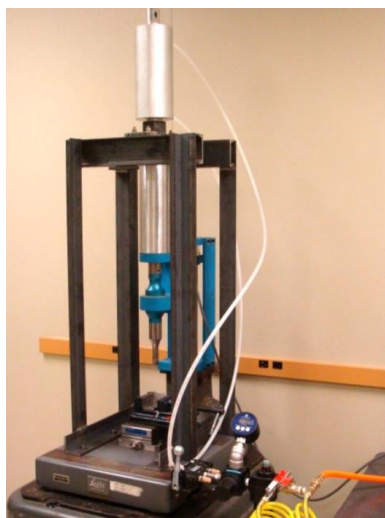


Figure 4.2 Pelleting Machine

Hydrolysis is carried out in 125-mL flasks in a water bath shaker (C76, New Brunswick Scientific, Edison, NJ, USA) at 50 °C for 48 h. The agitation speed of the water bath shaker is 110 rpm. After 24 h and 48 h of hydrolysis, sugar yield in the biomass samples are determined by analyzing the supernatant from the hydrolysis slurry

using an HPLC system (Shimadzu, Kyoto, Japan). HPLC is an analytical tool for separating and quantifying components in complex liquid mixtures. The input parameters studied in hydrolysis are shown in Table 4.1. Three types of biomass with three size distributions are used as the input after pretreatment. The hydrolysis duration is also considered another input with two different settings (24 h and 48 h). Two runs are executed in the experiments for each combination. Sugar yield per unit biomass input is measured as the output of the experiment. The sugar yield per unit energy consumption in preprocessing is also calculated and analyzed as output.

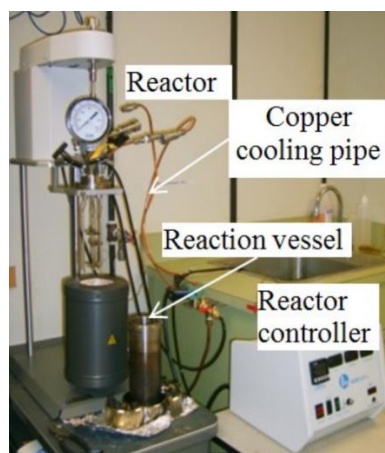


Figure 4.3 Pretreatment Reactor

Table 4.1 Parameters Studied for Sugar Yield in Hydrolysis

Parameter	Level 1	Level 2	Level 3
Particle Size (A)	1mm	2mm	4mm
Biomass Type (B)	Corn Stover	Wheat Straw	Big Bluestem
Hydrolysis Duration (C)	24 hr	48hr	

The general mathematical model of the sugar yield regarding the input size distribution of biomass particles can be illustrated by equation (1):

$$\begin{aligned}
 y_{ijk} &= \mu + \tau_i + \beta_j + \gamma_l + \varepsilon_{ijk} \\
 i &= 1, 2, 3 \\
 j &= 1, 2, 3 \\
 l &= 1, 2 \\
 k &= 1, 2
 \end{aligned} \tag{1}$$

where y_{ijk} is the k th replicate of the observed experimental result (sugar yield) given the i th level of the parameter A (size distribution), j th level of parameter B (biomass type), l th level of parameter C (hydrolysis duration): μ is the overall mean effect of the sugar yield: τ_i is the effect of the i th level of parameter A: β_j is the effect of the j th level of parameter B: γ_l is the effect of the l th level of parameter C: and ε_{ijk} is a random error component (Nrel.gov, 2013).

The hypotheses can be formulated as follows:

$$\begin{aligned}
 H_0 : \tau_1 = \tau_2 = \tau_3 &= 0 \\
 H_1 : \text{at least one } \tau_i &\neq 0
 \end{aligned} \tag{2}$$

$$\begin{aligned}
 H_0 : \beta_1 = \beta_2 = \beta_3 &= 0 \\
 H_1 : \text{at least one } \beta_i &\neq 0
 \end{aligned} \tag{3}$$

$$\begin{aligned}
 H_0 : \gamma_1 = \gamma_2 &= 0 \\
 H_1 : \text{at least one } \gamma_i &\neq 0
 \end{aligned} \tag{4}$$

Equation (2) describes the hypothesis that all size distribution effects are the same against the hypothesis that at least one size distribution effect is different from the rest ones. Equation (3) describes the hypothesis that all the biomass type effects are the same against the hypothesis that at least one biomass type effect is different from the rest ones.

Equation (4) describes the hypothesis that the hydrolysis duration effects are the same against the hypothesis that at least one is not same as the rest ones.

4.1.2. Experimental Results and Analysis. The experimental results of sugar yield are illustrated in Table 4.2.

Table 4.2 Experimental Results Regarding Sugar Yield

Biomass type	Particle size (mm)	24hr (g glucose/1 g dry biomass)		48hr (g glucose/1 g dry biomass)	
Corn stover	1	0.183	0.177	0.207	0.201
	2	0.198	0.186	0.216	0.203
	4	0.178	0.188	0.195	0.199
Wheat straw	1	0.17	0.179	0.168	0.187
	2	0.191	0.19	0.199	0.186
	4	0.147	0.164	0.158	0.175
Big blue stem	1	0.2	0.204	0.215	0.224
	2	0.245	0.244	0.267	0.266
	4	0.197	0.19	0.222	0.22

The results are analyzed using Minitab as shown in Figure 4.4. It can be noted that all three factors are highly significant to the sugar yield. The interaction terms of biomass type/particle size and biomass type/hydrolysis time are also significant. After removing the insignificant terms, the reduced model can be obtained as shown in Figure 4.5.

Thus, it can be concluded that the null hypotheses in equations (2), (3), and (4) can be rejected: that is, different settings of particle size, biomass type, and hydrolysis duration may lead to different sugar yields. The model adequacy has been examined as

shown in Figure 4.6, Figure 4.7, and Figure 4.8. It can be seen that the model adequacy is not violated.

Analysis of Variance for Sugar Yield, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F
Biomass Type	2	0.0143127	0.0143127	0.0071564	139.79
Particle Size	2	0.0058629	0.0058629	0.0029314	57.26
Hydrolysis Time	1	0.0021314	0.0021314	0.0021314	41.63
Biomass Type*Particle Size	4	0.0020498	0.0020498	0.0005124	10.01
Biomass Type*Hydrolysis Time	2	0.0004771	0.0004771	0.0002385	4.66
Particle Size*Hydrolysis Time	2	0.0000216	0.0000216	0.0000108	0.21
Biomass Type*Particle Size* Hydrolysis Time	4	0.0001288	0.0001288	0.0000322	0.63
Error	18	0.0009215	0.0009215	0.0000512	
Total	35	0.0259056			

Source	P
Biomass Type	0.000
Particle Size	0.000
Hydrolysis Time	0.000
Biomass Type*Particle Size	0.000
Biomass Type*Hydrolysis Time	0.023
Particle Size*Hydrolysis Time	0.812
Biomass Type*Particle Size* Hydrolysis Time	0.648
Error	
Total	

S = 0.00715503 R-Sq = 96.44% R-Sq(adj) = 93.08%

Figure 4.4 ANOVA Model of Sugar Yield

Analysis of Variance for Sugar Yield, using Adjusted SS for Tests

Source	DF	Seq SS	Adj SS	Adj MS	F
Biomass Type	2	0.0143127	0.0143127	0.0071564	160.24
Particle Size	2	0.0058629	0.0058629	0.0029314	65.64
Hydrolysis Time	1	0.0021314	0.0021314	0.0021314	47.72
Biomass Type*Particle Size	4	0.0020498	0.0020498	0.0005124	11.47
Biomass Type*Hydrolysis Time	2	0.0004771	0.0004771	0.0002385	5.34
Error	24	0.0010718	0.0010718	0.0000447	
Total	35	0.0259056			

Source	P
Biomass Type	0.000
Particle Size	0.000
Hydrolysis Time	0.000
Biomass Type*Particle Size	0.000
Biomass Type*Hydrolysis Time	0.012
Error	
Total	

S = 0.00668279 R-Sq = 95.86% R-Sq(adj) = 93.97%

Figure 4.5 Reduced ANOVA Model of Sugar Yield

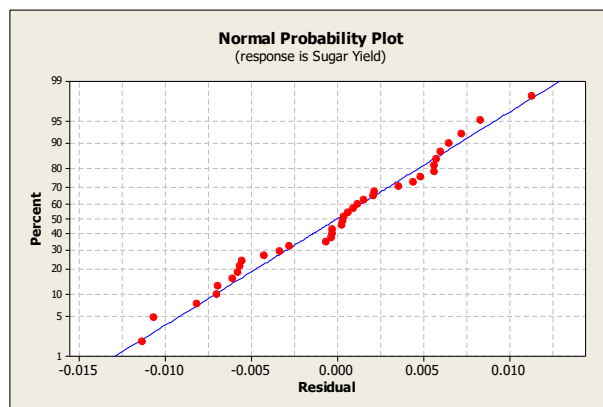


Figure 4.6 Adequacy Checking Using Normal Probability Plot

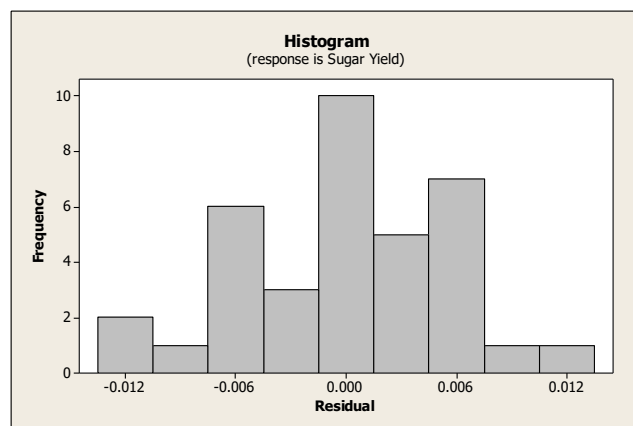


Figure 4.7 Adequacy Checking Using Histogram

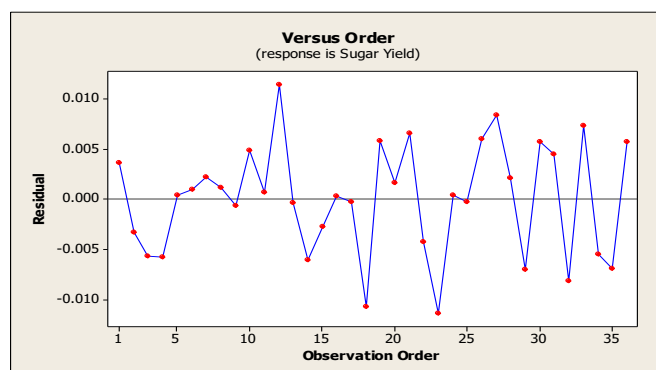


Figure 4.8 Adequacy Checking Using Residual versus Order

The significance regarding biomass type and hydrolysis duration matches common understanding. It needs to be noted that the particle size of the input biomass that is determined by biomass preprocessing also plays a significant role in sugar yield. To further check for the particle size that is different from others, Fisher's test is used. The results of Fisher's test are shown in Figure 4.9., where it can be seen that the sugar yield for particle size of 2 mm is significantly lower than for the other two sizes.

Grouping Information Using Fisher Method

size	N	Mean	Grouping
0	6	0.20900	A
-1	6	0.18550	B
1	6	0.17733	B

Means that do not share a letter are significantly different.

Figure 4.9 Fisher's Test Regarding Size Effects

Surface plots describing the relationships between sugar yield and particle size/hydrolysis duration for each type of biomass are generated as shown in Figure 4.10, Figure 4.11, and Figure 4.12. This figure also demonstrates that the biomass with the particle size using a 2 mm sieve in size reduction can lead to highest sugar yield.

4.2. ENVIRONMENTAL IMPACTS OF PELLETING

4.2.1. Analysis of Benefits and Impacts of Pelletting. Densification of cellulosic biomass into pellets can significantly increase the density of the feedstock, resulting in low transportation and storage costs (Leaver, 1984). Density of pelleted feedstocks can be 600-800 kg/m³, which is much higher than the bulk density of loose biomass (40-250

kg/m³) (Kaliyan & Morey, 2009; Mani et al., 2003). Meanwhile, pellets with the uniform size and shape are easier to handle using existing grain handling and storage infrastructures. Denser cellulosic pellets would allow ethanol producers to save money by utilizing the same equipment they use to transport and handle corn grain, including elevators, hoppers, and conveyor belts. Furthermore, transportation and handling costs of pelleted cellulosic biomass are much lower than those of baled or chopped cellulosic biomass, as shown in Table 4.3 (Kaliyan & Morey, 2009). The pellet transportation cost for large plants could be further reduced if pelleting plants are located close to growing fields (Krishnakumar & Ileleji, 2010).

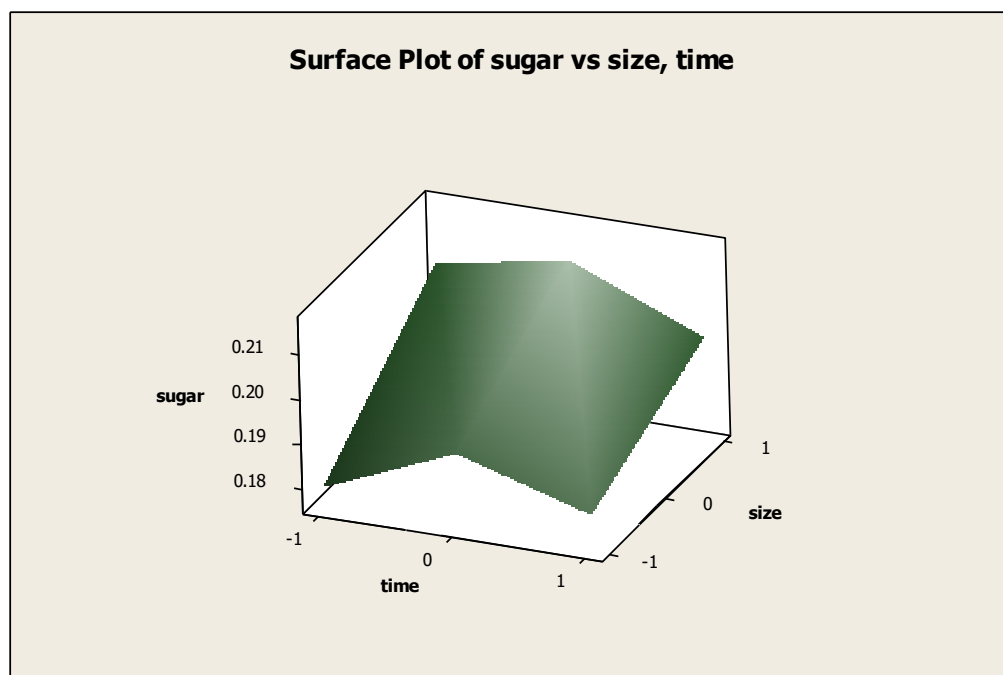


Figure 4.10 Surface Plot for Corn Stover

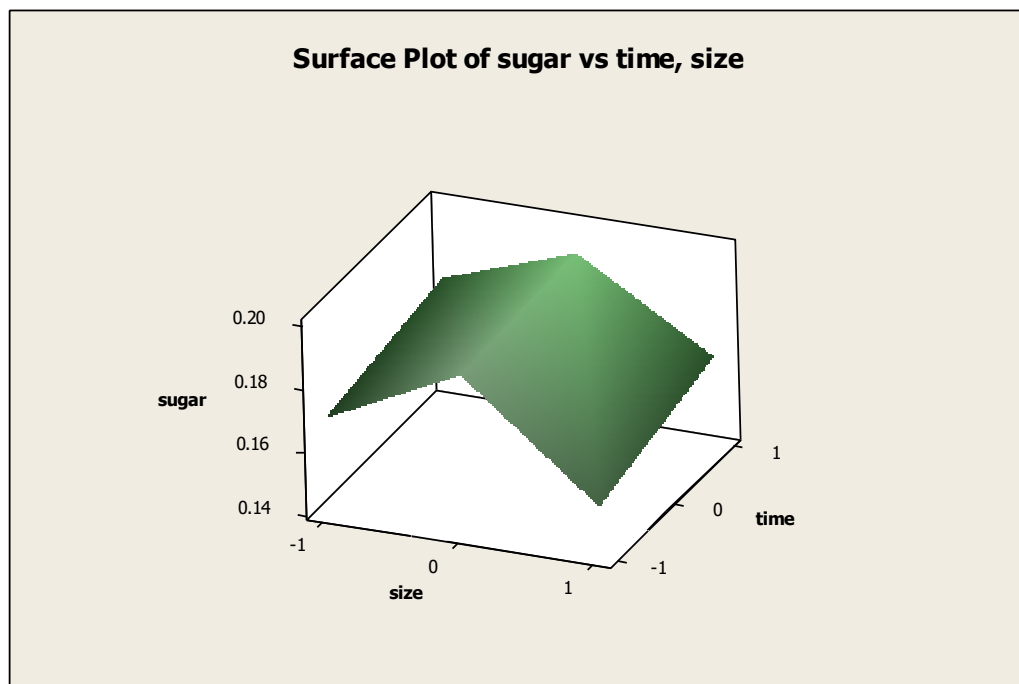


Figure 4.11 Surface Plot for Wheat Straw

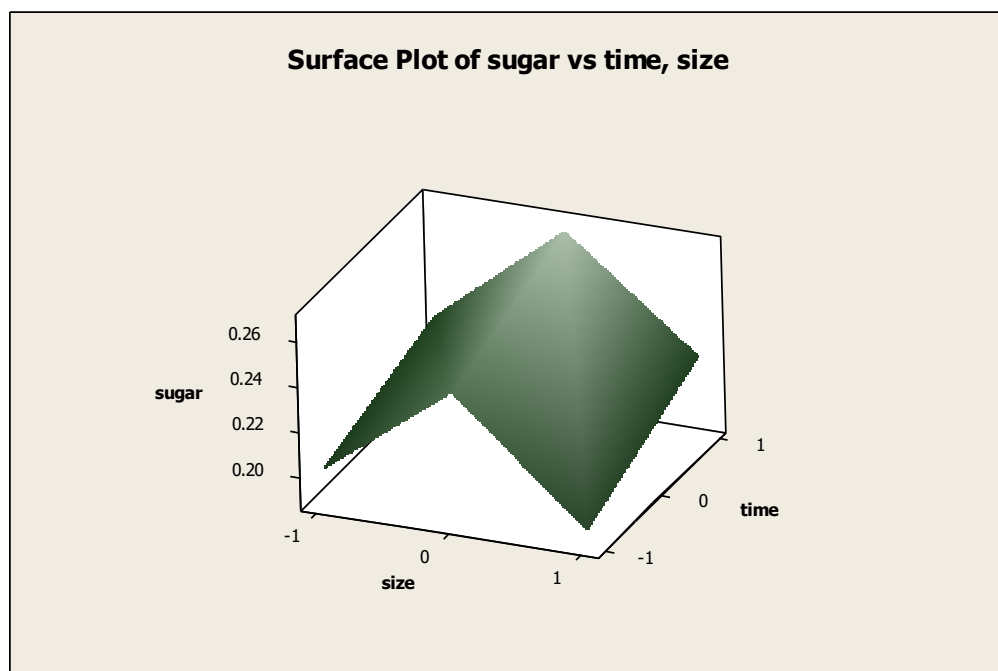


Figure 4.12 Surface Plot for Blue Bigstem

Table 4.3 Transportation and Handling Cost of Cellulosic Biomass Feedstock in Different Forms

Forms	Transportation cost (\$/dry ton)	Handling cost (\$/dry ton)
Baled	10	24.6
Chopped	16.3	21.8
Pelletized	4.5	13.4

Meanwhile, densification of cellulosic biomass into pellets is an energy intensive process after size reduction. During the densification process, the biomass is packed through elastic and plastic deformation (Mani et al., 2006b). Several technologies are currently developed to densify the biomass and are performed on a screw extruder, a briquetting press, a rolling machine, or a ring-die pelleting machine. Among them, the screw extruder is reported to consume the largest portion of energy (Tumuluru et al., 2011). In order to improve the biomass binding characteristics, milled biomass should be either heated at an elevated temperature (over 100 °C) where the lignin in the biomass can be melted to a natural binder or mixed with external binders like soluble sugars, fat, starch, or protein (Kaliyan & Morey, 2009).

