Green Design of a Cellulosic Bio-butanol Supply Chain Network with Life Cycle Assessment

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ABSTRACT

The incentives and policies spearheaded by the U.S. government have created abundant opportunities for renewable fuel production and commercialization. Bio-butanol is a very promising renewable fuel for the future transportation market. Many efforts have been made to improve its production process, but seldom has bio-butanol research discussed the integration and optimization of a cellulosic bio-butanol supply chain network. This study focused on the development of a physical supply chain network and the optimization of a green supply chain network for cellulosic bio-butanol. To develop the physical supply chain network, the production process, material flow, physical supply chain participants, and supply chain logistics activities of cellulosic bio-butanol were identified by conducting an onsite visit and survey of current bio-fuel stakeholders. To optimize the green supply chain network for cellulosic bio-butanol, the life cycle analysis was integrated into a multi-objective linear programming model. With the objectives of maximizing the economic profits and minimizing the greenhouse gas emissions, the proposed model can optimize the location and size of a bio-butanol production plant. The mathematical model was applied to a case study in the state of Missouri, and solved the tradeoff between the feedstock and market availabilities of sorghum stem bio-butanol. The results of this research can be used to support the decision making process at the strategic, tactical, and operational levels of cellulosic bio-butanol commercialization and cellulosic bio-butanol supply chain optimization. The results of this research can also be used as an introductory guideline for beginners who are interested in cellulosic bio-butanol commercialization and supply chain design.
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GENERAL AUDIENCE ABSTRACT

Renewable energy is one of the most effective tools to fight the threats of climate change, global warming, food price rising, and energy dependence. Cellulosic bio-butanol, a renewable alcohol-based biofuel, is a very promising energy candidate to support the fight for these threats. Due to its low water miscibility, similar energy content and octane number with gasoline, blending ability with gasoline in any proportions, and its directly utilization in gasoline engine, cellulosic bio-butanol is a potential candidate to replace gasoline. Unlike bioethanol, which only relies its fuel distribution on railway and tanker trucks, bio-butanol is compatible with not only railway and tanker trucks but also current pipeline based fuel distribution infrastructures. In order to increase the competitively of this promising energy candidate, the cellulosic bio-butanol is worth to be commercialized. An important step for the commercialization of cellulosic bio-butanol is the network design of its supply chain.

In this research, the supply chain network of cellulosic bio-butanol was constructed and optimized. The supply chain network of cellulosic bio-butanol was constructed by identifying the three important aspects of a supply chain network structure: structure dimension, participants in supply chain, and supply chain business process links. A) The structure dimension was identified by understanding the production process of bio-butanol. A case study was used to study the production process of cellulosic bio-butanol. B) The supply chain business process links were identified by conducting a survey on the logistics activities in bio-butanol supply chain. C) The participants of cellulosic bio-butanol supply chain were identified by identifying the physical infrastructure of cellulosic bio-butanol supply chain. The results of the literature review, case study and survey were analyzed to identify the physical infrastructure and the participants in the supply chain. It was found out that the supply chain network structure of cellulosic bio-butanol includes 4 tiers of horizontal structure: suppliers, producers, distributors, and customers. The suppliers refer to the local farmers and feedstock aggregators. The producers are the cellulosic bio-butanol production plants. The distributors are the fuel logistics companies and fuel distributors. The customers are the fuel companies. The cellulosic bio-butanol producers use contracts to connect with biomass suppliers, fuel distributors, and bio-butanol customers.

Based on the proposed network structure of cellulosic bio-butanol supply chain, the optimization of the green cellulosic bio-butanol supply chain network was conducted. A multi-objective linear integer programming model was developed to design the green cellulosic bio-butanol supply chain network. Life cycle analysis (LCA) and net present
value techniques were used in the proposed model to formulate the environmental and economic objective function. With the objectives of maximizing the economic profits while minimizing the greenhouse gas (GHG) emissions, the proposed model can optimize the location and the size of bio-butanol production plant. The model was applied using data from the state of Missouri (MO). The results showed that the optimal location of cellulosic bio-butanol production plant is in the southeastern region of MO. And the production size of bio-butanol production plant is based on the tradeoff between the economic and environmental objectives. The lower GHG emissions results in a smaller size of production plant.
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Reference
1 Introduction of the Study

The United States Energy Policy Act of 2005, the Energy Independent and Security Act of 2007, and the Food, Conservation, and Energy Act of 2008, shows U.S government support for renewable energy enterprises by providing preferential tax, incentive policies, and loans (Withers et al 2015). These acts largely encourage the renewable fuel industry to develop non-food cellulosic biofuel. In addition, the Renewable Fuel Standard (RFS), the Low Carbon Fuel Standard (LCFS), and the Renewable Identification Number system (RINs) which were stemmed from Energy Policy Act of 2005 also hasten the development of non-food cellulosic bio-butanol. The RFS requires an annual increasing amount of renewable fuel blended into transportation fuel. This requirement maintains a certain amount of renewable consumption each year, guaranteeing a portion of market share for renewable fuel. The LCFS supports the renewable fuel industry by working to reduce the carbon footprint of transportation. The RINs are used to track the production, use, and trade of biofuel to ensure the implementations of RFS requirements. Combined, the incentive policies by U.S government have created a good opportunity for commercialization of renewable fuel.

With these strong policies as the backup force, the development and commercialization of non-food cellulosic biofuel should have become a booming industry. Paradoxically, the real status of the cellulosic biofuel producers is not as ideal as what was expected. The publication (Withers et al 2015) analyzes why so many current cellulosic biofuel projects were cancelled or shutdown and concludes the industry has been hampered by various external and internal barriers. Among these barriers, suppliers and third-party issues are one of the main external barriers while strategic issues are one of the most important internal barriers. The supplier barrier refers to the feedstock logistics costs and facility location. The third-party issues include the partnership with feedstock supply and distribution channels. The strategic issues are fundamental since it has to consider not only the revenue of the bio-fuel, but also the commercialization of byproducts and co-products (Withers et al 2015). Each of these barriers can cause the shutdown or cancellation of a biofuel refinery or a cellulosic biofuel project. Therefore, removing these barriers is critical for the commercialization of non-food cellulosic biofuel industry.

The supply chain network design (SCND) is an option to remove barriers and to further commercialize the non-food cellulosic bio-fuel industry. Supply chain network design refers to the design and optimization of the physical network structure of a supply chain. It is one of the most significant steps to design a new supply chain since it can impact all of the tactical and operational decisions that follow (Farahani et al 2014). The traditional SCND can deal with the above barriers because it can economically optimize not only the locations, numbers and capacities of the facilities within the network, but
also the associate amount and transportation mode of upstream and downstream material flow inside the supply chain (Autry et al 2013).

A well-designed traditional supply chain network can help entrepreneurs to make better decisions. However, recently the bioenergy industry has realized the significance of sustainable development (Hopwood et al 2005) and the government has issued policies to press the fuel industry to develop more sustainably (Withers et al 2015). Therefore, traditional SCND is not enough for bio-fuel commercialization and a more long-lasting strategy to satisfy the requirements for future sustainable development is required. Hence, green supply chain network design (GSCND) could be a wiser choice, because it can not only optimize the economic performance of a supply chain, but also improve its environmental performance.

The goal of this research is to design a green cellulosic bio-butanol supply chain network with maximum economic and environmental benefits. In this research, the network structure of a bio-butanol supply chain was constructed and an optimization model for bio-butanol supply chain network design was developed. This research project consists of three major parts. In the first phase the related publications about supply chain management, optimization method, cellulosic biofuel, and sustainable supply chain network design were reviewed to construct a comprehensive information framework for the future research. In the second phase, the necessary information about bio-butanol supply chain was gathered and the supply chain network structure of cellulosic bio-butanol was constructed. To gather this information, a case study was conducted to study the production process of cellulosic bio-butanol in the integrated bio-refinery research facility of the national renewable energy laboratory (NREL) and an online survey among the cellulosic bio-fuel companies was conducted to study the logistics activities in the bio-butanol supply chain. In the last phase, a mathematical model was developed to optimize the cellulosic bio-butanol supply chain network. By applying this model, the optimal locations, numbers, and capacities of the facilities inside the cellulosic bio-butanol supply chain network can be determined with the objective of maximizing profits and minimizing greenhouse gas emissions.
2 Problem Statement and objectives

Bio-butanol is becoming increasingly recognized as an alternative fuel option. For example, in 2007, three policies: Renewable Identification Number’s (RIN’s), Low Carbon Fuel Standard (LCFS), and the U.S Renewable Fuel Standard (RFS2) all promoted the development of cellulosic biofuel (Fueling Growth 2013). The RFS2 requires a minimum volume of renewable biofuel blended into transportation fuel, and bio-butanol, which is qualified as renewable biofuel under RFS, is allowed to be blended into gasoline (USDOE 2015). The LCFS requires the reduction of carbon intensity during the entire life cycle of transportation fuel (Fueling Growth 2013), which can encourage the development of alternative fuel with lower carbon intensity like bio-butanol. The RINs refers to a 38-digit number which is assigned to one gallon of renewable biofuel in order to track its production, usage, and trade. It can operate as a commodity that can be sold and purchased (Yacobucci 2013). RINs are generated to check whether the bio-refineries produce enough biofuel to meet the federal biofuel-use mandates (Parker 2013), which can ensure the market demand for renewable biofuel. These three policies emphasize the importance of environmental protection by encouraging the production of renewable biofuel, and increasing the potential demand for cellulosic biofuel in the future market. Furthermore, the U.S Clean Air Act (CAA) points out that bio-butanol can be legally blended into transportation fuel at up to 10% which provides a direct pipeline for the commercialization of bio-butanol (Slating & Kesan 2012). In addition, bio-butanol made of inedible feedstock can provide a tremendous economic benefit for industry, because its feedstock does not need to compete with food offers (Dürre 2007).

However, the shutdown or cancellation of some bioethanol projects (Withers et al 2015) have led investors to hesitate investing in bio-butanol projects. This is because bioethanol and bio-butanol share some of the same characteristics, such as the same upstream supply chain activities, the same raw materials, and the same usage as a fuel addictive. Without support from investors, the commercialization of biofuels and specifically bio-butanol will never get off the ground. In order to alleviate hesitations of those possible investors and to further commercialize cellulosic biofuel, external and internal barriers of cellulosic biofuel commercialization should be removed (Withers et al 2015).

The barriers of bio-butanol commercialization should be clarified first before they can be removed. The barriers of bio-butanol commercialization include seasonal availability of cellulosic biomass, the low use ratio of biomass compositions, natural resource (land and water) requirements, cultivation practices, logistics cost, et. al. must be addressed (Morone & Pandey 2014). Among these barriers, transportation logistics is a critical issue to successfully commercialize the biofuel (not just bio-butanol) industry from cellulosic biomass since it is the most expensive and challenging issue in
the bio-butanol industry, therefore logistic and supply chain planning play an important role in the success of cellulosic bio-butanol commercialization (Rentizelas et al 2009). Although traditional supply chain network design is a good tool to mitigate or even remove this logistic barrier to some extent, it is still may not be enough to both attract and reassure investors. To intrigue cautious investors, a more sustainable strategy is necessary. In order to remove these barriers and further commercialize the cellulosic fuel bio-butanol, a well-designed green supply chain network is a persuasive tool for those potential investors.

Literature review is a good path to study the green supply chain network design. However, research focusing on environmental or green supply chain network design of bio-butanol is insufficient. For example, Eskandarpour et al. (2015) reviewed 87 papers about sustainable supply chain network design. Only 6 papers discussed the supply chain network design of bio-ethanol (Akgul et al. 2012, Corsano et al. 2011, Giarola et al. 2012, Mele et al. 2009, You and Wang 2011, You et al. 2012). However, none of them discussed bio-butanol supply chain network design. Due to the advantages of using bio-butanol as an alternative energy supply, such as environmental protection, fuel performance, and transportation convenience, bio-butanol has sufficient superiority over bioethanol. Therefore, the green supply chain network design of cellulosic bio-butanol needs to be further researched.
2.1 Goals and Objectives

The goal of this dissertation is to design a green supply chain network for cellulosic bio-butanol. By designing a green supply chain network for cellulosic bio-butanol, the production process, logistic activities, and physical supply chain structure can be identified to achieve not only economic but environmental performance. This information provides the basic structure of a cellulosic bio-butanol supply chain, and can act as an introductory guideline for beginners who are interested in cellulosic bio-butanol commercialization. In addition, a green supply chain network design can provide ideal locations of production plants or warehouses, the best size of production plants or warehouses, and transportation methods within the supply chain network with minimum costs and environmental impact. In turn, investors can use this tool to set up their own cellulosic bio-butanol supply chain network. Furthermore, a well-designed supply chain network can help the decision making activities in strategic, tactical and operation level of cellulosic bio-butanol commercialization and optimization of the cellulosic bio-butanol supply chain.

In response to the goal, the following objectives were defined:

• Objective 1: evaluate the production process of the bio-butanol industry
• Objective 2: map logistics activities in the bio-butanol supply chain
• Objective 3: identify the physical infrastructures in the bio-butanol supply chain network
• Objective 4: develop a mathematical model for green bio-butanol supply chain network design.

Lambert et al. (2000) pointed out that participants of a supply chain, the network structural dimension, and the supply chain business process links are the three aspects of the supply chain network structure, as shown in Fig. 2.1. The network structure dimension is identified in objective 1, the supply chain business process links are identified in objective 2. The participants of a supply chain are identified in objective 3. By these 3 objectives, the supply chain network structure of cellulosic bio-butanol supply chain can be constructed.
Fig. 2.1 Construction of bio-butanol supply chain network

The reasons for defining these four objectives are illustrated in the following sections.
2.1.1 Objective 1: Evaluate the production process of the bio-butanol industry

The design of a green supply chain network first requires the understanding of the network structure of the cellulosic bio-butanol supply chain. The structure dimension is one of the three aspects of a supply chain network structure (Lambert et al. 2000). Structure dimension includes horizontal structure, vertical structure, and horizontal position of the focal company (Lambert et al. 2000). Horizontal structure refers to the number of tiers across the supply chain, such as how many tiers of suppliers and how many tiers of customers exist. The vertical structure refers to the numbers of suppliers or customers in each tier. The horizontal position refers to the position of the company across the supply chain (Lambert et al. 2000). To identify the structure dimension of cellulosic bio-butanol supply chain, it is necessary to understand the production process of cellulosic bio-butanol, as shown in Fig. 2.2. The production processes not only dictate the needed equipment and material for bio-butanol production, but also shine light on the material flow inside the bio-butanol industry. The material flow refers to the flow of material from supplier sites to customer sites. Through understanding the material flow, the number of tiers of suppliers and customers can be easily identified. In addition, the position of the bio-butanol company across the supply chain can also be known from the material flow. Furthermore, it is clear to see how many suppliers and customers are in each tier by understanding the material or equipment needed for producing cellulosic bio-butanol. Therefore, the production process of cellulosic bio-butanol industry provides key insights into the structure dimension of a cellulosic bio-butanol supply chain. With the structure dimension, the first step of constructing the network structure of cellulosic bio-butanol supply chain is completed.

![Fig. 2.2 The rationality of objective 1](image-url)
2.1.2 Objective 2: Map the logistics activities in the bio-butanol supply chain

The supply chain business processes link seeks to understand the web of business transactions that must occur to procure raw materials and deliver and sell a product. The supply chain business processes include five major parts: procurement, manufacturing, delivery, sales, and marketing (Lambert et al. 2000). To link these business processes together requires an understanding of the logistic activities in the supply chain, as shown in Fig. 2.3. The key logistic activities include procurement, inventory management, traffic and transportation, warehousing and storage, materials handling, logistics communications, customer services, et. al. (logistics, Wikipedia 2017). In other words, for the bio-butanol industry, the logistics activities include the acquisition of major feedstock, the delivery and storage of feedstock before production and after production processes, and the sale of the final product. The business process link between procurement and manufacturing can be obtained from information on feedstock sourcing methods. Similarly, the business process link between manufacturing, delivery, and sales is known from product transportation methods. Finally, the process link between sales and marketing can be obtained from customer service data. Therefore, through understanding the logistic activities of cellulosic bio-butanol supply chain, the business process links of cellulosic bio-butanol supply chain can be known.

![Diagram of Objective 2, Logistic Activities, and Business Process Links]

**Fig. 2.3 The rationality of objective 2**
2.1.3 Objective 3: Identify the physical infrastructure of bio-butanol supply chain

The final step of constructing the supply chain network structure is to identify the participants within a supply chain. “The participants of a supply chain include all companies and organizations with whom the focal company interacts directly or indirectly through its suppliers or customers, from point of origin to point of consumption” (Lambert et al 2000). In other words, the participants include feedstock suppliers, product manufacturers, distributors, retailers or customers. By identifying the physical infrastructure, the participants in the supply chain can be identified, as shown in Fig. 2.4. The physical infrastructure of a supply chain includes feedstock harvest field, feedstock delivery agent, feedstock storage site, product manufacturing site, product storage site, product delivery agent, and product retail site. The feedstock harvest sites identify the feedstock suppliers. The feedstock storages sites and product manufacturing sites indicate who the manufacturers are. The feedstock delivery agents and product delivery agents identify who the distributors are. The product retail sites tell who the retailers or customers are. The participants in a supply chain are identified by understanding the physical infrastructures within that supply chain. Therefore, with the information of physical infrastructures in cellulosic bio-butanol supply chain, the members of cellulosic bio-butanol supply chain can be known. And further the network structure of cellulosic bio-butanol supply chain can be obtained.

![Diagram](image-url)

**Fig. 2.4 The rationality of objective 3**
2.1.4 Objective 4: Develop a mathematical model for green bio-butanol supply chain network design

Through objective 1 to objective 3, the network structure of cellulosic bio-butanol supply chain is constructed. However, the seasonal availability of feedstock, the high maintenance cost, and the high logistic cost of biomass biofuel supply chain are some of the main factors that might be impeding the commercialization and large-scale production of cellulosic bio-butanol (Baños et al. 2011). The traditional supply chain network design can optimize the material flow and minimize the supply chain related cost by providing the number, location and size of the warehouses and production plants (Eskandarpour et al. 2015). Besides the economic issues, environmental issues are also needed to be considered. Since the quality revolution of the 1980s and the supply-chain revolution of the 1990s, it has become clear that the best supply chain management configuration involves the integration of environmental management with ongoing operations (Srivastava 2007). Green supply chain network design, which combines the supply chain network with environmental performance metrics (Miranda-Ackerman et al. 2017), can provide an optimal supply chain network with minimum supply chain costs and limited environmental impact, as shown in Fig. 2.5. From this objective, the cellulosic bio-butanol investors can learn how to optimize their supply chain network with minimum cost and environmental impacts. By developing a successful mathematical model, the optimal location and size of production site and the optimal transportation methods in the supply chain can be determined. Meanwhile, the output of a mathematical model can encourage investors to invest more to this industry by giving them a tool for development.

Fig. 2.5 The rationality of objective 4
3 Literature review

3.1 Background of Bio-butanol and its supply chain activities

3.1.1 Bio-butanol

Butanol is a four-carbon alcohol that can be used as fuel and solvent. Butanol has four possible isomers: n-butanol, 2-butanol, iso-butanol, and tert-butanol. Generally, bio-butanol refers to iso-butanol specifically since only iso-butanol was selected by BP and DuPont for commercialization. Bio-butanol or bio-based butanol fuel, which sometimes also be called bio-gasoline, refers to an alcoholic biofuel that has been produced from many kinds of biomass, sugar, food processing waste, and household waste.

Bio-butanol can be considered as a renewable fuel and has been qualified under the Renewable Fuel Standard. Since bio-butanol is a very promising fuel in the future transportation fuel market, many efforts were made to improve its production process to lower its production cost, increase its yield, and further boost its commercialization process (Cheng et al 2012, Yadav et al 2014, Cai et al 2013, Elbeshbishy et al 2015, Su et al 2015). In addition, researchers also developed mathematic models to optimize the cellulosic feedstock transportation to reduce feedstock transportation cost and optimize transportation mode (Maung et al 2013, Xie et al 2014, Haque et al 2014).

3.1.2 Current Bio-butanol usage

The current global demand for bio-butanol is exceeding 1.2 billion gallons per year and it has been valued over $6 billion annually (Wood 2016). Bio-butanol can not only be blended into gasoline directly but also be used to produce renewable hydrocarbon, diesel, and jet fuel. Although theoretically bio-butanol could be used as both transportation fuel and fuel additive, practically no vehicle in production is approved for using 100% bio-butanol. Therefore, the bio-butanol is widely used as a kind of gasoline blender. The ASTM D77862 fuel quality standard shows that bio-butanol can be blended with gasoline up to 12.5%. In addition, a 16% bio-butanol blended gasoline is equivalent to E10 (a 10% ethanol blended gasoline), which indicates that using bio-butanol as a blender can save more gasoline that using ethanol under the same fuel property requirement.

Instead of being used as fuel, bio-butanol can also be used as feedstock for chemistry and solvent for industry, for example, coatings, fibers, resins, plasticizing agents, food grade extractive agents, medications, herbicides, different chemical intermediates, and etc.
3.1.3 Bio-butanol feedstock

The feedstock of bio-butanol can significantly impact its cost and production technology (Visioli et al 2014). Taking the Cathay Industrial Biotech in China as an example, the feedstock purchase cost accounts for more than 70% of the total butanol production cost (Xue et al 2013).

Theoretically, bio-butanol can be made from biomass, sugar, food processing waste, and household waste as aforementioned. Although there are some companies using waste as their fuel feedstock, such as Butalco GmBH which plans to use municipal solid waste and industrial waste stream to produce ethanol, practically there are very limited companies using food processing waste and household waste. Bio-butanol feedstock can be roughly divided into two types: the first generation bio-butanol feedstock and the second generation feedstock. The first generation bio-butanol feedstock includes sugar, starch, and whole grain. Among them, the most common feedstock are sugar cane and corn. The second generation bio-butanol feedstock, which is also known as non-food cellulosic biomass, refers to any source of carbon that can be renewed fast in the Carbon Cycle, such as lignocellulose, hemicellulose or lignin. The second generation bio-butanol feedstock might involve dedicated energy crops (such as switchgrass), residues from forestry and agriculture (such as waste wood, pulp, corn cobs, corn stalks, and sugarcane bagasse). It is worth to mention that algae, considered as the third generation biofuel feedstock, has entered the mainstream feedstock due to higher yield but lower resource input.

Compared with the first generation bio-butanol feedstock, the second generation feedstock has more advantages. First, since the first generation feedstock is mainly food crop, continuously producing first generation bio-butanol in a large scale may lead to food price rise and further threat the food supply (Laursen 2006, Naik et al. 2010). In addition, from the environmental point of view, second generation bio-butanol feedstock takes good use of waste from agriculture and forest, reducing the environmental cost of dealing with this waste.

3.1.4 Bio-butanol storage

At the iso-butanol production plant, the refined fuel-grade iso-butanol is generally stored in a few large above ground storage tanks (AST), or specifically the iso-butanol ASTs. Bio-fuel in the ASTs is shipped to the fuel refineries or terminals to be blended with gasoline. The blended gasoline is stored in the iso-butanol blended ASTs and shipped to gas stations. Fuel at gas stations is stored in the underground storage tanks (UST), which can be accessed by the fuel pumps. Neither iso-butanol nor the gasoline blended with iso-butanol shows instability under the normal condition of storage. The > 240 minutes’ induction period oxidation test convinced its stability in underground storage tank, vehicle tank, and laboratory vessel. However, some additional
implementations are required for the storage of bio-butanol and its gasoline blend. For example, (Butamax et al 2010),

- Avoid excessive heat and any potential source of ignition
- Avoid any highly reactive ingredient, such as oxidant and reductant.
- Store the fuel in the isolated and approved areas
- Avoid static electrical discharge and any source of ignition from storage tanks when pumping and sampling.
- Avoid the fuel contact with hot surface
- Avoid the fuel leak from the pressurized fuel pipes
- Never weld, solder or braze empty containers since they may still contain some flammable product residues and vapor.

3.1.5 Cellulosic bio-butanol production

Currently, in the case of industrial cellulosic bio-butanol production, the bio-butanol production flow includes 4 steps. A pretreatment step is done first, then an enzymatic hydrolysis step is conducted to hydrolyze the cellulosic biomass into monosaccharides. After that, a process of anaerobic fermentation is proceeded to convert the sugars into iso-butanol by using certain microorganisms (Wang et al 2015). Finally, a purification process is used in order to distil the iso-butanol, because the fermentation process not only produce butanol but also generate other byproducts such as acetone and ethanol.

The method of cellulosic bio-butanol production can be roughly divided into two types: direct microbial conversion (DMC) and simultaneous saccharification and fermentation (SSF). In DMC, the enzyme production, enzyme hydrolysis, and fermentation are completed in one single step. While in SSF, the cellulose hydrolysis and bio-butanol fermentation are completed together in a single vessel, and enzyme production is carried out as a separate process. These two major production methods can further evolve into several segmentations, such as catalytic pyrolysis and hydro-treating to hydrocarbons, dilute acid hydrolysis, fermentation to acetic acid, and chemical synthesis, enzymatic hydrolysis and consolidated bioprocessing (Brown et al 2012). Among this small segmentations, the most economical one is consolidated bioprocessing (CBP) (Lynd et al 2005), since it can simultaneously complete the enzyme production, hydrolysis and fermentation in one single step and save more than 50% of the production cost comparing with the other production configurations such as SSF (Olson et al 2011).

3.1.6 Bio-butanol transportation

Currently, since the 100% bulk fuel-grade iso-butanol is still under the road testing and cannot be used as a vehicle biofuel yet, the information of 100% bulk fuel-grade iso-butanol transportation cannot be accessed. Based on this situation, the following transportation mode is just feasible for the gasoline-blended iso-butanol fuel. The transportation of iso-butanol fuel can be divided into two types based on the difference
of blending locations. For the iso-butanol fuel blended at the refineries, the iso-butanol is first transported from bulk iso-butanol ASTs to refineries by marine cargo, railway tanker cars or tanker trucks, then blended with gasoline in the refineries. The blended fuel is distributed by pipeline to the fuel terminals, then be shipped to the retail sites by tanker trucks. While for the other type, which is blended in the fuel terminals, the iso-butanol is transported from the bulk iso-butanol ASTs to the fuel terminals by marine cargo, railway tanker cars or tanker trucks. The iso-butanol fuel is blended with gasoline which is transported from the refineries to the same terminals via pipeline. After they blend with each other with a certain proportion, the blended fuel is shipped to retail sites by tanker trucks.

3.1.7 U.S. Bio-butanol producers

Although bio-butanol is a promising transportation fuel, investors are still very cautious at their investing. So the number of large-scale bio-butanol production plants are not as many as expected. Table 3.1 lists the current U.S. bio-butanol producers. As shown in the table, the number of bio-butanol producer in the U.S are still very limited.

<table>
<thead>
<tr>
<th>Company Name</th>
<th>Brief Introduction</th>
<th>Feedstock</th>
<th>Location</th>
</tr>
</thead>
</table>
| Gevo         | -Plans to modify existing ethanol plants for butanol production  
               -Uses a novel biocatalyst for reduction of by-product creation, yielding more butanol in a continuous process  
               -Butanol produced in a continuous process rather than a batch process  
               -Use of a modified strain of E.Coli | Corn  
               Wheat  
               Sorghum  
               Barley  
               Sugarcane  
               Non-food-Cellulosic feedstock. | Agri-Energy LLC  
               502 S Walnut Ave, Luverne, Minnesota, US |
| Butamax      | -A fully resourced and committed biofuel company providing the technology to cost-effectively produce bio-butanol for the long term.  
               -Developing a comprehensive licensing package to supply current ethanol operations with new technology enabling the production of bio-butanol. | Corn starch  
               corn  
               sugarcane | 4500 US-14, Lamberton, Minnesota, US |
3.2 Supply Chain Management

The research of supply chain management (SCM) has gained much attention during the last few decades and this trend keeps increasing in both academic and industrial areas (Naslund et al 2010).

For the definition of SCM, different views are held from different perspectives. For example, the Global Supply Chain Forum (GSCF) presented their definition of SCM from a vertical perspective. They defined the SCM as the synthesis of pivotal business processes from end consumer to initial suppliers which provides information, products and services that add value for other stakeholders and customers (Lambert et al 1998). However, the Council of Supply Chain Management Professionals (CSCMP) gave a SCM definition from a two-dimensional perspective. CSMP defined the SCM as an integration of both supply and demand management internally and externally, which means the SCM should include the management and plan of every activity related to procurement and sourcing, transportation and all other logistics manage activities, the collaboration and coordination among the source suppliers, intermediate agencies, third-parties, and customers (Stock et al 2009).

Besides the general definitions above, different branches of learning may have different explanations on SCM. In the field of industry, Villa (2001) considered SCM as an industrial term and Villa claimed the SCM should combine the issues of management and technology, starting from manufacturing design, using suppliers’ contraction and outsource, multi-locations inventories, and the third party logistics coordination for decentralized product manufacturing.

In the field of business, researchers also provided their understanding of SCM. Swaminathan et al. (1998) defined SCM as a semiautonomous and autonomous business entities network in which all entities work corporately to synthesize distribution, manufacture and procurement activities for one or more related product´s families. Gunasekaran (2004) defined SCM as a competitive tactic for synthesizing suppliers and customers with the goal of improving flexibility and responsiveness of organizations and manufacturing. Based on Gunasekaran’s definition of SCM, Langley et al. (2008) gave a more specific illustration. They defined SCM as a tool aiming at managing and testing supply chain networks. The logic for this concept is to reduce the costs and satisfy the needs of customers. A significant goal is to help the corporate become more competitive in the global marketplace regardless of how the market changes. Janvier-James (2011) summarized the definition of supply chain management as a tool to make the firms be fast and dependable, cost-saving, and flexible enough to satisfy the requirements of customers. Besides that, Drake (2012) in his book Global Supply Chain Management, presented an extension to the scope of SCM. He stated that every activity in the supply chain should take the requirements of customers into
consideration and take the satisfaction of customers as their ultimate goal. From this point of view, it can be seen that the scope of SCM is extended from synthesizing only the internal resources to synthesizing the internal and external resource. The goal of SCM is also changed from simply improving the company’s efficiency and profitability to maximizing the customer’s satisfaction, then the company’s core competitiveness can be maintained or improved.

Based on these different definitions of SCM from different aspects, the meaning of SCM can be explained as a tool aiming at improving the customer’s satisfactions and core competence of a company, which is implemented by utilizing various technologies and synthesizing the internal and external recourse of a company. The internal resource refers to every resource inside the company, including labor force, manufacturer and service. The external resource refers to every third party recourse, including third party logistic and suppliers. The technology of SCM may refer to the skills of multi-agent coordination or lean manufacturing.

3.2.1 Supply chain operations reference model

Supply chain operation reference (SCOR)-model, which was developed and endorsed by Supply-Chain Council since 1996, is a supply chain process reference model being used to illustrate the business processes associated with all phases of customer’s demand satisfaction. There are six macro processes included in the SCOR model: plan, source, make, deliver, return, and enable. Although it spans from all customer interactions to all market interaction, including all physical materials transportation, it is still not a perfect enough. Because the scope of SCOR-model does not include all the activities in the areas of demand generation, research and development, product development, and some other process of post-delivery customer support. Also, the model does not attempt to teach a particular organization how to tailor its systems or conduct its business. The structure of the model composes of four primary sections: performance, processes, practices, and people. Among them, the performance of SCOR refers to set up standard metrics to describe the performance attributes of reliance, responsiveness, agility, cost, and asset management; the processes in SCOR involves in the standard descriptions of management activities and activity relationship; the practices section in the model is about the management practices that produce important improved process performance in emerging, best, standard, and declining practices; the people part defined the skills that are necessary to perform supply chain activities. Apart from these four main sections, there is a new added section for special applications in Green SCOR, but this part has not been thoroughly tested (Steward 1997, supply chain council 2012).

3.2.2 History of SCM

Drake (2012) briefly described some significant factors and milestone in the evolution of SCM. The area of SCM derives from the huge manufacturing firms of the late 19th
century when the large firms could have their own supply chain to complete their vertical integration. The supply chain covers raw materials, finished productions, and distribution channels. In 20th century, these vertically integrated firms began to improve their core competencies by eliminating some ancillary functions. When it came to 1960s, the main business functions involved in SCM evolved into independent departments which had the right to make decisions by themselves. However, these departments only cared about their own profits instead of considering the profits of the whole supply chain. Until 1970s, these firms realized the necessity to integrate these internal linked functions together. In 1980s, to achieve a higher competitiveness, some firms started to integrate the internal materials management process with the external physical distribution process. Ten years later, these firms truly synthesized all the logistics processes including sourcing, producing, and delivery.

3.2.3 Problems in SCM

<table>
<thead>
<tr>
<th>Problem</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Demand forecasting</td>
<td>Predicting the possible demand for a product or a service based on its previous demand data and the current trends (Demand forecasting, Wikipedia, 2016).</td>
</tr>
<tr>
<td>Scheduling problem</td>
<td>Determining when to start a job on a resource under certain constrains (Błażewicz et al 2007).</td>
</tr>
<tr>
<td>Inventory control</td>
<td>Cooperating and managing the supply, storage, distribution, and recording the materials to maintain just enough product for current needs (Inventory Control, Merriam-Webster, 2016).</td>
</tr>
<tr>
<td>Transportation problem</td>
<td>Optimizing the pattern of product distribution from certain points of origin to different destinations (Transportation problem, Wikipedia, 2016).</td>
</tr>
<tr>
<td>Supplier relationship management</td>
<td>Managing all interactions with third party agents of a companies in order to gain maximum benefits (Supplier relationship management, Wikipedia, 2016).</td>
</tr>
<tr>
<td>Customer relationship management</td>
<td>Managing and analyzing customer interactions and data throughout the customer lifecycle in order to improve the relationships with customers and gain more benefits (Customer relationship management, TechTarget, 2016)</td>
</tr>
<tr>
<td>Supply chain performance</td>
<td>Indicating the situation of the supply chain system so that the administrators could have a well understanding of the supply chain and further improve the overall performance (Charan et al 2008).</td>
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</tbody>
</table>
The definitions of SMC problems are shown in Table 3.2. An accurate demand forecasting could help an organization to obtain high profit. Additionally, effective information sharing between retailers and manufacturers could help to mitigate the negative effect of demand uncertainty. Yue (2002) analyzed the value of sharing data within a supply chain in two scenarios: The Make to Order Scenario and the Make to Stock Scenario. The first scenario is less possible to occur, because the company could not get benefit if the manufacture’s forecast was not accurate enough; while the second scenario would be more possible to occur. Cachon and fisher (2000) analyzed the value of information sharing in a model of one manufacturer, multiple retailers, and uncertainty consumer demand. The authors concluded that it is more valuable to implement information technology to smooth and accelerate the physical flow of products through the supply chain than just using it to expand the flow of information. Chen et al. (2000) analyzed the bullwhip effect in a simple two-stage supply chain and stated that the demand information centralizing could highly decrease the uncertainty in expansion. EI-Telbany et al (2008) applied a particle swarm optimization method to forecast the short-term electricity demand in Jordan. In order to test the feasibility of the method, the authors use a backpropagation algorithm as a comparison. The result shows that the particle swarm optimization is more feasible due to its efficiency of searching large spaces and better capability of global search for vest forecast model. Yu et al (2011) proposed a hybrid algorithm to estimate the primary energy demand of China. The hybrid algorithm is based on Particle Swarm Optimization and Genetic Algorithm. The algorithm utilizes factors like GDP, population, economic structure, urbanization rate, to optimize the coefficients of three forms of the model (quadratic, linear, and exponential).

Inventory management is also an indispensable part in the SCM, since it covers the aspect of logistics, operations, marketing, finance, and information systems (Sprague, Sardy, 2009). For example, in the aspect of finances, inventory management may associate with carrying, ordering, stock out, and capacity associated costs (Arnold et al. 2008). In relation to operations, inventory management need to manage the stock at an optimal level and determine the quality of this inventory to satisfy customer demands and the needs of manufacturing (Bayraktar, 2012). Managing inventory needs to balance the carrying cost and ordering cost carefully (Klms, 2013), so it is very necessary to describe the term with economic order quantity (EOQ).

EOQ is the order quantity of minimizing total inventory holding and ordering costs, and also a fundamental approach to address the inventory problem (Ford 1990). The fundamental model for optimizing the EOQ was first proposed by Harris, presented by the squire root of the quotient of double annual demand quantity times the setup cost over annual holding cost. This model can work only when all the following assumptions were satisfied: constant ordering cost and purchase price, known and uniform demand rate, fixed lead time, instantaneous replenishment, and only involve one product. So,
many researchers made effort to develop the extension of traditional EOQ model in order to address some of these unrealistic assumptions. For example, Wilson’s EOQ model was developed to accommodate the quantity discounts (Wilson, 1934), and Malakooti’s multi-criteria EOQ model could be used to minimized the total cost, order quantity, and shortages (Malakooti, 2013). Mekel (2014) used a quantitative method of forecasting calculation with double exponential smoothing models to predict the level of demand from 2013 to 2014, through deciding the safety level and re-order point, the inventory quantities and re-order point could be known. Besides, the author used EOQ calculation to know the economic order quantity of raw materials. 

Another aspect of managing the inventory was to control the stock. For example, Yue (2002) constructed two models derived from a pipeline hedging method to evaluate the reduction of safety stock when redesigning a manufacturing process. Model one was used to study the product family with single product and focused on operation re-sequencing. Model two was used to study the product family with two products and focused on the merging of operation. The result showed that both the merging and re-sequencing model could significantly minimize the safety stock level. Singh and Kumat (2011) proposed an efficient method to minimize the total cost of a supply chain. The method is based on Genetic Algorithm to determine the most probable shortage level and additional stock level for inventory optimization. Liou et al (2013) introduced the Stackelberg equilibrium framework to maximize the total benefit of vendors in a one seller, one buyer, finite horizon, and multi-period inventory model. The framework is restricted by minimizing the total cost to an acceptable level. Liou concluded that the Stackelburg equilibrium could obtain the optimal condition, and the optimal replenishment policy could also be found by a numerical algorithm and some examples. Varga et al (2013) proposed a regional gradient-based PSO to address inventory problem in a complex supply chain. In order to validate its feasibility in dealing inventory problem, the authors applied this method in a multi-echelon system with two warehouse. The result showed that the improved algorithm is simple enough to be applied in decision support and flexible enough to deal with complex situations.

SCM needs to deal with the scheduling problem, a very typical problem in combinatorial optimization. Generally, scheduling problem studied the distribution of limited resources to tasks for a certain period (Conway et al. 2003). However, in SCM, the scheduling problem deals with the administration of machines and jobs in order to improve the performance of supply chain. The state task network (STN) method may be the most popular approach to model a production system that has multiple products produced from shared resources (Kondili et al 1993, Shah et al 1993). This method can be represented by a graph with three elements: state nodes, task note, and arcs between states and tasks. The state nodes denote raw materials, intermediates, and finished products; the task nodes represent the processes from one state to another; and the arcs are the flow of materials. (Bose et al 2009). Another basic approach is the resource-
constrained project scheduling problem (RCPSP). The RCPSP can be applied to model many real-world problem, such as production process, school timetable, and airport renovation. Given a time horizon, some activities can be scheduled so that the scarce resource capacities are respected and a certain objective function can be optimized (Brucker et al 2012). Dawande (2006) tried to coordinate the conflicts in schedules from manufacturers and distributors by studying two practical scenarios in which the manufacturer hopes to minimize the unproductive time while the distributor hopes to minimize the customer cost and inventory holding cost respectively. The results shown that a profit of cooperation occurred when the dominant party compromised on giving up the individually optimal schedule. Zhong (2008) investigated the scheduling problem with transportation, he used a polynomial-time approximation algorithm with certain worst case ratios to minimize the maximum job completion time through several goods delivery cases which from a simple scenario of one manufacture to one customer transportation to a scenarios of a transportation network among manufacturers, third party logistics service and customers. At last, he proposed a polynomial-time heuristic algorithm with a tight bounded worst case ratio of 2. Ullrich (2012) studied the makespan (the time spend on the whole production line) by listing and comparing eight scheduling scenarios from a four stage supply chain, in which the most promising scenario is a combinatorial scheduling approach that considers the supply chain as a flow shop, while the simplest scenario is a separate scheduling of four stages. The author concluded that a combinatorial supply chain approach based on Johnson’s algorithm is unreasonable when taking the cost of coordination into consideration, because in the first stage, applying the shortest process time would lead to near-optimum makespan.

The forecast problem, inventory problem and scheduling problem should be interwoven with each other throughout the SCM. These problems are all based on one pivot problem, that is, information accuracy. Accurate information could help to solve these problems by providing the true and timely order data, reducing redundant information, and presenting customers’ feedback (Drake 2012). Although many relative previous literatures did mention its importance, detailed study is a few. Given the significance of information accuracy, the future researchers may need to pay more attentions to it.

Transportation, which serves as an essential link between the company and its suppliers and customers, is undoubtedly an important issue in SCM, because if one level in supply chain undergo delays and problems, the performance of downstream members to serve their customers are impacted. (Goldsby et al 2014). In SCM, the transportation problem refers to minimize the total transportation cost of shipping goods from some origins to certain destinations. The transportation problem is also very important in the supply chain optimization, because according to the 23rd annual states of logistic report from council of SCM professionals, transportation costs account for 64% of the total logistic costs, 33% of the inventory cost, and 4% of the administrative cost (Bravo et al
These proportions indicate the significance of optimizing the transportation problem in SCM. The transportation problem can be solved by greedy heuristic and mathematical problem. The greedy heuristic is an iterative algorithm. In each iteration, a minimum unit of transportation cost is selected and applied to the maximum possible transportation unit. It is important to know that the maximum transportation units are the minimum production available and minimum shipment required. Although this method is easy to operate, but it cannot guarantee an optimum solution (Langevin et al 2005). The mathematical problem transforms the transportation problem into a linear programming problem. Then by the use of optimization software the problem can be solved. The mathematical approach could be applied to deal with large and complex real world transportation problem (McCarl et al 2004). For example, Uzorh et al (2014) applied a linear programming method to solve a transportation problem from Coca Cola Company of Nigeria. The objective is to minimize the transportation cost and optimize transportation schedule between four plants and five depots. The objective function is the sum of transportation cost from plants to depots, the problem is solved by the use of TORA software package. Tierney et al (2014) used a novel integer programming model to optimize the inter-terminal transportation (ITT) problem. The ITT problem is the transportation of containers between terminals within one port. The paper proposed an IP model to minimize container delivery delay and optimize vehicle routes and contain flow of two ports from Germany and Netherlands. The model was solved by CPLEX.

Customer relationship management (CRM) is used to help the enterprises to create the customized servers on the individual basis, so that, the relationships with all the involved parties can be enhanced and maintained. This individual basis comes from fairness and trust (Nguyen et al 2012). Nowadays, the competition among enterprises are on longer the competition of individual companies in certain field. It is the integrated competition base upon production development and design, product manufacture, distribution, retail, sales, and service. It is also the competition of high quality market occupation, which means the competition of customers’ loyalty among supply chains (Tang 2008). According to this trend, the CRM should be integrated into the entire supply chain management rather than being as an individual part (Li et al 2013). Customer relation management is to manage an organization’s interrelationship with current and potential customers. One aspect of the CRM is the customer segmentation, the company can divide the customers into different groups, based on one or more features, such as age and gender. And then calculate the data to obtain useful information (Nettleton 2014). For example, the clients can be separated into two major groups: new clients and clients/ex-clients. The company can attract the potential new clients by designing and executing some campaigns, providing good quality products and service; and win the ex-clients by providing discount. By the use of these actions, the company can improve their relationship with their customers (Nettleton 2014). Many companies have the trend to develop the CRM systems, for example, they
would set up a telephone or internet call center equipped with a data capture system. This system can obtain client data from its large client database and provide this data to the sales and customer service staff, so that the sales and customer staff can take good use of this information to achieve greater success in commercial dealings. The CRM system can also help the company to exploit personalized treatment, since it can provide the information about customer preference, earning situations, and so on. Personalized treatment refers to treat the customer as if he or she is the only customer. Thanks to this special service, company can provide better service and products to their customers, and further gain a longer customer loyalty (Nettleton 2014).

According to Schuh et al (2014) the true supplier relationship management (SRM) includes managing all interactions between supplier and the organizers. More specifically, SRM includes the systematic, comprehensive evaluation of the suppliers’ capabilities and assets of overall business strategy; the determinations of what activities should be taken in terms of different suppliers; and the execution and planning of every interaction with suppliers (Hughes 2010). A well-functioned SRM can provide the organizers with competitive advantage, better brand development, cost reduction, good efficiency and effectiveness, and supply side risks reduction or mitigation (O’Brien 2014). The problems of SRM include supplier selection problem, supplier development problem, and supplier evaluation problem (Schiele 2007). Supplier development includes all the activities initiated by a buyer to improve the performance of its suppliers (Krause et al 1998). Krause et al (2000) summarized four useful supplier development strategies: competitive pressure (employ multiple suppliers); evaluation and certification system (evaluate the performance of suppliers and give feedback to the suppliers); Incentive (motivate the suppliers by offering incentives); direct involvement (make investment to suppliers). Various multi-criteria decision making methods were proposed for solving supplier selection, such as analytic network process, data envelopment analysis, genetic algorithm, mathematical programming, and their hybrids (Ho et al 2010). For example, Ding et al (2005) applied a genetic algorithm for supplier selection, in which the method presented possible configurations of the chosen suppliers, including the transportation modes. Hong et al (2005) proposed a mixed integer linear programming model to tackle the supplier selection problem. This model maximizes the revenue by determining optimum number of supplier and order quantity. Wadhwa et al (2007) addressed the supplier selection problem by applying a multi-objective programming model. In this model there are three objective functions which are used to minimize the price, lead time, and rejects respectively. These three solutions are compared by weighted objective method, compromise programming, and goal programming method. Besides, the multiple criteria decision making method can also be applied to address the supplier evaluation problem, since there are various criteria of evaluating the suppliers’ performance, such as quality, delivery, price or cost, technology, manufacturing capability, reputation, service, flexibility, and etc. (Ho et al 2010). For example, Chu et al (2012) solved the supplier evaluation problem by using
a multi-level multi-criteria decision making method under fuzzy environment. In their research, the criteria are categorized into two sub-criteria: quantitative and qualitative, then the quantitative criteria are further divided into cost and benefit ones. They maximize the benefit and minimize the cost. Finally, the supplier is evaluated by both qualitative criteria and the fuzzy numbers which represent the importance weights of all the criteria.