In reality, the actual cost savings obtained in transportation by using pellets instead of bales or chopped biomass is dependent on the distance of preprocessing facility from the farms (Krishnakumar & Ileleji, 2010). Ileleji also pointed out that in some scenarios, as much as 50% of the original feedstock could be lost in the pelleting process. At the end, the cost of converting corn stover and switchgrass into pellets outweighed the transportation and storage savings (Ileleji, 2010).

Similarly, the net benefits from environmental perspective due to the use of pelleting also needs to be carefully examined in practice. The potential reduced and incurred GHG emissions due to the use of pelleting need to be quantitatively measured. Let ΔR_k and ΔA_k be the incurred GHG emission reduction and increment, respectively, for a certain process k due to the use of pelleting. Thus, the total net emissions for all the involved processes can be formulated as

$$\sum_k (\Delta R_k - \Delta A_k) \quad (5)$$

To find the quantitative solution for equation (5), research needs to be implemented to include the identification of the different process k whose GHG emissions may be influenced by the adoption of pelleting technology, the possible input factors in each process k that may influence the GHG emissions, etc. In this section, as an initial trial, we would like to focus on the transportation process in the supply chain of biofuel manufacturing to see the net benefits regarding GHG emission reduction. A numerical case study is implemented in Section 4.3.2 to provide some initial insights of the research in this area.

4.2.2. Case Study. As illustrated in the Idaho National lab report (Inldigitallibrary.inl.gov, 2013; Hess et al., 2009a), a typical supply chain for the biomass looks like a hub style network, as shown in Figure 4.13.

The preprocessing plant is modeled as a hub (referred to as the “depot”); and multiple bio-refinery plants are modeled as different delivery points with demand of biomass. One fleet with a few trucks are used to transport biomass from the preprocessing unit to different bio-refinery plants.



Figure 4.13 A Typical Supply Chain of Biomass

The transportation routes of the vehicles are first identified using a heuristic algorithm by Clarke and Wright (Clarke & Wright, 1964), which is briefly described below. This heuristic is based on the initial understanding about the cost saving between two scenarios of transportation routes, as illustrated in the Figure 4.14. One location of depot (indexed by o) and two locations of customers (indexed by i and j) are included. In the location of depot, the goods required by the customers are stored and the fleet of trucks is deployed. In the customer locations, the demand of the goods needs to be satisfied by shipping the goods from the depot.

Let C_{oi} , C_{oj} , and C_{ij} be the transportation cost between the locations denoted by the corresponding subscripts. Two scenarios of the routes are defined as follows. In Scenario 1: Assign a separate truck with the respective load to each customer location. The total transportation cost will be $2(C_{oi}+C_{oj})$. In Scenario 2: Assign one truck with the load to satisfy the demand from both customers to go through customer i and customer j . The transportation cost will be $C_{oi}+C_{oj}+C_{ij}$. The cost saving between the two scenarios could therefore be $C_{oi}+C_{oj}-C_{ij}$. We first compare the cost savings between two scenarios for each pair of the biorefinery plants, i.e., dispatch two trucks to two biorefinery plants,

and dispatch one truck to go through these two plants. The steps of the algorithm are outlined as follows:

Step 1: Rank pairs of customers i and j in ascending order of transportation cost.

Step 2: Start from the top of the ranked list. Include link (i, j) in a vehicle route provided that the vehicle load capacity is not exceeded. If vehicle capacity is exceeded, then move on to the next link, and assign it to a new vehicle.

Step 3: Go back to Step 2 until the list is exhausted or all collection points are assigned.

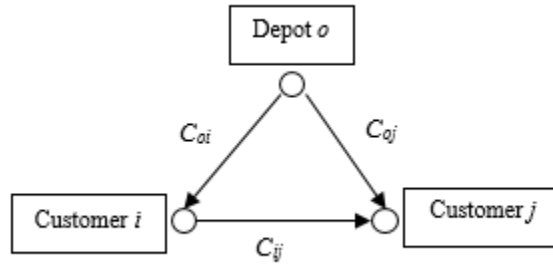


Figure 4.14 Scheduling Algorithm Example

We assume that all trucks are equally efficient, all trucks have same load capacity, and traffic-related delays are neglected. Let h be the index of the transportation trip identified by the aforementioned algorithm, m_h be the total mass of the biomass loaded on the truck, ρ be the density of the biomass, and V be volume of the truck. Then, m_h can be calculated by equation (6):

$$m_h = \rho V \quad (6)$$

In addition, we also assume that the emissions per distance of the truck are a linear function of the load carried by the truck, and the emission of the truck in a trip is proportional to its travel distance. Let e^0 be the emissions of the truck per unit distance without load, α be the rate of the increase of emissions per unit of load added to the truck, and e_h be the emissions of the truck per unit distance with load on the trip h . Therefore, e_h can be formulated by equation (7):

$$e_h = e^0 + \alpha m_h \quad (7)$$

Let l_h be the distance of trip h , and thus the total emission E_h for this trip can be calculated by equation (8).

$$E_h = e_h l_h \quad (8)$$

Let E be the total emissions from all the transportation trips, which can be calculated by equation (9)

$$E = \sum_h E_h \quad (9)$$

Based on the previous model, we consider a supply chain system as shown in Figure 4.15 including one preprocessing unit and five biorefinery plants. The distances between the depots (location o) and the biorefineries are shown in Table 4.4.

The preprocessing plant is modeled as a hub (referred to as the “depot”); and multiple bio-refinery plants are modeled as different delivery points with demand of biomass. One fleet with a few trucks are used to transport biomass from the preprocessing unit to different bio-refinery plants.

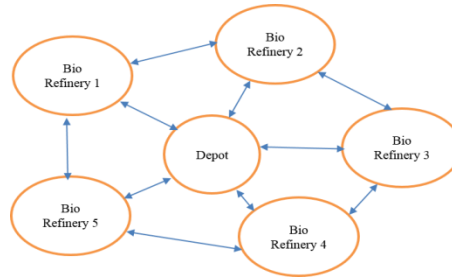


Figure 4.15 Biomass Supply Chain System

The preprocessing plant is modeled as a hub (referred to as the “depot”); and multiple bio-refinery plants are modeled as different delivery points with demand of biomass. One fleet with a few trucks are used to transport biomass from the preprocessing unit to different bio-refinery plants.

The transportation routes of the vehicles are first identified using a heuristic algorithm by Clarke and Wright (Clarke & Wright, 1964), which is briefly described below. This heuristic is based on the initial understanding about the cost saving between two scenarios of transportation routes, as illustrated in the Figure 4.15. One location of depot (indexed by o) and two locations of customers (indexed by i and j) are included. In the location of depot, the goods required by the customers are stored and the fleet of trucks is deployed. In the customer locations, the demand of the goods needs to be satisfied by shipping the goods from the depot.

The density of the biomass without pelleting is set to 200 kg/m^3 (441 lbs/m^3). The density of the biomass after pelleting is set to 700 kg/m^3 (1543.25 lbs/m^3). The volume capacity of one truck is set to 20 m^3 . The load capacity of one truck is 15,000 lbs.

Maximum weight of non-pelletized biomass that can be loaded on a truck is 8,820 lbs. Maximum weight of pelletized biomass that can be loaded on a truck is 15,000 lbs,

which can be obtained by finding the minimum between $(1543.25 \text{ lbs/m}^3 \times 20 \text{ m}^3)$ and 15,000 lbs.

Table 4.4 Transportation Distances (Miles) between Different Location Pairs

	o	1	2	3	4	5
o		100.5	91.2	67.2	21.3	67.2
1			30	33.6	80.7	61.8
2				33.6	75	75
3					47.4	42.3
4						47.4

The daily demand of the biorefinery plants is shown in Table 4.5.

Table 4.5 Daily Demand at Different Biorefineries

	1	2	3	4	5
Daily demand (pounds)	5600	8000	2800	7400	4800

The fuel efficiency of the truck is set to 5mpg with no load and 3mpg with full load. Fleet for delivery trucks is assumed to have an average emission factor of 22.2 lbs of CO₂ per gallon of diesel consumed (Carbonfund.org, 2018). The value of e^0 is set as 4.44 lbs /mile and α is set as .0002.

We use a fix standard cost of 2 \$/mile for transportation and handling combined as these costs are mostly dictated by the freight companies. Using the routing method by Clarke and Wright (Clarke & Wright, 1964), we generate the transportation plan for

scenarios both with and without pelleting as shown in Table 4.6 and Table 4.7, respectively.

Table 4.6 Travel Route of Transporting the Biomass with Pelleting

Travel Route	
Trip 1	Depot- Bio refinery 1- Bio refinery 2- Depot.
Trip 2	Depot- Bio refinery 3- Bio refinery 4- Bio refinery 5- Depot.

The total emissions for two scenarios are shown and compared in Table 4.8 and Table 4.9. It can be seen that approximately 233 lbs GHG emissions can be reduced.

Table 4.7 Travel Route of Transporting the Biomass without Pelleting

Travel Route	
Trip 1	Depot- Bio refinery 1- Bio refinery 3- Depot.
Trip 2	Depot- Bio refinery 2- Depot.
Trip 3	Depot- Bio refinery 4- Depot.
Trip 4	Depot- Bio refinery 5- Depot.

Table 4.8 Emissions during Transportation with Pelleting

Trip #	Link	Distance (miles)	Weight (pounds)	Emission (pounds)
1	(0,1)	100.5	13600	719.58
1	(1,2)	30	8000	181.2
1	(2,0)	91.2	0	404.928
2	(0,3)	67.2	15000	499.968
2	(3,4)	47.4	12200	326.112
2	(4,5)	47.4	4800	255.960
2	(5,0)	67.2	0	298.368
Total emission (lbs.)				2686.116

Table 4.9 Emissions during Transportation without Pelleting

Trip #	Link	Distance (miles)	Weight (pounds)	Emission (pounds)
1	(0,1)	100.5	8400	615.06
1	(1,3)	33.6	2800	168
1	(3,0)	67.2	0	298.368
2	(0,2)	91.2	8000	550.848
2	(2,0)	91.2	0	404.928
3	(0,4)	21.3	7400	126.096
3	(4,0)	21.3	0	94.572
4	(0,5)	67.2	4800	362.88
4	(5,0)	67.2	0	298.368
Total emission (lbs.)				2919.12

The energy consumed in the pelleting process is 180 kWh/ton (Sun et al., 2014), and 1.55 lbs of CO₂ is produced per kWh (Wiley, 2009). Based on these two parameters, the emissions generated in the pelleting process are calculated as shown in Table 4.10.

Table 4.10 Emissions in Pelleting Process

	Total demand (pounds)	Energy consumed (kWh)	CO ₂ emission (pounds)
Daily demand	28600	2335.08	3619.37

The emissions due to the pelleting process (shown in Table 4.10) far exceeds the savings in the GHG emissions of approximately 233 pounds. Thus, there is a net increase in GHG emissions due to the pelleting process. It implies that more research is needed to further improve the feasibility of pelleting in biofuel manufacturing regarding environmental impacts. Such research can include the redesign of supply chain system,

integrate the emission concerns into the objective when developing routing algorithm, etc.

The algorithm that can reduce the cost may not necessarily lead to a considerable reduction regarding the GHG emissions. Multi-objective models considering both cost effectiveness and environmental sustainability need to be developed for the transportation planning.

4.3. SUMMARY OF INITIAL STUDY OF SECOND GENERATION BIOFUEL SUPPLY CHAIN

In this section, we conduct experiments in cellulosic biofuel manufacturing from preprocessing (size reduction and pelleting) to bioconversion (pretreatment and hydrolysis) to examine the interaction between preprocessing and bioconversion. We focus on the relationships between sugar yield and particle size. The experimental results are analyzed. Particle size plays a significant role in determining sugar yield. This section also analyze the benefits and impacts due to the adoption of pelleting process in transportation of biofuel manufacturing processes. An existing technique is applied to a numerical case study in order to examine the influence of pelleting process on GHG emissions in transportation.

For future work, more experiments on different particle sizes need to be conducted. For example, the center point between 1 mm and 2 mm, and between 2 mm and 4 mm, can be added to the experiment to determine if curvature exists. The sugar yield per energy consumption from preprocessing to bioconversion can be examined. In addition, analysis regarding cost effectiveness can also be implemented to study the influences of the input parameter settings on the overall cost of the entire manufacturing

procedure. Further, a more systematic investigation based on the case study in this research can be implemented. The design of experiment method can be used to consider multiple case scenarios to further quantify the pelleting impacts model in biofuel manufacturing. The critical parameters that will influence the net benefits need to be identified to provide a useful tool to check both economic and environmental feasibility of pelleting process in biofuel manufacturing.

5. ANALYTICAL MODEL OF SECOND GENERATION BIOFUEL SUPPLY CHAIN

In this section, we propose a biofuel supply chain model using second generation biofuel manufacturing technology considering the existing bio-refinery infrastructure and farms to examine the environmental and economic impacts when switching the biofuel manufacturing technology from first to second generation. Both distributed and centralized supply chain restructuring strategies are considered. AFEX is used as the chemical pretreatment method due to the aforementioned advantages of AFEX mentioned in section 2.2.2.

The goal of this section is to explore the economic viability and environmental impact of using corn stover to replace corn grains in producing bioethanol following two supply chain restructuring strategies. The total cost and emission for each of the two strategies are formulated, optimized, and compared to the cost and emission of the bioethanol produced using first generation manufacturing technology. The models identify the location and capacity of the preprocessing center (for distributed strategy), along with the transportation quantities between nodes in the supply chain. A case study using existing farms, bio-refinery plants, and fuel demand in the state of Missouri in the United States is implemented.

The remainder of the section is organized as follows: Section 5.1 introduces the modeling methods for both corn-sourced and corn stover-sourced supply chain network. Section 5.2 introduces a case study using relevant data of Missouri in the United States. Section 5.3 demonstrates the results of the case study along with sensitivity and

stochastic analysis. Finally, conclusions are drawn and future work is proposed in Section 5.4.

5.1. PROPOSED MODEL

In this section, the methods to estimate the cost and emission for the corn-sourced and corn stover-sourced biofuel supply chain are introduced. The notations used are provided in the notation list as follows.

Notations:

List of indexes of the model

Index	Description
i	index of the farms
j	index of the candidate preprocessing centers
k	index of the bio-refinery plants

List of variables of the model

Variable	Description
<u><i>Binary decision variables</i></u>	
x_j	binary decision variable to denote if candidate preprocessing center j is selected or not
y_j	corn stover handling capacity (tons/year) of preprocessing center j

Continuous nonnegative decision variables

$b_{f_i p_j}$	amount of corn stover (tons) transported from farm i to preprocessing center j
$b_{f_i b_k}$	amount of corn stover (tons) transported from farm i to bio-refinery plant k
$b_{p_j b_k}$	amount of preprocessed corn stover (tons) transported from preprocessing center j to bio-refinery plant k

List of parameters of the model

Parameter	Description
<u>Cost related parameters</u>	
a^{sC}	cost per unit yearly capacity (\$/ton) for building a chemical pretreatment system
b^{sC}	fixed cost (\$) for building a chemical pretreatment system
F_j	selling price (\$/ton) of animal feed obtained from the secondary products of chemically pretreated biomass in preprocessing center j in the distributed supply chain built by pathway 1
G_P	investment (\$) of a single system for physical densification in the preprocessing center
o^{cF}	operating cost (\$/ton) of hydrolyzed corn mash in fermentation process at bio-refinery plant
o^{cH}	operating cost (\$/ton) of milled corn mash in hydrolysis process at bio-refinery plant

o^{cM}	operating cost (\$/ton) of corn milled in milling process at bio-refinery plant
o^{sC}	operating cost (\$/ton) of corn stover processed in chemical pretreatment
o^{sF}	operating cost (\$/ton) of hydrolyzed corn stover slurry in fermentation process
o^{sH}	operating cost (\$/ton) of preprocessed corn stover slurry in hydrolysis process
o^{sP}	operating cost (\$/ton) of corn stover processed in physical densification
P_i^c	selling price (\$/ton) of the corn sold by farm i to bio-refinery plants
P_i^s	selling price (\$/ton) of the corn stover sold by farm i to preprocessing centers
$T_{f_i p_j}^{su}$	cost (\$/truck/mile) of corn stover transported from farm i to preprocessing center j
$T_{p_j b_k}^{sp}$	cost (\$/truck/mile) of preprocessed corn stover transported from preprocessing center j to bio-refinery plant k
$T_{f_i b_k}^c$	cost (\$/truck/mile) of corn transported from farm i to bio-refinery plant k
z_j	selling price (\$/ton) of preprocessed corn stover at preprocessing center j

Emission related parameters

α	rate of GHG emission increase (lbs. of CO ₂ /mile) when unit load is added to a truck in transportation
e^0	GHG emission (lbs. of CO ₂ /mile) of transportation truck per unit distance without load

e^{cF}	GHG emission (lbs. of CO ₂ /ton) of hydrolyzed corn mash in fermentation process
e^{cH}	GHG emission (lbs. of CO ₂ /ton) of milled corn mash (mixture of milled corn and water) in hydrolysis process
e^{cM}	GHG emission (lbs. of CO ₂ /ton) of corn grain in milling process
e^{sC}	GHG emission (lbs. of CO ₂ /ton) of corn stover processed in chemical pretreatment
e^{sF}	GHG emission (lbs. of CO ₂ /ton) of hydrolyzed corn stover slurry in fermentation process
e^{sH}	GHG emission (lbs. of CO ₂ /ton) of preprocessed corn stover slurry (mixture of preprocessed corn stover and water) in hydrolysis process
e^{sP}	GHG emission (lbs. of CO ₂ /ton) of corn stover processed in physical densification

Transportation related parameters

B_{ik}	amount of corn (tons) transported from farm i to bio-refinery plant k
$D_{f_i p_j}$	distance (miles) from farm i to preprocessing center j
$D_{p_j b_k}$	distance (miles) from preprocessing center j to bio-refinery plant k
$D_{f_i b_k}$	distance (miles) from farm i to bio-refinery plant k

Capacity related parameters

δ_j^s	percentage of the post chemical pretreated corn stover from preprocessing center j that is sold back to the farms as the animal feed in the distributed supply chain built by pathway 1
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g_p	yearly capacity of a physical densification system in preprocessing center
K	maximum corn stover intake capacity (tons/year) for preprocessing centers
M^c	maximum mass of corn grain (tons) that can be transported by a truck
M^{sp}	maximum mass of densified corn stover (tons) that can be transported by a truck
M^{su}	maximum mass of corn stover (tons) that can be transported by a truck
Q_i	capacity (tons) of the corn stover can be supplied by farm i
W_k^s	preprocessed (chemically and physically) corn stover handling capacity (tons) at bio-refinery plant k

Process related parameters

β^{cH}	mass transition factor from corn mash to hydrolyzed corn slurry in hydrolysis process in bio-refinery plant
β^{cM}	mass transition factor from corn to corn mash in milling process in bio-refinery plant
β^{sC}	mass transition factor from corn stover to chemically pretreated corn stover in chemical pretreatment process in the preprocessing center in supply chain
β^{sH}	mass transition factor from pre-hydrolyzed corn stover slurry to hydrolyzed corn stover slurry in hydrolysis process
β^{sL}	mass transition factor from preprocessed corn stover to pre-hydrolyzed corn stover slurry
β^{sP}	mass transition factor in physical densification process in the preprocessing center in the distributed supply chain

σ_k^c	bioethanol conversion coefficient (gallons per ton of milled corn) at bio-refinery plant k when corn is used as feedstock
σ_k^s	bioethanol conversion coefficient (gallons per ton of preprocessed corn stover) at bio-refinery plant k when preprocessed corn stover is used

Miscellaneous parameters

N	a large real number
r	annual discount rate
T	lifetime (years) of the preprocessing center

5.1.1. Corn Stover-Sourced Biofuel Supply Chain Using Distributed

Preprocessing Strategy. In this section, corn stover-sourced biofuel supply chain model with two pathways of distributed preprocessing center deployment strategy is introduced.

5.1.1.1. Pathway 1: chemical pretreatment and physical densification in

preprocessing center. In this section, the corn stover-sourced distributed biofuel supply chain model considering pathway 1 is formulated. In the model, both chemical pretreatment and physical densification are conducted in the proposed preprocessing facility. The objective is to identify the locations for building the preprocessing centers, the capacities of the preprocessing centers, and the material flows, that minimize the emission and cost of the bioethanol produced under the various constraints (e.g., bioethanol demand needs to be met). The objective function is formulated by equation (1) through a conventional weighted sum method with two weights w_1 and w_2 between zero

and one assigned to two objectives. Note that the superscript “sd1” is used to denote the notations used in distributed corn stover-based supply chain in pathway 1.

$$\min_{x_j^{sd1}, y_j^{sd1}, b_{f_i p_j}^{sd1}, b_{p_j b_k}^{sd1}} w_1 E^{sd1} + w_2 C^{sd1} \quad (1)$$

In equation (1), E^{sd1} is the total emissions in biofuel manufacturing when corn stover is used as the feedstock. It consists of the emission of the transportation of corn stover from farms to preprocessing centers, the emission due to the preprocessing activities of chemical pretreatment and densification at preprocessing centers, the emission of the transportation of preprocessed corn stover from preprocessing centers to bio-refinery plants, and the emission due to the bioconversion activities of hydrolysis and fermentation at bio-refinery plants. E^{sd1} can be calculated by equation (2).

$$\begin{aligned} E^{sd1} = & \sum_i \sum_j [(e^0 + \alpha M^{su}) \cdot D_{f_i p_j} + e^0 D_{f_i p_j}] \left\lceil b_{f_i p_j}^{sd1} / M^{su} \right\rceil \\ & + \sum_j [e^{sC} \sum_i b_{f_i p_j}^{sd1} + e^{sP} \beta^{sC} (1 - \delta_j^s) \sum_i b_{f_i p_j}^{sd1}] \\ & + \sum_j \sum_k [(e^0 + \alpha M^{sp}) \cdot D_{p_j b_k} + e^0 D_{p_j b_k}] \left\lceil b_{p_j b_k}^{sd1} / M^{sp} \right\rceil \\ & + \sum_k [e^{sH} \beta^{sL} \sum_j b_{p_j b_k}^{sd1} + e^{sF} \beta^{sH} \beta^{sL} \sum_j b_{p_j b_k}^{sd1}] \end{aligned} \quad (2)$$

where $\lceil \cdot \rceil$ is ceiling function. In equation (1), C^{sd1} is the total cost when corn stover is used as the feedstock in biofuel manufacturing, it can be calculated by equation (3).

$$C^{sd1} = \sum_k C_k^{sd1} \quad (3)$$

where C_k^{sd1} is the cost incurred in bioethanol production using preprocessed corn stover at bio-refinery plant k , which can be calculated by equation (4). It consists of the cost for

purchasing preprocessed corn stover by bio-refinery plant k from preprocessing centers, the cost for transporting preprocessed corn stover from preprocessing centers to bio-refinery plant k , the cost for the corn stover bioconversion (i.e., hydrolysis and fermentation) at bio-refinery plant k , and the inventory cost for holding the raw material of preprocessed corn stover at bio-refinery plant k (the inventory level is maintained so that $1/d$ annual production requirement can be satisfied).

$$C_k^{sd1} = \sum_j z_j b_{p_j b_k}^{sd1} + \sum_j \left[b_{p_j b_k}^{sd1} / M^{sp} \right] D_{p_j b_k} T_{p_j b_k}^{sp} + o^{sH} \beta^{sL} \sum_j b_{p_j b_k}^{sd1} + o^{sF} \beta^{sH} \beta^{sL} \sum_j b_{p_j b_k}^{sd1} + \frac{h^{sp}}{d} \sum_j b_{p_j b_k}^{sd1} \quad (4)$$

Correspondingly, the cost per unit of bioethanol produced at bio-refinery plant k can be obtained by equation (5).

$$PP_k^{sd1} = C_k^{sd1} / TP_k^{sd1} \quad (5)$$

where TP_k^{sd1} is the total bioethanol produced in gallons using preprocessed corn stover at bio-refinery plant k , which can be calculated by equation (6).

$$TP_k^{sd1} = \sigma_k^s \sum_j b_{p_j b_k}^{sd1} \quad (6)$$

The constraints are formulated as follows.

$$PP_k^{sd1} \leq PP_k^c, \forall k \quad (7)$$

$$\sum_j b_{f_i p_j}^{sd1} \leq Q_i, \forall i \quad (8)$$

$$\sum_i b_{f_i p_j}^{sd1} \leq y_j^{sd1}, \forall j \quad (9)$$

$$\sum_k b_{p_j b_k}^{sd1} \leq \beta^{sP} \beta^{sC} (1 - \delta_j^s) y_j^{sd1}, \forall j \quad (10)$$

$$\sum_j b_{p_j b_k}^{sd1} \leq W_k^s, \forall k \quad (11)$$

$$NPV_j^{sd1} > 0, \forall j \quad (12)$$

$$b_{f_i p_j}^{sd1}, b_{p_j b_k}^{sd1}, y_j^{sd1} \geq 0 \quad (13)$$

$$x_j^{sd1} \in \{0, 1\} \quad (14)$$

$$b_{f_i p_j}^{sd1} \leq N x_j^{sd1}, \forall i, \forall j \quad (15)$$

$$b_{p_j b_k}^{sd1} \leq N x_j^{sd1}, \forall j, \forall k \quad (16)$$

$$y_j^{sd1} \leq N x_j^{sd1}, \forall j \quad (17)$$

$$\sum_k TP_k^s = D \quad (18)$$

$$x_j^{sd1} \leq N y_j^{sd1}, \forall j \quad (19)$$

$$y_j^{sd1} \leq K, \forall j \quad (20)$$

Constraint equation (7) specifies the economic feasibility of using preprocessed corn stover instead of milled corn in bioconversion by bio-refinery plant k . Constraint equation (8) illustrates that the corn stover supply capacity at each farm should not be

violated. Constraint equation (9) shows that the total amount of incoming corn stover from various farms cannot be larger than the designed capacity in terms of handling corn stover at preprocessing center j . Constraint equation (10) demonstrates that the total amount of preprocessed corn stover sold by the preprocessing center j cannot be larger than the maximum production capacity of preprocessed corn stover considering the process efficiencies of both chemical pretreatment and physical densification as well as the secondary products of animal feed after chemical pretreatment. Constraint equation (11) denotes that the total amount of preprocessed corn stover purchased by each bio-refinery plant cannot exceed its corresponding preprocessed corn stover processing capacity. In equation (12), NPV_j^{sd1} is the net present value of the project of building and running preprocessing center j throughout its lifetime. It requires that the net present value be larger than zero. Constraint equation (13) shows the non-negativity constraints for the decision variables of the preprocessing center capacities and material flows. Constraint equation (14) demonstrates that the decision variable x_j^{sd1} is binary. Constraint equation (15) ensures that the transportation amount from farm i to preprocessing center j is set to zero if the preprocessing center j is not selected. Constraint equation (16) ensures that the transportation amount from preprocessing center j to bio-refinery plant k is set to zero if the preprocessing center j is not selected. Constraint equation (17) ensures that the capacity of preprocessing center j is set to zero if the preprocessing center j is not selected. Constraint equation (18) ensures that the overall produced bioethanol can satisfy the total demand. Constraint equation (19) excludes the possibility that the capacity of preprocessing center j is zero when the location j is selected for building the preprocessing center. Constraint equation (20) limits the annual handling capability of

corn stover of preprocessing center j to a maximum capacity according to existing technological capability.

In equation (12), NPV_j^{sd1} can be calculated by equation (21).

$$NPV_j^{sd1} = -CS_j^{sd1} + \sum_{t=3}^{T+2} \frac{\text{Profit}_j^{sd1}}{(1+r)^t} \quad (21)$$

In equation (21), CS_j^{sd1} is the discounted setup cost of preprocessing center j . It can be calculated by equation (22).

$$CS_j^{sd1} = (I_j^{sd1} / 3) + (2I_j^{sd1} / 3(1+r)) \quad (22)$$

where I_j^{sd1} is the total initial setup cost of preprocessing center j . It consists of the setup costs for both chemical pretreatment (AFEX) system and physical densification system, which can be calculated by equation (23). Typically, the first two years are used to build the preprocessing center from scratch. One third of the initial investment is required in the first year and the remaining two thirds are required in the second year (Carolan et al., 2007).

$$I_j^{sd1} = [(a^{sC} y_j^{sd1}) + x_j^{sd1} b^{sC}] + G^P \cdot \{[y_j^{sd1} \beta^{sC} (1 - \delta_j^s)] / g^P\} \quad (23)$$

In equation (21), Profit_j^{sd1} is the yearly profit of preprocessing center j which is assumed to be fixed throughout the lifetime based on the current demand of biofuel. It can be calculated by subtracting the cost of purchasing corn stover by preprocessing center j , the cost of corn stover transportation between farms and preprocessing center j , and the operational cost of preprocessing center j from the yearly revenue of the

preprocessing center j . It can be calculated by equation (24).

$$\begin{aligned} \text{Profit}_j^{sd1} = & z_j^{sd1} \sum_k b_{p_j b_k}^{sd1} + F_j \delta_j^s \beta^{sC} \sum_i b_{f_i p_j}^{sd1} - \sum_i P_i^s b_{f_i p_j}^{sd1} - \sum_i \left[b_{f_i p_j}^{sd1} / M^{su} \right] D_{f_i p_j} T_{f_i p_j}^{su} \\ & - o^{sC} \sum_i b_{f_i p_j}^{sd1} - o^{sP} \beta^{sC} (1 - \delta_j^s) \sum_i b_{f_i p_j}^{sd1} \end{aligned} \quad (24)$$

Note that, the raw material inventory cost for holding corn stover at preprocessing center is not considered. The literature foresees that third party supply harvesters will enter into the existing biofuel supply chain, offering the service of corn stover harvesting and storage to enhance a steady supply of feedstock (Garino and Mends, 2018, Mertens et al., 2018) with a relatively low storage cost for holding baled corn stover (Hess et al., 2009b). The selling price of corn stover from farms typically includes the storage cost (University of Missouri Extension Commercial Agriculture Program, 2012). It implies that the inventory of corn stover at preprocessing center can be potentially managed by a Vendor Managed Inventory (VMI) mode, and thus inventory holding cost is not included in (24). While for the bio-refinery plant in distributed supply chain model, the raw material inventory of preprocessed stover is considered as shown in equation (4) since the bio-refinery plant is more far away from the farms in the distributed supply chain compared to the preprocessing center and the uncertainty of supply may be augmented. This assumption also holds for the pathway 2 model.

5.1.1.2. Pathway 2: densification at preprocessing centers and AFEX at bio-refinery plants. In this section, the formulation of the corn stover-sourced distributed biofuel supply chain built by pathway 2, i.e., the physical densification is implemented at the newly constructed preprocessing center, while the AFEX is carried out at the existing bio-refinery plant, is introduced. Note that the superscript “ $sd2$ ” is used

to denote the notations used in corn stover-based distributed pathway 2 supply chain.

The objective can be similarly formulated as equation (25).

$$\min_{x_j^{sd2}, y_j^{sd2}, b_{f_i p_j}^{sd2}, b_{p_j b_k}^{sd2}} w_1 E^{sd2} + w_2 C^{sd2} \quad (25)$$

Similarly, E^{sd2} can be calculated by equation (26). Note that processing emissions include AFEX, hydrolysis, and fermentation at bio-refinery plant k . In equation (25), C^{sd2} can be calculated by equation (27)

$$\begin{aligned} E^{sd2} = & \sum_i \sum_j [(e^0 + \alpha M^{su}) \cdot D_{f_i p_j} + e^0 D_{f_i p_j}] \left[b_{f_i p_j}^{sd2} / M^{su} \right] + \sum_j [e^{sp} \sum_i b_{f_i p_j}^{sd2}] \\ & + \sum_j \sum_k [(e^0 + \alpha M^{sp}) \cdot D_{p_j b_k} + e^0 D_{p_j b_k}] \left[b_{p_j b_k}^{sd2} / M^{sp} \right] \\ & + \sum_k [e^{sc} \sum_j b_{p_j b_k}^{sd2} + e^{sh} \beta^{sl} \beta^{sc} \sum_j b_{p_j b_k}^{sd2} + e^{sf} \beta^{sh} \beta^{sl} \beta^{sc} \sum_j b_{p_j b_k}^{sd2}] \end{aligned} \quad (26)$$

$$C^{sd2} = \sum_k C_k^{sd2} \quad (27)$$

where C_k^{sd2} is the annual cost at bio-refinery plant k that considers the annualized AFEX setup cost, densified corn stover purchase cost by bio-refinery plant k from preprocessing center j , densified corn stover transportation cost from preprocessing center j to bio-refinery plant k , operational costs including AFEX, hydrolysis, and fermentation, and raw material inventory holding cost to hold the densified corn stover. It is calculated by equation (28).

$$\begin{aligned}
C_k^{sd2} = & G_C^{sd2} \left[\frac{r}{1 - (1+r)^{-(T+1)}} \right] + \sum_j z_j^{sd2} b_{p_j b_k}^{sd2} + \sum_j \left[b_{p_j b_k}^{sd2} / M^{sp} \right] D_{p_j b_k} T_{p_j b_k}^{sp} \\
& + o^{sC} \sum_j b_{p_j b_k}^{sd2} + o^{sH} \beta^{sL} \beta^{sC} \sum_j b_{p_j b_k}^{sd2} + o^{sF} \beta^{sH} \beta^{sL} \beta^{sC} \sum_j b_{p_j b_k}^{sd2} + \frac{h^{sp}}{d} \sum_j b_{p_j b_k}^{sd2}
\end{aligned} \quad (28)$$

Note that in equation (28), unlike in the pathway 1 supply chain where the setup of the preprocessing center takes two years since it is built from scratch, here, the AFEX system is intended to be built in existing bio-refinery plant with available infrastructure and facility, thus, we assume the setup time is one year.

In equation (28), G_C^{sd2} is the setup cost for the chemical pretreatment (AFEX) system, which can be calculated by equation (29). The capacity of the AFEX system is determined by the capacity of the corresponding bio-refinery plants.

$$G_C^{sd2} = (a^{sC} (W_k^s / \beta^{sC})) + b^{sC} \quad (29)$$

The cost per unit gallon of bioethanol produced through corn stover following pathway 2 in bio-refinery plant k can be obtained by equation (30).

$$PP_k^{sd2} = C_k^{sd2} / TP_k^{sd2} \quad (30)$$

where TP_k^{sd2} is the total gallons of bioethanol produced using preprocessed corn stover at bio-refinery plant k , which can be calculated by equation (31).

$$TP_k^{sd2} = (\beta^{sC} \sigma_k^s) \sum_j b_{p_j b_k}^{sd2} \quad (31)$$

The constraints are formulated as shown below. Most of these constraints are similar to the ones in pathway 1 except the NPV calculation and the selling capacity of

preprocessed corn stover since only physical densification is included in the preprocessing center and no animal feed sold back is considered.

$$PP_k^{sd2} \leq PP_k^c, \forall k \quad (32)$$

$$\sum_j b_{f_i p_j}^{sd2} \leq Q_i, \forall i \quad (33)$$

$$\sum_i b_{f_i p_j}^{sd2} \leq y_j^{sd2}, \forall j \quad (34)$$

$$\sum_k b_{p_j b_k}^{sd2} \leq \beta^{sP} y_j^{sd2}, \forall j \quad (35)$$

$$\sum_j b_{p_j b_k}^{sd2} \leq (W_k^s / \beta^{sC}), \forall k \quad (36)$$

$$NPV_j^{sd2} > 0, \forall j \quad (37)$$

$$b_{f_i p_j}^{sd2}, b_{p_j b_k}^{sd2}, y_j^{sd2} \geq 0 \quad (38)$$

$$x_j^{sd2} \in \{0, 1\} \quad (39)$$

$$b_{f_i p_j}^{sd2} \leq N x_j^{sd2}, \forall i, \forall j \quad (40)$$

$$b_{p_j b_k}^{sd2} \leq N x_j^{sd2}, \forall j, \forall k \quad (41)$$

$$y_j^{sd2} \leq N x_j^{sd2}, \forall j \quad (42)$$

$$\sum_k TP_k^{sd2} = D \quad (43)$$

$$x_j^{sd2} \leq Ny_j^{sd2}, \forall j \quad (44)$$

$$y_j^{sd2} \leq K_2, \forall j \quad (45)$$

In equation (37), NPV_j^{sd2} can be calculated by equation (46).

$$NPV_j^{sd2} = -CS_j^{sd2} + \sum_{t=3}^{T+2} \frac{\text{Profit}_j^{sd2}}{(1+r)^t} \quad (46)$$

In equation (46), CS_j^{sd2} can be calculated by equation (47).

$$CS_j^{sd2} = (I_j^{sd2} / 3) + (2I_j^{sd2} / 3(1+r)) \quad (47)$$

where I_j^{sd2} only consists of the setup cost of physical densification system, which can be calculated by equation (48). In equation (46), Profit_j^{sd2} can be calculated by subtracting the cost of purchasing corn stover from farms by preprocessing center j , the cost of corn stover transportation between farms and preprocessing center j , and the operational cost of preprocessing center j , from the revenue of the preprocessing center j as shown in equation (49).

$$I_j^{sd2} = G^P \cdot [y_j^{sd2} / g^P] \quad (48)$$

$$\text{Profit}_j^{sd2} = z_j^{sd2} \sum_k b_{p_j b_k}^{sd2} - \sum_i P_i^s b_{f_i p_j}^{sd2} - \sum_i \left[b_{f_i p_j}^{sd2} / M^{su} \right] D_{f_i p_j} T_{f_i p_j}^{su} - o^{sP} \sum_i b_{f_i p_j}^{sd2} \quad (49)$$

5.1.2. Corn Stover-Sourced Biofuel Supply Chain Using Centralized

Preprocessing Strategy. In this section, we establish the model to estimate the cost and emission per gallon of bioethanol produced in bio-refinery in corn stover-sourced AFEX centralized biofuel supply chain. A superscript “ sc ” is used to denote the corresponding notations used in this model. The objective can be similarly formulated by equation (50). The decision variable is the transportation quantity of corn stover from farm j to bio-refinery plant k .

$$\min_{b_{f_i b_k}^{sc}} w_1 E^{sc} + w_2 C^{sc} \quad (50)$$

In equation (50), E^{sc} is the total emission incurred, which can be calculated by equation (51). It includes the emissions incurred by corn stover transportation from various farms to bio-refinery plants, and corn stover processing through pretreatment, hydrolysis and fermentation at bio-refinery plants.

$$\begin{aligned} E^{sc} = & \sum_i \sum_k [(e^0 + \alpha M^{su}) \cdot D_{f_i b_k} + e^0 D_{f_i b_k}] \left[b_{f_i b_k}^{sc} / M^{su} \right] \\ & + \sum_k [e^{sc} \sum_i b_{f_i b_k}^{sc} + e^{sH} \beta^{sL} \beta^{sc} \sum_i b_{f_i b_k}^{sc} + e^{sF} \beta^{sH} \beta^{sL} \beta^{sc} \sum_i b_{f_i b_k}^{sc}] \end{aligned} \quad (51)$$

In equation (50), C^{sc} is the total cost, which can be calculated by equation (52).

$$C^{sc} = \sum_k C_k^{sc} \quad (52)$$

where C_k^{sc} is the annual cost at bio-refinery plant k that includes annualized AFEX setup cost, corn stover purchase cost by bio-refinery plant k from farm i , corn stover

transportation cost from farm i to bio-refinery plant k , and the operational costs including AFEX, hydrolysis, and fermentation. It is calculated by equation (53).

$$\begin{aligned}
 C_k^{sc} = & [(a^{sC} (W_k^s / \beta^{sC})) + b^{sC}] \left[\frac{r}{1 - (1 + r)^{-(T+1)}} \right] + \sum_i P_i^s b_{f_i b_k}^{sc} \\
 & + \sum_i \left[b_{f_i b_k}^{sc} / M^{su} \right] D_{f_i b_k} T_{f_i b_k}^{su} + o^{sC} \sum_i b_{f_i b_k}^{sc} + o^{sH} \beta^{sL} \beta^{sC} \sum_i b_{f_i b_k}^{sc} \\
 & + o^{sF} \beta^{sH} \beta^{sL} \beta^{sC} \sum_i b_{f_i b_k}^{sc}
 \end{aligned} \tag{53}$$

Note that, inventory cost for holding raw materials of corn stover is not considered in equation (53) since bio-refinery plant in this centralized supply chain model is located immediately downstream to the farms, the raw material inventory holding can be similarly managed by a VMI mode through the involvement of third party harvesting and storage service providers.