Performance measures are also important to the effectiveness of SCM, because it functioned as an indicator to the situation of the SCM so that the relative manager could have a well understanding of the supply chain and further improve the overall performance of the supply chain (Charan et al 2008). According to Neely (2004), the fundamental processes of supply chain performance measures includes: design measurement system; implementation; manage through measurement; and refresh the measurement system. Designing the measurement system lies in choosing the right measures; implementation means the access to right data, political and culture issues; managing through measurement requires an internally cultural shift; refreshing the measurement system aims at making the measurement system up to date. It is very necessary to understand the supply chain performance metrics. Gunasekaran et al (2004) provided a relatively comprehensive framework for the supply chain (SC) performance metrics, which is summarized in Table 3.3.
<table>
<thead>
<tr>
<th>SC activity/process</th>
<th>Strategic</th>
<th>Tactical</th>
<th>Operational</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Plan</strong></td>
<td>Perceived customer value; order lead time; budget variances; cost of processing information; total cycle time; total cash flow time; product development cycle time; net profit Vs productivity ratio.</td>
<td>Customer consulting time; forecast techniques accuracy; Product development cycle time; planning process cycle time; productivity of human resource; order entry methods.</td>
<td>Productivity of human resource; Order entry method.</td>
</tr>
<tr>
<td><strong>Source</strong></td>
<td></td>
<td>Supplier delivery performance; supplier lead time; Supplier pricing; purchase order cycle time; cash flow method efficiency; supplier booking in procedures.</td>
<td>Supplier pricing; purchase order cycle time.</td>
</tr>
<tr>
<td><strong>Make/Assemble</strong></td>
<td>Range of products and services</td>
<td>Defects percentage; capacity utilization; operation cost per hour; economic order quantity utilization.</td>
<td>Defects percentage; human resource of productivity; operation cost per hour.</td>
</tr>
<tr>
<td><strong>Deliver</strong></td>
<td>Flexibility of service system; effectiveness of distribution planning schedule</td>
<td>Flexibility of service system; delivery invoice method efficiency; delivery reliability; distribution planning schedule efficiency; percentage of finished goods in transit</td>
<td>Goods delivery quality; on time delivery; delivery invoice method efficiency; urgent delivery percentage; number of faultless delivery; delivery reliability</td>
</tr>
</tbody>
</table>
3.2.4 Components of SCM

The components of supply chain management, which is developed from the classic version of SCM elements proposed by Lambert and Cooper in 1997, is summarized in Fig. 3.1.

Cooper et al. (1997) identified nine components in SCM and categorized them into five physical technical components and four managerial behavioral components. The physical technical components are product flow structure, communication and information flow structure, work flow structure, organization structure and planning and control methods. The four managerial behavioral components include culture, risk and reward structure, power and leadership structure, and management methods. Lambert et al. (2000) improved Cooper’s theory by depicting the components of the SCM as three interrelated elements: network structure of supply chain, the business processes of supply chain, and the management components of supply chain. The structure contains the relevant participants and links between each of them; the business processes are a set of activities, such as customer relationship management, demand management, customers service management, order fulfillment, procurement, manufacture flow management, returns, etc. that generate a certain value output to customers; and the management components are integration and management across the supply chain.
Many researchers tried to specify the details of the network structure of supply chain. Lambert et al. (2000) pointed out that practitioners in supply chain, network structural dimension, and supply chain business processes links are the three aspects of supply chain network structure. Mills et al (2004) proposed four perspectives of analyzing the supply chain network: upstream, downstream, static network, dynamic network. The upstream concerns how to deal with suppliers; the downstream concerns how to deal with customers; the static network considers how the effectiveness of the supply chain is developing and how to improve without altering the structure of network; the dynamic network considers how to improve the company’s position in the current network and how to create a new supply chain network structure. Dong et al (2005) implied that a structure of supply chain network may have four elements: supplier sites, which purchase raw materials from outside suppliers; fabrication site, which transforms raw materials into components; assembly site which assemble the components into semi-finished products and finished products; and distribution site which delivers the products to customers and warehouses. Stock et al (2009) proposed that the network of supply chain management should consist of raw material suppliers, production facilities, logistics, marketing, purchasing, and relevant systems that facilitate the materials flow, services, funds flow, information flow, and customer satisfaction. D’Ignazio et al (2014) summarized that the network of supply chain is a very significant structure since it manages the distributions and productions of goods, involving spatially dispersed customers, retailers, distributors and manufacturers.

The understanding of the concept of SCM has shifted from the understanding of the management of logistics across the supply chain to the management and integration of key business process in supply chain. (Lambert et al 2000) The relevant research about business process of supply chain is illustrated as follows. Cooper et al. (1997), Lambert et al. (1998) and Croxton et al. (2001) proposed the following key business processes: customer service management, customer relationship management, demand management, order fulfillment, product development and commercialization, returns management, supplier relationship management, and manufacturing flow management. Later on the Global Supply Chain Forum (2005) selected new product development, demand management, and customer relationship management as the basis of the business processes of supply chain. Siddiqui (2010) studied the Oracle E-Business Suite and found some modules that could be applied to manage the supply chain business process such as: procurement, manufacturing, logistics, order management, and marketing and sales. These five modules also implied five components of business process in supply chain, which are procurement, manufacturing, logistics, order management, and marketing and sales.

The management components of supply chain also gained the attention by other researchers. Lambert et al (2000) identified 9 management components for successful management of supply chain. They were organization structure; work structure;
planning and control; information flow facility structure; product flow facility structure; power and leadership structure; management method; culture and attitude; and risk and reward structure. Chow et al. (2008) summarized three management components of supply chain: supply chain competencies, supply chain practices, and supply chain concerns. Kumar et al. (2013) also hold the same point of view as Chow. They tested the research model and found that there are some positive direct relationships among those three components, and further concluded that the effect of supply chain practices on the performance of supply chain has the greatest indirect effects. Chao et al. (2012) stated that the SCM components should include partnership management, coordination management, supply chain information, and supply chain integration. They studied the impact of SCM components on logistics service performance and concluded that supply chain integration, coordination, and partnership have significant effects on logistic performance, but supply chain information do not have effect on logistic performance.

The above literatures were based on the classic version of SCM elements proposed by Lambert and Cooper in 1997. Besides that, some researchers also proposed their own understanding of SCM components from a different point of view. For example, Fleischmann et al. (2003) proposed a supply chain framework that contained the strategic, tactical, and operational analysis for decision making at long term, mid-term, short-term respectively. The strategic component concerned the structure and design of the supply chain and would have an effect over several years; the tactical component was an outline of regular operation, it referred to tactical planning from half to one year; the operation component specified every activity and specific instructions for direct implementation and control. Chen et al. (2009) claimed that the supply chain integration is a core component of supply chain management. Supply chain integration involves linking the functions and process of business across and within organizations into a cohesive and highly performed business model. Vierasu et al. (2011) classified the components of supply chain into two categories according to their importance of determining the performance of supply chain. The primary components are facilities, transportation, and inventory, and the secondary components are production location, information, and price. They also pointed out these six components are interrelated and could not act independently.

3.3 Non-food cellulosic biofuel

Cellulose, which can be produced by every living plant on the earth, is a kind of polymer that consists of many glucose molecules. Glucose is a kind of simple sugar which can be used to produce ethanol through fermentation (Mosier 2015). Biofuel is a kind of newly sustainable energy, which can be defined as biomass based products derived from renewable resources, like bagasse, wood, or corn, Biofuel can also be defined as products that are chemically transformed from biomass to produce bio-oil, charcoal, biogas and ethanol (Brito Cruz et al. 2014). As a combination of the cellulose and
biofuel, the non-food cellulosic biofuel is the biofuel that produced from grasses, wood or the inedible parts of plants. Only biofuels converted from cellulosic feedstock, such as switchgrass, miscanthus, corn stover, forest residues, or short-rotation woody crops, could be counted into the category of cellulosic biofuels (Tyner, 2013). The renewable fuel standard classifies the renewable fuel into four categories and uses a D-code to identify the fuel type. Table 3.4 shows the details of these four fuel type.

| Table 3.4 Fuel Classification under Renewable Fuel Standard |
|---------------------------------|-----------------|-----------------|--------------------------|
| Fuel                           | Code  | Lifecycle GHG Reduction | Example Feedstock          |
| Cellulosic biofuel             | D-3   | ≥ 60%                        | cornstover, wood chip, miscanthus, biogas |
| Biomass-based diesel           | D-4   | ≥ 50%                        | soybean oil, canola oil, waste oil, animal fats |
| Advanced biofuel               | D-5   | ≥ 50%                        | Sugarcane                  |
| Total renewable fuel           | D-6   | ≥ 20%                        | Corn Starch                |

The lifecycle GHG reduction in Table 3.4 is compared to a 2005 petroleum baseline as mandated by Energy Independence and Security Act of 2007. According to the table the nonfood cellulosic biofuel is belong to D-3 category based on the feedstock it used.

Fuel ethanol production in the U.S exceeded 7.5 billion gallons in 2012, double what it was 8 years earlier. This increased demand for domestic produced liquid fuel impacts the animal feed supply from corn because production of every unit of fuel ethanol would consumed about 10% of domestic produced corn (Mosier 2015). In addition, using food crops to produce ethanol raises crisis of environmental aggregation (Pimentel et al 2005), food security (Baek et al 2014) and energy security (Ang et al 2015). In order to mitigate this crisis, federal and many state government agencies developed new energy strategies, such as the Energy Independence and Security Act of 2007 and Farm Bill of 2008, to emphasize the importance of using various renewable energy source, such as tidal; wind; solar; geothermal; and biomass. Among these various renewable energy resources, Biomass is very popular, since it is the only renewable resource that could be converted into many kinds of transportation fuels especially ethanol (Dwivedi et al 2009). In addition, U.S owns a very large cellulose biomass production base (Perlack et al 2005, Dwivedi et al 2009). Research conducted by the U.S. Department of Agriculture and U.S. Department of Energy showed that annually at least 1 billion tons of cellulose biomass can be collected and processed from corn stover, straw, and wood wastes. This amount of cellulose biomass can produce 67 billion gallons of ethanol, which is equal to 30% of U.S gasoline consumption (Mosier 2015). Furthermore, using cellulosic biofuel as a substitute for gasoline could promote rural development, reduce greenhouse gas emission, and obtain energy independence.
Therefore, extending the application of non-food cellulosic biofuel is feasible in the U.S.

The non-food cellulosic biomass can produce many kinds of biofuel such as bio-ethanol, renewable diesel, pyrolysis bio-oil, bio-butanol, and etc. The following sections discuss the detail of each of them.

3.3.1 Bio-ethanol

In the first generation of bioethanol production, bio-ethanol was produced from crops, such as sugar cane and maize. However, in the second generation production process, the raw materials of the bio-ethanol were shifted to a cheaper, more accessible and renewable resource—the lignocellulosic biomass (Kootstra et al 2009). The production process of lignocellulosic bioethanol contain five steps: pretreatment, saccharification, fermentation, distillation and dehydration (Morales et al 2015). Bio-ethanol is extensively applied as a fossil fuel additive in the U.S, partly because it can be mixed with gasoline in any combination. Currently, it can be approved as a 10% mixture for all vehicles, an 85% mixture for flex-fuel vehicles, and a 15% mixture for all vehicles with the model year from 2001. Besides, it can also be used as the pure vehicle fuel in specially designed engines (Morales et al 2015). In addition, bio-ethanol has a very low freezing point, so it can be utilized under the low temperature (Yue et al 2013). However, several disadvantages of bioethanol hamper its wider applications. The bioethanol can completely miscible with water, which means it can separate from the blended gasoline when certain amount of water was found in the pipeline or storage tank. What’s worse, the bioethanol can also corrode the wall of pipeline, which cause the transportation problem of bioethanol, therefore many U. S pipeline operators strongly prohibit the utilization of ethanol and ethanol blended gasoline. (Bunting et al 2010).

3.3.2 Renewable diesel

According to Energy Policy Act of 2005, renewable diesel is the diesel fuel that derived from biomass using a thermal depolymerization procession. Renewable diesel satisfies the registration requirements of fuels and fuel additives established by Environmental Protection Agency under section 211 of Clean Air Act, and it also satisfies the requirement of the American Society of Testing and Materials D975 or D396. Conventionally, the fossil diesel alternative is bio-diesel, a biofuel that produced from food grade vegetable oil or animal fatty by transesterification process (Canakci et al 2008). However, the raw material cost of biodiesel is so high that it prevents the further extension of biodiesel (Sorate et al 2015). Therefore, a new kind of fossil diesel alternatives was proposed to address this problem. This new alternative is renewable diesel, whose raw materials can be obtained in non-edible oil seed plants (Borugadda et al 2014). The method of producing diesel fuel from lignocellulosic biomass was proposed by Huber et al (2005), which is about producing the liquid alkanes by using an aqueous-phase procession of biomass-derived carbohydrates. However, the
commercialized production method of renewable diesel is not available at this time, so it cannot tell much more about the production of renewable diesel from cellulosic biomass (Van Gerpen et al 2014).

3.3.3 Pyrolysis bio-oil

Pyrolysis bio-oil is dark brown, free glowing organic liquid that is produced by rapidly and simultaneously fragmenting and depolymerizing lignin, cellulose, and hemicellulose with rapidly increasing temperature (Mohan 2006). Most organic residues or biomass wastes, such as bagasse, switchgrass, wood, crop straw, peanut hulls, sawdust, and poultry litter, can be used to produce pyrolysis bio-oil, (Guo et al 2015). Crude pyrolysis bio-oil is highly moisture and acidic, so it is unstable, viscous, corrosive, immiscible with hydrocarbon fuel, low in energy density, and hard to ignite (Czernik et al 2004). Therefore, before being used as the petrol distillate fuel alternative, this crude oil need to reduce the moisture content and acidity further improve the heating value and storage ability, (Guo et al 2015). The updated bio-oil can be served as alternative for fuel oil or diesel in power static appliances, such as boilers, furnaces, engines, and electric generators (Mohan 2006). The major advantages of pyrolysis bio-oil include (Jahirul et al 2012):

- CO2 balance is positive in biomass fuel
- Can be used in both small-scale and large power generation system
- Relatively easy to store and transport
- High-energy density compares to biomass gasification energy

However, commercial production and application of pyrolysis bio-oil as a petrol fuel substitute still has some technological challenges (Guo et al 2015). For example, the major challenge is to improve the competitiveness of pyrolysis bio-oil by maximizing pyrolysis oil yield and energy recovery. Other challenges may include the control of primary emissions of pyrolysis oil combustion and the establishment of standards or specifications for both pyrolysis oil and combustion systems (Lehto 2012).

3.3.4 Bio-butanol

Renewable energy sources are an attractive option for ensuring future energy security (Sharma et al 2013), since it can reduce the fossil fuel dependency and mitigate climate change (Cherubini et al 2011). Therefore, researchers devote a lot to study and develop new energy, such as ethanol and biodiesel. However, a very potential energy substitute, bio-butanol, has been overlooked (Kenneth 2010). Bio-butanol is an alcoholic fuel that can be used as the direct replacement for gasoline, due to its low water miscibility, similar energy content and octane number with gasoline, blending ability with gasoline in any proportion, and its directly utilization in gasoline engine (Kumar et al 2009, Gu et al 2012). Just like second generational bio-ethanol, bio-butanol is also a renewable fuel that can be produced from lignocellulose biomass through acetone butanol ethanol
(ABE) fermentation (García et al 2011). Besides that, compare to ethanol, butanol has the following advantages (Dürre 2007):

- Bio-butanol can be directly used in pure form or blended in any concentration with gasoline, while bio-ethanol can only be blended up to 85% or used as pure form in specially designed engines.
- When using bio-butanol as pure vehicle fuel or gasoline extender, there is no need to make any modification of existing car.
- Bio-butanol is safer to handle, because it has a lower vapor pressure than bio-ethanol.
- Bio-butanol can be blended with gasoline at the refinery before storage and distribution, because it is not hygroscopic; while bio-ethanol could only be blended with gasoline just before use.
- Since bio-butanol is immiscible with water, it is less likely to contaminate the groundwater if it spills; while bio-ethanol is completely miscible with water and will cause water-pollution when it spills.
- Unlike bio-ethanol, bio-butanol is less corrosive, so it can be used in infrastructure, such as pipelines, tankers, filling station, pumps, and etc.
- Bio-butanol has a higher mileage/gasoline blend ratio based on its higher energy content.
- Compare to bio-ethanol, bio-butanol has a more similarity quantity of the caloric value, octane number and air-fuel ratio with real gasoline, which means bio-butanol is more similar with gasoline in characteristics.

However, there still existing some issues in the productions and utilizations of bio-butanol (Jin et al 2011):

- The production of bio-butanol is quite low. The production rate of bio-butanol yield from ABE fermentation is 10-30 times lower than the bio-ethanol produce from yeast ethanol fermentation process.
- Although bio-butanol has a higher energy density than other low-carbon alcoholic biofuel, its heating value is still lower than the real gasoline or diesel fuel, so it needs to increase the fuel flow when it uses as a fossil fuel substitute.
- Bio-butanol is a kind of alcohol-based fuels, so it still cannot compatible with some fuel system components, and may cause gas gauge reading mistakes in vehicles with capacitance fuel level gauging.
- Bio-butanol may create more greenhouse gas emissions per unit motive energy extracted compare to bio-ethanol, due to it contains fewer octane number. Higher octane number means greater compression ratio and efficiency, and higher engine efficiency can achieve less greenhouse gas emissions.
- The higher viscosity of bio-butanol may lead to a potential corrosive or aggradation problem when it was used in Spark-ignition engines.
From the above illustration, we can see that although bio-butanol still need some further developments, since it still has some issue. However, compare to the other lignocellulose bio-fuel it has much more advantages, such as compatibility with infrastructure and relatively less pollution. Therefore, with further improvements or upgrade, the bio-butanol are believed to be the next generation biofuel, since it can reduce the carbon footprint, mitigate the supply and price fluctuation during the transportation sectors, relieve the energy security problem, and provide related job opportunities to improve social equality (Yue et al 2014).

3.4 Sustainability

Since the increasing threats of climate change and global warming was sprawling, people began to realize the significance of sustainable development. The word sustainability could be traced from Latin, which meant maintain, support, or endure. The World Commission on Environmental and Development (1987) defined sustainability as the economic practices that satisfy the needs of current generations but no compromising the ability of future generations to satisfy their needs. During the past few decades, the concept of sustainability has changed and became more specified and practical. For instance, the focus of the sustainability was shifted from merely focusing on environmental issues to pursuing the tripartite of environmental, economic, and social performance. (Foerstl et al 2010) Besides that, under different situations, sustainability can be explained in different ways. Berns et al (2009) claimed that there is not a single established definition for sustainability. For example, when apply sustainability in industrial business, it contains triple bottom line: economic, society, and environment (Elkington 1997); but when it some to the urban sustainability, the components increases to four: ecology, economics, politics, and culture (Paul 2015). In supply chain management, sustainability is called green supply chain management or sustainable supply chain management. (Ashby et al 2012)

3.4.1 Sustainable supply chain management

Previously, supply chain management and sustainability were two independent disciplines. However recently, in order to mitigate the climate change, protect the current living environment without violating the profit of next generations, it is necessarily to integrate the sustainability into supply chain management (Seuring et al 2008). As mentioned above, in the area of industrial business, sustainability adopts the triple button line approach, so as the supply chain management. Ciliberti et al (2008) defined the sustainable management of supply chain as the management of considering the economic, environmental, and social dimensions. Similarly, Wittstruck et al (2011) defined the sustainable supply chain management as an extension to the traditional SCM through adding social and environmental aspects. Also, there are other definitions with more specified details. Carter et al (2008) defined the sustainable SCM as the
scientifically coordination of economic, environmental, and social issues in business activities, aiming at improving the long-term economic performance of the whole supply chain. Besides, Seuring et al (2008) stated that sustainable SCM should not only managing information, materials and capital flow along with cooperation among companies in the supply chain, but also considering the three dimensions of sustainable development which were derived from stakeholder and customer requirements. What’s more, Ahi and Searcy (2013) reviewed 12 definitions of Sustainable SCM and 22 definitions of Green SCM, averred that sustainable supply chain management (SSCM) is an extension of green supply china management (GSCM). The SSCM has seven characteristics: economic focus, environmental focus, stakeholder focus, social focus, resilience focus, volunteer focus and long-term focus. Briefly, the SSCM is to minimize the supply chain cost or maximize the supply chain profits and simultaneously avoid the adverse effects on environment and society. Or say, the SSCM is to enrich the tradition SCM with the considerations of social and environmental impacts. Therefore, the following sections are focused on introducing the social and environmental aspect of SSCM.

3.4.2 Social aspect of sustainable supply chain management

It is easy to understand the functions and concepts of environmental and economic dimensions, but the social aspect still needed to be illustrated, though it is still under developing (Benoi’t-Norris 2014). The social aspect in SSCM may include the problems of social justice and human rights, such as social auditing, codes of practices, social equity, labor condition, and human right actions. Besides, the social aspects in sustainable supply chain network decision helps the stakeholders (customers, employees, and local communities) to have a better evaluation on the supply chain, and helps the decision makers to obtain a consistency between quantitative and qualitative decisions (Eskandarpour et al 2015). Social responsibility is a totally multi-disciplinary and multi-stakeholder issue. Its impacts are often naturally qualitative. Therefore, it is difficult to model social sustainability by using the relative quantitative indicators (Pishvavee et al 2012). In this case, the multi-criteria decision method (MCDM) is a feasible method to address the social sustainability problem based on its characteristics. However, how to select the most suitable criteria and how to incorporate them into the mathematical models are still under development (Eskandarpour et al 2015).

3.4.3 Environmental aspect of sustainable supply chain management.

Integrate the environmental aspect into SSCM needs to deal with the problems of which environmental performance metrics should be involved and how to put them into the mathematical models or optimization methods (Eskandarpour et al 2015). The environmental performance metrics include carbon footprint (commonly indicate the GHG emissions), waste generation, energy use, material recovery, and etc. (Eskandarpour et al 2015). The modeling methods include Life Cycle Analysis (LCA),
Analytic Hierarchy Process (AHP), Data Envelopment Analysis (DEA), Analytic Network Process (ANP), equilibrium models, simulation, etc. (Brandenburg et al 2014). Among these methods, the most widely used approach is LCA, based on its easy integration into optimization model (Eskandarpour et al 2015). Therefore, it is very necessary to introduce the LCA method. The LCA evaluates the environmental impacts in the scope of the whole product life cycle from raw materials to final disposal or recycling (Khasreen et al 2009). It also evaluates the inputs, outputs, and potential environmental effects of a production system throughout its manufacturing processes, life-cycle, and all pertinent supply chain decisions (Pieragostini et al 2012). According to ISO 14040 and 14044 standards, the LCA has four main steps: goal and scope definition, inventory analysis, impact assessment, and interpretation (ISO 2006).

3.4.3.1 Life Cycle Analysis

Life cycle analysis (LCA) refers to a qualitative environmental estimation and assessment of the life cycle of a product (Rebitzer et al 2004). The framework of LCA including objective definition, inventory analysis, impact assessment, and interpretation are discussed in the following paragraph. Fig. 3.2 is the summary of the LCA framework based on ISO 14040.

![Fig. 3.2 Framework of Life cycle Analysis](image)

The first step of LCA is to set up a well-defined objective of the study, then the functional units and boundaries could be defined. The boundary based on different phases of a product can be classified into four types: cradle-to-grave (from raw materials to disposal or recycle), cradle-to-gate (from raw materials to factory gate), gate-to-gate (manufacturing gate to deliver, transportation to another manufacturing gate, and etc.), and gate-to-grave (from factory gate to disposal) (Eskandarpour et al 2015). For example, the main goal of LCA on biofuels is to estimate the environmental impacts on the system under examination and to quantify the ecological benefits from the substitution of the reference system. Then its boundary can be the cradle-to-grave scope (Singh 2013). Functional unit serves as a reference unit to measure the performance of a product system (ISO 2006). Depending on the goal of study, the functional unit must be represented in terms of per unit output. The function unit can
also be categorized into four types: input unit related, output unit related, unit agriculture land, and unit time (Cherubini and Strømman 2011).

The inventory analysis should be based on the data on the physical outputs and inputs of the processions in the production system, considering product flows and elementary flows (Singh and Olsen 2011). The core issue of inventory analysis contains standardized data collection and estimation as well as pertinent data validation. After collecting the initial data, the system boundaries are decided by excluding the subsystems and materials flows or including the new unit processes. The data validation serves as a tool to improve data quality (Jensen et al. 1997).