The constraints for this model include economic feasibility for each bio-refinery plant, corn stover supply capability of each farm, bio-refinery plant biomass handling capability, non-negativity of transportation amount, and total biofuel demand satisfaction. The details of these constraints are formulated as follows.

$$PP_k^{sc} \leq PP_k^c, \forall k \tag{54}$$

$$\sum_k b_{f_i b_k}^{sc} \leq Q_i, \forall i \tag{55}$$

$$\sum_i b_{f_i b_k}^{sc} \leq (W_k^s / \beta^{sC}), \forall k \tag{56}$$

$$b_{f_i b_k}^{sc} \geq 0 \quad (57)$$

$$\sum_k TP_k^{sc} = D \quad (58)$$

In equation (58), TP_k^{sc} is the total bioethanol in gallons that can be produced using corn stover in bio-refinery plant k , which can be calculated by equation (59). In equation (54), PP_k^{sc} is the cost per gallon of bioethanol produced at bio-refinery plant k . It can be calculated by equation (60).

$$TP_k^{sc} = \sigma_k^s \beta^{sc} \sum_i b_{f_i b_k}^{sc} \quad (59)$$

$$PP_k^{sc} = C_k^{sc} / TP_k^{sc} \quad (60)$$

5.2. CASE STUDY

The effectiveness of the proposed corn stover-sourced supply chain model considering two restructuring strategies will be examined using the relevant data of the state of Missouri in the United States. In this section, all the input data used in the case study are introduced. Missouri is located on the “corn belt” in the Midwest of the United States. Approximately 18 million tons of corn is produced in the state each year (University of Missouri Extension, 2018). It ranks 3rd and 13th in biodiesel and bioethanol production capacities, respectively, in the United States (Eia.gov, 2015).

Corn and Corn Stover Supply from Farms

The data of the corn and corn stover supply in Missouri is obtained from National Agricultural Statistics Service (NASS) provided by the Department of Agriculture of the

United States (2012) (USDA, 2012). There are 63 out of a total of 115 counties planting corn in Missouri. Each county is modeled as a pseudo “farm” providing corn and corn stover to the biofuel supply chain. The latitude and longitude of the center of each county is used to approximately represent the location of each pseudo “farm”. Note that this “centralization” assumption has been widely used in literature (Muth et al., 2014, Mertens et al., 2018) for simplifying the model. To offset the possible error of this assumption, a tortuosity factor is typically used to adjust the physical distance (Kim & Dale, 2005, Sultana & Kumar, 2014). So in this section, we use a tortuosity factor with the value of 1.27 to obtain the adjusted transportation distance to deal with the possible errors due to using this “centralization” assumption (Sultana & Kumar, 2014).

The literature has indicated that a stable and continuous biomass supply is a complex process with different influencing factors (i.e., willingness, coordination, supply reliability, participation, and economic context) (Mertens et al., 2018). Complex interplays exist among these five factors under four different coordination scenarios (Mertens et al., 2018). However, it’s hard to quantitatively capture the complicated correlations among the five factors so that the variations of biomass supply and price can be exactly quantified. Therefore, in this section, we consider the variations of the supply and price of corn and corn stover from historical records in the past five years (University of Missouri Extension Commercial Agriculture Program, 2012) to model and examine such uncertainties. Specifically, the corn and corn stover supplies of each county are randomly drawn from a uniform distribution with the mean value equal to the average of the past five years and a bandwidth of 22% in both directions (University of Missouri Extension Commercial Agriculture Program, 2012). Here we assume that the corn stover

supply is same as corn supply (Luo et al., 2009). The corn selling price is drawn from another uniform distribution with mean of \$180/ton that is equal to the average of the past five years and a bandwidth of 5% in both directions, *i.e.*, \$171-\$189/ton (Balaman et al., 2018; Garino & Mends, 2018). The average price of corn stover after taking into account the corn stover collection and storage cost in the future is \$60/ton; and it is expected to fluctuate between \$55 and \$65 per ton (Dairy.missouri.edu, 2018; Kim & Dale, 2016).

The mean of the annual supply capacity of corn and corn stover and the farm location in Missouri are summarized in Table 3.12. The counties with corn planting and corresponding corn supply quantity are extracted from (USDA, 2012). The latitude and longitude of the center of each county are identified by (Latlong.net, 2018). The available corn stover supply is 60% of total corn stover (Luo et al., 2009; Kesharwani et al., 2018; Kesharwani et al., 2019a). The selling price of AFEX chemically pretreated corn stover that is sold back to the farms as animal feed is set at \$171/ton (Agfax.com, 2018).

Bio-refinery Plant

There are six bio-refinery plants in Missouri with yearly capacities from 20 to 60 million gallons of bioethanol per year (Renewable Fuels Association, 2017). The locations of these bio-refinery plants as well as of the farms where corn is planted in the state of Missouri are shown in Figure 5.1. The location and capacity of each plant is given in Table 3.11 (Ethanolrfa.org, 2017; Poet.com, 2018a; Poet.com, 2018b; Goldentriangleenergy.com, 2018; Midmissourienergy.com, 2018; Showmeethanolllc.com, 2018; Icmbiofuels.com, 2018). Parameters for the hydrolysis and fermentation in bio-refinery plants are summarized in Table 5.1 (Hardwick & Glatz,

1989; Sun & Cheng, 2002; Lin & Tanaka 2006). The operating cost of corn milling is \$8.5/ton (Bitra et al., 2009a). The emissions from corn milling are 17.05 lbs. CO₂/ton (Wiley, A., 2009; Dabbour et al., 2015).

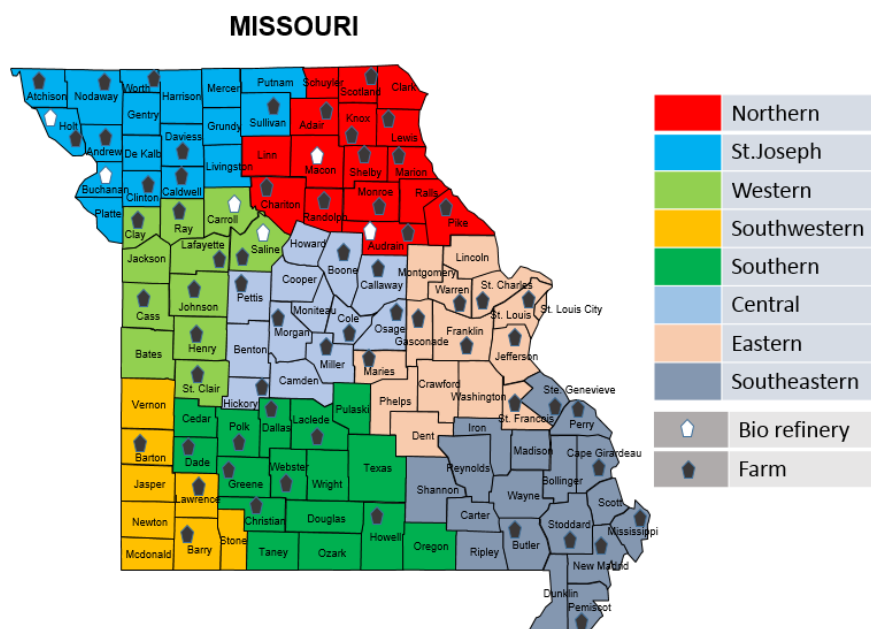


Figure 5.1 Farms and Bio-Refinery Plants in Missouri

Table 5.1 Conditions for Hydrolysis and Fermentation of Corn and Corn Stover

Process	Substrate	Enzyme	loading	pH	Temp (degree centigrade)	Reference
Hydrolysis	Corn	α -Amylase	Broth contains 1 gm KH ₂ PO ₄ and 200 μ L high temperature α -Amylase, Liquozyme, at 1.26g/mL, per liter	4.2	60-70	(Xu et al., 2018)
	Corn stover	Accelerase 1500	0.5 mL/g cellulose	--	50	(Xu et al., 2018)
Fermentation	Corn, corn-stover	Saccharomyces cerevisiae	--	5.5	30	(Lin and Tanaka, 2006)

Bioethanol Demand

The total biofuel demand in Missouri was 308.86 million gallons in 2015, which was roughly 20% of the total gasoline demand (Eia.gov, 2015). Most of the biofuel demand is assumed to be satisfied by E85 (Kesharwani et al., 2018), which consists of 85% bioethanol and 15% gasoline by volume. Thus, the total bioethanol demand in Missouri is 262.5 million gallons. The bioethanol yield from one ton of corn is 98 gallons (Fsa.usda.gov, 2018), which can be translated into annual demand for milled corn of 2.678 million tons. The bioethanol yield from one ton of chemically pretreated and physically densified corn stover is set at 100 gallons, since the corn stover ethanol yield ranges from 70-130 gallons/ton in literature (Ekşioğlu et al., 2009; Koundinya, 2018; Bals et al., 2011; Tumbalam et al., 2016; Aden & Foust, 2009). It can be translated into annual demand for preprocessed corn stover of 2.625 million tons.

Preprocessing Center

Each corn planting county is considered a candidate location for a preprocessing center, since the preprocessing centers are typically co-operative financial institutions held by the farmers (Carolan et al., 2007). The latitude and longitude of the center of each county is used to approximately represent the location of each candidate. The lifetime of the preprocessing centers of both pathways is 25 years (Ng & Maravelias, 2015, Ng & Maravelias, 2017). Typical technical parameters of AFEX and densification are summarized in Table 5.2 for illustration (Carolan et al., 2007; Kesharwani et al., 2017a; Kesharwani et al., 2017b).

The selling price of chemically and physically preprocessed corn stover at a preprocessing center in pathway 1 is \$175/ton (Kim & Dale, 2016). The selling price of

physically preprocessed corn stover at a preprocessing center in pathway 2 is \$95/ton (Kim & Dale, 2016; Bals et al., 2011). The chemical AFEX pretreatment in pathway 2 is assumed to be built at each of the six existing bio-refinery plants in Missouri. We assume a mass conversion efficiency of 95% for both chemical pretreatment and physical densification.

Table 5.2 Conditions for AFEX Pretreatment and Densification Processes

Process	Substrate	Input	Process 1	Output	Process 2	Output	Reference
AFEX	Corn stover (loose or pelletized)	Pressure = 20 atms. ; temp = 20 degree centigrade	AFEX reactor (90 degree centigrade, 20 atms. Pressure)	Pretreated corn stover slurry	Ammonia column (pressure = 3 atms., top temperature = 28 degree centigrade; bottom temperature = 135 degree centigrade)	Dry pretreated corn stover	(Carolan et al., 2007)
Densification	Corn stover	Density = 200 kg/m ³	Grinding, drying, hammer milling	Corn stover with particle size = 2 mm	Pelleting	Density = 700 kg/m ³	(Kesharwani et al., 2017a; Kesharwani et al., 2017b)

For pathway 1, 25% corn stover pretreated in AFEX will be transferred to secondary products and sold back as animal feed to the farms (Carolan et al., 2007). The setup costs (including both capital and installation) and emissions for the different processes involved in the physical and chemical preprocessing of biomass are shown in Table 5.3.

The operating cost (including maintenance and taxes) of AFEX is \$69.77/ton of corn stover (Bals et al., 2011). The physical densification system usually consists of grinding, drying, hammer milling, and pelleting equipment, the typical capacity of such equipment is 1.5 ton/hr (Alibaba.com, 2017). Assuming 2800 working hours in a year, g_p

is set to be 4200 tons per year. The operating cost (including maintenance and taxes) of physical densification is \$29.8/ton (Mani et al., 2006a).

Table 5.3 Setup Costs and Emissions of Physical and Chemical Preprocessing

Process	Setup cost	Reference	Emission (lbs. of CO ₂ /ton)	Reference
Grinding	\$23,134/machine	(Jacobson et al., 2014)	8.8	(Bitra et al., 2009a; Wiley, 2009)
Drying	\$4,570/machine	(Jacobson et al., 2014)	17.05	(Wiley, 2009; Mani et al., 2004)
Hammer-milling	\$14,737/machine	(Jacobson et al., 2014)	11.16	(Wiley, 2009, Alibaba.com, 2017)
Pelleting	\$45,010/machine	(Jacobson et al., 2014)	136	(Kesharwani et al., 2017a; Wiley, 2009)
AFEX	$a^{sC} = \$14.8375/(\text{ton}/\text{year}/\text{machine});$ $b^{sC} = \$5.225 \times 10^6/\text{machine}$	(Carolan et al., 2007, Jacobson et al., 2014)	341.25	(Carolan et al., 2007; Wiley, 2009; Teymouri, 2017)

Transportation

The transportation cost and emission related parameters are listed in Table 5.4.

Table 5.4 Transportation Costs and Emission Related Parameters

	Distance range (mile)	Cost for corn and corn stover pellets (\$ per mile per truck)	Cost for corn stover (\$ per mile per truck)	Reference
Transportation cost	Less than 25	3.12	1.74	(Ekşioğlu et al., 2009)
	Between 25 and 100	5.72	3.19	
	More than 100	7.8	4.35	
	Parameter	Value		Reference
Transportation emission	e^0	4.44 lbs. of CO ₂ /mile		(Kesharwani et al., 2017a; Schroeder et al., 2007; Engineeringtoolbox.com, 2017)
	α	0.074 lbs. of CO ₂ /mile/ton		
	M^c	55.75 tons		
	M^{su}	22.3 tons		
	M^{sp}	55.75 tons		

5.3. RESULTS AND SENSITIVITY ANALYSIS

5.3.1. Results. The results are as discussed below.

Corn-Sourced Scenario

In the corn-sourced supply chain, the total demand of bioethanol in Missouri is proportionally allocated to each of the six bio-refinery plants according to respective capacities. Similarly, the demand for corn in each bio-refinery plant is proportionally allocated to each of the 63 farms in Missouri, according to the capacity of each farm (Kesharwani et al., 2018). 500 replications are run with different prices and supplies of the corn from various farms. The resultant cost and emissions are illustrated in Table 5.5. The average unit cost is \$2.30 per gallon. It falls in the estimation range of the unit cost for corn based bioethanol production (i.e., \$1.89-\$3.59 per gallon) (Muth et al., 2014).

Table 5.5 Performance of the Corn Sourced Supply Chain

	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Mean	603,567,475	4,891,616,936	262,531,000	2.30	18.63
Half width of 95% CI	508,281	204,338	-	.002	.001

Distributed Pathway 1 Corn Stover Sourced Scenario (Quality Depot)

The maximum capacity of the preprocessing center is 70,000 tons/year (Jacobson et al., 2014). Equal weights for both objectives are used (i.e., w_1 and w_2 are set as 0.5). 500 replications with different prices and supplies of the corn stover from various farms is run to solve the proposed corn stover-sourced distributed biofuel supply chain problem formulated in pathway 1. The resultant cost and emission of the supply chain are

illustrated in Table 5.8. As can be seen through comparison with Table 5.6, the cost per unit production is reduced by 10%, while the emission per unit production has a significant increase of 37%.

Table 5.6 Performance of the Corn Stover Sourced Distributed Supply Chain in Pathway 1

	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Mean	543,852,062	6,853,317,839	262,531,000	2.07	26.10
Half width of 95% CI	258,203	345,213	-	.001	.00034
Reduction Compared to corn-based supply chain	9.8%	-38%	-	10%	-37%

On average, 56 counties are selected for building the preprocessing centers with respective capacities. Table 5.7 shows the resultant locations selected and corresponding capacities from one replication. Most of the selected counties are required to build a preprocessing center with capacity equal to or very close to the capacity upper bound. The counties that are not selected by the model for building preprocessing centers are typically with a low corn stover supply capacity and surrounded by other low stover supply counties. Dallas County (County code 31) can be an example. The farm capacity is 1.3 kilo-tons, and it is surrounded by Hickory (County code 32, farm capacity 6.6 kilo-tons), Polk (County code 39, farm capacity 5.8 kilo-tons), Greene (County code 54, farm capacity 4.6 kilo-tons), Webster (County code 57, farm capacity 4.2 kilo-tons), and Laclede (County code 33, farm capacity 5.2 kilo-tons) counties.

The details of financial performance of a typical preprocessing center with capacity of 70,000 tons/year built in Sullivan County (County code 14) are provided in Table 5.8. Note that the AFEX setup cost and physical densification setup cost are calculated using equation (23) along with the identified y_j and x_j in Table 5.7 and the parameters with respect to the setup cost of AFEX and physical densification equipment (grinding, drying, hammer milling, and pelleting) shown in Table 5.3. The revenue, processing cost, transportation cost, raw material cost, and profit are calculated using equation (24).

Table 5.7 Optimal Average Preprocessing Center Capacities in the Pathway 1 Supply Chain

County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI
1	70,000	--	17	70,000	--	33	0		49	70,000	--
2	70,000	--	18	70,000	--	34	67,480	1,146	50	0	
3	70,000	--	19	70,000	--	35	67,900	1,049	51	68,002	1,015
4	70,000	--	20	70,000	--	36	70,000	--	52	0	
5	70,000	--	21	70,000	--	37	70,000	--	53	67,076	1,028
6	70,000	--	22	70,000	--	38	70,000	--	54	60,550	2,043
7	70,000	--	23	70,000	--	39	70,000	--	55	68,022	1,015
8	70,000	--	24	70,000	--	40	70,000	--	56	0	
9	70,000	--	25	70,000	--	41	70,000	--	57	0	
10	70,000	--	26	70,000	--	42	70,000	--	58	66,808	1,024
11	70,000	--	27	70,000	--	43	0		59	63,288	1,166
12	70,000	--	28	70,000	--	44	58,026	1,089	60	70,000	--
13	70,000	--	29	70,000	--	45	70,000	--	61	64,402	1,134
14	70,000	--	30	70,000	--	46	60,841	1,007	62	58,616	989
15	70,000	--	31	0		47	26,691	2,983	63	70,000	--
16	70,000	--	32	70,000	--	48	70,000	--			

*Zero capacity means the county is not selected to build a preprocessing center

Table 5.8 Average Financial Performance of a 70,000 tons/year Preprocessing Center in the Distributed Supply Chain Built in Pathway 1

Parameter	Value
AFEX Setup Cost (\$)	6,234,544
Physical Densification Setup Cost (\$)	1,487,500
Total setup cost (\$)	7,722,044
Revenue per year (\$)	10,803,743
Processing cost per year (\$)	5,628,918
Transportation cost per year (\$)	157,364
Raw material cost per year (\$)	3,721,419
Profit per year (\$)	1,296,042

As can be seen from Table 5.10, the transportation cost is much less than the processing cost and the raw material cost. This can be largely explained by the amount (in kilo-tons) and pattern of transportation between the farms and the preprocessing centers as shown in Figure 5.2. Most of the biomass produced by the farm is supplied to the preprocessing center built in the same county. This is because the model tries to keep the transportation cost and emission at the minimum by sourcing most of the biomass locally.

In cases, where the selected preprocessing center has exhausted the corn stover supply from the farm in the same county, it sources the balance from the counties which have surplus supply with a lower cost (highlighted by blue color in Figure 5.2). For example, as shown in Figure 5.3, the preprocessing center in Worth County (County code 10) first utilizes around 40 kilo-tons of corn stover available from the farm located in the same county, and then sources the remaining from the farm in the neighboring Nodaway County (County code 8) which has a surplus supply with a capacity of 379 kilo-tons as well as a shorter transportation distance.

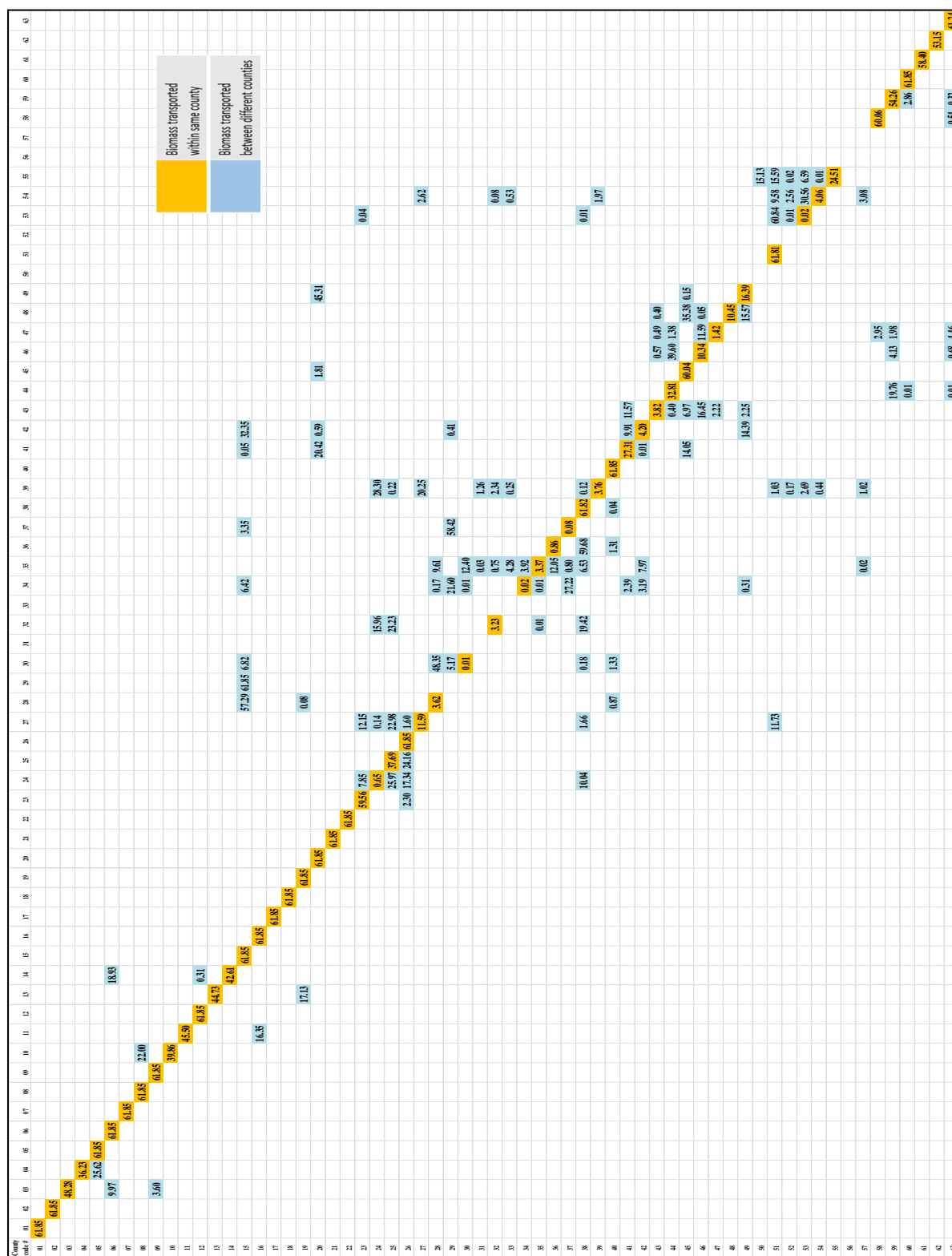


Figure 5.2 Average Corn Stover Transportation Amount from Farms to Preprocessing Centers in Kilo-Tons in the Pathway 1 Supply Chain

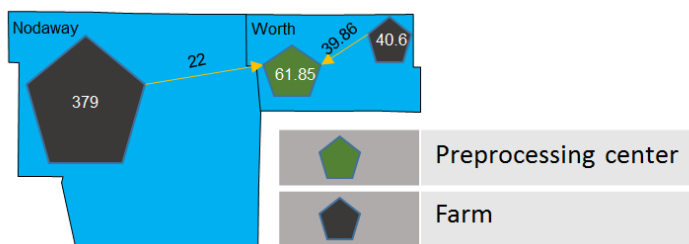


Figure 5.3 Worth County Sourcing the Surplus Demand

The average transportation amounts in kilo-tons between the preprocessing centers and the bio-refinery plants are illustrated in Table 5.9. Most of the preprocessing centers serve a single bio-refinery plant or at most two bio-refinery plants, depending on capacity, geographical proximity, and the demand of the bio-refinery plant. The bio-refinery plant with the lowest production capacity (bio-refinery plant 2, 20 million gallons per year) sources the preprocessed biomass from three preprocessing centers. The bio-refinery plant with the highest production capacity (bio-refinery plant 6, 60 million gallons per year) sources the preprocessed biomass from sixteen preprocessing centers.

Distributed Pathway 2 Corn Stover Sourced Scenario (Conventional Depot)

The maximum capacity of a preprocessing center in the distributed supply chain built in pathway 2 is set to be 52,500 tons/year, considering the fact that the center does not need to process biomass for animal feed as it does in pathway 1 (where the capacity is 70,000 tons/year). Equal weights for both objectives are used (i.e., w_1 and w_2 are set as 0.5) along with the other relevant parameters to run the mixed integer linear program to solve the proposed corn stover-sourced distributed biofuel supply chain problem formulated in pathway 2. 500 replications are run with different prices and supplies of

corn stover from different farms. 60 counties are selected for building preprocessing centers with respective capacities in a certain replication as shown in Table 5.10. The resultant cost and emission are shown in Table 5.11.

Table 5.9 Average Preprocessed Corn Stover Transported from Preprocessing Center to Bio-Refinery Plants in the Pathway 1 Supply Chain (Kilo-Tons)

Biorefinery code #						Biorefinery code #					
1 2 3 4 5 6						1 2 3 4 5 6					
County Code #						County Code #					
1	47.4					33					
2	47.4					34	47.4				
3	47.4					35	47.4				
4	47.4					36	47.4				
5	47.4					37					
6	47.4					38					
7	47.4					39	47.4				
8	47.4					40					
9	44.1 3.3					41	47.4				
10	47.4					42	47.4				
11	47.4					43					
12	47.4					44	35.2				
13	47.4					45	47.4				
14	47.4					46	43.6				
15	47.4					47	45.7				
16	47.4					48	47.4				
17	47.4					49	47.4				
18	47.4					50					
19	47.4					51	47.4				
20	47.4					52					
21	47.4					53	47.4				
22	47.4					54	47.4				
23	47.4					55	47.4				
24	47.4					56					
25	47.4					57					
26	47.4					58	47.4				
27	47.4					59	47.4				
28	47.4					60	47.4				
29	33.6					61	36.1				
30	47.4					62	37.5				
31						63	43.9				
32	47.4						3				

Table 5.10 Optimal Preprocessing Center Capacities in Pathway 2 Distributed Supply Chain

County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI	County Code #	Capacity* (tons/day)	Half width of 95% CI
1	52,500	--	17	52,500	--	33	14,243	215	49	52,500	--
2	52,500	--	18	52,500	--	34	52,500	--	50	17,208	197
3	52,500	--	19	52,500	--	35	52,500	--	51	52,500	--
4	52,500	--	20	52,500	--	36	52,500	--	52	4,313	78
5	52,500	--	21	52,500	--	37	52,500	--	53	52,500	--
6	52,500	--	22	52,500	--	38	52,500	--	54	52,500	--
7	52,500	--	23	52,500	--	39	52,500	--	55	52,500	--
8	52,500	--	24	52,500	--	40	52,500	--	56	3,144	34
9	52,500	--	25	52,500	--	41	52,500	--	57	5,670	284
10	52,500	--	26	52,500	--	42	52,500	--	58	52,500	--
11	52,500	--	27	52,500	--	43	52,496	8	59	52,500	--
12	52,500	--	28	52,500	--	44	52,500	--	60	0	
13	52,500	--	29	52,500	--	45	52,500	--	61	0	
14	52,500	--	30	52,500	--	46	52,500	--	62	0	
15	52,500	--	31	52,463	47	47	36,650	897	63	45,651	843
16	52,500	--	32	52,500	--	48	52,500	--			

*Zero capacity means the county is not selected to build preprocessing center

Table 5.11 Performance of the Distributed Corn Stover Sourced Supply Chain in Pathway 2

	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Mean	556,882,330	6,604,038,135	262,531,000	2.12	25.16
Half width of 95% CI	302,236	428,362	-	.004	.0002
Reduction compared to corn-based supply chain	7.7%	-35.1%	-	7.8%	-34.9%

The details of the financial performance a typical preprocessing center in Johnson County (County code 25) with an annual capacity of 52,500 tons are provided in Table 5.12.

Table 5.12 Average Financial Performance of a 52,500 Tons/Year Preprocessing Center Intended to be Built in Pathway 2 of the Distributed Supply Chain

Parameter	Value
Physical Densification Setup Cost (\$)	1,137,500
Revenue per year (\$)	4,738,125
Processing cost per year (\$)	1,422,273
Transportation cost per year (\$)	194,981
Raw material cost per year (\$)	2,675,672
Profit per year (\$)	445,199

As can be seen in Table 5.12, similar to the results shown in Table 5.8, the transportation cost is much less than the processing cost and the raw material cost. The detailed average transportation amounts (in kilo-tons) and the corresponding transportation pattern between the farms and the preprocessing center are illustrated in Figure 5.4.

The average transportation amounts in kilo-tons between the preprocessing centers and the bio-refinery plants are illustrated in Table 5.13. Similar to the insights from Table 5.9, most of the preprocessing centers serve a single bio-refinery plant or at most two bio-refinery plants, depending on the capacity, geographical proximity, and the demand at the bio-refinery plant. The bio-refinery plant with the lowest production capacity (bio-refinery plant 2, 20 million gallons per year) sources the preprocessed biomass from three preprocessing centers. The bio-refinery plant with the highest

Figure 5.4 Average Corn Stover Transportation Amount from Farms to Preprocessing Center in Kilo-Tons in Pathway 2 Distributed Supply Chain

Centralized AFEX Supply Chain

In this model, equal weights for both objectives are used (i.e., w_1 and w_2 are set as 0.5) along with the other relevant parameters to run the mixed integer linear program to solve the proposed corn stover-sourced biofuel supply chain problem formulated using centralized strategy. 500 replications with different prices and supplies of corn stover in various farms are experimented. The resultant cost and emission are shown in Table 5.14.

Table 5.14 Performance of the Corn Stover Sourced Centralized Supply Chain

Centralized supply chain model	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Mean	439,390,173	6,085,729,801	262,531,000	1.67	23.18
Half width of 95% CI	284,036	315,027	-	.001	.0002
Reduction compared to corn-based supply chain	27.2%	-24.2%	-	27.4%	-24.4%

The transportation amounts in kilo-tons between the farms and the bio-refinery plants in a certain replication are illustrated in Table 5.15. All the bio-refinery plants source the corn stover from their own county or neighboring counties depending on the capacity of bio-refinery, farm capacity, geographical proximity, and price of corn stover. For example, the bio-refinery plant situated in Buchanan County (bio-refinery code 5, 50 million gallons per year) sources the corn stover from the neighboring counties of Andrew (County code 1), Clay (County code 4), Clinton (County code 5), and Holt (County code 7). The bio-refinery plant with the lowest production capacity (bio-refinery plant 2, 20 million gallons per year) sources the corn stover from a single county.

5.3.2. Sensitivity Analysis. The results of the sensitivity analysis are below.

Distributed Pathway 1 Corn Stover Sourced Scenario (Quality Depot)

Sensitivity analysis is conducted to examine the variations of the performance of distributed pathway 1 model due to the variations of different input factors. The price and supply of corn stover is fixed for the sensitivity analysis in this section. The performance variations due to varying the weights assigned to two objectives are illustrated in Table 5.16. It can be observed that the cost decreases and emission increases as the problem starts to weight cost more than emission. The total number of nodes selected remains fairly constant. The cost per unit of bioethanol produced and the emissions per unit of bioethanol produced also remain fairly constant.

Table 5.16 Performance of the Distributed Supply Chain in Pathway 1 with Different Weight Combinations

Cost Weight	Emission Weight	Total number of pre-processing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
0.1	0.9	56	544,172,595	6,852,798,321	262,531,000	2.07	26.10
0.25	0.75	56	543,748,816	6,852,926,919	262,531,000	2.07	26.10
0.5	0.5	56	543,546,385	6,853,063,940	262,531,000	2.07	26.10
0.75	0.25	56	543,370,113	6,853,488,187	262,531,000	2.07	26.11
0.9	0.1	56	542,437,382	6,856,566,572	262,531,000	2.07	26.12

The performance variations due to varying the percentage of preprocessed biomass sold as animal feed (δ_j^s) are illustrated in Table 5.17. It can be seen that both overall and unit cost and emission increase with an increase in δ_j^s , the number of nodes selected for building preprocessing centers also increases with an increase in δ_j^s . When δ_j^s goes up, more biomass is required and hence the model starts opening up more nodes to meet this demand. Each new node incurs a new setup cost and hence the cost goes up. Meanwhile, additional processing and transportation are incurred, and hence the emission goes up, too. The overall performance of the supply chain is fairly sensitive to the variation of δ_j^s . Therefore, the variation, especially the increase of δ_j^s should be considered cautiously by practitioners, although such an increase can lead to a higher income for the preprocessing center.

Table 5.17 Performance of the Supply Chain in Distributed Pathway 1 with Different Percentages of Preprocessed Biomass Sold as Animal Feed

δ_j^s	Total number of pre-processing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Combined secondary income at the preprocessing centers from animal feed (\$)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
15%	49	541,071,910	6,693,707,892	75,811,091	262,531,000	2.06	25.50
20%	52	541,385,779	6,767,647,626	107,399,045	262,531,000	2.06	25.78
25%	56	543,546,385	6,853,063,940	143,198,727	262,531,000	2.07	26.10
30%	60	546,082,802	6,957,665,047	184,112,649	262,531,000	2.08	26.50

The performance variations due to the combined variations of both selling price of secondary product of animal feed (F_j) and δ_j^s are shown in Table 5.18. As can be

observed, fluctuation in F_j influences the design of the supply chain in terms of the number of nodes, and has an influence on the total cost and the total emission of the supply chain. It also affects the combined revenue generated by selling the secondary product of animal feed for the preprocessing centers. The δ_j^s , has a very pronounced effect on the design of the supply chain and its performance, as discussed above. A combination of a lower selling price (\$160 per ton) for the secondary product and a higher production volume (30%) may decrease the revenue of some of the preprocessing centers and the constraint of a positive NPV (see constraint equation (12)) cannot be met.

Table 5.18 Performance of the Distributed Supply Chain in Pathway 1 with Different Prices of Secondary Product of Animal Feed and Percentages of Preprocessed Biomass Sold as Animal Feed

F_j	δ_j^s	Total number of preprocessing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Combined secondary income at the preprocessing centers from animal feed (\$)	Total production (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
180	30%	60	545,911,217	6,952,526,555	193,802,789	262,531,000	2.08	26.48
180	20%	54	538,546,724	6,765,124,860	113,057,627	262,531,000	2.05	25.77
160	30%	Infeasible						
160	20%	52	546,486,335	6,779,190,846	100,490,335	262,531,000	2.08	25.82

The performance variations due to varying the selling price of chemically and physically pretreated biomass by the preprocessing centers to the bio-refinery plants are as shown in Table 5.19. As can be observed, the decrease in this price leads to an infeasibility due to the violation of net present value constraint. The increase in this price causes a slight modification in the design of the supply chain in terms of the number of preprocessing centers intended to be built. The overall cost of the supply chain and the

cost of unit production increase with an increase in this selling price as expected. Meanwhile, there is a slight decrease in the overall emission of the supply chain with an increase in this selling price, and thus the emission of unit production stays constant. The economic performance is more sensitive to the variation of the selling price of the preprocessed biomass than the environmental performance.

Table 5.19 Performance of the Distributed Supply Chain in Pathway 1 with Different Prices of Chemically and Physically Preprocessed Biomass Sold to the Bio-Refinery Plants

Preprocessed corn stover selling price (\$/ton)	Total number of pre-processing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
165	Infeasible					
175	56	543,546,385	6,853,063,940	262,531,000	2.07	26.10
185	57	579,947,523	6,851,262,280	262,531,000	2.21	26.10

The performance variations due to varying the inventory holding level of the bio-refinery plants are shown in Table 5.20. As can be observed, there exist the variations of total cost and total emissions, while the unit cost and the unit emission seem not very sensitive to the variation of inventory holding level.

Table 5.20 Performance Comparison for Distributed Supply Chain in Pathway 1 with Different Raw Material Inventory Levels at Bio-Refinery Plants

Inventory holding level	Total cost (\$)	Total emission (lbs. of CO ₂ /gal)	Total preprocessing center sites selected	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Weekly inventory	543,546,385	6,853,063,940	56	2.07	26.10
Monthly inventory	546,312,720	6,852,809,078	56	2.08	26.10

Pathway 2 Corn Stover Sourced Scenario (Conventional Depot)

Sensitivity analysis is conducted to examine the variation of the performance of distributed pathway 2 model due to the variations of different input factors. The performance variations due to varying the weights assigned to two objectives are illustrated in Table 5.21. Similar to pathway 1, it can be observed that the cost decreases and emission increases as the problem starts to weight cost more than emission. While the unit cost, unit emission, and the total number of nodes selected for building preprocessing center remain fairly constant.

Table 5.21 Performance of the Distributed Supply Chain in Pathway 2 with Different Weight Combinations

Cost Weight	Emission Weight	Total number of pre-processing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
0.1	0.9	61	558,561,396	6,602,931,203	262,531,000	2.13	25.15
0.25	0.75	60	557,205,303	6,603,723,306	262,531,000	2.12	25.15
0.5	0.5	60	556,856,659	6,603,928,051	262,531,000	2.12	25.16
0.75	0.25	60	555,494,781	6,606,437,152	262,531,000	2.12	25.16
0.9	0.1	60	555,494,781	6,606,438,105	262,531,000	2.12	25.16

The performance variations due to varying the selling price of physically pretreated biomass by the preprocessing centers to the bio-refinery plants are shown in Table 5.22. As can be observed, the reduction of this selling price leads to infeasibility due to the violation of the net present value constraint (see constraint A(12)). The number of preprocessing centers intended to be built decreases with an increase of selling price. The overall cost of the supply chain increases due to an increase in the raw material cost. The emission of the supply chain decreases as the model reduces one preprocessing center and this causes a corresponding decrease in transportation emission.