Impact assessment aims at expressing the output of complex environmental analysis into a few environmental impacts of interest. Mid-point (theme) oriented life-cycle impact assessment (LCIA) methods include many kinds of impacts, such as greenhouse effect, climate change, stratospheric ozone depletion, natural resource depletion, aquatic toxicity, human toxicity, eutrophication, acidification, etc. Endpoint (damage) oriented methods converge the mid-point categories into fewer categories of damage, such as human health related damages, ecosystem health related damages, and resource damages (Eskandarpour et al 2015). The midpoint approach is a typical method since it provides much more results of impact category indicator. The endpoint approach uses its easily understandable damage categories to provide results with a lower interpretive uncertainty level (Yi et al 2011). In the mathematic model, both midpoint and endpoint categories can be used in environmental assessment, and either exhaustive LCA or partial LCA approaches can be employed in the model (Eskandarpour et al 2015).

Several commonly used or relatively new LCIA methods are necessary to be introduced, such as Eco-indicator 99, IMPACT 2002+, and ReCiPe. Eco-indicator 99 aggregates 11 impact categories (organic substances, inorganic substances, climate change, ionizing radiation, ozone layer depletion, eco-toxic emissions, combined effect of acidification and eutrophication, land occupation and land conversion, extraction of minerals, and extraction of fossil fuels) into 3 damage-oriented categories: resource, ecosystem quality, and human health. Then all the environmental impacts are measured as one single metric (Goedkoop et al 2000).

IMPACT 2002+ links the overall life cycle inventory results, such as elementary flows and other interventions, through 14 midpoint categories (human toxicity, respiratory, ionizing radiations, ozone layer depletion, photochemical oxidation, aquatic eco-toxicity, terrestrial eco-toxicity, terrestrial acidification or nitrification, aquatic acidification, aquatic eutrophication, land occupation, global warming, non-renewable energy, and mineral extraction), to 4 endpoint categories: resource depletion, climate change. Human health, and ecosystem quality. The environmental impact is indicated by the sum of the 4 endpoint indicators (Jolliet et al 2003). Both Eco-indicator and
IMPACT 2000+ are widely-used methods, while the ReCiPe is no so popular because it is a new method and just be published in 2008 (Eskandarpour et al 2015).

ReCiPe gathers 18 midpoint categories (climate change, ozone depletion, terrestrial acidification, freshwater eutrophication, marine eutrophication, human toxicity, photochemical oxidant formation, particulate matter formation, terrestrial eco-toxicity, freshwater eco-toxicity, marine eco-toxicity, ionizing radiation, agricultural land occupation, urban land occupation, natural land transformation, water depletion, mineral resource depletion, and fossil fuel depletion) into 3 endpoint indicators: resource surplus cost, ecosystems, and human health, and present a single score as a result (Goedkoop et al 2009). Among them, the score from Eco-indicator 99 and ReCiPe can be easily transformed into an environmental objective function (Eskandarpour et al 2015). The scores or results of the above LCIA methods can be obtained by using the SimaPro 6.0 LCA software (Contreras et al 2009). However, exhaustively utilization of LCIA approach is costly, time consuming, and requires professional knowledge of environmental management and experiments (Pishvaee et al 2012). So instead of using exhaustive LCIA approach, many researchers prefer to borrow only one or a few impact categories and integrate them into the mathematical model directly (Eskandarpour et al 2015).

The step of interpretation is to analyze the results provided by inventory analysis and impact assessment, and then come out the conclusions and recommendations falling into the scope and goal of the study (Lo Giudice et al 2014). According to ISO 14040, the interpretation should contain the following 3 components: the identification of core issues coming from the LCA methods; the evaluation of the study taking the comprehensiveness, sensitiveness, and consistency into account; and conclusions, limitations, as well as recommendations (ISO 14040). The complexity of interpretation is caused by the variety of goals, which includes the improvement of performance, recommendation for some actions, decision of a more in-depth LCA objectives (Reap et al 2008). From the perspective of quantitative analysis, the performance of LCA interpretation highly relies on the accuracy of interpretation. Errors of the inventory analysis and impact assessment can be accumulated to impact the accuracy of interpretation, so it is very necessary to prevent these errors. Theoretically, the use of iterative analysis can detect the error source in some cases, but in practices not all error can be matched to a causal source. Especially in the case of mathematical analysis process, the error can be resulted from the uncertainty such as mechanical failures or the use of computation methods (Chang et al 2014). Therefore, many researchers are interested in proposing some methods to improve the result of LCA interpretation. For example, Benetto et al (2008) proposed a modified NAIADE, a fuzzy multi criteria method, to support the LCA interpretation result and uncertainty evaluations. The characteristic of this method lies in considering the capability of integrating fuzzy and stochastic criteria, as well as probabilistic uncertainty evaluations.
3.4.3.2 EPA regulations of GHG emissions

Besides the LCA method, it is also very necessary to know the regulations of GHG emissions from the supply chain when integrating the environmental issues in the SCM. In this case, the regulations from the U.S. Environmental Protection Agency (EPA) can be good references when considering environmental aspect of SCM.

EPA is an agency aiming at protect human health and the environment (Our Missions, EPA, 2016). In order to protect the environment, EPA is taking commonsensible steps to developing standards to reduce the GHG emissions from mobile and stationary sources under the Clean Air Act. Clean Air Act (CCA) is a federal law that used to regulate the air emissions from mobile and stationary sources (The clean Air Act 2004). Since from Table 4, cellulosic biofuel has the lifecycle GHG emissions threshold reduction of at least 60% comparing to the 2005 EPA estimated gasoline GHG emissions baseline. This baseline is estimated to be 93.08 carbon dioxide emitted per mega joule of fuel (g CO₂ e/MJ) (EPA 2010). According to a report prepared by Baland and Unnasch (2015), the GHG emissions thresholds of different renewable fuel type can be calculated in terms of g CO₂ e/MJ. Since the energy density of butanol fuel is 29.2 MJ/L (Butanol fuel, Wikipedia, 2016), therefore the GHG emissions threshold can be transform into g CO₂ e/L. The GHG emissions threshold of different renewable fuel type can be summarized in Table 3.5.

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>GHG reduction</th>
<th>Threshold</th>
<th>Threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulosic biofuel</td>
<td>≥ 60%</td>
<td>37.23 g CO₂ e/MJ</td>
<td>1087.11 g CO₂ e/L</td>
</tr>
<tr>
<td>Biomass-based diesel</td>
<td>≥ 50%</td>
<td>46.54 g CO₂ e/MJ</td>
<td>1358.97 g CO₂ e/L</td>
</tr>
<tr>
<td>Advanced biofuel</td>
<td>≥ 50%</td>
<td>46.54 g CO₂ e/MJ</td>
<td>1358.97 g CO₂ e/L</td>
</tr>
<tr>
<td>Total renewable fuel</td>
<td>≥ 20%</td>
<td>74.46 g CO₂ e/MJ</td>
<td>2174.23 g CO₂ e/L</td>
</tr>
</tbody>
</table>

Under the Renewable Fuel Standard Program 2 published by EPA in 2010, the lifecycle analysis of the renewable bio-fuel includes the following processes (EPA 2010):
- Feedstock agriculture
- Feedstock transport
- Feedstock processing and bio-fuel production
- Biofuel transport and distribution
- Biofuel tailpipe emissions

3.5 Sustainable supply chain network design

Before going into the sustainable supply chain network design, it is necessary to introduce some basic ideas about supply chain network design. Supply chain network
design (SCND) is to design a supply chain’s physical network structure. It is one of the most significant stage in designing a new supply chain since it can impact all the following tactical and operational decisions (Farahani et al 2014). The SCND aims at designing an effective network structure for the entities of a new supply chain or redesigning an existing network in order to increase the total value. Therefore, various decisions need to be made during this process. For instance, Simchi-Levi and Kaminsky (2004) stated that SCND can be used to deal with the strategic decisions, such as locations, size, and type of their facilities, as well as some tactical decisions, like distribution and inventory control policies. In addition, Autry et al (2013) in their book pointed out that the SCND is a discipline which can be applied to determine the optimal size and location of the facilities as well as the flow through these facilities (Autry et al 2013). Furthermore, Farahani et al (2014) proposed that besides making strategic and tactical decisions, SCND can be evolved into a more comprehensive tool, which can be used to make operational decisions like customer demand fulfillment, pricing, and provide service level, called comprehensive SCND.

Recently, because of a growing concern of the environmental performance and social responsibilities of business operation, the supply chain network design is shifting to sustainable supply chain network design (SSCND) (Devika et al 2014). Therefore, SSCND may refer to determining the optimal size and location of facilities as well as the flows through these facilities, simultaneously improving the environmental performance or social responsibilities or both.

To get further access of SSCND, it is required to clarify some questions (Eskandarpour et al 2015):

- What environmental and social performance measurements should be used in the SSCND?
- How to integrate the environmental and social factors into the mathematical models?
- Which optimization method and tool should be adopted in the SSCND?

3.5.1 Environmental performance measurements

Up to now, the carbon footprint is a common terminology to measure the environmental performance of a supply chain which is often quantified as the greenhouse gases (GHG) emissions. GHG emission is defined as the total amount of GHG emitted from the firms or supply chains (Eskandarpour et al 2015). Theoretically, every type of GHG emission should be involved in measuring the carbon footprint. However, for some practical and economic reasons, CO2 and CH4 emissions become the main indicator to measure the carbon footprint (Wright et al 2011). Usually, GHG emission do not need to be calculated explicitly, but it can be estimated by the quantity of consumed energy (Harris et al 2011) or an economic input-output analysis from some recent Error Input / Output (EIO) studies (Pourmohammadi et al 2008). Besides, there are many commonly-used
environmental metrics available to be adopted in different type of supply chains. For example, the waste generated (Lira-Barragán et al 2011; Pishvaee et al 2012; Eskandarpour et al 2013), energy utility (Papapostolou et al 2011; Corsano et al 2011; Mohammadi et al 2014), and material recovery (Minciardi et al 2008; Harraz et al 2011; Amin et al 2013).

3.5.2 Social performance measurements

The social responsibility measurement should be considered from three aspects: work conditions, societal commitment, and customer issues. In the aspect of work conditions, the employment, which means the number of job position created, is a significant indicator, since many researchers prefer to use this metric to measure the social responsibilities. For example, Mota et al (2015), Devika et al (2014), and Yue et al (2014) introduced the position creation into their mathematical model to measure the social aspect of their supply chain network design. Also, based on the different characteristics of different supply chains, other indicator like the damage to workers (exposure to hazardous environment) should be considered (Dehghanian et al 2009). The societal commitment is about improving populations’ health, culture, and education (Datta 2012). To measure the societal commitment, the local development policies (Dehghanian et al 2009), the impact of supply chain on real estate (Bouzembrak et al 2013), and healthcare accession equity (Beheshtifar et al 2015) could be used. Last, the customer issue includes all the impacts that would affect customers (Eskandarpour et al 2015). For example, the product risks from using different recycle materials (Dehghanian et al 2009).

3.5.3 Sustainable supply chain network design model

According to a comprehensive literature review on supply chain network design (SCND) conducted by Farahani et al (2014), there are many models of SCND proposed in recent publications. Therefore, different decisions can be made through SCND. One of most significant decisions is to locate the facilities of different tires in the chain. Besides, according to a detailed literature review on sustainable SCND proposed by Eskandarpour et al (2015), SCND is the combination of academic facility location problem and practical SCND problem, since it can not only deal with many issues in logistics network, multiple period, product, technology, transportation mode and facility type, but also integrate them with capacity constraints, tactical decisions, and product flow. In addition, SCND may also make some other decisions, such as partnership selection, distribution network selection, and etc., rather than just determine the transportation mode, resources allocation, as well as the number, location, type, and capacity of the facilities (Barbosa-Póvoa 2014). Therefore, additional discussions of the model of partner selection and distribution network selection are shown below.
3.5.3.1 Models for supplier or customer selection

Yeh and Chuang (2011) proposed a multi-objective mixed-integer non-linear programming model to select the partner for a green supply chain network. The model has four objectives which include product quality, time, cost and green appraisal score. Two multi-objective genetic algorithms are used to find the Pareto-optimal solutions and solve the conflicting objectives. Sha et al (2006) proposed a systematic model for partner selection and production/distribution planning in supply chain network design. In this paper, the authors developed a novel multi-phase mathematical method which is based on genetic algorithm, analytical hierarchy, and multi-attribute utility theory to simultaneously optimize the suppliers and customer selection. The model has five phases, the first is to estimate the efficiencies of the potential corporations according to their yield rate, demand factor, and capacity by using the genetic algorithm; the second is to find the corporations which has a high yield rate according to the result of last phase; the third phase is to calculate the priority of each criteria for partner selection by using analytical hierarchy; the forth is to construct the single utility function of each criteria using multi-attribute utility theory and integrate them with two-way consideration; and the last phase is to design the nearly optimal supply chain network and obtain the feasible supply chain network solution by using genetic algorithm. Cakravastia et al (2002) proposed a two-stage mix integer linear programming model for supplier selection in SCND. In the model, the limitations of each potential suppliers’ capacity are considered. The objective is to minimize the customer dissatisfaction, which is measured by the delivery lead time and price. This model works in two decision making levels: operational and strategic, in which the former is about optimizing the production and logistic activities of every potential supplier, the other is about evaluating the potential suppliers and determining the final configuration of supply chain network.

3.5.3.2 Models for distribution network selection

Selim and Ozkarahan (2006) designed a supply chain distribution network model by using a novel and generic interactive fuzzy goal programming-based (IFGP-based) solution approach to determine the optimum numbers, capacities, and locations of warehouses and plants. The IFGP-based solution method has six main steps: the first is to develop a linear programming formulation; the second is to obtain the efficient solutions which is used to construct the membership functions in the objective; the third is to use the upper and lower bounds of the objective to define the membership functions; the forth step is to develop the problem formulation using the modified fuzzy and operator; then the next is to obtain the compromise solution, if the decision maker accepts this solution, then stop, otherwise continue to step 6; the sixth is about asking whether the decision maker wants to modify the coefficient of compensation and the membership functions in the objective, if so then turn to step three. Ahmadi-Javid and Hoseinpour (2015) proposed a mix-integer non-linear programming model to solve a
profit-maximization location-inventory problem (PM-LAP) under price-sensitive demands in a multi-commodity supply chain network. The problem includes the decisions of optimal location and order size of the facilities, the allocation of customers to distribution centers, as well as the selling prices of different commodities. The objective of the model is to maximize the overall income minus the overall cost which includes fixed distribution setup cost, procurement cost, transportation cost, and the inventory cost. Constraints in this model is to arrange the relationship among customers, distribution centers, and commodities. In order to solve this mathematic model, a Lagrangean relaxation algorithm is used. In this algorithm, the hard constraints in the formulated model are relaxed and multiplied by Lagrangean multipliers. Then they are added to the objective function in order to generate a new model which is easier to solve than the original one. The feasible solution of the original model can be obtained based on the optimal solution from the new model. Amiri (2006) developed a mixed-integer linear programming model in order to solve the distribution network design problems of a supply chain system with a minimum cost. The problems include the decisions of optimal locations, capacities, and numbers of production plants and distribution warehouses, as well as the optimal strategy for transporting the products to warehouses, to production plants, and to customers from warehouses. In this paper, a Lagrangean relaxation technique is used to obtain the feasible solutions and the lower bounds for the optimum solution to the distribution network problem. A sub-gradient optimization method is used to generate good Lagrangean multipliers. This heuristic procedure composed of two different steps: one is to use a relevant solution from Lagrangean relaxation to decide which warehouse is going to open and their capacities to satisfy the demand of customers; the other is to use another relevant solution from Lagrangean relaxation to decide which production plant is going to open and their capacities to satisfy the needs from opened warehouses.

3.5.3.3 Models for sustainable supply chain network design

By the use of SSCND model, the environmental and social issues can be integrated into the traditional SCND. The SSCND model is about integrating the environmental or/and social factors into the traditional SCND mathematical models.

Just like the traditional SCND model, which usually uses the cost or profits as the quantized value in the mathematical model to measure the economic performance of a project (Autry et al 2013), the SSCND model also need some quantized value to measure their environmental or social performance and formulate the mathematic model. Therefore, knowing the metrics of measuring sustainable SCM helps to select the environmental or social factors for the SSCND model. According to a literature review of Ahi and Searcy (2015), at the end of 2012 there are 2555 different metrics from 445 articles about green supply chain management and sustainable supply chain. However, most of the metrics are only used once which means there exist a highly disagreement in metrics selection. However, he also pointed out that there still exists
some commonly used metrics, such as quality, air emissions, greenhouse gas emissions, energy use, and energy consumptions, which are all be used more than 20 times. For example, Elhedhli and Merrick (2012) developed a linear programming model for green SCND. In their model, the greenhouse gas emission is used as an environmental performance measures and embedded into the objective function. Wang et al (2011) developed a bi-objective mixed-integer optimization programming model and applied it in the green SCND of a global procurement center in a Chinese world-class company. In their model, the CO2 emissions is the only environmental metrics used in the objective function. Comas Martí et al (2015) used an assignment-based formulation to design an environmental supply chain network. The model includes not only the environmental impacts, but also the inventory level, demand uncertainty, transportation mode, and geographical differences of procurement costs. In their formulation, the carbon emissions of each supply chain process is measured as a metrics for environmental performance.

In SCND model, the main decision variables include facilities locations, facilities sizes, technology selection, and transportation model selection. Since the flows within the supply chain network are usually modeled as continuous constrain, the formulations of SCND model are often mix-integer mathematical programming model, which can be either linear or nonlinear (Eskandarpour et al 2015). The category of objective function includes single objective and multi objectives. The objective models can be divided into deterministic model and stochastic model (Eskandarpour et al 2015).

3.5.3.4 Single objective model

In the single objective model, there are two approaches to integrate environmental factors into the SCND model. The simplest way is to directly integrate the environmental factors into the objective function. In this way, the environmental factors are multiplied by a certain weight and then added into the objective function. For example, the environmental indicator GHG emission can be first converted into the monetary equivalent and then aggregated into the economic objective function, so that a single objective function can reflect both economic and environmental dimensions. While the alternative way is to put the environmental factors into constrains. In this way, the objective function is mainly focus on the economic factors while constrains focus on the environmental factors. For example, in constrains, the GHG emissions of each activity in the supply chain are limited to a certain authorized level (Eskandarpour et al 2015).

3.5.3.5 Multi-objective model

The multi-objective model is a mathematical model which has at least two objective functions. In this model, the economic, environmental and social issues can all be formulated as the objective functions. Amount the objective functions, there exist a trade-off which can make it possible to obtain a single optimum solution in this system.
Therefore, to solve this model, the first step is to optimize the objective functions independently and obtain the solutions which is called Pareto optimal. Then improving any objective without deteriorating others. If there isn’t additional preference on these objectives, then the weight of each Pareto optimal solution is considered equivalent. If there is a preference towards a certain objective, then more weight is added to this objectives (Devika et al 2014). The details of this optimization model are illustrated with examples as follows.

3.5.3.6 Deterministic multi-objective linear models

Mota et al (2015) proposed a generic multi objective Mixed Integer Linear Programming model for a closed-loop SCND which simultaneously considers the economic, environmental, and social aspects. In this model, costs, environmental assessment, and social assessment are formulated as three objective functions. Besides, materials flow, demand, return, vehicles and facilities capacity, and operations such as maximum travelling distance per time period are classified into five major types of constrains. The economic objective function is to maximize the sum of fixed setup cost, raw material cost, transportation cost, outsourced transportation cost, and product recovery cost. The social objective function is to maximize the created job position. The environmental objective function is to minimize the environmental impact of production, transportation, and entities installation. In order to solve to environmental objective function, first, the Life Cycle Inventory of production, transportation mode, and installation of entities are retrieved form Ecoinvent databases and assessed via the software SimaPro 7.3.2. Next, the environmental impacts of these three activities are determined from the Life Cycle Inventory and then be used as the input data for the mathematical model. After that, the overall environmental impacts of three activities are determined by multiplying the impacts by their relative variables. Finally, the results from the last step are aggregated into one single score by the ReCiPe 2008 methodology, and then be minimized. The model is the sum of different regional factors times the number of job created at that region. To complete the multi objective approach, the $\varepsilon$-constraint method is applied because of its applicability and simplicity. The $\varepsilon$-constraint is about optimizing one of the objective functions by putting other objectives into constrains. For example, when optimizing the economic function, the following equations are formulated:

$$\min f_1(x)$$
$$\text{s.t. } f_2(x) \leq f_2^{\min}(x) + k\Delta\varepsilon_2$$
$$f_3(x) \geq f_3^{\min}(x) + k\Delta\varepsilon_3$$
$$x \in S$$
$$k = 0, ..., n$$
\[ \Delta \varepsilon_i = \frac{f_i^{\text{max}} - f_i^{\text{min}}}{n}, i = 2,3 \]

In order to solve the problem, a lexicographic optimization method is applied. This method can introduce some appropriate surplus or slacks variables into constrains and objective functions on the basis of \( \mathcal{E} \)-constraint method. The following equations are the transformed model:

\[
\begin{align*}
\min & \quad (f_1(x) + \text{eps} \times (s_2 + s_3)) \\
\text{s. t.} & \quad f_2(x) + s_2 \leq f_2^{\text{min}}(x) + k\Delta \varepsilon_2, \\
& \quad f_3(x) - s_3 \geq f_3^{\text{min}}(x) + k\Delta \varepsilon_3, \\
& \quad x \in S \text{ and } s_i \in R^+, \\
& \quad k = 0, ..., n, \\
\Delta \varepsilon_i = \frac{f_i^{\text{max}} - f_i^{\text{min}}}{n}, i = 2,3,
\end{align*}
\]

where \text{eps} denotes a very small number (usually between \(10^{-3}\) and \(10^{-6}\), so that it does not affect the objective function).

Devika et al (2014) also developed a MILP model to design a sustainable closed-loop supply chain network. There are three objective functions in the model: economic, environmental, and social. The economic objective function is to minimize the difference between costs and savings. The costs include the setup cost of facilities, purchasing cost, manufacturing cost, holding cost, transportation cost, assignment cost, and collection cost, while the savings include product recovering, remanufacturing, recycling, and reuse market sale. The environmental objective function is to minimize environmental impacts and maximize the environmental benefits. The social objective function is to focus on maximizing the job creation of each activity in the supply chain and minimizing the workers’ damages which come from the facilities set up, products manufacturing and products handling. Constraints of the model involve the capacities of manufacturing centers and suppliers, the number of facilities, the maintaining of products flow, demands satisfaction, technology applications. To obtain the solution, the paper proposed three different hybrid methods: HIV (the hybrid of adapted imperialist competitive algorithm (ICA) and variable neighborhood search (VNS) algorithm), TIV (the hybrid of two-phase ICA and VNS), and NIV (Nested ICA and VNS). In order to test the effectiveness and efficiency of the results, these three methods are compared with each other, and examined by some benchmark methods. The result shows that the NIV has a better performance.

### 3.5.3.7 Deterministic multi-objective non-linear model

Yue et al (2014) proposed a multi-objective mixed integer linear fractional programming (MILFP) model to address the network design problem of a sustainable
cellulosic bioelectricity supply chain. In this large-scale model there are 29 constrains, in which the biomass supply system, preprocessing stage, conversion stage and sale situation are modeled. The model has three objective functions: economic, environmental, and social. The economic objective function is to minimize the difference the costs and government incentives. The cost in the economic objective function include the facilities setup cost and the cost of biomass acquisition, routine operation, equipment maintenance, inventory management, and inter-site transportation. The environmental objective function uses the GHG emission from the different activities of the supply chain minus the carbon. The social objective function is about maximizing the local employment opportunities created by setup this supply chain. In order to obtain the solution, the \( \varepsilon \)-constraint method is used at the beginning to get the better approximation of the Pareto optimization solution, then two tailored solution methods (the parametric algorithm and the reformulation linearization algorithm) are applied to solve the MILFPs. The specific details of parametric algorithm are be showed in Fig. 3.3. The reformulation linearization refers to changing the MILFP problem into its equivalent MILP problem. The optimal solutions of the MILP problem are converted into the form of original variables. The Fig. 3.4 shows the transformation of variables between the original MILFP and the equivalent MILP.