Table 5.22 Performance of the Distributed Pathway 2 Supply Chain with Different Prices of Physically Preprocessed Biomass Sold to the Biorefinery Plants

Preprocessed corn stover selling price (\$/ton)	Total number of preprocessing sites selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
85	Infeasible					
95	60	556,856,659	6,603,928,051	262,531,000	2.12	25.16
105	59	583,470,359	6,603,857,325	262,531,000	2.12	25.15

The performance variations due to varying the inventory holding level of the bio-refinery plants are shown in Table 5.23. Similar to the observation from Table 5.20, although there exist the variations of total cost and total emissions, the unit cost and the unit emission seem not very sensitive to the variation of inventory holding level.

Table 5.23 Performance Comparison for Distributed Pathway 2 Model with Different Raw Material Inventory Levels at Bio-Refinery Plants

Inventory holding level	Total cost (\$)	Total emission (lbs. of CO ₂ /gal)	Total preprocessing center sites selected	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Weekly inventory	556,856,659	6,603,928,051	60	2.12	25.16
Monthly inventory	559,547,764	6,603,658,999	60	2.13	25.15

Centralized AFEX Supply Chain

Sensitivity analysis is conducted to examine the variations of the performance of centralized AFEX supply chain model due to the variation of different weights assigned to two objectives as illustrated in Table 5.24. It can be observed that the model is fairly insensitive to the variation of the weights.

Table 5.24 Performance of the Distributed Supply Chain in Pathway 1 with Different Weight Combinations

Cost Weight	Emission Weight	Total number of farms selected	Total cost (\$)	Total emission (lbs. of CO ₂)	Total production of the supply chain (gal)	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
0.1	0.9	18	439,290,902	6,085,418,465	262,531,000	1.67	23.18
0.25	0.75	18	438,721,583	6,085,426,788	262,531,000	1.67	23.18
0.5	0.5	18	438,721,583	6,085,426,974	262,531,000	1.67	23.18
0.75	0.25	18	438,721,583	6,085,427,353	262,531,000	1.67	23.18
0.9	0.1	18	438,721,583	6,085,427,233	262,531,000	1.67	23.18

5.4. COMPARISON AMONG THREE MODELS IN TWO STRATEGIES

The overall performance comparison among three models are shown in Table 5.25. As can be seen, all the three models are better than the corn sourced supply chain in terms of cost, but worse with respect to emission. The centralized strategy can reduce the unit production cost by 27.39%, while increasing the emission by 24.42% compared to the corn sourced supply chain. It is better than the two models using distributed strategy in terms of both cost and emission. Between the two models using distributed strategies, pathway 1 model outperforms pathway 2 model in terms of unit cost, while pathway 2 model is superior to pathway 1 model in terms of unit emission.

Table 5.25 Performance Comparison

Supply Chain	Total cost (\$)	Total emission (lbs. of CO ₂)	Total bioethanol production (gal)	Cost per unit production (\$/gal)	Emission per unit production (lbs. of CO ₂ /gal)
Corn sourced (baseline) Mean	603,567,475	4,891,616,936	262,531,000	2.30	18.63
Half width of 95% CI	508,281	204,338	-	.002	.001
Corn stover sourced (Distributed pathway 1) Mean	543,852,062	6,853,317,839	262,531,000	2.07	26.10
Half width of 95% CI	258,203	345,213	-	.001	.00034
Corn stover sourced (Distributed pathway 2) Mean	556,882,330	6,604,038,135	262,531,000	2.12	25.16
Half width of 95% CI	302,236	428,362	-	.004	.0002
Corn stover sourced (Centralized) Mean	439,390,173	6,085,729,801	262,531,000	1.67	23.18
Half width of 95% CI	284,036	315,027	-	.001	.0002

The decomposition of the cost incurred in producing bioethanol in bio-refinery plants is given in Table 5.26 for the three models under two strategies. The biomass purchase cost in pathway 1 model is much higher than pathway 2 model and centralized model. This difference is mainly due to additional processes (both chemical pretreatment and physical densification) that are imposed on the corn stover purchased by bio-refinery plants in pathway 1 model. The reductions of purchase cost in pathway 2 model and centralized model are largely offset by the increase of the operating cost compared to pathway 1 model. In pathway 1, the feedstock purchase cost of bio-refinery largely covers the processing cost for chemical pretreatment and physical densification, and thus, the operating cost in bio-refinery plant is much lower than the remaining two models.

Through Table 5.26, it can be seen that the superiority with respect to cost effectiveness of the centralized strategy in the case of Missouri is mainly contributed by a much lower transportation cost compared to the two models using distributed strategy. This is mainly due to a lower biomass collection distance in centralized strategy. The existing bio-refinery plants in Missouri are built in the areas with large amounts of biomass supply. While, with two models using distributed strategy, due to the capacity limitation of the preprocessing center with the current technology, most of the counties will need to build a preprocessing center to satisfy the final demand (if we assume “one center in one county” when formulating the model), thus, the bio-refinery plant requires to source preprocessed corn stover from most of those centers. Therefore the transportation cost incurred to bio-refinery plants under the distributed strategy is much higher than the centralized one in this case.

Table 5.26 Cost Decomposition in Bio-Refinery Plants for Three Corn Stover-Sourced Supply Chain Model

Supply chain model	Total cost (\$)	Transportation cost (\$)	Feedstock purchase cost (\$)	Inventory cost (\$)	Annualized cost of AFEX (\$)	Operating cost (\$)
Distributed pathway 1	543,852,062	33,724,219	450,719,690	862,291	-	58,545,861
Distributed pathway 2	556,882,330	32,190,956	257,554,111	907,675	7,973,559	237,888,594
Centralized	439,390,173	9,099,259	162,784,329	-	8,068,439	237,888,594

The decomposition of the emissions incurred when using corn stover for producing bioethanol is demonstrated in Table 5.27 for the three models under two strategies. It can be seen that the major source of emissions is the main production processes for second generation biofuel manufacturing including AFEX, physical

densification, and bioconversion (i.e., hydrolysis and fermentation). The centralized AFEX supply chain can lead to lowest emissions due to nonstop transportation along shorter distances between farms and bio-refinery plants, in comparison to the two pathways in distributed strategy. The process emissions in centralized AFEX supply chain are lower than the two pathways when distributed strategy is used because physical densification is not needed. Emissions of the pathway 1 supply chain are higher than the pathway 2 supply chain because more stover is handled in the pathway 1 supply chain for providing the animal feed. The production of animal feed in the pathway 1 supply chain can generate additional income and thus reduce the overall operation cost while increasing emissions.

Table 5.27 Decomposition of Emissions in the Corn Stover Supply Chain

	Transportation emissions (CO ₂ lbs)	Total process emissions (CO ₂ lbs)	AFEX emissions (CO ₂ lbs)	Densification emissions (CO ₂ lbs)	Bioconversion emissions (CO ₂ lbs)
Pathway 1 supply chain	91,760,637	6,762,843,137	1,203,239,537	434,620,699	5,124,982,902
Pathway 2 supply chain	78,723,958	6,525,517,361	943,038,987	457,495,472	5,124,982,902
Centralized AFEX supply chain	17,707,912	6,068,021,889	943,038,987	--	5,124,982,902

To further examine the influence of the capacity limitation of the preprocessing center, we run additional sensitivity experiments that vary the capacity bound of the preprocessing center with a proportionally augmented fixed investment cost in distributed supply chain model to approximately examine the performance when multiple preprocessing centers can be built in one county. The results are shown in Tables 5.28 and 5.29.

Table 5.28 Sensitivity Analysis for Preprocessing Capacity Bounds for Distributed Pathway 1 Model

Supply Chain	Total setup cost of the preprocessing centers (\$)	Total transportation cost of bio-refinery (\$)	Total preprocessing center built	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Current capacity bound (Mean)	432,715,421	33,724,219	56	2.07	26.10
200% capacity bound (Mean)	461,792,546	11,491,052	30	2.02	25.89
300% capacity bound (Mean)	468,410,242	9,079,779	21	2.02	25.86

Table 5.29 Sensitivity Analysis for Preprocessing Capacity Bounds for Distributed Pathway 2 Model

Supply Chain	Total setup cost of the preprocessing centers (\$)	Total transportation cost of bio-refinery (\$)	Total preprocessing center built	Cost per unit production (\$)	Emission per unit production (lbs. of CO ₂ /gal)
Current capacity bound (Mean)	63,202,475	32,190,956	59	2.12	25.15
200% capacity bound (Mean)	61,207,475	11,797,092	33	2.04	24.96
300% capacity bound (Mean)	61,645,500	2,238,448	23	2.03	25.02

When allowing multiple preprocessing centers to be built in a county (i.e., the capacity is doubled or tripled as shown in Tables 5.28 and 5.29), the transportation cost of bio-refinery plant can be reduced along with a relatively small variation of the setup cost of preprocessing centers (since the number of centers intended to be built decreases proportional to the increase of the capacity bound) for both pathways. A closer look further reveals that the cost per unit of bioethanol production can be significantly reduced when doubling the center capacity bound, while it is not very obvious when the capacity bound increases from 200% to 300%. Although the bio-refinery transportation cost can be further reduced when the capacity bound increases from 200% to 300%, the reduction percentage is much less than the one when the capacity bound is doubled from current bound to 200%. While for the unit emission, the variations are not that obvious compared

to the unit cost. In pathway 1, the capacity bound increase leads to a decrease of the unit emission. In pathway 2, no obvious variation trend of the unit emission can be identified with the increase of the capacity bound.

5.5. SUMMARY OF SECOND GENERATION BIOFUEL SUPPLY CHAIN OPTIMISATION

In this section, we propose a corn stover-sourced biofuel supply chain considering two strategies for conducting preprocessing operation to restructure the existing supply chain and offer cellulosic feedstock for bio-refinery in second generation bioethanol manufacturing. Two major performance measures (i.e., cost and emission) from economic and environmental perspectives are modeled as the optimization objective using a mixed integer linear program to select the locations for building preprocessing centers, the capacity of the preprocessing centers, and the material flows. A case study is conducted based on the state of Missouri in the United States.

The results of the case study show that all three models from two restructuring strategies investigated in the case study are more cost effective but less environmentally friendly than first generation corn-based biofuel supply chain. Specifically, the centralized strategy outperforms the distributed one with a larger cost reduction and a less emission increase. It reduces the unit cost by 27.39% while increasing the unit emission by 24.42% compared to the corn-sourced supply chain. On the other hand, pathway 1 and pathway 2 models under the distributed strategy can reduce the unit cost by 10% and 7.8%, while increasing the unit emission by 36.5% and 34.9%, respectively, compared to the corn-sourced supply chain. These results reveal that the major impedance to such a replacement may be from the perspective of environmental sustainability.

The results of the case study allow us to obtain the insights into how the economic and environmental concerns vary when restructuring the supply chain infrastructure for switching first generation to second generation biofuel manufacturing. Using the state of Missouri as a case, the environmental performance in terms of GHG emissions is worse. This is mainly due to additional preprocessing operations to handle cellulosic biomass. It implies that further research focusing on the methods that can effectively reduce the GHG emissions in preprocessing is urgently needed to facilitate the wide adoption of second generation biofuel manufacturing technology.

As for the economic performance, all three models from two strategies for corn stover-sourced supply chain outperform the existing corn-sourced supply chain. This is mainly contributed by the cost saving due to the use of cellulosic biomass instead of corn grains, which can cover the additional cost for preprocessing. Specifically, centralized strategy is superior to the distributed one due to the fact that the existing bio-refinery plants in Missouri are located in the areas with abundant biomass supply. Their production capacities are not high enough to exhaust the supply in surrounding areas with a short collection distance. It matches the observations from the literature in terms of the threshold conditions of handling capacity and biomass collection distance to determine the superiority between centralized and distributed strategies (Muth et al., 2014). It also implies the significance of considering the existing infrastructure of the supply chain when implementing the switch from first generation to second generation biofuel manufacturing. The option of centralized strategy should not be excluded when the existing bio-refinery infrastructure has been built with an appropriate handling capacity in the area with a high production amount of corn. The physical densification for the corn

stover may not be needed if the collection distance can be short enough so that the negative impact due to a lower density of corn stover in transportation can be offset.

Also, the increase of the capacity of the proposed preprocessing center seems to be an effective path to improve the competitiveness of the distributed supply chain. The number of such centers intended to be built can be reduced, with more preferable location selections, considering the existing bio-refinery plants to reduce the transportation cost.

The first generation biofuel may lead to the destruction of wild lands and pastures to grow corn, soybean and other crops, which may have additional negative effects on the environment. Similar effects on the wild land of second generation biofuel manufacturing should be less evident since the biomass feedstocks are non-edible crop matter with high availability from existing farms. While, since the scope of this section does not include crop planting and harvesting, the emissions in such earlier biomass production stages are not included. The corn stover harvesting might have negative impacts, such as soil compaction, and increased emission, especially when a two or three pass harvesting system is used. Even for a one-pass harvesting system, the emission impact is not clear when corn stover is used on a large scale for second generation biofuel manufacturing.

For future work, the research scope can be expanded to include the harvesting and planting system so that a more accurate comparison between first and second generation biofuel supply chain can be systematically implemented, especially focusing on environmental interests. The complex interrelationships of the price, supply, and target customers between corn and corn stover when switching from first generation to second generation biofuel manufacturing could be further quantified. The uncertainties in terms of the operations during the lifetime period should be integrated into the model when

examining the model performance. The conflicts between different participators in the supply chain need to be analyzed and the overall benefit allocation should be explored. In addition, the potential risks that may affect different sections of the biofuel supply chain need to be considered and further studied to identify the resilience of given supply chain configurations. A mixed biomass source including both corn and corn stover in the supply chain can also be one interesting direction.

6. ECONOMIC VIABILITY AND ENVIRONMENTAL IMPACT INVESTIGATION OF CO-FERMENTATION IN BIOFUEL MANUFACTURING

The main limitation of second generation biofuel production is the low glucose concentration in the biomass slurry after hydrolysis and the low ethanol concentration post fermentation, which render the production of second generation biofuels commercially unviable. Furthermore, a pretreatment process that disrupts the lignin structure of the cellulose is required as an extra step compared to first generation biofuel production, this will cause additional emissions and increase the cost (Xu et al., 2018; Yang & Wyman, 2008).

To reduce the competition between food and fuel, as well as boost the low cellulosic ethanol concentration, a hybrid process of co-fermentation that integrates both first and second generation biofuel production technologies has been proposed. In co-fermentation, a mixture of biomass for fermentation is generated by combining starchy feedstock (the first generation) with the slurry of the post hydrolysis cellulosic feedstock (the second generation). The resulting mixture is then put through simultaneous sacchrification and fermentation (SSF), where the ethanol is produced from the fermentation of the mixture caused by microorganisms such as yeasts (Lin & Tanaka, 2006). A typical bioethanol production through co-fermentation of corn and corn stover is shown in Figure 6.1. The advantages of co-fermentation are the resulting increase in glucose concentration of the cellulosic biomass slurry after hydrolysis and the higher ethanol concentration post fermentation (Xu et al., 2018).

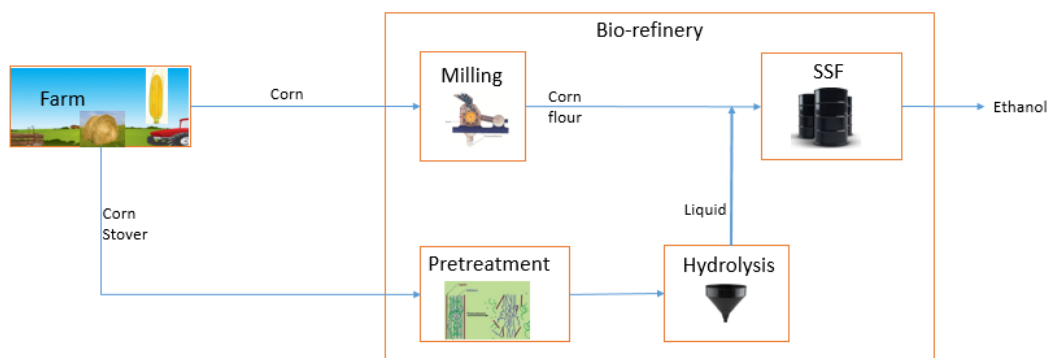


Figure 6.1 Co-Fermentation of Corn and Corn Stover for Bioethanol Manufacturing

In this section, the economic and environmental performance of large scale adoption of co-fermentation technology is examined and compared to first and second biofuel production technologies. Mathematical models that calculate the cost and emission per gallon of ethanol produced for three different biomass feedstock options (i.e., corn grains, corn stover, and mixed corns and corn stover) are proposed to systematically and quantitatively evaluate the economic feasibility and the environmental footprint. To the best of our knowledge, this is the first study of the economic viability and environmental impact of the co-fermentation technique. The rest of the section is organized as follows. The models for the three biofuel production options using three different biomasses are introduced in Section 6.1. In section 6.2, a case study comparing the results with respect to economic and environmental performance among the three options is presented, using relevant data collected in the state of Missouri in the United States. Conclusions are discussed and future work is proposed in Section 6.3.

6.1. BIOETHANOL PRODUCTION MODELS USING THREE OPTIONS

Notations:

List of indexes of the model

Index	Description
j	index of farms in supply chain
k	index of biorefinery plants in supply chain

List of variables of the model

Variable	Description
<i>Continuous nonnegative decision variables</i>	
b_{jk}^c	transportation amount of corn (in ton) from farm j to biorefinery plant k for producing bioethanol
b_{jk}^s	transportation amount of corn stover (in ton) from farm j to biorefinery plant k for producing bioethanol

List of parameters of the model.

Parameter	Description
<i>Cost related parameters</i>	
o^{cM}	operating cost per ton of corn in milling process

o^{cH}	operating cost per ton of corn milled in hydrolysis process
o^{cF}	operating cost per ton of corn in fermentation process
o^{sP}	operating cost per ton of corn stover in pretreatment process
o^{sH}	operating cost per ton of corn stover in hydrolysis process
o^{sF}	operating cost per ton of corn stover in fermentation process
o^{csF}	operating cost per ton of mixture of corn and corn stover in co-fermentation process
p_j^c	selling price (\$/ton) of the corn sold by farm j to biorefinery plant
p_i^s	base selling price (\$/ton) of the corn stover sold by farm i to biorefinery plant
T_{jk}	cost (\$/mile/truck) biomass feedstock transported from farm i to biorefinery plant k

Emission related parameters

e^0	GHG emission of transportation truck per unit distance without load
e^{cM}	GHG emission per ton of corn in milling process
e^{cH}	GHG emission per ton of corn in hydrolysis process
e^{cF}	GHG emission per ton of corn in fermentation process
e^{H0}	GHG emission per ton of corn stover burned in the farms

e^{H21c}	GHG emission per ton of corn through the corn harvesting equipment in the first pass of the two-pass harvesting system
e^{H21s}	GHG emissions per ton of stover through the stover harvesting equipment, used in the first pass of the two-pass harvesting system
e^{H22}	GHG emission per ton of stover baled in the second pass in two-pass harvesting system
e^{H31}	GHG emission per ton of corn harvested in the first pass of the three-pass harvesting system
e^{sP}	GHG emission per ton of corn stover in pretreatment process
e^{sH}	GHG emission per ton of corn stover in hydrolysis process
e^{sF}	GHG emission per ton of corn stover in fermentation process
e^{csF}	GHG emission per ton of mixture of corn and corn stover in co-fermentation process
α	rate of GHG emission increase per unit distance when unit load is added to the truck in transportation

Transportation related parameters

D_{jk}	distance from farm j to biorefinery plant k
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Capacity related parameters

M_c	maximum mass (tons) of corn grain that can be transported by a truck
M_{su}	maximum mass (tons) of corn stover that can be transported by a truck

W_k^c capacity of intake of corn at biorefinery plant k

W_k^s capacity of intake of corn stover at biorefinery plant k

Process related parameters

R ratio of weight percentage of corn to corn stover in co-fermentation

β_k^c conversion efficiency (gallons/ton) of ethanol production through corn at biorefinery

β_k^s conversion efficiency (gallons/ton) of ethanol production through corn stover at biorefinery

β_k^{cs} conversion efficiency (gallons/ton) of ethanol production through co fermentation of corn and corn stover at biorefinery

γ_k^{cMH} mass transition factor of corn after milling in bioethanol production using corn at biorefinery

γ_k^{cHF} mass transition factor of corn after hydrolysis in bioethanol production using corn at biorefinery

γ_k^{sPH} mass transition factor of corn stover after pretreatment in bioethanol production using corn

Miscellaneous parameters

K total bioethanol demand in gallons

6.1.1. Corn-Sourced Biofuel Supply Chain. In this section, we establish a model to estimate the cost and emission per gallon of bioethanol produced in a biorefinery with corn-sourced biofuel supply chain. The objective is formulated by equation (1). The

decision variables are the transportation amounts from farms to bio-refineries: $b_{fjb_k}^c$

is the quantity of corn stover from farm j to bio-refinery plant k :

$$\min_{b_{fjb_k}^c} w_1 E^c + w_2 C^c \quad (1)$$

In equation (1.1), C^c is the total cost, which can be calculated by equation (2):

$$C^c = \sum_k C_k^c \quad (2)$$

where C_k^c is the total cost for producing bioethanol at bio-refinery plant k which includes the material purchase cost, the transportation cost, the raw material (corn) holding cost, and the operation costs of milling, hydrolysis and fermentation. It can thus be calculated by equation (3).

$$\begin{aligned} C_k^c = & \sum_j P_j^c b_{fjb_k}^c + \sum_j \left[b_{fjb_k}^c / M^c \right] D_{fjb_k} T_{fjb_k} + \frac{h^c}{50} \sum_j b_{fjb_k}^c \\ & + o^{cM} \sum_j b_{fjb_k}^c + o^{cH} \beta^{cL} \beta^{cM} \sum_j b_{fjb_k}^c + o^{cF} \beta^{cH} \beta^{cL} \beta^{cM} \sum_j b_{fjb_k}^c \end{aligned} \quad (3)$$

where $\lceil \cdot \rceil$ is the ceiling function. We assume the biorefinery plant stocks enough raw corn grain inventory to satisfy a one-week production requirement (assuming 50 weeks of production per year).

In equation (1), E^c is the total emission, which can be calculated by equation (4):

$$E^c = \sum_k E_k^c + \sum_j E_j^c \quad (4)$$

where E_k^c is the total emission incurred by producing bioethanol while using corn at bio-refinery plant k , which can be calculated by equation (5). It includes the emissions incurred by corn transportation from various farms to bio-refinery plant k and corn processing through milling, hydrolysis and fermentation at bio-refinery plant k . Note that we assume that the truck used for transportation will be empty on its return trip:

$$E_k^c = \sum_j [(e^0 + \alpha M^c) \cdot D_{f_j b_k} + e^0 D_{f_j b_k}] \cdot \left[b_{f_j b_k}^c / M^c \right] + e^{cM} \sum_j b_{f_j b_k}^c + e^{cH} \beta^{cL} \beta^{cM} \sum_j b_{f_j b_k}^c + e^{cF} \beta^{cH} \beta^{cL} \beta^{cM} \sum_j b_{f_j b_k}^c \quad (5)$$

where E_j^c is the emission amount incurred by providing corn to the biorefinery as well as the emissions due to corn harvesting, and burning of excess corn stover at a farm. E_j^c can be calculated using equation (6). We assume the conventional three pass harvesting system. In this system, corn is harvested in the first pass. Then corn stover is windrowed in the second pass. Finally corn stover is baled in the third pass. In a corn sourced supply chain, the second and third passes do not occur as there is no demand for the corn stover:

$$E_j^c = e^{H31} \sum_k b_{f_j b_k}^c \quad (6)$$

where e^{H31} is the emission per ton of corn harvested in the first pass of the three-pass harvesting system. The total bioethanol in gallons that can be produced using corn in bio-refinery plant k can be calculated by equation (7):

$$TP_k^c = \sigma_k^c \sum_j b_{f_j b_k}^c \quad (7)$$

The constraints for this model include the corn supply capability of each farm, bio-refinery plant's corn handling capability, non-negativity of transportation amount, and total biofuel demand satisfaction.

$$\sum_k b_{f_j b_k}^c \leq Q_j, \forall j \quad (8)$$

$$\sigma_k^c \beta^{cM} \sum_j b_{f_j b_k}^c \leq W_k, \forall k \quad (9)$$

$$b_{f_j b_k}^c \geq 0 \quad (10)$$

$$\sum_k TP_k^c = D \quad (11)$$

6.1.2. Corn-Stover-Sourced Biofuel Supply Chain Using Centralized

Preprocessing Strategy. In this section, we establish a model to estimate the cost and emission per gallon of bioethanol produced in a biorefinery utilizing a corn-stover-sourced AFEX centralized biofuel supply chain. A superscript s is used to denote the corresponding notations used in this model. The objective can be formulated by equation (12). The decision variables are the transportation amounts of corn stover from farms to

bio-refineries: $b_{fjb_k}^s$ is the amount of corn stover transported from farm j to bio-refinery plant k :

$$\min_{b_{fjb_k}^s} w_1 E^s + w_2 C^s \quad (12)$$

In equation (12), E^s is total emissions incurred, which can be calculated by equation (13):

$$E^s = \sum_k E_k^s + \sum_j E_j^s \quad (13)$$

where E_k^s is the total emissions incurred by producing bioethanol using corn at bio-refinery plant k , including the emissions incurred by corn stover transportation from various farms to bio-refinery plants and corn stover processing through pretreatment, hydrolysis and fermentation at bio-refinery plants. It can be calculated by equation (14):

$$\begin{aligned} E_k^s = & \sum_j [(e^0 + \alpha M^{su}) \cdot D_{fjb_k} + e^0 D_{fjb_k}] \left[b_{fjb_k}^s / M^{su} \right] \\ & + e^{sC} \sum_j b_{fjb_k}^s + e^{sH} \beta^{sL} \beta^{sC} \sum_j b_{fjb_k}^s + e^{sF} \beta^{sH} \beta^{sL} \beta^{sC} \sum_j b_{fjb_k}^s \end{aligned} \quad (14)$$

We assume a two-pass harvesting system. In the first pass, the corn is harvested and the corn stover is windrowed. This is achieved by two separate equipment assemblies, one after the other. One is used for corn harvesting, while the other is used for stover windrowing. In the second pass, the amount of corn stover equivalent to the demand from the farm is baled and sent to the bio-refineries. The remaining amount is either sent to the animal feed industry, kept on the field for maintaining soil organic carbon level, or burnt in the open field. Note that we only consider the emissions

contributed by the corn stover sent as feedstock to the bio-refineries. In equation (13),

E_j^s is the emissions relevant to farm j incurred by providing corn stover to the biorefinery, which includes the emissions due to corn stover harvesting. This can be calculated using equation (15):

$$E_j^s = e^{H21s} \sum_k b_{f_j b_k}^s + e^{H22} \sum_k b_{f_j b_k}^s \quad (15)$$

where e^{H21s} is the emissions per ton of stover produced by the stover harvesting equipment, used in the first pass of the two-pass harvesting system. Similarly, e^{H22} is the emissions per ton of stover baled in the second pass.

In equation (12), C^s is the total cost, which can be calculated by equation (16):

$$C^s = \sum_k C_k^s \quad (16)$$

where C_k^s is the annual cost of bio-refinery plant k , which includes the annualized AFEX setup cost, corn stover purchase cost by bio-refinery plant k from farms, corn stover transportation cost from farms to bio-refinery plant k , raw material (stover) holding cost, and the operational costs including AFEX, hydrolysis, and fermentation. This is calculated by equation (17). Note that when calculating the annualized setup cost, we assume that the installation time is one year:

$$\begin{aligned}
C_k^s = & [(a^{sC} (W_k^s / \beta^{sC})) + b^{sC}] \left[\frac{r}{1 - (1 + r)^{-(T+1)}} \right] + \sum_j P_j^s b_{f_j b_k}^s \\
& + \sum_j \left[b_{f_j b_k}^s / M^{su} \right] D_{f_j b_k} T_{f_j b_k} + \frac{h^s}{50} \sum_i b_{f_j b_k}^s + o^{sC} \sum_j b_{f_j b_k}^s \\
& + o^{sH} \beta^{sL} \beta^{sC} \sum_j b_{f_j b_k}^s + o^{sF} \beta^{sH} \beta^{sL} \beta^{sC} \sum_i b_{f_j b_k}^s
\end{aligned} \tag{17}$$

The total bioethanol in gallons that can be produced using corn stover in bio-refinery plant k can be calculated by equation (18):

$$TP_k^s = \sigma_k^s \beta^{sC} \sum_j b_{f_j b_k}^s \tag{18}$$

The constraints for this model include corn stover supply capability of each farm, bio-refinery plant's stover handling capability, non-negativity of transportation amount, and total biofuel demand satisfaction:

$$\sum_k b_{f_j b_k}^s \leq Q_j, \forall j \tag{19}$$

$$\sigma_k^s \beta^{sC} \sum_j b_{f_j b_k}^s \leq W_k, \forall k \tag{20}$$

$$b_{f_j b_k}^s \geq 0 \tag{21}$$

$$\sum_k TP_k^s = D \tag{22}$$

6.1.3. Ethanol Production through Co-Fermentation Using Corn and Corn

Stover. In this section, we establish a model used to estimate the cost and emission required to produce a unit of ethanol through co-fermentation using both corn and corn stover. A superscript “cs” is used to denote the corresponding notations used in this

model. The objective is to identify the material flows of corn and stover between the farms and the bio-refinery plants that can minimize the cost and emission of the bioethanol produced under various constraints (e.g., bioethanol demand needs to be met).

This can be formulated by equation (23):

$$\min_{b_{fjb_k}^c, b_{fjb_k}^s} w_1 E^{cs} + w_2 C^{cs} \quad (23)$$

The cost of the production of ethanol through co-fermentation at biorefinery plant k includes annualized AFEX setup cost, purchase cost, transportation cost, inventory holding cost, and processing cost as shown in equation (24). The processing cost consists of the cost of milling operation for corn, the cost of the pretreatment operation for corn stover, the cost of the hydrolysis operation for corn stover, and the cost of simultaneous sacchrification and fermentation of the mixture of the hydrolyzed slurry of corn stover and milled corn water solution.

$$\begin{aligned} C_k^{cs} = & [(a^{sC} (W_k^s / \beta^{sC})) + b^{sC}] \left[\frac{r}{1 - (1 + r)^{-(T+1)}} \right] + \sum_j (P_j^c b_{fjb_k}^c + P_j^s b_{fjb_k}^s) \\ & + \sum_j \left[b_{fjb_k}^c / M^c \right] D_{fjb_k} T_{fjb_k} + \sum_j \left[b_{fjb_k}^s / M^{su} \right] D_{fjb_k} T_{fjb_k} + \frac{h^c}{50} \sum_j b_{fjb_k}^c \\ & + \frac{h^s}{50} \sum_j b_{fjb_k}^s + o^{cM} \sum_j b_{fjb_k}^c + o^{sC} \sum_j b_{fjb_k}^s + o^{sH} \beta^{sL} \beta^{sC} \sum_j b_{fjb_k}^s \\ & + o^{csF} \sum_j (\beta^{cL} \beta^{cM} b_{fjb_k}^c + \beta^{sH} \beta^{sL} \beta^{sC} b_{fjb_k}^s) \end{aligned} \quad (24)$$

The total cost of ethanol production through co-fermentation can be calculated by equation (25):

$$C^{CS} = \sum_k C_k^{CS} \quad (25)$$

We assume a two-pass harvesting system. In equation (23), E_j^s is the emissions relevant to farm j incurred by providing corn and stover to the biorefinery which includes the emissions due to corn and stover harvesting. E_j^s can be calculated using equation (26):

$$E_j^{CS} = e^{H21c} \sum_k b_{f_j b_k}^c + e^{H21s} \sum_k b_{f_j b_k}^s + e^{H22} \sum_k b_{f_j b_k}^s \quad (26)$$

where e^{H21c} is the emission per ton of corn produced by the corn harvesting equipment in the first pass of the two-pass harvesting system. The emissions relevant to the biorefinery plant k include the emissions of transportation and processing at biorefinery plant k , which can be calculated by equation (27):

$$\begin{aligned} E_k^{CS} = & \sum_j [(e^0 + \alpha M^c) \cdot D_{f_j b_k} + e^0 D_{f_j b_k}] \left[b_{f_j b_k}^c / M^c \right] \\ & + \sum_j [(e^0 + \alpha M^{su}) \cdot D_{f_j b_k} + e^0 D_{f_j b_k}] \left[b_{f_j b_k}^s / M^{su} \right] \\ & + e^{cM} \sum_j b_{f_j b_k}^c + e^{sC} \sum_j b_{f_j b_k}^s + e^{sH} \beta^{sL} \beta^{sC} \sum_j b_{f_j b_k}^s \\ & + e^{csF} \sum_j (\beta^{cL} \beta^{cM} b_{f_j b_k}^c + \beta^{sH} \beta^{sL} \beta^{sC} b_{f_j b_k}^s) \end{aligned} \quad (27)$$

The total emission due to ethanol production through co-fermentation can be calculated by equation (28):

$$E^{cs} = \sum_k E_k^{cs} + \sum_j E_j^{cs} \quad (28)$$

The equivalent gallons of the bioethanol that can be produced using such co-fermentation in biorefinery plant k can be calculated by equation (29):

$$TP_k^{cs} = \sigma_k^{cs} \sum_j (\beta^{cM} b_{f_j b_k}^c + \beta^{sC} (R b_{f_j b_k}^s)) \quad (29)$$

The constraints are formulated as follows:

$$\sum_k b_{f_j b_k}^c \leq Q_j, \forall j \quad (30)$$

$$\sum_k b_{f_j b_k}^s \leq Q_j, \forall j \quad (31)$$

$$\sigma_k^{cs} (\beta^{cM} \sum_j b_{f_j b_k}^c + \beta^{sC} R \sum_j b_{f_j b_k}^s) \leq W_k, \forall k \quad (32)$$

$$b_{f_j b_k}^c, b_{f_j b_k}^s \geq 0 \quad (33)$$

$$\sum_j b_{f_j b_k}^c = R \sum_j b_{f_j b_k}^s, \forall k \quad (34)$$

$$\sum_k TP_k^{cs} = D \quad (35)$$

Constraints equation (30) and (31) illustrate the supply capacity at each farm for corn and corn stover respectively. Constraint equation (32) illustrates the demand capacity of bio-refinery plant k . Constraint equation (33) illustrates that the transportation amounts of corn and corn stover from farm j to bio-refinery plant k are non-zero. Constraint equation (34) illustrates the constraint of the ratio of corn and corn stover required for the co-fermentation method. Constraint equation (35) ensures that the total amount of produced bioethanol can satisfy the total demand.

6.2. CASE STUDY

In this section, we build a case based on data from the state of Missouri in the United States by utilizing the models proposed in Section 2 to examine the cost and emission of biofuel production using three different feedstocks. Missouri is located in the corn belt of the United States, produces approximately 2 million tons of corn annually and ranks 3rd and 13th in biodiesel and bioethanol production capacities, respectively, in the United States (USDA, 2012; U.S. Energy Information Association, 2017).

Corn and Corn Stover Supply from Farms

The data detailing corn and corn stover supply in Missouri is obtained from National Agricultural Statistics Service (NASS) of the U.S. Department of Agriculture (USDA, 2012). Sixty three out of 115 counties in Missouri plant corn out as shown in Figure 5.1 (Kesharwani et al., 2018). In this case study, each county is modeled as a pseudo “farm,” providing corn and corn stover to the biofuel supply chain. The latitude and longitude of the center of each county is used to approximately represent the location

of each pseudo “farm” so that the distance between the farm and the biorefinery plant can be calculated.

The yearly corn supply (unit: ton) available for ethanol production from each farm is given in Table 3.12. Note that 60% of corn produced is available for ethanol production (Uptownsheep.com, 2018), while 60% of corn stover produced is available for ethanol production (Economides, 2018). The average price of corn is around \$180/ton (Balaman et al., 2018). We assume that the price fluctuates around \$180/ton with a bandwidth of 5% in both directions, (i.e., \$171-\$189/ton). The average base price of corn stover is \$60/ton and is expected to fluctuate between \$55 and \$65 per ton (Corn-stover in Missouri, 2018). The selling prices of corn and corn stover from different farms are randomly drawn from the uniform distributions of $U(171, 189)$, and $U(55, 65)$, respectively, as shown in Table 6.1.

The emission resulting from corn harvesting is 203.61 lbs CO₂/ton (Romm, 2008; Marland & Turhollow, 1991). The emission resulting from changes in land use due to additional planting of corn is 16.89 lbs CO₂/ton (Kendall & Chang, 2009). The cost of fertilizer input needed to restore soil quality per unit of corn stover removed for biofuel production above the maximum allowable limit is \$15/ton (Hettinga et al., 2009).

Biorefinery Plant

There are six biorefinery plants in Missouri as shown in Figure 5.1, with yearly bioethanol production capacities ranging from 20 to 60 million gallons (Renewable Fuels Association, 2017). Bioethanol production capacity and location of each plant is given in Table 3.11 (Goldentriangleenergy.com, 2018; Icmbiofuels.com, 2018;

Midmissourienergy.com, 2018; Poet.com, 2018a; Poet.com, 2018b; Showmeethanolllc.com, 2018).

The unit operating costs of the corresponding processes in corn-based, corn-stover-based, and co-fermentation biofuel manufacturing are shown in Table 6.1. For the corn and corn-stover-based processes, the unit operating cost parameters are obtained from (Shapouri & Gallagher, 2002) and based on energy consumption cost being the leading contributor to the operating cost in hydrolysis and fermentation (Shapouri & Gallagher, 2002). For co-fermentation, the weight ratio of corn and corn stover in co-fermentation is 1:1 (Xu & Wang, 2017). Due to the lack of existing data of the operating cost of co-fermentation in literature, the unit operating cost is inferred through weighted average of corn and corn stover used in the co-fermentation.

The unit emissions of the corresponding processes of corn-based, corn-stover-based, and co-fermentation biofuel manufacturing are shown in Table 6.2. Similarly, for co-fermentation, the unit emission is inferred by the weighted average of corn and corn stover used in co-fermentation.

Table 6.1 Operating Costs for the Processes at Biorefinery Plants

Operation	Feedstock	Cost (\$/ton)	Reference
Milling	Corn	0.15	(Shapouri & Gallagher, 2002; Kim & Dale, 2005)
Hydrolysis	Corn	5.64	(Shapouri & Gallagher, 2002; Kim & Dale, 2005)
Fermentation	Corn	0.67	(Shapouri & Gallagher, 2002; Kim & Dale, 2005)
Pretreatment	Corn-stover	80	(Bals et al., 2011)
Hydrolysis	Corn-stover	8.42	(Aden et al., 2002)
Fermentation	Corn-stover	1	(Aden et al., 2002)
Co-fermentation	Corn and corn-stover	0.853	

The mass transition factors between two successive processes in corn-based, corn-stover-based, and co-fermentation biofuel manufacturing are listed in Table 6.3.