3.5.3.8 Multi-objective model coupled with LCA and Input-Output analysis

You et al (2012) proposed a model which combines the LCA, Input-Output analysis and a multi-objective, multi-period mixed integer linear programming model to design the network of a sustainable cellulosic bio-ethanol supply chain. The model has three objective functions and 40 constrains. The economic objective function is to minimize the difference between the costs and benefits. The costs include the setup cost, biomass harvest cost, biomass drying cost, ethanol production cost, transport cost and inventory cost, while the benefits include the byproduct and biofuel selling incentives. The environmental objective function is to minimize the GHG emission of every activity throughout the supply chain. The values of the relative parameters are obtained from the Argonne GREET Model, the Aspen Plus process models, the U. S Life Cycle Inventory Database and relative literatures. The social objective function in this model is to maximize the local job opportunities resulted from this supply chain. The relative parameters are obtained from IMPLAN Professional model by using 2002 state data. This model is solved by a \( \varepsilon \)-constraint method.
3.5.3.9 Stochastic model

In some particular cases, some factors which are not deterministic and known, such as customer demand, transportation cost, waste generation, and emission generation, are also needed to be considered when designing the supply chain network. In these cases, stochastic programming may come into use. A stochastic model refers to using probability to model the scenario which contains uncertainties. For example, Giarola et al (2012) generated a mixed-integer linear two-stage stochastic programming model in order to maximize the profits and minimize the GHG emissions of a multi-echelon and multi-period bioethanol supply chain network. In this network, the biomass cost and carbon cost are uncertain. In addition, Verma et al (2013) also used a two-stage stochastic programming method to determine the location and stockpile of equipment.
in the oil-spill response facilities for South coast of Newfoundland in Canada. A standard form of a two-stage stochastic integer program is shown below:

$$\min_x C^T x + E_P [Q(x, w)]$$

$$\text{S.t. } Ax = b,$$

$$x \in \mathbb{R}_{+}^{n_1-p_1} \times \mathbb{Z}_{+}^{p_1}$$

Where

$$Q(x, w) := \min_y q^T y$$

$$\text{S.t. } Wy = h - Tx,$$

$$y \in \mathbb{R}_{+}^{n_2-p_2} \times \mathbb{Z}_{+}^{p_2}.$$ 

In the above model, W is a matrix which is assumed to be deterministic. The symbol $n_1, n_2, p_1, p_2$ are nonnegative integers with $p_1 \leq n_1$ and $p_2 \leq p_2$, the variable $x$ refers to the first-stage decisions and $y$ refers to the second-stage decisions, and $\omega$ represents the uncertain data for the second-stage (the parameters $q$, $h$, $T$ are actual realization of the random data) with known distribution $P$ (Ahmed 2011).

3.6 Optimization Methods

Sadegheih (2009) stated that optimization is a process of regulating the characteristics of inputs of an experiment, device, or mathematical process to obtain a maximum or minimum result. Optimization methodologies can be divided by three categories: heuristic approach, mathematical programming, and multi-criteria decision analysis. More specifically, heuristic approaches include genetic algorithm (GA), Particle swarm optimization (PSO), binary honey bee foraging (BHBF); mathematical programming includes linear programming (LP), integer programming (IP), mixed integer linear program (MILP); Multi-criteria decision analysis contains multiple attribute decision analysis (MADA) and multiple objective decision analysis (MODA) (Winston 2003).

3.6.1 Heuristic approach

3.6.1.1 Genetic algorithm

Genetic algorithm (GA) is a biological evoluational abstraction or model based on the theory of natural selection (Holland 1975, De Jong 1975). Genetic algorithms are the most widely adopted optimization algorithms in modern nonlinear optimization, since they have the excellent ability to deal with the parallelism and complex problems. However, the inappropriate choices in GA such as the misuse of population size, the incorrect formulation of a fitness function, the infeasible selection criteria of new population, and the improper choice of important parameters, can lead to the
convergence failures and meaningless results. (Yang 2014). The applications of GA in different areas are shown as followed.

Zhang et al (2014) applied the GA to a functional areas layout optimization problem of railway logistic parks. After understanding the whole relationship of the different functional areas, the authors addressed the functional area layout problem by constructing a mathematical model. Then used GA to solve the problem on Matlab. The model was tested by a practical example and the result showed that the application of GA in the layout optimization model can largely improve the quantifiable accuracy. Khoshahval et al (2012) combined the genetic algorithm (GA) with the Hopfield Neural Network (HNN) to develop a hybrid optimization method and applied this method to the burnable poison placement (BPP) problem in order to increase the qualities of results. In this problem, the objective function is to minimize the radial power peaking with an increasing burnable poison worth. They compared the efficiencies of GA, HNN and hybrid optimization methods and concluded that the hybrid optimization method is the best in solving the BPP problem. Wikaisuksakul (2014) deployed a multi-objective GA with the fuzzy c-means method to solve the data clustering problem. This new approach can solve data clustering when the prior knowledge on the clusters number is unknown. In addition, this method can simultaneously optimize both the overlap-separation criteria and fuzzy Jm index criteria. The author encoded a string of real-coded values to represent the cluster centers and found that this algorithm can handle the well-separated, hyper-spherical and overlapped clusters from real life and synthetic data set when comparing with the existing multi-objective and single-objective clustering techniques. Lovinger et al (2014) proposed a hypothesis of GA, that is, if a GA can optimize the parameters which have an important impact on the effectiveness and efficiency, then it can provide an automatic and rapid optimization. They tested their hypothesis by using a GA to solve the general optimization functions and take the time of solving problems as a measurement of GA’s effectiveness. They obtained the improvements of an average 947% on training sets and 440% on testing set and concluded that an optimized GA can remain general enough to solve adaptive systems problem effectively.

3.6.1.2 Particle swarm optimization

Particle swarm optimization (PSO), which is proposed by Kennedy and Eberhart in 1995, is an evolutionary stochastic algorithm for solving discrete and continuous optimization problems. Since it is inspired by swarm behavior in nature, like bird flocking and fish schooling, it belongs to the class of swarm intelligence techniques for solving optimization problems (Kennedy et al 2001). The PSO is very easy to implement because it uses real-number randomness and global communication in swarm particles, no encoding and decoding into binary strings. It has many variants and can be combined with other algorithms to create hybrid algorithms. Base on its
simplicity and flexibility, PSO can be applied to almost every area in optimization, design application, computational intelligence (Yang 2014).

The PSO algorithm finds the optimal solutions by modeling the location searching activities of the swarm particles. The movement of a particle composes of two components: the deterministic and the stochastic. Each particle has a trend to move randomly or to a better location. When a particle moves to a better location, it can update this location as its new current best location. Each time during this process, there exists a current best location for all particles. The particles keep moving until they find the global best location from all current best locations (Yang 2014). The researches about PSO is described as follows.

López et al. (2008) developed a binary PSO method to find the optimal location of forest residues biomass power plants and supply areas for the biomass plants. The location problem is formulated as a nonlinear optimization problem. And the objective function is to optimize the profitability index. The authors also conducted a contrast experiment to test the efficiency between the PSO and GA methods. The result shows that the PSO method converge faster and had a lower computational cost. AlRashidi et al (2010) applied a PSO to minimize an error with respect to the estimated model parameters for yearly peak load prediction in an electrical power system. The result obtained from this method is compared with the result using the least error squares estimation technique. The result of contrast experiment shows that the PSO method is better. Sun et al (2013) presented a two-swarm cooperative particle swarm optimization (TCPSO) to improve previous canonical PSO algorithm. This new approach not only has a better balance between the convergence speeds and the diversities, but also can find the global optimum in a large search interval. This method adopts two particle swarms, which have a clear division of their works as a slave and a master. The former particles can be updated regardless the current velocities. The latter particle must be updated based on the former one. The dimension of each particle learns from the same dimension of its complementary particles, which makes the slave particles concentrate to the local optimal and further accelerates the convergence. Tanweer et al (2015) developed a new PSO algorithm with two learning strategies and call it Self Regulating Particle Swarm Optimization algorithm. In this new method, one strategy uses a self-regulating inertia weight which is used by the best particle for better exploration, the other strategy uses the self-perception on the global search direction which is used by the other particles for solution space intelligent exploitation. These two strategies let SRPSO obtain faster convergence and better solutions in most of the situations. Moreover, according to a statistic analysis, the performance of SRPSO on CEC2005 problems is better than other SPO methods within a confidence interval of 95%. Lim et al (2015) developed a new PSO variant called the PSO with dual-level task allocation to balance the exploitation and exploration search processes. In this new approach, the two tasks allocation modules refer to the dimension-level and the individual-level task
allocation modules. The dimension-level module assigns different search strategies to their complementary dimensional components of a particle; while the individual-level module acts as a backup learning phase to PSO-DLTA. The authors compared this new variant with several recently published algorithms on 25 benchmark and two engineering design problems, and found that the PSO-DLTA has a better reliability, searching accuracy and efficiency.

3.6.1.3 Binary honey bee foraging

Binary Honey bee foraging (BHBF) is a new optimization calculation tool based on particles swarm, which is inspired by the swarm behavior of honey bee. The algorithm of BHBF is like the forage activity of honey bee swarms. For example, there are a few groups of bee foraging for better honey location in a collective manner, meanwhile there are a few scouting bees researching for the same thing but randomly. They use the waggle dance at the hive to share the information, so when bees return from foraging and scouting, they can update their information and reallocate themselves. (Vera et al 2010).

Vera et al (2010) used this method to help the investors to determine the optimal location, power plant size and biomass supply area of the olive tree biomass production industry in Spain. In this publication, the Profitability Index (PI), that is, the ratio between the initial investment and net present value, is set as the fitness function. The result shows that the optimal location of the power plant corresponds to coordinate is X=49, Y=97 in Úbeda, the optimal plant size is 2MW (PI=3.3122), the biomass supply area is 161.3343 km2. Quijano et al (2010) introduced a honey bee social foraging model to create an algorithm which is used to solve a set of dynamic resource allocation problems. They proved that (1) If several HBF algorithm is used to solve the same dynamic resource allocation problems, they can use a Nash equilibrium and an evolutionarily stable strategy. (2) The allocation strategy is globally optimal for a multiple and single algorithm.

3.6.1.4 Biogeography-based optimization

Biogeography-based optimization (BBO) is a population-based meta-heuristic optimization algorithm based on the equilibrium theory of island biogeography. It mainly composes of mutation operation, migration operator, and migration model (Simon 2008). A few examples of current research about BBO are discussed as follows.

Xiong et al (2013) proposed a multi-strategy ensemble biogeography-based optimization (MsEBBO) based method for economic dispatch problems. Generally speaking, the no free lunch theorem in optimization means almost all algorithms have the similar average performance on the set of all problems. According to this no free lunch theorem, the MsEBBO has three extensions to the three components of BBO. First, adopting a sinusoidal-curve-based nonlinear migration model; second, presenting a backup migration operator by using a backup strategy to combine blended operator
and perturb operator to strengthen the exploitation abilities; third, applying a similar backup strategy for MsEBBO mutation operator which Lévy local search and differential mutations are embedded. Through this mutation operator, the MsEBBO is fast enough to escape from perform efficient search and local optima within global range. The authors tested the MsEBBO performance on four economic dispatch problems with various complexities and found that the MsEBBO can not only have a good balance between exploitation and exploration, but also gain a high quality solution. Khoshahval et al (2014) proposed a new BBO method for the optimization problem of loading pattern in pressurized water reactors. The new method uses the migration operator to share information among problem solutions. By conduct a contract experiment on BBO and PSO, the authors found that the BBO has a faster convergence but need more computational time than PSO. Niu et al (2014) proposed a biogeography-based optimization algorithm with mutation strategies (BBO-M) to identify the model parameters of solar cells and fuel cells efficiently. The new algorithm improves the global searching capability of the original algorithm by incorporating the BBO algorithm structure with both the chaos theory and the mutation motivated from the differential evolution algorithm. The authors conducted numerical experiments on ten benchmark functions with fifty dimensions and showed that BBO-M can produce high quality solutions and fast convergence rate.

3.6.2 Mathematical programming

3.6.2.1 Linear Programming

Arora (2012) defined the linear programming (LP) as an optimal design problem with constraint functions or a linear cost in the design variables. A linear programming model is the mathematical programming models with linear constrains and a linear objective function (Meyer et al 2014).

There are various algorithms for LP, however, the most fundamental method is Dantzig’s simplex method which is mentioned in nearly every textbook talking about LP. The method was designed in the summer of 1947 by George Dantzig. The main idea of this simplex method is to continually improve (increase or decrease) the value of the cost function by Gauss-Jordan elimination procedure. This procedure proceeds one basic feasible solution to the other, until it reaches the optimal (maximum or minimum) value or concludes that it is an unbound LP (Arora 2012). In many cases, an initial basic feasible solution is not at hand. At this time, some techniques can be applied to obtain the initial basic feasible solution (Bazaraa et al 2009). Generally, there are two widely used techniques to start the simplex method, which are two-phase method and Big-M method. The two-phase method uses two steps to eliminate the artificial variables which is added to the LP system when transforming the inequality constrains to a standard form. The first step is to drop the artificial variables into zero or concluding that the original LP has no feasible solutions; the second step is to minimize.
the original objective function value by pivoting the basic feasible solution from phase I. While the Big-M method is another way to eliminate the artificial variables. In this method, a large coefficient (denoted by M) is assigned to each artificial variables, then move the artificial variables out of the basis by using simplex methods. The iteration will continue until it finds the optimal solution for the original problem (Bazaraa et al. 2009).

It is now very popular to apply the LP into the area of biomass SCM (Ryu et al. 2004, Kanyalkar et al. 2005, Oh et al. 2006). Many researchers prefer to use the algorithm of Dijkstra, a graph searching algorithm, to solve the single-source shortest path problem when the cost of the edge path are all non-negative. The result of this algorithm are presented as a shortest path tree. (Dijkstra 1959). For example, Perpiña et al (2009) developed a methodology using geographic information system based on Dijkstra algorithm to determine the optimal location of a bioenergy plant network. The objective is achieved by computing the transportation distance, transportation costs, and transportation time between all potential conversion sites and biomass production sites. Panichelli et al (2008) conducted a GIS-based approach to select the optimal locations for biomass torrefaction plants and gasification facilities when considering resource competitions and biomass farm gate price. The locations of gasification facilities are obtained by minimizing the marginal costs of torrefied wood supplier to gasification plants, while the locations of torrefaction plants are obtained by applying a simplified Dijkstra algorithm. The LP can be used to address allocation problem, Dicoraro et al. (2008) used a linear programming optimization procedure which is based on energy flow optimization model (known as EFOM) to evaluate the contributions from energy efficiency actions and distributed generation productions. This method shows the feasibility of generation allocations between distributed generation and large scale generation. It also shows an optimal energy efficiency technologies diffusion in the objective of reducing operational cost and environmental impacts.

There are some gaps in the application of LP:

- There are less publications focusing on the application of LP on biomass supply chain.
- The application of LP in supply chain is limited, since it is just able to solve some simple problems.
- In some cases, the LP cannot work well just by its own, it has to combine with other mathematical programming.

3.6.2.2 Integer Programming

Integer programming (IP) model is a mathematical model which some or all of its decision variables are integers. (Meyer et al. 2014) Although integer programming can be categorized into linear IP and non-linear IP, in general, the term IP refers to integer linear program, since an IP is derived from the LP which has the integer values on some
or all of the variables. (Bosch et al 2005) The integer linear programming problem is a discrete optimization problem: \( \min \left\{ cx : Ax=b, \ x \in \mathbb{N} \right\} \). In this equation, \( c \) and \( b \) represent the integer vectors of appropriate dimensions, \( A \) denotes an \( m \times n \) integer matrix, and \( \mathbb{N} \) is the set of nonnegative integers. (Loera et al 2008).

The most commonly used method for solving the IP is branch and bound (BB) (Land et al 1960). Now, there are many versions of BB algorithm, such as fast BB algorithm (Somol et al 2004), adaptive BB algorithm (Nakariyakul et al 2007), and GPU-accelerated BB algorithm (Chakroun 2013). Although the variant of this algorithm can be different, their core concepts are the same. The core of basic branch and bound algorithm is an exhaustive search, that is, image the systematic enumeration of candidate solutions as a tree with roots, and the running of this algorithm is just like tracing the structure of the tree. The roots represent the subsets of the candidate solutions. Before running the algorithm, the root is checked against lower and upper estimated bounds of the optimal solution. Candidate solutions are added into the tree structure as a deeper root based on the outcome of the previous algorithm, the candidate that cannot produce a better solution is discarded from the tree structure. This algorithm will not stop until no more solutions can be added into the tree. (Fukunage et al 1977).

Another popular method for solving IP is cutting plane method (Gomory 1958). The first step of this method is to solve the IP as a LP by dropping the integer requirement, if the feasible solutions are not all integer, the method will use a hyperplane as an additional linear constraint and add it into the iteration tableau to update the tableau. The hyperplane is used to cut the set of solutions into two parts: the integer variables and the non-integer variable. After that, solve the modified LP and repeat this above process until all the variables are integers. (Jeroslow 1979) Besides that, there are other methods to solve the IP, such as branch and cut (Crowder et al 1983) method which synthesizes the method of BB and cutting plane and greatly improve the basic BB algorithm; branch and price (Barnhart et al 1998) which is a hybrid of column generation methods BB algorithm.

The IP models can be used to solve many problems in SCM, including supply chain design, planning, scheduling, and resource assignment. For example, Judd et al (2010) developed an IP model in a bioenergy SCM to select the optimal locations of the storage facilities and the optimal allocation of the farm to these facilities by the use of two binary integer variables. Kim et al (2011) presented a model based on a two stage mixed integer stochastic program for the optimal design of a biomass-supply-chain network in the Southeastern region of the United States under uncertainties. The uncertainty presents themselves as many stochastic model parameters which have impacts on the design and profitability of the supply chain. To tackle this parameters, the authors used a two stage mixed integer stochastic program in which the first stage is the capital investment decision including the location and size of each plant, while the second stage is the resource decision of the biomass and product flow in each scenario.
IP has a history over fifty years, and it has been used to solve many difficult problems. Nowadays, by the use of modern computer, the IP can be used to solve problems from a wider variety of areas, based on the efficient algorithms and accurate data. Since now, the IP can help to optimize the bioenergy supply chain management, its application in the sustainable biofuel supply management can be seen not so far.

3.6.2.3 Mixed integer linear program.

Mixed integer linear program (MILP) is a hybrid of LP and IP, it has integer decision variables, linear objective function and constrains (Meyer et al 2014). The group of MILP can be divided into two parts: pure integer linear program which all of its variables are integer and binary linear integer program which all of its variables are 0 or 1. Its main solving methods are similar to the IP which were mentioned above. Those methods are mostly branch-and-bound method and cutting plane method.

As analyzed above, both LP and IP can address the optimization problems in bio-energy supply chain and have a great application potential in the SCM. The MILP, which is the combination of LP and IP, can be applied in nearly every stage across the biomass or bioenergy supply chain, from strategic decision making level to tactical decision making level and to operational decision making level. For example, in the strategic decision making level, Dal-Mas et al (2011) presented a dynamic spatial explicit and multi echelon MILP modeling framework to assess the risks on investment and economic performances of a biomass-based ethanol supply chain. A case of corn-to-ethanol production supply chain in North Italy is used in order to support the effectiveness of MILP application in biofuel supply chain. Giarola et al (2013) developed a general MILP modelling framework to make planning decisions and strategic designs in a multi-echelon and multi-period ethanol supply chain. A case of the future potential Italian biomass-based ethanol production is used to prove effectiveness of MILP in the strategic decision level. Ann et al (2014) applied a MILP method to design a cellulosic biofuel supply chain. The supply chain design includes the determinations of facilities capacities, locations and technologic types along with a strategic plan for materials flow about storage, transportation, and production. Besides, in the level of tactical decision, Marvin et al (2011) optimized a lignocellulose biomass to ethanol supply chain in the Midwestern United States by using MILP. This optimization involves the determination of optimal capacities and locations of bio-refineries. Osmani et al (2014) proposed a two-stage stochastic MILP to optimize a sustainable lignocellulose based biofuel supply chain. This optimization involves the selection of optimum location of bio-refinery and choice of optimum conversion technology. Finally, in the operational decision level, Dyken et al (2010) developed a MILP model for basic elements in a biomass supply chain encompassing demand, supply, storage, and processing of different types of biomass. Papapostolou et al. (2011) proposed a MILP for the optimum operation and design of biofuel supply chain to facilitate the decision making in different planning and operational issues. This model
is an integrated method which considers both economic and technical parameters that affecting the performance of the biofuel value chain.

Based on the large number of publications about the MILP application in biofuel SCM, it is safe to conclude that the MILP is an excellent and powerful tool to address the problems in the biofuel SCM. Besides that, being the hybrid of IP and LP, MILP inherits the advantages of both of them, which enable its application in every stage of the entire supply chain.

3.6.3 Multiple criteria decision analysis.

Multiple criteria decision analysis (MCDA) is a mathematical tool and decision aid which helps the decision makers to make a judicious choice by comparing different scenarios and alternatives under many conflicting criteria (Roy 1996). Based on different types of criteria, the MCDA can be classified into two distinguished parts: multiple attribute decision analysis (MADA) and multiple objective decision analysis (MODA). (Malczewski 1999).

In MADAs, attributes are used as categorization criteria to select the optimum alternatives or to rank the alternatives in descending order of preference (Wang et al 2009). In spatial MODA, the attributes act as the criteria map layers in a geographic information system (GIS). Then, the capabilities of MADA and GIS techniques are combined to synthesis the data and the preference of the decision maker into sortable unidimensional alternative decision values. Shi et al (2008) applied a MADA approach to estimate the feasibility of building a new biomass power plants as well as select the optimal location in Guangdong, China. The attributes are the location of raw material harvest field and the efficiency score calculated by a distance decay function. Kahraman et al (2009) used the fuzzy MADA method to determine the best renewable energy alternative in Turkey. This methodology is the integration of axiomatic design (AD) principles and analytic hierarchy process (AHP). Zhang et al (2011) used the MADA to determine the optimal location of conversion facility in a woody biomass to biofuel supply chain based on the attributes of the population census, distributions of village and city, county boundaries, pulpwood distribution in the county, and transportation networks.

Multiple objective decision analysis is another form of MCDA in which the determination of best alternatives is mainly based on multiple conflicting objectives (Parnell 2008). The main idea of MODA can be simplified as adding weight on each objectives of an objectives echelon-tree according to the preferences of decision makers and importance of the objectives. The final decision is determined by the rank of weight on each objective. Zamboni et al (2009) used a MODA technique associated with a MILP modelling framework to optimize the conflict objectives between environmental and economic performance of a bioethanol production supply chain. The economic objective determines facilities location, biomass cultivation site, transportation system,
and ethanol production capacity with minimum cost. The environmental objective minimizes greenhouse gas emission by applying a well to tank approach to evaluate the impact of supply chain on global warming over its entire life time. Mele et al (2011) combined MODA with MILP and used it to optimize a sugar-ethanol supply chain. In this problem, the mainly conflict objectives are the environmental and economic performance of the entire supply chain.

It is necessary to introduce the term of multi-objective optimization method, a special area of MCDA. The multi-objective optimization method is concerned as a mathematical optimization method which has the ability to optimize more than one objective functions simultaneously. Generally, this method is used to optimize the objective functions which is conflicted with each other. Solving multi-objective optimization problem is like approximating to or computing all the representative set of Pareto optimal solution. The Pareto optimal solution exists when no objective function value can be improved without degrading some objective values (Miettinen 1999). The multi-objective optimization method can be used in the strategic decision making level, for example Zangeneh et al (2009) applied a multi-objective optimization algorithm to generate a Pareto set of optimal planning scheme in Distributed generation expansion planning by considering different objective function. However, the optimal planning scheme is chosen by using a Monte Carlo Simulation. Soroudi et al. (2010) used a long term dynamic multi-objective planning model associated with an Immune-GA based method to address the Distributed Generation (DG) planning and formulated problems. This model can not only optimize the costs and the emissions objectives, but also provide the optimal scheme of placement, sizing, and timing of investment on network reinforcement and DG units over the planning period.