Table 6.2 Emission for the Processes at Biorefinery Plants

Operation	Feedstock	Emission (lbs. of CO ₂ /ton)	Reference
Milling	Corn	17.05	(Shapouri & Gallagher, 2002; Kim & Dale, 2005; Electric Power Monthly, 2018)
Hydrolysis	Corn	126.89	(Shapouri & Gallagher, 2002; Kim & Dale, 2005; Electric Power Monthly, 2018)
Fermentation	Corn	633.63	(Shapouri & Gallagher, 2002; Kim & Dale, 2005; Electric Power Monthly, 2018)
Pretreatment	Corn-stover	341.25	(Dabbour et al., 2015; Carolan et al., 2007; Teymouri, 2017)
Hydrolysis	Corn-stover	188.70	(Electric Power Monthly, 2018; Ray & Behera, 2011)
Fermentation	Corn-stover	641.14	(Electric Power Monthly, 2018; Ray & Behera, 2011)
Co-fermentation	Corn and corn-stover	637.79	

Bioethanol Demand

The total biofuel demand in Missouri was 308.86 million gallons in 2015, which was roughly 20% of the total gasoline demand (Eia.gov, 2018b). Most of the biofuel demand is satisfied by E85 (Kesharwani et al., 2018), which consists of 85% bioethanol and 15% gasoline by volume. Thus, the total demand for bioethanol in Missouri is 262.5 million gallons.

Table 6.3 Mass Transition Factors between the Processes at Biorefinery Plants

Upstream Process	Downstream Process	Feedstock	Mass transition factor	Reference
Milling	Hydrolysis	Corn	2.33	(Bothast & Schlicher, 2005; Anval.net, 2018)
Hydrolysis	Fermentation	Corn	1	(Ray & Behera, 2011; Humbird et al., 2010)
Pretreatment	Hydrolysis	Corn-stover	2.25	(Humbird et al., 2010)
Hydrolysis	Fermentation	Corn-stover	1	(Ray & Behera, 2011; Humbird et al., 2010)
Milling	Co-fermentation	Corn and corn-stover	2.33	(Bothast & Schlicher, 2005; Anval.net, 2018)

The bioethanol yield from one ton of corn is 110 gallons (Articles.extension.org, 2017), which can be translated into the annual demand of corn of 2.386 million tons. While the bioethanol yield from one ton of corn stover is 84 gallons (Tumbalam et al., 2016), which can be translated into the annual demand of preprocessed corn stover of 3.125 million tons. The bioethanol yield from one ton of mixture of corn and corn stover is 100 gallons (Xu & Wang, 2017).

Transportation

The transportation cost rates are listed in Table 5.6 (Kim & Dale, 2005; Kesharwani et al., 2017a; Schroeder et al., 2007; Engineeringtoolbox.com, 2017)

6.3. RESULTS

The biomass transportation amounts of the three sourcing strategies are shown in Table 6.4, 6.5, 6.6, and 6.7.

6.4. COMPARISON AMONG THREE MODELS

The comparison of unit cost and unit emission of the three strategies is shown in Table 6.8. As can be seen from Table 6.8, the co-fermentation supply chain has a fairly competitive cost advantage compared to the low-cost corn stover sourced supply chain.

It is able to achieve this while mitigating the increase in emission caused by switching from corn to corn stover feedstock.

6.5. SUMMARY OF TECHNIQUE OF COFERMENTING FIRST AND SECOND GENERATION BIOFUELS

In this section, we analyzed the cost and emission related performance for three different feedstock sourcing strategies in bioethanol manufacturing. We evaluated the co-fermentation technique and compared its economic and environmental performance with corn sourced and corn stover sourced scenarios. A numerical case study using the data from the State of Missouri in the United States was conducted. The results of the case study show that co-fermentation can strike a balance in both cost and emission performance between corn and corn-stover-sourced biofuel manufacturing. Thus, this technique provides an economic advantage and mitigates the environmental impact caused by transitioning from the starchy feedstock of corn grain to a cellulosic feedstock of corn stover.

For future work, the scale of the case study can be expanded to include multiple states on the “corn-belt” of the United States. The proposed mathematical model can be further utilized as a platform to optimize the structure of the biofuel supply chain such that the desired performance measures can be optimized.

Table 6.5 Average Stover Transportation from Farms to Bio-Refinery Plants in the Corn-Stover-Sourced Supply Chain (Kilo-Tons)

County Code #	Biorefinery code #						County Code #
	1	2	3	4	5	6	
1					150.4		33
2		210.5					34
3						49.5	35
4							36
5					123.7		37
6							38
7					252.2		39
8							40
9						119.9	41
10							42
11	46.5						43
12						227.8	44
13	45.9						45
14							46
15				278.5			47
16							48
17	67.4						49
18							50
19	168.6						51
20				186.1			52
21							53
22	155.9						54
23							55
24							56
25							57
26						7.3	58
27							59
28							60
29				61.7			61
30							62
31							63
32							

Table 6.6 Average Corn Transportation from Farms to Bio-Refinery Plants in the Co-Fermentation Supply Chain (Kilo-Tons)

County Code #	Biorefinery code #						County Code #
	1	2	3	4	5	6	
1					150.4		33
2							34
3							35
4							36
5					112.8		37
6							38
7							39
8		105.3					40
9							41
10							42
11							43
12							44
13							45
14							46
15				263.2			47
16							48
17							49
18							50
19	86.2						51
20							52
21							53
22	155.9						54
23							55
24							56
25							57
26			78.3			244.9	58
27							59
28							60
29							61
30							62
31							63
32							

Table 6.8 Performance Comparison

Supply Chain	Total cost (\$)	Total emission (lbs. of CO ₂)	Total bioethanol production (gal)	Cost per unit production (\$/gal)	Emission per unit production (lbs. of CO ₂ /gal)
Corn sourced	541,493,815	4,589,839,974	262,531,000	2.06	17.48
Corn stover sourced	432,498,820	5,961,808,603	262,531,000	1.65	22.71
Co-fermentation	444,982,169	4,980,507,105	262,531,000	1.69	18.97

7. CONCLUSION AND FUTURE WORK

7.1. CONCLUSION

Compared to the existing literature, the proposed models in this dissertation have the advantages that 1) they consider the existing infrastructure in biofuel supply chain when investigating both economic and environmental impacts for the switch from first generation biofuel to second generation biofuel manufacturing; 2) different supply chain restructuring strategies are modeled and examined for offering a systematic comparison for the decision maker; and 3) the results are based on the analytical optimization model to provide an achievable best performance of the supply chain using different strategies.

This dissertation is expected to fill, to some extent, the gap of a systematic performance comparison between first and second generation biofuel supply chain. It provides a modeling tool to enhance the optimal use of bioenergy sources considering economic viability and environmental sustainability towards a green energy system. Both overall performance of the entire supply chain and interests of individual participators in the supply chain are considered. It is expected to serve the readers (including academic peers, policy makers, government agencies, business owners, etc.) who are interested in further enhancing the transition from traditional fossil fuel to renewable biofuel.

7.2. FUTURE WORK

Many assumptions have been made to simplify the proposed model in this section, which leaves many open research issues that invite deeper investigations from the peers in the future.

Inclusion of Harvesting System

The harvesting system is not included in the scope of this dissertation, which may incur an inaccurate estimation from both economic and environmental perspectives. In the United States, it is reported in the literature that currently corn stover is harvested using three-pass systems (Cook & Shinnars, 2011). In three-pass systems, corn grain is harvested in the first pass, followed by windrowing corn stover in the second pass, and finally corn stover is baled in the third pass (Cook & Shinnars, 2011).

The selling price of corn stover for biofuel manufacturing used in this dissertation is estimated considering corn stover collection and storage cost when using existing three-pass harvesting systems for second generation biofuel manufacturing (Kim & Dale, 2016; Langholtz et al., 2016). We set the constraint that no more than 60% of corn stover can be removed from the farms, so that no additional cost for additional fertilizer will be incurred considering possible soil degradation (Cardona & Sánchez, 2006; Ng et al., 2018). Therefore, most of the costs due to harvesting have been largely considered in the models with the existing harvesting system.

The emissions due to the additional fertilizers can be ignored due to the constraint of no more than 60% corn stover removal. The emissions from the fuel use during harvesting depend largely on the equipment used and time required. Specifically, compared to first generation biofuel manufacturing where corn grain needs to be collected, the time spent and fuel consumed from the operations of stover windrowing and baling need to be quantified in future research to estimate additional emissions from stover collection.

The existing three-pass harvesting systems typically are corn grain prioritized since the farmers gain most of their profit from selling the corn grain. If they harvest both corn grain and corn stover in a single pass, it may delay the grain harvest which may result in a potential business loss. When the production of cellulosic ethanol is commercialized on a large scale, there will be a constant demand for corn stover from the bio-refinery plants. Thus, it is reasonable to foresee that farmers will be interested in harvesting both corn and corn stover with a fewer pass harvesting system (e.g., a two-pass or a one-pass system) with less fuel consumption and harvesting time, since both grain and stover have the opportunity to bring in profits. Two-pass harvesting system refers to simultaneously harvesting grain and windrowing stover in the first pass, followed by the baling of stover in the second pass. In one-pass systems, both grain and stover are harvested in a single pass (Cook & Shinnars, 2011).

Generally, a one-pass system takes less time to complete the collection of both corn and corn stover compared to a two-pass system (Cook & Shinnars, 2011). However, it requires investment for new equipment, while most of the equipment in a one-pass system is still in prototype stage since one-pass systems are not in full-fledged commercial use (Milhollin et al., 2011). In addition, the selection of chopping or baling for storing the collected stover will lead to different cost superiorities between one-pass and two-pass systems (Vadas & Digman, 2013). Thus, the advantage in terms of cost effectiveness between one-pass and two-pass systems is not clear. Furthermore, both one-pass and two-pass harvesting systems, especially the one-pass system, will reduce the field drying time and moisture of stover may increase (Wendt et al., 2018). This will lead to additional transportation cost and dry matter loss, which influences stover cost. The

possible influence on supply chain performance of this cost variation due to increased moisture is additionally discussed in “Stover Moisture.”

From an environmental perspective, there exist performance variations between various harvesting techniques. One-pass systems generally have the least collection time; however, the new equipment required in one-pass systems may have a higher power rating, and thus the advantage in terms of fuel consumption is not clear compared to multi-pass systems. Further, the use of different baling/chopping strategies will lead to different emissions’ superiorities (Vadas & Digman, 2013). The two-pass system is considered more feasible for the stover collection in second generation biofuel manufacturing (Cook & Shinnars, 2011). Some research focusing on different baling/chopping strategies in two-pass systems has been reported. For example, the two-pass bale system has fuel use comparable to conventional three-pass bale systems, while the two-pass chop system uses around 50% more fuel (Vadas & Digman, 2013).

It seems that for the existing harvesting systems, the research focusing on environmental issues is lagging behind the research focusing on economic concerns. Therefore, the emissions due to the harvesting operations have been left out of the scope of this dissertation considering the existing harvesting system. While for the harvesting system with fewer passes that may be possibly adopted to accommodate the large scale cellulosic biofuel production in the future, both cost and emission studies are not completed. More investigation on the variations of cost and emission is needed to validate the possible options of harvesting system switch.

Uncertainty Modeling

The uncertainties in the supply chain modeling consist of the concerns from various aspects such as supply, demand, facility operation performance, and some other external influencing factors. In this research, the uncertainty of the performance of the facilities involved in the supply chain (e.g., equipment degradation) is not considered when evaluating the lifetime performance. The demand uncertainty is not considered, either. The existing literature has indicated that the demand for stover stays practically fixed by the capacity of bio-refinery plants in the given region (Golecha & Gan, 2016). The supply uncertainty due to non-constant participation willingness of farmers when offering corn stover to the biofuel supply chain is examined using stochastic analysis with varied inputs of corn stover supply and corn stover price. The complex relationships among the supply amount, selling price, and some other external economic factors such as gas price are simplified through separately extracting the price and supply amount from the respective distributions built using the recent historical records of Missouri, while the possible correlation between price and supply is not considered.

The results from the case study offer 95% confidence intervals for the unit cost and unit emission with a fairly narrow width, which shows the performance on unit production is not very sensitive to the variations of the price and supply amount modeled in this section. This is mainly due to 1) not all uncertainty sources are considered in the analysis, and 2) the raw data used for modeling the variation of price and supply are from a local area (i.e., Missouri) in recent years (in past four to five years) with a less fluctuation range.

Future research considering more uncertainty factors and using more historical data for a broader area should be implemented to strengthen the robustness of the model. A mathematical model that can quantitatively reveal the relationships between different input factors with uncertainties needs to be derived. In addition, the issue of corn demand “post-replacement by corn stover” should also be studied. Since a large amount of corn is especially planted and used for biofuel production rather than food, a new target customer group for selling these “replaced corn” needs to be carefully investigated. The selling outlets of the replaced corn and the corresponding price could influence the willingness of the farmers to offer corn stover for biofuel manufacturing, especially in the areas with a mature system of first generation biofuel manufacturing and supply.

Conflicts between Different Participators

In the model presented in this section, the overall performance of the supply chain is optimized while considering the interests from different individual participators in the supply chain. Corresponding constraints (e.g., the NPV constraint for the preprocessing center) are used in the formulation, which may reduce the number of feasible solutions of the problem. The interests from different parties in the supply chain may have mutual conflicts. For example, the motivation of bio-refinery plants in the supply chain is largely represented by a more cost effective alternative feedstock of corn stover instead of corn. The interests of the preprocessing centers are preserved by a larger amount of income when selling the preprocessed feedstock to bio-refinery plants.

Different constraint relaxation options can be experimented in future research to examine and compare the overall benefits to the entire supply chain and the possible

gains and losses to different individual participators. The policy of overall benefit allocation and cross subsidization can be further explored.

Redundant Corn Stover Handling

The redundant corn stover is typically burned (Ghani et al., 2018). In the United States, around 6% of the corn stover is used for livestock and other industries (Kim & Dale, 2004), and around 40% of the corn stover is required to maintain the organic carbon levels of soil (Luo et al., 2009). This means that approximately 54% of the corn stover may be burned in open fields. When the feedstock for bioethanol production is switched from corn to corn stover, more corn stover will be consumed and the amount of burning could be reduced. It is estimated that 4,850 lbs of CO₂ emission is incurred by burning one ton of corn stover (Cao et al., 2008). If this redundant corn stover handling is considered, the comparison of unit emission between the three proposed supply chains and the corn-sourced supply chain is as illustrated in Table 7.1. The unit emission of corn-sourced supply chain is much higher than the result when redundant stover handling is not considered. It can be seen that a reduction of 52%, 38%, and 37% can be achieved in the unit emission by the pathway 1, pathway 2, and centralized AFEX supply chains compared to the corn-sourced supply chain. The pathway 1 supply chain outperforms the pathway 2 and centralized AFEX supply chains because of the additional stover consumed for secondary product of animal feed at the preprocessing centers.

Stover Moisture

The existing three-pass harvesting system can offer the stover in the U.S. cornbelt region with the moisture level typically around 15-20% (Jacobson et al., 2014). The densification and AFEX equipment used in the depots is capable of handling this level of

moisture (Jacobson et al., 2009). As mentioned earlier, the harvesting systems with fewer passes will be preferred in the future to accommodate the stover collection in second generation biofuel manufacturing. One main drawback, especially for one-pass systems, is the reduced field drying time, which results in a higher moisture level. This main negative impact is worth analyzing further (i.e., increased stover cost due to the increased moisture level) although one-pass systems are not commercially available now. Therefore, a sensitivity analysis considering two higher stover price possibilities (i.e., \$80 and \$100 per ton) for all three supply chain models is implemented. The performance variations are shown in Tables 7.2 to 7.4.

Table 7.1 Emission Comparison when Redundant Stover Handling is Considered

Supply Chain	Emissions of the supply chain (not including redundant stover handling) (lbs. of CO ₂)	Corn stover used for biofuel production	Corn stover burned (tons)	Emissions due to burning of corn stover (lbs. of CO ₂)	Total emissions (supply chain plus redundant stover handling) (lbs. of CO ₂)	Total bioethanol production (gal)	Total unit emission (lbs. of CO ₂ /gal)	Reduction
Corn sourced	4,891,616,936	0	5,794,256	28,102,141,600	32,993,758,536	262,531,000	125.68	--
Pathway 1	6,853,317,839	3,957,729	1,836,527	8,907,155,950	15,760,473,789	262,531,000	60.03	52%
Pathway 2	6,604,038,135	2,908,931	2,885,325	13,993,826,250	20,597,864,385	262,531,000	78.46	38%
Centralized AFEX	6,085,729,801	2,763,484	3,030,772	14,699,244,200	20,784,974,001	262,531,000	79.17	37%

Note that, in the pathway 1 and pathway 2 supply chain models, the increase in corn stover price leads to the violation of the NPV constraints for the preprocessing centers. Therefore, selling prices of preprocessed stover (in both the pathway 1 and

pathway 2 supply chains) and animal feed (in the pathway 1 supply chain) are increased accordingly to cover the increase in raw material cost and to maintain a similar profit level for the preprocessing center. It can be seen that with the increase of stover purchase price due to increased moisture with the use of single-pass harvesting system, the unit emission can largely stay constant, while the unit cost is quite sensitive to this variation. In the pathway 1 supply chain, when corn stover price increases to \$80 per ton, the unit cost is increased to \$2.28, which is very close to the unit cost in the corn-sourced baseline model. When stover price is increased to \$100 per ton, the unit cost exceeds the baseline model of the corn-sourced supply chain. A similar trend can be seen from the pathway 2 and centralized AFEX supply chain models. Specifically, the increase of the stover farmgate price leads to the pathway 2 supply chain less economically competitive compared to the corn-sourced baseline model. While the centralized AFEX model can still keep the advantage of unit cost when compared to the baseline model although a significant increase of the unit cost. It is because the centralized AFEX supply chain has a much lower unit cost with the stover farmgate price considering the existing harvesting systems compared to the two pathway supply chains under the distributed strategy.

In addition, the selection of baling or chopping for stover storage also influences moisture level and feedstock stability. Earlier research has indicated that when the chopped logistic system is used combined with a two-pass harvesting system and stover is stored in bulk format in silage bags, it could result in the lowest farmgate price of stover (Cook and Shinnars, 2011; Vadas and Digman, 2013). The dry matter loss associated with ensiled biomass in storage is significantly less compared to high moisture bales stored aerobically in existing three-pass systems. Additionally, such storage can

reliably limit the risks of loss from fire in storage and preprocessing operations (Wendt et al., 2018).

Table 7.2 Performance of the Pathway 1 Supply Chain with Different Stover Purchase Prices

Corn stover price (\$/ton)	Unit cost (\$/gal)	Unit emission (lbs. of CO ₂ /gal)	Selling price of preprocessed corn stover (\$/ton)	Selling price of animal feed (\$/ton)	Total revenue (\$)	Total raw material cost (\$)	Transportation cost (\$)	Processing cost (\$)	Total profit (\$)
60	2.07	26.10	175	171	555,548,412	204,739,332	7,930,434	311,888,256	30,990,390
80	2.28	26.10	191.5	194	623,708,023	273,284,318	7,930,434	311,888,256	30,605,015
100	2.48	26.10	212	218	692,491,145	341,829,305	7,930,434	311,888,256	30,843,150

Table 7.3 Performance of the Pathway 2 Supply Chain with Different Stover Purchase Prices

Corn stover price (\$/ton)	Unit cost (\$/gal)	Unit emission (lbs. of CO ₂ /gal)	Selling price of preprocessed corn stover (\$/ton)	Total revenue (\$)	Total raw material cost (\$)	Transportation cost (\$)	Processing cost (\$)	Total profit (\$)
60	2.12	25.16	95	262,531,000	158,122,216	5,260,955	78,805,578	20,342,251
80	2.32	25.16	114.2	315,589,897	211,011,866	5,260,955	78,805,578	20,511,498
100	2.52	25.16	133.3	368,372,445	263,901,516	5,260,955	78,805,578	20,404,396

Table 7.4 Performance of the Centralized AFEX Supply Chain with Different Stover Purchase Prices

Corn stover price (\$/ton)	Unit cost (\$/gal)	Unit emission (lbs. of CO ₂ /gal)
60	1.67	23.18
80	1.88	23.18
100	2.09	23.18

This implies that moisture issues and storage strategy, when the harvesting systems with fewer passes are used in the future, need to be well addressed. Otherwise, the cost advantage in second generation biofuel will be significantly weakened.

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VITA

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