The MCDA method is a good tool for decision making when there exist multiple conflict objectives in the problem and multiple conflict disagreements among the decision makers. It can compare the different criteria and rank them out. This property makes this method suitable to address the problems occurred in biofuel SCM. Since optimizing the whole supply chain can involve many conflict criteria and consider many different aspects, such as social responsibilities, economic, and environmental. In many case, the decision makers have to consider and weight many complex factors to determine which one is the most impending. Especially, now the sustainability of supply chain draws more and more attention among governments and many entrepreneurs hope to seek a good solution to balance relationship among the social responsibility, environmental friendless and economic profitability of their supply chain. Therefore, the MCDA may have huge potential applications in the SSCM.

3.6.4 Combination of hybrid optimization Methods

Optimization models can be combined with each other to generate a new hybrid optimization method in order to better solve some complex problems and meet some
special needs. For example, Cai et al. (2009) used an optimization method to solve a complex problem about long-term planning of renewable energy management system and obtain some useful solutions for energy systems management planning. This is an inexact community-scale energy model, which integrates the interval linear programming, MILP and chance-constrained programming techniques. Its solutions prove a desire management planning with a maximized system reliability, a maximized energy security and minimized system costs, which can help the decision makers to select the desired policies under a variety of constrains. In this example, the hybrid optimization model is good at making wiser decisions under many limitations, which indicates that the hybrid method can deal with many complex problems. Besides, this hybrid method can also be applied to solve other systems such as biochemical management system or food management system because those systems are also need to be managed under many constrains. Sadegheih (2009) used an optimization model which is developed by using MIP, GA and SA to design an optimal network structure of system transmission planning with the minimum costs of carbon emissions. In this model, the GA is used to simplify the iteration. This hybrid method can not only optimize the network planning system, but also take environmental issues into consideration, which indicates a multi-functional characteristic of hybrid optimization method. Rentizelas et al. (2010) developed a hybrid optimization method to overcome the restrictions posed by the intricacy of the optimization problem in order to figure out the locations of a bioenergy facilities that optimizes the system-wide investment and operational costs in Greece. The location problem is modeled as a non-linear optimum problem with objective function of investment yield. The result shows that when solving this specific problem, the hybrid optimization method is better than the stochastic method and the sequential quadratic programming. This is a good case to illustrate 1+1>2, the performance of using hybrid optimization method is better than using a single optimization method when dealing with the same problem. Dai and Zheng (2015) propose a hybrid optimization method in order to solve a complex under-uncertainty, multi-echelon, multi-product, and multi-period closed-loop supply chain network design model. The hybrid optimization method combines Monte Carlo simulation embedded hybrid genetic algorithm, fuzzy programming and chance-constrained programming together, so that the network structure of the closed-loop supply chain and the uncertainty issue can both be determined and addressed. In addition, by using this hybrid optimization method, the problem can obtain a global optimum result with maximized profit and less computational time. This case shows the strong ability of hybrid optimization method because it can solve very complex problem even under many uncertainties but still shows an excellent performance.
3.7 Mathematical Optimization software

In the modern era, optimization problems are the real-world problems which can be seen in many different areas, such as business, engineering, science, and mathematics (Chandrakantha 2012). For example, assuming assigning 50 people to 50 positions, the benefit of person i to position j is represented by \( y_{ij} \). Each person only has one position, and each job must be filled. This problem includes 100 restrictions, 2500 activities and 50! different position solutions (Dantzig 2002). It is obvious that this problem is difficult to solve by hand. However, with the mathematical optimization software, the real-word problem can be solve. The problem can be formulated into a mathematical model by using a proper programming language, and be solved by the optimization software. And the (Funaki 2009). In this manner, optimization software is easy to input data, specify constrains, perform optimization, and visualize result, especially for many large problems (Souza 2014).

There are more than 40 types of software can optimize mathematical problem. Among them, this paper only selects 5 types of software to analyze. Table 3.6 provided the information about this six mathematical optimization software and their supporting problem types.

Table 3.6 shows the programming languages and type of supporting problems of six popular optimization software. Among them, AMPL and CPLEX are highly popular software. AMPL is used to describe and solve very complex problems for large scale optimization and scheduling problems (Fourer et al 2002). According to NEOS statistics, AMPL is the most popular optimization software because the similarity of its syntax to the mathematical notation in optimization problems, the wide adaptability of problem types, and free for academic and noncommercial users. Besides, CPLEX also earns its popularity by its wide adaptability and multi-language interface. CPLEX is good at addressing integer programming, very large linear program problems through either dual or primal variants of simplex method or barrier interior point method. (Mittelmann 2007)
<table>
<thead>
<tr>
<th>Name</th>
<th>Problems</th>
<th>Language</th>
<th>Advantages</th>
<th>Disadvantages</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMPL</td>
<td>Modeling, LP, NP, MIP, MINP, MIQP, MIQCP</td>
<td>C++, Java, Python</td>
<td>Can exchange data with external data sources. Supports a wide range of problem types. Allows separation of model and data. Support re-use and simplify the construction of large-scale problems</td>
<td>Commercial software, needs to be purchased.</td>
</tr>
<tr>
<td>CPLEX</td>
<td>Modeling, IP, LP, MILP, MIQP, MIQCP, MISOCP</td>
<td>C, C++, C#, Java, Python</td>
<td>Free for academic use. Supports a wide range of problem types. Very fast running time. Flexible interface. Could solve large-scale and complex problems. Support wide variety of program languages;</td>
<td>Commercial software, needs to be purchased;</td>
</tr>
<tr>
<td>GAMS</td>
<td>Modeling, LP, NP, MIP, QCP</td>
<td>C, Fortran</td>
<td>Straightforward and understandable syntax. Solve large-scale and complex model efficiently. Full constrain equation automatically</td>
<td>Not convenient for nonprofessional user solving small problems</td>
</tr>
<tr>
<td>MATLAB</td>
<td>LP, NP, QP</td>
<td>C, C++, Java, Fortran, Python</td>
<td>Relatively easy to learn; Relatively quick in performing matrix operations; Easier to fix errors.</td>
<td>Commercial software. Its interpreted language result it in a slower speed than compiled language;</td>
</tr>
<tr>
<td>Excel</td>
<td>LP, IP, MILP, NP</td>
<td>--</td>
<td>Easy to learn; Good enough to solve many tasks</td>
<td>Poor computational performance on large scale models; Hard to debug</td>
</tr>
</tbody>
</table>
3.8 Supply Chain Management Applications

3.8.1 SCM applications on forest products

Forest products include various types, from standing timber and logs, to solid wood products such as lumber and different panels, and to fiber products such as paper and paperboard (Adams et al 2013). There are many successful applications of SCM in these forest products, Table 3.7 is the summary of the important applications of SCM in forest products.

Table 3.7 important applications of supply chain management in forest products

<table>
<thead>
<tr>
<th>SCM method</th>
<th>Application example</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supply chain</td>
<td>Facilities configuration design</td>
<td>Huang et al (2010)</td>
</tr>
<tr>
<td>based analysis</td>
<td>Manufacturing system design</td>
<td>Mansoornejad et al (2010)</td>
</tr>
<tr>
<td></td>
<td>Business process optimization</td>
<td>Windisch et al (2013)</td>
</tr>
<tr>
<td></td>
<td>Economic impact evaluation</td>
<td>Alam et al (2014)</td>
</tr>
<tr>
<td>SCOR model</td>
<td>logistic processes optimization</td>
<td>Schnetzler et al (2009)</td>
</tr>
<tr>
<td>MILP</td>
<td></td>
<td>Gunnarsson et al. (2004)</td>
</tr>
<tr>
<td>GIS-based model</td>
<td></td>
<td>Tahvanainen et al. (2011)</td>
</tr>
</tbody>
</table>

In SCM, strategic long-term decisions, such as the decisions of type of product, technology, number, location and size of each facility, are made. Supply chain based analysis that helps to make long-term decisions can be used as a supply chain tool to analyze and evaluate a company’s long-term strategies. Besides, the applications of supply chain based analysis in forest bio-refinery is emerging (Mansoornejad et al 2013). For example, Huang et al (2010) developed a process model which can simulate the integrated forest bio-refinery under different scenarios to determine the best configuration of the bio-refinery. They used this model to compare the economic benefit of three integrated forest bio-refinery scenarios: conventional Kraft pulping process, pulp mill-based integrated forest bio-refinery with pre-extracted hemicelluloses and short fiber based ethanol production, and pulp mill-based integrated forest bio-refinery hemicelluloses extraction prior to pulping. The result shows that the second scenario has a better economic benefit under a fixed feedstock throughput. Mansoornejad et al (2010) proposed a systematic hierarchical method which integrating product portfolio design into supply chain design in order to construct a decision making framework for forest bio-refinery. In this method, manufacturing flexibility design, process/product
portfolio design, and supply chain design are integrated together by a margins-based supply chain operating policy. The supply chain based analysis method is applied to help a P&P mill implementing forest bio-refinery. Windisch et al (2013) applied supply chain analysis method to analyze the forest biomass supply chains in Finland and Germany in order to identify business processes and stakeholders of supply chain. 268 projects in Germany and 213 projects in Finland have been studied in this case. The results show a considerable difference in supply chain process in these projects. Although the results are company specific and cannot be generalized directly, each supply chain does reflect the feature of its operational country. Therefore, this method can be further applied into the in-depth analysis of forest biomass supply chain and treated as a step towards holistic cost calculation as well as business process optimization approaches on supply chain level.

In addition, the SCOR model is also a diagnostic method for SCM. It enables the companies to understand their business process and to identify the critical feature that improve the level of customer satisfaction (Ntabe et al 2015). The SCOR model is widespread in industry (Schnetzler et al 2009) and the following is an example of its application on forest product. Schnetzler et al (2009) proposed a modified SCOR model, whose standardize process elements are modified in terms of wood supply, delivery, harvest, and forest planning, to describe and standardize the second level of woody supply chain in technical timer production. This model can generate a mapping of forest reality and depict the differences of different levels in detailed, which means this method can be a first step towards standardized and improved inter-organizational logistic processes in the woody supply chain.

The following outcomes are also from the researches about SCM in forest products. Hudson (2000) studied the wood fuel supply chain in England by carrying out the trials on compaction system of the Swedish Bala Press baling system in England from 1996 to 1997. He found that greater productivity can result in less supply costs. This results were introduced into a number of harvesting systems. Gunnarsson et al. (2004) studied a large Swedish bioenergy-fuel-supplying entrepreneur and used a large MILP model to solve the supply chain problems. In this case, the supply chain problems include methods of transporting and storing the forest residues to fulfill the demand of heating plants; the time and location of converting the residuals into forest fuel; whether contracting the additional harvest areas and saw-mills or not; the flow of goods from saw-mills and import harbors; and the decision of using which terminal. Carlsson et al. (2005) studied a pulp production company in Sweden and described five major cases that focus on improving the wood flow chain management. They concluded that the optimization models used in these cases have a huge potential in providing better decisions for the company in the future. Windisch et al. (2010) investigated two forest owners’ associations (FOA) of forest fuel procurement to find out whether modern SCM applications can increase the profitability of forest fuel procurement operations.
The profitability is determined by the cost-benefit analysis which using the net present value methodology. It turns out that the benefits are far exceed the cost over a period of ten years. The results also show that a huge potential cost saving in forest fuel purchases is feasible if improving the work flows and reducing the work input. Tahvanainen et al. (2011) created a GIS-based model for energy wood supply chain and simulated the costs for several energy wood supply chains in a certain area of eastern Finland in order to find the optimal transportation method. The authors finally concluded that for distances within 60 kilometers, truck transportation of end-facility and loose residues is the best choice, while for longer distances, roadside chipping with chip truck transportation is the optimal selection.

3.8.2 SCM application on cellulosic biomass based biofuel

There are many successful applications of SCM in cellulosic biomass biofuel, Table 3.8 is the summary of important applications of SCM in cellulosic biomass biofuel.

<table>
<thead>
<tr>
<th>SCM Method</th>
<th>Application</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic Model</td>
<td>Facility location selection of corn bio-ethanol</td>
<td>Rendon-Sagardi et al. (2014)</td>
</tr>
<tr>
<td>Supply chain based analysis</td>
<td>Supply chain network design and Inventory control of a bio-refinery</td>
<td>Ekşioglu et al. (2009)</td>
</tr>
<tr>
<td></td>
<td>Transportation problem of a lignocellulos biomass supply chain</td>
<td>Sultana et al. (2011)</td>
</tr>
<tr>
<td></td>
<td>Output optimization of a rice straw power plants consider environmental issues</td>
<td>Shafie et al. (2014)</td>
</tr>
<tr>
<td>Risk Analysis</td>
<td>Climate-related hazard mitigation of a cellulosic bio-fuel supply chain</td>
<td>Langholtz et al. (2014)</td>
</tr>
<tr>
<td>Static MILNP</td>
<td>Post-disaster Recovery of a bio-fuel supply chain network</td>
<td>Poudel et al. (2016)</td>
</tr>
<tr>
<td>Mathematical model</td>
<td>Supply chain network design of a bio-energy conversion plant</td>
<td>Gan and Smith (2011)</td>
</tr>
<tr>
<td></td>
<td>Demand forecasting of a bio-ethanol supply chain</td>
<td>Huang et al (2010)</td>
</tr>
<tr>
<td></td>
<td>Logistic process optimization of a switchgrass-based biofuel supply chain</td>
<td>Zhang et al. 2013</td>
</tr>
<tr>
<td>MILP</td>
<td>Scheduling problem</td>
<td>Dunnett et al (2007)</td>
</tr>
</tbody>
</table>
The details of these applications are discussed in the following paragraphs. In the field of cellulosic biomass and biofuel, the SCM can help a company to make a wiser decision in the initial strategic planning stage. For example, Rendon-Sagardi et al. (2014) analyzed an ethanol supply chain by developing a system dynamic model in order to determine whether the biofuel production should be developed in Mexico. The model explores five scenarios and evaluates the availability of areas for sowing grain sorghum and sugarcane crops, the possible decline in carbon dioxide emissions, and the productivities of ethanol and fuel. The model concerns the parameters and trends impacting the energy and agricultural industries, and provides valuable information about the conditions of Mexican fossil fuel and biofuel productions and supply in the future. The obtained results show that Mexico will face a fuel crisis in the future and the biofuel availability will collaborate little to meet the fuel demand of Mexico in the future. This is an example of applying supply chain analysis method to make long-term decisions for a bioethanol supply chain. Through developing a dynamic model to simulate several scenarios, decisions can be made based on the information provided by analyzing simulation results. Ekşioğlu et al. (2009) proposed a model that could be used to design a biomass to bio-refinery supply chain, and tested this model in Mississippi State. It was found that the supply chain generated by this model has better impacts on decisions about number, size and location of the bio-refinery, and the inventory problems of biomass. This case is about applying supply chain network design model to design the biofuel supply chain in the initial strategic planning stage. The result of the Mississippi case indicates the well-performance of this application. Langholtz et al. (2014) studied climate risk management for the cellulosic biofuels supply chain in the U.S. in order to mitigate the impacts of climate-related hazard on the cellulosic biofuels industry. The authors pointed out that there are opportunities and strategies across the supply chain to improve adaptive capacity in response to the risk. In particular, the influence of climate change can be altered by the expansions of cellulosic feedstock like woody biomass and perennial grasses. Moreover, increases in feedstock development, extension, and logistic can create better opportunities to support the sustainable development of the bioenergy industry in the United States. This case is also a good example of using supply chain analysis method to make long-term decisions. By understanding the mechanism of how the feedstock alert climate change, the decisions of increasing cellulosic feedstock development, extension, and logistic can be made by the cellulosic biofuel industry. Poudel et al. (2016) combined a spatial static model with mixed integer nonlinear programming (MILNP) model to design a pre-disaster planning model for a bio-fuel supply chain network. This model is used to strengthen the links among the facilities inside the supply chain network against disasters as well as minimize the transportation cost involved in the supply chain network. The post-disaster connectivity maximization is achieved by using a spatial static model developed from real world data, and the cost minimization is achieved by using the MILNP model. They validated the feasibility of the model by applying this
model in the case in Mississippi and Alabama. The results show that this model can save 0.27 dollar per gallon when the disaster occurs. This study is a very proactive research, since supply chain network has a long-term impact, therefore, preventing or minimizing the disaster damage in SCND is very significant. This study takes the post-disasters network connectivity into consideration when designing the supply chain network, ensures an easier conduction of post-disaster and less pay in post-disaster rescue. From the above examples, it can be concluded that using supply chain management method can help the cellulosic biofuel producers to make better long-term decisions in the strategic planning stage.

In addition, since the economic benefit is what companies care most, there are many researchers trying to use supply chain management method to improve economic benefits of the bioenergy companies. For example, Gan and Smith (2011) developed a generic framework, which can determine the optimal size of bioenergy conversion plant, cost of bioenergy production, as well as feedstock supply radius, to minimize the cost of both energy conversion and feedstock production. This supply chain management tool is used in a case of producing cellulosic bioethanol and generating electricity from biomass. The application shows that this tool can elucidate the relationship among activities in bioenergy supply chain and provide strategies for enhancing the bioenergy cost competitive. In this case the economic cost of a bioenergy conversion plant is minimized by applying supply chain network design method. Sultana et al. (2011) analyzed multiple feedstock transportation methods of three types of lignocellulosic biomass (wheat straw, corn stover, forest biomass) to determine the optimal delivery costs. It was found that the delivery cost of a single type of biomass is higher than the mix of agricultural and woody biomass feedstock, which had an optimal combination of 30% in bales and 70% in woody chips. In this case, the economic benefit is improved through analyzing the biomass supply chain to determine the optimum combination percentage of feedstock delivery. Huang et al (2010) proposed a mathematical model for bioethanol supply chain strategic planning and applied this model in a case of California to evaluate the economic potential and facilities requirement of bioenergy production. They found that with a well-designed supply chain, the production cost can be stable at a very low cost: $1.1 per gallon. In addition, Dunnett et al (2007) used a state-task network approach to develop a multi-period MILP and applied this model to design the supply chain and operational scheduling of the biomass to heat company. The application of this model helps the company to achieve 5-25% improvement on cost minimization goal. The above two cases both indicate the effect of a well-designed supply chain on economic benefits. From the above examples, it can be concluded that SCM can help the bioenergy company to minimize the cost by optimizing the transportation cost, scheduling, and the intra-system configuration.

Apart from considering the economic benefit, current business operators also need to consider the environmental performance. Therefore, researchers are also trying to use
SCM to improve the environmental performance. For example, Shafie et al. (2014) analyzed the aspects of logistic cost and supply potential in a rice straw supply chain from Malaysia to determine the optimal output of rice straw power plants. They used carbon emissions and environmental impacts as the references and concluded that allocating a small power plant of 10 MW can help to protect the environment. They also predicted that Malaysia can generate power on a small scale (no more than 12 MW) using rice straw as feedstock for electricity. This case indicates that the SCM can not only benefit the company economically, but also can improve the environmental performance. Zhang et al. (2013) constructed an integrated mathematical model to make the optimum logistic decision of a switchgrass-based biofuel supply chain with a minimum cost. The feasibility of the method is tested by applying the optimized supply chain in the state of North Dakota in U.S. The case study result shows that by using this SCM optimization method, the marginal land for switchgrass feedstock production can be reduced by 39% and still 100% satisfying the annual gasoline energy equivalent requirement of North Dakota. From the above cases, SCM can be successfully applied to improve both economic and environmental performance of cellulosic biomass based biofuel industry.

From the cases shown above, using SCM can help the cellulosic biofuel companies make long-term decisions in the initial strategic planning stage (Rendon-Sagardi et al. 2014, Ekşioğlu et al. 2009, Langholtz et al. 2014), improve economic performance in the strategic planning stage (Gan and Smith 2011, Huang et al. 2010, Dunnett et al. 2007), improve economic benefit in the operational stage (Sultana et al. 2011), and improve both economic and environmental performance (Shafie et al. 2014, Zhang et al. 2013).

3.9 Summary of literature review

Supply chain management is a business process to effectively manage the activities of the whole supply chain of a company. The activities of the whole supply chain not only include the vertical supply chain, such as resource planning, feedstock sourcing, product manufacturing, product delivering, and customer services, but also include the horizontal supply chain, such as the collaborations with supplier, third party agents and customers (Lambert et al 1998 and Stock et al 2009).

Although researchers hold different opinions on what elements should be included in supply chain management (Cooper et al. 1997, Lambert et al. 2000, Fleischmann et al 2003 and Vierasu et al. 2011), most of them agreed that network/organization structure is an important element in the supply chain management (D’Ignazio et al 2014). The supply chain network structure contains the participants in supply chain, supply chain business process links, and supply chain network dimension (Lambert et al 2000).
Supply chain network structure can impact all of the decision making activities in a supply chain (Farahani et al. 2014).

The power of a well-designed supply chain network is remarkable, because it impacts all the following tactical and operational decisions (Farahani et al. 2014). Supply chain network design is the tool to design a feasible network structure for a supply chain. It can not only determine the optimal size and location of each facility, but also determine the cash flow and material flow among these facilities (Autry et al. 2013). According to the quality revolution of the 1980s and the supply-chain revolution of the 1990s, it has been clear that the best supply chain management needs to integrate environmental management with ongoing operations (Srivastava 2007). Green supply chain network design is a good practice of integrating environmental management into supply chain network design (Miranda-Ackerman et al. 2017). In green supply chain network design, both economic and environmental performance can be optimized simultaneously. The economic performance can be quantified as cost or profits (Autry et al. 2014) and the environmental performance is usually quantified as greenhouse gas emissions (Ahi and Searcy 2015).

Based on different objectives and different situations, there are different types of green supply chain network design models. These models can be categorized into single objective model, multi objective model, deterministic model, and stochastic model. In single objective model, environmental factors can be directly integrated into the objective function or set as constrains. Single objective model is used when there is no conflict between environmental objective and economic objective, such as the case that both economic cost and energy consumption need to be minimized, or the case that both economic cost and greenhouse gas emissions need to be minimized (Eskandarpour et al. 2015). In multi-objective model, both the economic and environmental factors can be formulated as the objective functions. The multi-objective model is used when there is a tradeoff between economic and environmental objective, such as the case that needs to maximize the profits but minimize the greenhouse gas emissions (Mota et al. 2015). In deterministic model, customer demand, transportation cost, feedstock cost, emissions, and etc., are known. While in stochastic models, these data are uncertain. Therefore, the model selection should be based on the actual situations and considerations.

There are quite a few optimization methods available for supply chain network design. The categories of optimization methods include heuristic approach, mathematical programming, multiple criteria decision analysis, and hybrid optimization method. Heuristic approach can be considered as a shortcut and it can find a good solution in reasonable time. However, it cannot guarantee to find the optimal solution. Heuristic approach is used when the problem is complicated and solving the problem is time-consuming. Mathematical programming is the classic optimization method which can provide an optimal solution. Multiple criteria decision analysis (MCDA) is a
mathematical tool which helps the decision makers to make a judicious choice by comparing different scenarios and alternatives even under conflicting criteria (Roy 1996). Hybrid optimization method is generated by combining two of the existing optimization method together. It can be applied to solve some complex problems or to meet some special needs. Similar as model selection, the adoption of optimization methods is also based on the actual situations and considerations.

Optimization software is used when it is difficult to solve the optimization model under human capability. By using optimization software, the real-world problem can be described into a mathematical objective function by using a proper programming language. In order to obtain the optimum output, the variables can be represented as the parameters and constrains can be added into the program (Funaki 2009). There are more than 40 types of software available to optimize mathematical problems. Table 3.6 provides the information about six commonly used mathematical optimization software and the applied problem types.

Considering the topic of this dissertation, bio-butanol related topics have also been reviewed. Bio-butanol is a four-carbon alcohol that can be produced from lignocellulose biomass through acetone butanol ethanol (ABE) fermentation (García et al. 2011). Bio-butanol is considered as a type of renewable fuel and has been qualified under the Renewable Fuel Standard. Similar but superior to bio-ethanol, bio-butanol can not only be blended into gasoline with higher proportion, but also has lower volatility, lower vapor pressure, less hygroscopicity, less corrosiveness, and water immiscibility (Dürre 2007). The American Society for Testing and Materials (ASTM) D7862 fuel quality standard shows that bio-butanol can be blended with gasoline up to 12.5%. In addition, a 16% bio-butanol blended gasoline is the legal fuel equivalent to E10 (a 10% ethanol blended gasoline), which indicates that using bio-butanol as a blender can save more gasoline than using ethanol under the same fuel property requirement (AFDC 2016). In addition to its usage as fuel additive, bio-butanol can also be used as a direct replacement of gasoline based on its direct usage in unmodified gasoline engines and diesel engines (Kumar et al. 2009, Gu et al. 2012, Yun et al. 2016). Furthermore, bio-butanol cannot only be transported by tanker truck and rail, but also be potential to be transported through the existing pipeline infrastructure (AFDC 2016).

Because bio-butanol is a very promising fuel in the future transportation fuel market, many efforts were made to improve its production process (Cheng et al. 2012; Yadav et al. 2014; Cai et al. 2013; Elbeshbisy et al. 2015; Su et al. 2015; Kumar et al. 2017). However, research rarely goes outside of the production process and studies the whole supply chain of bio-butanol. Although Morone and Pandey (2014) published a literature review paper that integrates all the stages of butanol production together, they seldom talked about the integration of bio-butanol supply chain.
4 Methodology

4.1 Overview of methodology

All objectives of this research project can be addressed by their corresponding method. The overview of the method design is shown in Fig. 4.1. As indicated in Fig 4.1, the research goal is generated based on the information from literature review and industrial background. To achieve this goal, a mathematical programming model needs to be developed. A case study was adopted to gather the information on the production process of the cellulosic bio-butanol industry and identify the structure dimension of the supply chain network. A questionnaire survey was utilized to map the logistic activities of the bio-butanol supply chain and identify the business process links of the supply chain. After that, the secondary data and results from the case study and questionnaire survey were analyzed to identify the physical infrastructure of cellulosic bio-butanol supply chain network and determine the participants of the supply chain network. Finally, a mathematical model was developed to design a green cellulosic bio-butanol supply chain network.

Fig. 4.1 Overview of the study design (Methodology)
4.2 Methods for objective 1: Evaluate the production process of the bio-butanol industry

Objective 1 sought to understand the production process of the bio-butanol industry. To achieve this objective, a case study methodology was used. Case study refers to the analysis of persons, events, decisions, projects, policies, institutions, and other systems which can be studied by one or more methods. The case is an object that can provide an analytical framework (Thomas 2011). Case study is a method of social science research. Compared with other forms of social science research, case study is mostly preferred when in the situations of: (1) answering “why” or “how” research questions; (2) the behavioral events that researchers cannot or nearly cannot control; and (3) contemporary phenomenon. Generally, case study can be applied in many disciplines, such as psychology, sociology, business, anthropology, marketing and etc. A case study can also be used to investigate the structure of a certain industry, including its organizational and managerial processes (Yin 2013). In this objective, case study was adopted to address a series of “why” research questions by observing the managerial process of several industries.

4.2.1 Design of the method

According to the theoretical framework of case study design proposed by Yin (2013), the case study should contain five major components which include research questions, research propositions or research purpose, unit of analysis-the “case”, linking data to propositions, and criteria for interpreting a case study’s finding (Yin 2013).

4.2.1.1 Research Question

What are the production processes in the bio-butanol industry?

4.2.1.2 Research Propositions or Research Purposes

Research propositions can benefit any case study, but not every case study needs to have the propositions, such as exploratory research when the experience, knowledge, and information was very limited (Baxter et al 2008). In this project, the related information from literature was not enough, so a proposition cannot be drawn. Instead, an exploratory study can have research purposes (Yin 2013). The research purposes of this case study are:

- Identify the equipment and facilities involved in the cellulosic bio-butanol supply chain network
- Identify the production processes involved in the cellulosic bio-butanol supply chain network.
- Identify the material flow involved in the cellulosic bio-butanol supply chain network
4.2.1.3 Units of analysis: the “cases”

Since the real operating cellulosic bio-butanol company was not open for visiting, the selection of the “cases” is very critical. The integrated bio-refinery research facility (IBRF) of national renewable laboratory (NREL) has the capability of producing various type of cellulosic bio-fuel. It also has the experiences of producing cellulosic bio-butanol. Therefore, the unit of analysis of this case study was the IBRF.

4.2.1.4 Linking Information to Research Purpose and Criteria for Interpreting a Study’s Findings

This case study observed the production processes of the IBRF and collects information on how the IBRF acquires their raw material, treats the raw material, produces the major product, and manages the major product and any byproducts. Based on the collected information and considering the similarity between bioethanol and bio-butanol production, the production process of the cellulosic bio-butanol supply chain network can be identified. Finally, the information from this case study was summarized and used for further objectives.

4.2.2 Proposed activities

This case study was achieved by conducting an observation on the IBRF. Observation was focused on the bio-fuel production, feedstock and fuel storage, feedstock and fuel transportation, as well as production plant location selection.

During the visit, the production processes of a cellulosic biofuel production were tracked from raw material acquirement to product production and finally to the product transportation. The observation process took half day due to the visiting limitation of NREL. During the observation, the answers of the following questions were ascertained to record a comprehensive process flow of the supply chain:

- How was feedstock acquired?
- What was the time, frequency, and volume for purchasing feedstock?
- How many feedstock storage sites were there, where were they located, and how large should they be?
- How was the location of production plant chosen? Describe the surrounding area of the bio-refinery.
- How was biofuel produced?
- What was the production yield of bio-butanol from a t/kg biomass?
- How was biofuel stored?

The arrangement of the case study is listed in the following table. The Table 4.1 includes the expected outputs from the case study and their associated activities.

<table>
<thead>
<tr>
<th>Table 4.1 the outline of activities and output in the case study</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activities</td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th>Observe the layout of the bioethanol production plant</th>
<th>Determine the facilities contained in the bioethanol production plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Observe whether there are any harvesting site inside or near the production plant or ask the relevant staff how they get the raw material</td>
<td>Determine the method of feedstock acquisition</td>
</tr>
<tr>
<td>Observe their feedstock storage site and ask the relevant staff how they treat the feedstock before manufacturing</td>
<td>Determine the feedstock pretreatment method, as well as the size and capacity of the storage site</td>
</tr>
<tr>
<td>Question the relevant staff or the professors in the production plant</td>
<td>Determine the production processes</td>
</tr>
<tr>
<td>Observe whether there are ASTs or storage site for co-products in the productions and visit their storage site or directly ask the relevant how they treat the major product or co-product</td>
<td>Determine the methods of major products and co-products storage, as well as the size and capacity of the ASTs</td>
</tr>
<tr>
<td>Observe whether there are any railroad near the production plant or tanker truck in the production plant or ask the relevant staff how they ship their major feedstock and the frequency of shipping out the final products</td>
<td>Determine the fuel distribution methods</td>
</tr>
<tr>
<td>Observe the whole manufacturing process of the production plant, from raw materials to final product and record all the activities occur in the production plant step by step.</td>
<td>Determine the material or production flow in the production plant</td>
</tr>
<tr>
<td>Question the relevant staff what is their annual yield and their production size</td>
<td>Determine the relationship among annual yield, feedstock input and production size</td>
</tr>
<tr>
<td>Interview the available expert or engineer inside the production plan</td>
<td>Determine the capital cost of the bio-refinery, holding cost of inventory storage, selling price of the products, and the methods to reduce the production cost</td>
</tr>
</tbody>
</table>

4.2.3 Limitations
- The cellulosic bio-butanol industries did not allow visitors.
• The time for visit was short, the information collected from the visit may be incomplete. To fulfill the missing information, the information from IBRF websites were also used.
• Although the IBRF has experiences in bio-butanol production, the production processes and equipment in the IBRF were not specific for cellulosic bio-butanol.
• The IBRF of NREL is a research facility, its production processes may be different from the production processes in commercial industry. The production processes in commercial industry should be the most cost-saving processes. However, for research facility, the cost is not the most critical consideration.

4.2.4 Expected outcomes of objective 1
• The type of facilities inside the bioethanol production plant
• The time, frequency, and volume of feedstock deliveries corresponding to the size of production plant
• The transportation mode of feedstock and biofuel
• The pretreatment of feedstock
• The surroundings of the bio-refinery
• The number, size and location of production plants corresponding to the volume of feedstock or annual production yield
• The method or process to produce biofuel
• The method to store the biofuel

4.3 Methods for objective 2: Map the logistics activities in the bio-butanol supply chain

Objective 2 was formulated to map the logistics activities in the bio-butanol supply chain. To achieve this objective, a survey was used to collect the necessary data. Responses from this survey may shine light on the behaviors and attitudes of decision makers within the supply chain. Modern online questionnaire tools make data collection and result analysis faster and easier. Statistics software such SAS, JUMP, and Excel ease the analysis of data. However, the design of questionnaires is a challenging process that requires many considerations (Wilson 2013).

4.3.1 Design of the method
4.3.1.1 Purpose of Questionnaire survey

This questionnaire was aimed at studying the logistics activities of the cellulosic bio-butanol supply chain and identifying the businesses processes links of cellulosic bio-
butanol supply chain network. Meanwhile, the attitudes of the cellulosic biofuel producers towards the environmental issues were gathered.

4.3.1.2 Sampling of Questionnaire survey

The goal of this questionnaire was to understand the logistic activities of cellulosic bio-butanol supply chain management, the population of this study should be the cellulosic bio-butanol producers. However, from table 1.1.1, only two companies are producing cellulosic bio-butanol as a renewable fuel in the U.S.: Butamax and Gevo. This small number of cellulosic bio-butanol producers cannot qualify as an appropriate sample size for a questionnaire survey. Due to the similar feedstock, usage and production facilities (Morone and Pandey 2014), existing ethanol production plants can cost-effectively be modified into butanol production plant by changing the distillation technology. Thus an expanded sample of ethanol production facilities were requested to take the questionnaire survey. Finally, the target population of this questionnaire survey included 15 cellulosic bio-ethanol production plants (including existing and proposed production plants) and 2 bio-butanol producers in the U.S. Limited by the population scale, the sample of interest was also the 15 second generation bio-ethanol producers and the 2 bio-butanol producer in the U.S.

4.3.1.3 Strategy to Gain the Highest Response Rate

To increase response rate, the design and implementation of the questionnaire followed the requirements from Tailored Design Method (TDM). According to TDM, the response rate will increase when the participants feel that the cost is low and the reward is high while understanding the source is trustworthy (Dillman et al 2009). The following elements were used in the questionnaire design:

- To lower the cost:
  1. Made all the questions relevant
  2. Made the question short and easy to complete
  3. Put the questionnaire in an online format
- To increase the reward:
  1. Showed positive regards and thank the respondents
  2. Asked the participants for help
- To build the trust:
  1. Told the participants the sponsorship of this survey is obtained from legitimate authority
  2. Showed appreciation in advance
  3. Assured participants that the information collected would be secure and confidential
  4. Explained the usage of the collected data
  5. Provided participants the contact information of the researcher
4.3.1.4 Questions in questionnaire

The questionnaire contained three sections which include basic information of the company, logistics activities of cellulosic bio-butanol supply chain, and environmental issues. The first section collected basic information on the company such as the location of the company, annual production yield, number of facilities, and annual biofuel sale. The second section asked questions on the logistics activities of the cellulosic supply chain, such as the purchase, storage, and transportation of the feedstock and fuel, as well as the criteria for selecting the location of the production plant. The last section focused on the environmental issues faced by the cellulosic bio-butanol companies. The question included whether companies value the balance between economic profits and environmental impact. These questions were almost all multiple-choice and ask for both closed-ended and open-ended responses. The specific questions of each sections are shown as follow:

- Basic information of the company:
  1. What’s the location of your production plant?
  2. What’s the annual cellulosic biofuel yield?
  3. What’s the unit price cellulosic bio-butanol?

- Supply chain management:
  1. How do you acquire the feedstock?
  2. Are you purchase the feedstock only one time in a year or you need to backorder feedstock several times?
  3. How do you acquire the vehicle for feedstock transportation?
  4. Where do you store the biofuel?
  5. What’s transportation methods are utilized to ship the biofuel from production plant to the ASTs?
  6. What kind of vehicle are you using to ship the biofuel from ASTs to fossil fuel refineries/terminals?
  7. How do you acquire the vehicle for biofuel transportation?

- Environmental issues:
  How much portion of economic profits do you want to pay for the related environmental issues?

4.3.1.5 Data analysis plan for the questionnaire survey

Since many of the questions were categorical multi-choice questions, categorical data analysis (CDA) was adopted to analyze the data collected from the questionnaire survey. For single variable questions, the results were known by counting the number of responses for each option (Cody 2011; Stokes et al 2012). For multiple variable questions, the results were analyzed by forming a contingency table and using the Fisher’s exact test to study the potential relationship among the selected choices (Fienberg 2007, Fisher 1922, Agresti 2002). It is necessary to mention that the
questionnaire involved the option of no response. That means that the condition of missing data will occur. In order to compensate for the missing data, multiple imputation technique was used. The multiple imputation is a statistical technique which uses two or more imputed values to replace the missing data. The imputed values follow a probability distribution which is determined by the observed data. (Carpenter and Kenward 2012). The overview of the data analysis plan is shown in Fig. 4.2.

![Fig. 4.2 Overview of Data Analysis Plan](image)

4.3.2 Proposed activities

The activities of the survey included 3 parts: information collection, online survey, and data analysis. At the very beginning, the information on the U.S cellulosic bio-butanol and cellulosic bio-ethanol companies were collected from online resources. The information of these companies includes name and contact information of the company administrators, major type of bio-fuel, and location of the company. The online survey included 3 recruitment activities. In the first recruitment activity, the invitation letters were sent out through email to the administrator of each cellulosic bio-fuel company. A sample of the invitation letter is shown in Appendix F: Invitation Letter for the Survey. After two weeks of the first recruitment activity, the reminder emails were sent out to the administrators who failed to complete the survey during the first round of contact. A third reminder email was sent out a week after the second recruitment. The data were analyzed after 1 week of the third recruitment. The timeline and the proposed activities were summarized in Table 4.2.

<table>
<thead>
<tr>
<th>Time</th>
<th>1 week</th>
<th>2 weeks</th>
<th>1 week</th>
<th>1 week</th>
<th>2 week</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activities</td>
<td></td>
<td>Online Questionnaire Survey</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

75
4.3.3 Limitations of the method

- There are only 17 companies in the U.S producing cellulosic bio-butanol and bioethanol.
- Objective 2 focused on mapping the logistic activities of a bio-butanol supply chain. The accuracy of the results was lower due to the survey sample including a large portion of cellulosic bioethanol producers.

4.3.4 Expected outcomes of objective 2

- The annual cellulosic biomass to biofuel yield
- The unit price of cellulosic bio-butanol
- The method and frequency of acquiring the feedstock
- The method of feedstock transportation
- The location of feedstock storage
- The location of feedstock preprocess
- The location of biofuel storage
- The method of biofuel transportation
- The factor of choosing the location of bio-butanol production site
- The weights of economy and environmental issues

4.4 Methods for objective 3: Identify the physical infrastructure of bio-butanol supply chain

Supply chain network refers to a complex web in which infrastructure can be cross-linked with each other by the flow of materials and information among them. Supply

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<table>
<thead>
<tr>
<th>Data Collection</th>
<th>1st Recruitment</th>
<th>2nd Recruitment</th>
<th>3rd Recruitment</th>
<th>Data analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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</table>
chain network design works to determine the optimal configuration of the supply chain with certain long-term objectives (Varsei and Polyakovskiy 2016). A well-designed supply chain network can not only reduce supply chain cost and improve service levels, but also improve the environmental performance of a company. With a well-designed supply chain network, a company can maintain its competitiveness for a long time. Since a well-designed supply chain network can achieve this wide variety of benefits, the design phase of a SC network should be processed very cautiously. In this dissertation, the results from literature review, case study and questionnaire survey are analyzed and cross-checked with each other to design the network. The network structure of the bio-fuel supply chain is shown in Fig. 4.3.

Fig. 4.3 Network structure of bio-fuel supply chain

4.4.1 Design of the methods
The analysis of a supply chain network included 3 parts: identifying the physical infrastructure of a cellulosic bio-butanol supply chain, identifying the participants within a cellulosic bio-butanol supply chain, and constructing the cellulosic bio-butanol supply chain network. The detailed information of these 3 parts are stated as followed.

4.4.1.1 Supply chain physical infrastructure identification.
The supply chain physical infrastructure includes the equipment and facilities needed for the supply chain network, such as warehouses, production plants, and distribution centers. The equipment for bio-butanol production can be identified from the results of objective 1. Other facilities, which were not included in the results of objective 1, can be identified from the literature review. In this part, the results of objective 1 and the literature review were analyzed and cross-checked with each other to provide the physical infrastructure of the cellulosic bio-butanol supply chain

4.4.1.2 Identification of supply chain participants
The supply chain participants refer to the companies and organizations who have direct and indirect involved in the supply chain (Lambert et al 2000). From the physical infrastructure of the cellulosic bio-butanol supply chain, the supply chain participants were easily identified. Furthermore, the function and associated costs of each participant were identified by analyzing the results of objective 1, objective 2, and the literature review.

4.4.1.3 Supply chain network structure construction
The supply chain network structure includes participants in the supply chain, network structural dimension, and supply chain business processes links (Lambert et al 2000). The network structure dimension was identified in objective 1. The supply chain business process links were identified in objective 2. The participants in the supply chain were identified by the physical infrastructure requirements of the supply chain
network. Results from objective 1, objective 2, and objective 3 provided data for understanding the flow of material, participants, the functions, equipment and associated costs of each member. The picture of the cellulosic bio-butanol supply chain network was visible.

4.4.2 Proposed activities

The results from objective 1 and objective 2 were analyzed together to construct the cellulosic bio-butanol supply chain network. The physical infrastructures of the cellulosic bio butanol supply chain were identified based on the literature review and the results of the two objectives. After that, the participants of the cellulosic bio-butanol supply chain network were also identified. The identification of supply chain participants was based on the information gathered on the physical infrastructures of cellulosic bio-butanol refining, literature review, and the results of objective 1 and 2. Finally, the supply chain network structure was constructed based on the information of the physical infrastructures and the participants of cellulosic bio-butanol supply chain network.

4.4.3 Limitations of the method

There is no previous research that discusses the cellulosic bio-butanol supply chain network design, so there is no direct reference with which to compare methodology and results.

4.4.4 Expected outcomes of objective 3

- The physical infrastructures (feedstock supplier, feedstock storage site, bio-butanol production plant, bio-butanol storage site, and bio-butanol blending site) of the bio-butanol supply chain network the transportation methods between these infrastructures
- The participants of cellulosic bio-butanol supply chain network
- The supply chain network structure of cellulosic bio-butanol
4.5 Methods for objective 4: Develop a mathematical model for green bio-butanol supply chain network design

Supply chain network design focuses on determining the optimal transportation methods and supply chain configuration, such as the location, number, capacity and types of facilities. The supply chain network design should be completed during the strategic phase of the supply chain management building, based on its long-term effects and inflexibility.

4.5.1 Design of the Method

In order to optimize this network, a multi-objective integer linear programming model was used to model the operation of the whole supply chain network. The research goal of this section was to optimize the supply chain network with economic and environmental objectives. Therefore, two objective functions (economic and environmental) were optimized simultaneously. The life cycle analysis (LCA) technique was used to formulate the environmental objective function. The net present value was used to formulate the economic objective function. The $\varepsilon$–constraint method was used to balance these two objectives. Before implementing the model, a pre-test was conducted in Excel with dummy data to check its feasibility and accuracy.

4.5.1.1 LCA Integration

Life Cycle Analysis (LCA) refers to a systematic process that can evaluate the environmental impact of every stage in a product’s life cycle from cradle to grave. To integrate the LCA approach with a mathematical model, four major phases are involved (You et al 2011). The first one is the goal and scope definition, in which the scope and performance measurements should be decided. Since greenhouse gas (GHG) emissions occur in nearly every stage of the cellulosic bio-butanol supply chain, it is a reasonable index for the environmental impact measurement of this network. Therefore, for this study, LCA is used to measure the GHG emissions of feedstock cultivation and harvest, feedstock storage, feedstock transportation, fuel production, and fuel transportation. The second phase is the inventory analysis, in which the data from Argonne GREET Model, the Aspen Plus process model, and the U.S Life Cycle Inventory Database can be utilized. In the third phase, the information gathered from the second phase is translated into a single indicator. In this case, the GHG emissions including the emissions of carbon dioxide, methane, and nitrogen dioxide are aggregated into single indicator called carbon dioxide equivalent emissions. The final phase is to analyze the results.
4.5.1.2 Net Present Value

The money at the present time is more valuable than the money in the future (Wikipedia 2017). Therefore, to estimate the profit of a project, the cash flow across different time periods should be treated differently. The net present value can help to achieve this goal since it can measure the profit within a period of time. The net present value can be calculated by subtracting the initial investments from the present values of cash flows over a period of time (Kurt 2003). The profit of a cellulosic bio-butanol project is different from year to year while the initial capital investment only occurs in the first year. Therefore, using net present value to formulate the economic objective function is a reasonable unit of measurement.

4.5.1.3 $\varepsilon$–Constraint Method

After integrating the environmental objective function with LCA, there is a tradeoff between the economic and environmental functions. In this dissertation, the $\varepsilon$-constraint method is used to solve this tradeoff. In order to use the $\varepsilon$-constraint method, one of the objective functions need to be transferred into constraints at the very beginning. In order to obtain the optimal solutions by $\varepsilon$-constraint method, the initial step is to obtain the upper and lower bound of the feasible solutions. The lower bound can be obtained by minimizing the environmental objective function subject to the relevant constraints. While the upper bound can be obtained by maximizing $ce + \chi \cdot ei$ subject to the objective functions and all constrains, where $ce$ is the economic objective function, $ei$ is the environmental objective function, $\chi$ is a very small value which is about $10^{-6}$. The final step is to maximize the economic objective function subject to all constraints and a new added constrain which is $ei \leq \varepsilon$, where $\varepsilon$ is obtained by dividing the range of feasible solutions into evenly distributed number of intervals (Mavrotas 2009).

4.5.1.4 Initial setup of the Model

In order to test the feasibility of constraints in the model, an optimization tool in Excel named Solver was used. The model was tested by listing the dummy data into an Excel worksheet and inputting constraints and objective function in the Solver dialog. Fig. 4.4 shows part of this preparatory work of the test. After the optimization, we got the result report, as shown in Fig. 4.5. If the model was wrong, Solver cannot output a reasonable result. Instead, it could be an invalid number or error message. For the model proposed in this dissertation, the economic objective value ($6,026,159,001$) and the environmental objective value ($460,296,673,416$ kg CO$_2$ eq) are both valid. The total supply chain profit for 5 years was 6 billion, which was also reasonable. That means the model was feasible to work.
For the time period setup, in order to investigate the impact of seasonal availability of the cellulosic feedstock, the length of the time period was set to be five years.

Although the supplier is located in the State of Missouri, there are no fuel refineries in that particular state according to the list of oil refineries published by Oil and Gas Journal. Therefore, the blending site of this supply chain network refers to the intrastate fuel terminals and (or) the nearest out-of-state fuel refineries depending on the distance between the production plant and those refineries and terminals. The locations of the blending site, the distance between the supplier and production plant, and the distance between the production plant and blending site were obtained by Google Maps.
shows how to get the distance information from google maps. From the graph, the distances between two locations are shown based on using different transportation vehicles.

![Google Map Data Test](image)

**Fig. 4.6 Google map data test**

In this case the major supplier and possible blending sites are located in the central area of the United States where the major transportation mode is inland transportation, such as rail road, pipeline, and trucks. For short-distance transportation, such as biofuel transport from production plant to ASTs, pipeline is referred. While for the long distance transportation, such as feedstock transportation from supplier to biofuel production plant and biofuel transportation from production plant to blending site, three types of modes were considered, including rail, large truck, and large tanker truck. The cost data involved in biomass transportation can be obtained from Searcy et al 2007. The Fig. 4.7, a screen shot from the paper of Searcy et al 2007, shows the transportation cost of straw or stove based on different transportation methods.
The GHG emission data for the environmental analysis of feedstock transportation, feedstock storage, fuel production, fuel storage, and fuel transportation were obtained from the GREET Model of Argonne National Laboratory. The Fig. 4.8 shows the data of GHG emissions of bio-butanol production from the GREET Model.

### Table 3

<table>
<thead>
<tr>
<th>Mode</th>
<th>Item transported</th>
<th>DWC1</th>
<th>Units</th>
<th>CPC2</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Truck</td>
<td>Straw/stover (2)</td>
<td>0.12</td>
<td>$/Actual t/m³</td>
<td>4.39</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td></td>
<td>Woodchips (2)</td>
<td>0.07</td>
<td>$/Actual t/m³</td>
<td>3.01</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td></td>
<td>Ethanol (9)</td>
<td>0.01</td>
<td>$/Actual t/m³</td>
<td>3.86</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td>Rail (2)</td>
<td>Straw/stover</td>
<td>0.025</td>
<td>$/Actual t/m³</td>
<td>14.15</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td></td>
<td>Woodchips</td>
<td>0.017</td>
<td>$/Actual t/m³</td>
<td>5.48</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td>Ship (8)</td>
<td>Straw/stover</td>
<td>0.01</td>
<td>$/Actual t/m³</td>
<td>54.01</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td></td>
<td>Woodchips</td>
<td>0.01</td>
<td>$/Actual t/m³</td>
<td>11.15</td>
<td>$/Actual t/m³</td>
</tr>
<tr>
<td>Pipeline</td>
<td>Biomass (7)</td>
<td>234 C.3.4 D.02</td>
<td>$/Dry t/m³</td>
<td>4.19×10⁶</td>
<td>C.3.4 D.02</td>
</tr>
<tr>
<td></td>
<td>Ethanol (10, 30)</td>
<td>4.13 C.2 D.03</td>
<td>$/Ethanol/kg</td>
<td>0</td>
<td>$/t Ethanol/kg</td>
</tr>
<tr>
<td></td>
<td>Ethanol (4, 10)</td>
<td>0.062 C.2 D.01</td>
<td>$/L/kg</td>
<td>0</td>
<td>$/L</td>
</tr>
</tbody>
</table>

1. Source data have been adjusted to consistent units and a common currency (USD, US dollars).
2. Pipeline capacity in metric tons of ethanol produced per day.
3. Pipeline capacity in liters of ethanol produced per day.

---

**Fig. 4.7** screen shot of a table about straw transportation costs in different transportation methods

**Fig. 4.8** data retrieved from GREET Model
4.5.2 Proposed activities

The proposed activities included 3 parts. The first part was to formulate the multi-objective linear integer programming model. The second part was to validate and test the model in Excel by using dummy data. After the feasibility of the model was verified, the model can be utilized. In part 3, the model was applied to design the sorghum stem bio-butanol supply chain network in MO. Through this application, the optimal location and production size of a bio-butanol production plant were determined with maximum profits and minimum GHG emissions.

4.5.3 Limitations of the methods

Based on the requirements of this DOE project, the sorghum producers in Missouri State were chosen as the major suppliers. Since the major supplier to this plant was a sorghum producer, the sorghum straw was selected as the feedstock. In addition, according to the requirements of this DOE project, the final product needed to be a cellulosic biofuel. Considering the pros and cons of the current existing cellulosic biofuels such as bioethanol, pyrolysis bio-oil, and bio-butanol, cellulosic bio-butanol was selected to be the final product depending on its higher blending compatibility with gasoline, lower volatility, lower vapor pressure, less hygroscopic, less corrosiveness, and water immiscibility.

4.5.4 Expected outcomes of objective 4

In objective 4, the MILP was used to design the bio-butanol supply chain network. The expected outcomes included a mathematical model for cellulosic bio-butanol supply chain network design and the results of the model application. The mathematical model can determine the optimal transportation method and the series of configuration parameters, such as the location, number, capacity and types of facilities required within the supply chain network.

The mathematical model was applied to a case study in the state of Missouri (MO). By applying this model, the tradeoff between feedstock availability and market availability of sorghum stem bio-butanol can be resolved. And the optimal transportation method, location and production capacity of the sorghum bio-butanol production plant in the state of MO were determined.
5 Results

5.1 Results of objective 1

Objective 1 was to develop an understanding of the production process of bio-butanol. To complete this objective, a visit to the Integrated Bio-refinery Research Facility (IBRF) at the National Renewable Energy Laboratory (NREL) in Denver, CO was conducted on April 26, 2017. During this visit, information was collected regarding the types of equipment used inside the biofuel production plant, various biomass sourcing methods, biomass storage locations, biomass pretreatment processes, bio-fuel production processes and bio-fuel storage methods. In addition, in order to provide a comprehensive view of the production process of the bio-butanol industry, secondary data were also collected. The information collected from the onsite visit and the secondary data were combined together as the results of objective 1. The detailed results of this objective are presented in the following sections based on the expected outcomes of objective 1.

5.1.1 Equipment inside the bioethanol production plant

5.1.1.1 Feedstock Storage Room

There are many ways to store feedstock, such as stacking bales outdoors, wrapping bale in plastic, or storing in covered buildings or pole barns. However, outdoor feedstock storage causes 5% to 15% dry matter losses. Therefore, indoor storage is preferred (EPA 2010). In IBRF, indoor storage was employed. The storage room was located in the basement of the IBRF building. In the central region of the storage room, two columns of double-layered-shelves were used to store different types of baled cellulosic biomass. The feedstock was packed into bags and stored on the upper and lower layers of the shelves.

In addition, the functions of the feedstock storage room included not only feedstock storage, but also feedstock pre-treatment. In order to improve the quality and stability of the production process, biomass production requires pretreatment processes to reduce water content and filter out contaminants (Holm-Nielsen and Ehimen 2016). In IBRF, some simple pretreatment processes, such as size reduction and contaminants cleaning, can be completed in the feedstock storage room. Inside the storage room, acids used in the feedstock pretreatment process, including hydrochloric acid (HCL) and sulfuric acid (H₂SO₄), were stored in the tanks beside the storage shelves. Additionally, the storage room was equipped with bulk bag unloaders, bulk storage hoppers, bulk feed conveyors, knife mills, train feed hoppers, and cyclones.

The basic pretreatment processes consisted of the following four steps. 1. The biomass was unloaded by the bulk bag unloader into the bulk storage hoppers. 2. The bulk feed
conveyor delivered the unloaded biomass to the knife mill. 3. The biomass was cut and separated into smaller sizes by the knife mill. 4. The milled biomass was sent out for pre-treatment process through a pneumatic conveyance system. The detailed information of the equipment used in these steps is shown in Table 5.1.

Table 5.1 Equipment inside storage room

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>Double layered-shelves</td>
<td>Biomass storage</td>
</tr>
<tr>
<td>Bulk bag unloaders</td>
<td>Unload biomass from large bags</td>
</tr>
<tr>
<td>Bulk storage hopper</td>
<td>Store the unloaded biomass</td>
</tr>
<tr>
<td>Bulk feed conveyor</td>
<td>Deliver the unloaded biomass to knife mill</td>
</tr>
<tr>
<td>Knife mill</td>
<td>Shrink the size of biomass</td>
</tr>
<tr>
<td>Train feed hopper</td>
<td>Collect the milled biomass</td>
</tr>
<tr>
<td>Cyclone</td>
<td>Remove char and tar</td>
</tr>
<tr>
<td>Pneumatic conveyance system</td>
<td>1. Transfer biomass between bulk storage and train</td>
</tr>
<tr>
<td></td>
<td>2. Feed hopper and between train feed hopper and</td>
</tr>
<tr>
<td></td>
<td>cyclone</td>
</tr>
</tbody>
</table>

5.1.1.2 Biochemical conversion pilot plant

The conversion pilot plant at the IBRF was used to pre-treat biomass and to produce bio-fuel. The conversion pilot plant is the primary area of IBRF. It includes two floors. The second floor was used to pre-treat biomass. The major feedstock pre-treating equipment included a vertical pre-treatment reactor system and a horizontal reactor system. The horizontal pre-treatment reactor system allowed the feedstock to be pre-treated with chemicals in a temperature ranging from 150 to 210°C. The vertical pre-treatment reactor system was equipped with two reactors, allowing the feedstock to be pretreated with chemicals at two temperatures ranges: 120 to 210°C and 120 to 180°C. Each of them has the capacity to pre-treat up to one dry ton of biomass per day. These two pre-treatment systems were connected to the feedstock storage room through a pneumatic conveyor system. This way, the milled biomass from the feedstock storage room was transferred to the pretreatment systems without further contamination.

The first floor of the pilot plant was used to convert the pre-treated biomass into various types of bio-fuel. The production flow inside the conversion pilot plant can be seen in Fig. 5.1. The equipment on this floor included a dynamic impregnator reactor system, high solids enzymatic hydrolysis reactors, fermentation systems, and a membrane filtration system. The dynamic impregnator reactor system is a multifunctional system.
designed for spraying, soaking, low-severity pre-treatment, enzymatic hydrolysis, fermentation, concentration/evaporation, and distillation. The high solid enzymatic hydrolysis reactors were used for enzymatic hydrolysis process. The biomass pre-treated by both systems was then delivered to the hydrolysis reactors to complete enzymatic hydrolysis. The hydrolyzed biomass was delivered to the fermentation systems to be converted into sugars, fuels, and chemicals. Finally, the membrane filtration system was used to recover the biofuels from the fermentation broth. The pipelines were used to transport materials and to connect these systems with each other. The equipment in the pilot plant was used to handle a wide range of biomass feedstock types and different pre-treatment processes. Further, there were several freezers outside of the building, which were used to store the cold fermentation materials.

![Flowchart](image.png)

**Fig. 5.1 Equipment in the conversion plant**

5.1.2 The reorder frequency and volume of feedstock corresponding to the size of production plant

Biomass, like agricultural residue, is available only at the time of harvest (Speight 2011). However, the bio-fuel producers need to produce bio-fuel continuously in a year, which therefore requires a continuous supply of biomass feedstock. To achieve a continuous supply of biomass, different companies have different inventory management plans.
Accordingly, the IBRF has the capacity to process two dry tons of biomass into several bio-fuels and chemicals per day. With this production capacity, they generally store seven days of biomass feedstock in their storage room. In addition, they have their feedstock delivered once a week to fulfill their inventory. The conversion pilot plant needs 14 dry tons of biomass per week to run continuously, which is how much they reorder on a weekly basis.

5.1.3 Pre-treatment of feedstock

As was stated before, biomass feedstock needs to be pre-treated before its conversion into biofuel. The pretreatment processes at the IBRF include two major types: physical pre-treatment and chemical pre-treatment. The physical pre-treatment is conducted first. This includes size reduction and dirt removal. In the feedstock storage room, after the biomass is unloaded into the storage hopper, the knife millers are used to cut and separate the feedstock biomass into smaller sizes. The milled biomass feedstock is then placed inside a cyclone to remove tar and char. After these physical pre-treatment processes, the chemical pre-treatment process is conducted. Here, several chemicals, such as acid, ammonia, alkali or etc., are mixed with biomass feedstock in the tube of the pre-treatment system. Then the mixture is heated from 120 to 210 °C inside the reactor vessel. If needed, the heated feedstock will go through a secondary heating process with a lower heating temperature in another reactor vessel.

5.1.4 Surroundings of bio-refinery

According to observations made outside the IBRF, there is nothing special around the bio-refinery. The conversion pilot plant was not operating during the time of visit, so it was hard to measure the average noise of the plant. It was also difficult to determine the amount of air pollution around the plant. However, based on observations form inside the IBRF, there are many pipelines and most of these pipelines are marked with “hot water”. A bio-refinery with an annual production of 100-million-gallon ethanol will consume 200 to 400 million gallons of water annually (National Research Council et al 2008). So it is reasonable to infer that the location of the bio-refinery must have easy and ready access to sufficient water resources.

5.1.5 Number, size and location of production facilities corresponding to the volume of feedstock or annual production yield

The IBRF converts different types of biomass into different types of bio-fuels and chemicals. Although IBRF has the capacity to convert two dry tons of biomass per day, the exact conversion rate of bio-fuel from biomass is hard to determine. Production yields for bio-fuel varies depending on the type of biomass used, different production processes used, and different pre-treatment processes used. Therefore, it is difficult to determine the annual production yield of a particular fuel from one onsite visit. However, I still collected useful data. To convert two dry tons of biomass feedstock a day, IBRF is equipped with two pre-treatment systems, each of them able to convert
one dry ton of biomass per day. Besides, they have four high solids enzymatic hydrolysis reactors and four primary 9,000-L fermentation vessels. At the location, the pretreatment systems are on the second floor of the conversion pilot plant. The hydrolysis reactors are in the first floor, directly underneath the two pre-treatment systems and fermentation systems.

5.1.6 The process of producing bio-fuel

In the IBRF, the process to produce bio-fuel includes five major steps. 1. At the beginning, knife mills are used to shrink the size of feedstock biomass and the cyclone is used to clean the feedstock biomass. 2. The biomass is delivered to the pre-treatment systems to go through the chemical pre-treatment process. The chemical pre-treatment method varies, including acid hydrolysis, alkaline hydrolysis, an organic solvation process, and more. (Morone and Pandey 2014). 3. The pre-treated biomass is treated with enzymes in the high-solid enzymatic hydrolysis reactor to make soluble sugars. This process is called enzymatic hydrolysis. 4. The soluble sugars from the hydrolysis reactors are delivered into the fermentation system to produce bio-fuel. 5. After the fermentation process, the membrane filtration system is used to separate bio-fuel from the fermentation broth. These five major steps are also used to produce bio-butanol (Morone and Pandey 2014, Dutton 2017). The process to produce cellulosic bio-butanol is summarized in Fig. 5.2. The figure also shows the seven different options for biomass pre-treatment, one traditional bio-butanol recovery option and three commercialized feasible options for bio-butanol recovery. It is also necessary to mention that the other two recovery options, which are absorption and treatment by a membrane reactor, are not economically feasible for industrial usage (Kaminski et al 2011).
5.1.7 Method to store the biofuel

Generally, bio-fuel is stored within ASTs. However, at the NREL, the bio-fuel product is used mainly for research purposes and therefore large volumes do not need to be stored. Therefore, there is no AST at the NREL.

5.1.8 Summary of results of objective 1

The data collected from the onsite visit are analyzed, and the material flows and production processes of a cellulosic bio-butanol supply chain are summarized in Fig. 5.3.
Fig. 5.3 material flow and production process of a cellulosic bio-butanol supply chain

At the beginning of the production process, a knife mill is used to shrink the size of the feedstock biomass. After that, the biomass is placed into the pre-treatment systems to go through the pretreatment process. The pre-treatment method varies, including acid hydrolysis, alkaline hydrolysis, an organic solvation process, and others. (Morone and Pandey 2014). The pre-treated biomass is then converted into soluble sugars using enzymes in the high-solid enzymatic hydrolysis reactor. The soluble sugars from the hydrolysis reactor are delivered into the fermentation system to produce bio-butanol. After the fermentation process, bio-butanol is separated from the fermentation broth by the membrane filtration system. Finally, the bio-butanol is stored inside ASTs, which are located near the production plant.
5.2 Results of objective 2

Objective 2 was to map the logistical activities of the bio-butanol supply chain. To complete this objective, an online survey of a sample of biofuel producers in the U.S. was conducted. In addition, secondary data were also used to supplement missing data from the survey. The population of the survey was composed of 15 advanced bio-ethanol producers and two bio-butanol producers. Seven responses were collected for a response rate of 41.18%. 85.7% of the responded companies are considered second-generation bio-ethanol producers, with the rest being cellulosic bio-butanol producers. In the category of bio-ethanol companies, 50% of them identify themselves as cellulosic bio-ethanol producer; the rest of them did not. They actually produce bio-ethanol by using feedstock such as crop residues, energy glass, or biomass crops, so these companies are identified as advanced bio-ethanol producers. The results of objective 2 are presented in the following sections based on the expected outcomes of this objective.

5.2.1 Annual cellulosic biomass to biofuel yield

The annual cellulosic biomass-to-biofuel yield is considered confidential by the companies. In addition, the biomass-to-biofuel yield varies depending on the different types or combinations of biomass and different production methods used. Therefore, it is difficult to gather accurate data. The only responses gathered from this survey was 41% to 60%, which was from one of the cellulosic bio-ethanol companies.

It is not feasible to estimate the conversion rate of bio-butanol by using the conversion rate of bio-ethanol; so secondary data are collected to supplement the missing data. The production yield of bio-butanol varies according to different biomass used, different production processes, and different pre-treatments. Table 5.2 shows the maximum bio-butanol yield from five types of biomass through the acetone–butanol–ethanol (ABE) fermentation process. The production yields of wheat straw, barley straw, corn stover, and switchgrass are gathered from Dutton (2017). The production yield is calculated from the production process of sulfuric acid pre-treatment, enzymatic hydrolysis, ABE fermentation, and membrane recovery. The production yield of sweet sorghum bagasse was collected from Qureshi et al. (2016). They developed a novel cellulosic butanol fermentation process. In this process, sweet sorghum bagasse is pre-treated by a liquid hot water (LHW) pre-treatment technique and produced through enzymatic hydrolysis and ABE fermentation. This production achieves a maximum ABE concentration of 16.88 g/L and hourly production yield of 0.34 g/L*h. This number is 0.04 g/L*h higher than the ABE production yield that uses acetic acid (AA) to pre-treat feedstock and utilizes a membrane recovery method to remove any inhibitors.
Table 5.2 Bio-butanol production yields from various types of biomass (Dutton 2017, Qureshi et al 2016)

<table>
<thead>
<tr>
<th>Type of biomass</th>
<th>ABE production yield</th>
<th>Hourly production yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wheat straw</td>
<td>25.0 - 28.2 g/L</td>
<td>0.63 - 0.71 g/L*h</td>
</tr>
<tr>
<td>Barley straw</td>
<td>26.6 g/L</td>
<td>0.39 g/L*h</td>
</tr>
<tr>
<td>Corn stover</td>
<td>26.3 g/L</td>
<td>0.31 g/L*h</td>
</tr>
<tr>
<td>Switchgrass</td>
<td>14.6 g/L</td>
<td>0.17 g/L*h</td>
</tr>
<tr>
<td>Sweet sorghum bagasse</td>
<td>16.88 g/L</td>
<td>0.34 g/L*h--</td>
</tr>
</tbody>
</table>

5.2.2 Methods and frequencies for acquiring feedstock

Data about feedstock acquisition methods were also collected through this survey. Fig. 5.4 shows the distribution of the particular feedstock sourcing method of each type’s producer. In Fig. 5.4, we can see that contracting with a third-party aggregator was the most popular feedstock sourcing method. It is necessary to mention that some companies were using hybrid methods which combine different feedstock sourcing methods. For example, 28.57% responders contracted with both local suppliers and third-party feedstock aggregators to source their feedstock.

![Fig. 5.4 Feedstock Sourcing Method Distribution](image)

The data about feedstock sourcing frequencies were also collected from the online survey. According to the responses, different companies reflected different feedstock
sourcing frequencies. The variety of sourcing frequencies included daily, monthly, yearly, and unknown sourcing frequencies. Some of the sourcing activities depended on the demand and feedstock availability. Others occur periodically based on the contract with suppliers.

5.2.3 Methods for feedstock transportation

The results of various feedstock transportation methods are shown in Fig. 5.5. Fig. 5.5 indicates that responders preferred suppliers to deliver their feedstock by truck for free. This means that feedstock transportation costs are paid by suppliers instead of the producers.

![Fig. 5.5 Distribution of feedstock transportation methods](image)

5.2.4 Location of feedstock storage

There are three options to store biomass feedstock (Zafar 2015):

- Hauling the biomass directly to the bio-refinery without storing it at the harvest site during harvest season.
- Storing the biomass at the harvest site and then transporting it to the bio-refinery as needed.
- Storing the biomass at a collective storage facility and then transport to the bio-refinery from the intermediate storage location.

Agricultural residues are available only at the time of harvest (Speight 2011), so the bio-fuel producers need to have a year’s worth of feedstock storage capacity. However, due to the low-energy density of the agricultural residues, storing a year’s worth of feedstock requires a large space, and storing all of them in the bio-fuel production site is impractical. In addition, storing the feedstock at farms also be problematic, since it can cause heating value reduction, biomass degradation, potential health risks, and low-
energy density as well as high-transportation costs due to high moisture content (Holm-Nielsen and Ehimen 2016). The third option is to use the secondary storage site. In this option, the harvested feedstock is moved to a secondary storage facility before being transported to the bio-fuel production site. The number of secondary storage sites is determined by the bio-refinery’s capacity bio-refinery and the density of feedstock production (EPA 2010). However, there is the additional cost of renting, building, or maintaining the secondary storage sites. Further, delivering the feedstock to secondary storage sites increases the transportation costs.

In order to see how producers deal with this problem, the survey included a question about the feedstock storage location. Fig. 5.6 shows the distribution of feedstock storage sites for each type of producer. The results indicate that storing the feedstock in the bio-refinery is adopted by all of the responders. In addition, it is necessary to mention that there was a company that uses two storage sites. They store the feedstock in both harvesting sites and secondary storage sites depending on the time of year.

Fig. 5.6 distribution of feedstock storage site

![Feedstock Storage Site Distribution](image)

5.2.5 Location of feedstock preprocess

The data regarding the feedstock pre-process locations were obtained from the survey. According to the survey results, responders highly agreed with the choice: preprocessing the feedstock at the production site. The results indicate that setting up the feedstock pre-process facilities in the production site is very common within the second-generation bio-fuel industry.

5.2.6 Location of bio-fuel storage

The data related to bio-fuel storage locations were also gathered from the survey. According to the survey results, responders highly agreed with the option of storing the bio-fuel in ASTs inside the production site. The results indicate that setting up the
storage sites of the bio-fuel in the ASTs inside the production site is very common for the second-generation bio-fuel industry.

5.2.7 Methods for bio-fuel transportation

The information about bio-fuel transportation methods, which include bio-fuel transportation vehicles and bio-fuel transportation destinations, was obtained through the survey. Fig. 5.7 illustrates the distribution of bio-fuel transportation vehicle choices. Both the railway and fuel tanker trucks are most commonly used as bio-fuel transportation vehicles. 28.57% of responders prefer to use railway only; 28.57% of responders prefer to use fuel tanker trucks only; 14.29% of responders prefer to use both. 71.43% of the responders contracted with a third-party distribution center to transport their bio-fuel. Therefore, contracting with third-party distribution centers to transport the bio-fuel through railway or fuel tanker trucks were the most commonly used methods for bio-fuel producers to transport biofuel.

![Graph showing distribution of bio-fuel transportation vehicle types]

**Fig. 5.7 distribution of bio-fuel transportation vehicle types**

As for the destination, all bio-ethanol producers (cellulosic and advanced) transport their bio-ethanol to fuel terminals. But cellulosic bio-butanol producers transport their final products directly to their customers.

5.2.8 The factors of choosing the location of production plant

The factors affecting the choice of a bio-refinery location were collected from the research. According to the collected responses, the factors for choosing the location of the production plant are similar among producers. Most of the respondents considered feedstock availability and market availability as critical factors. The market here refers to the bio-fuel and co-product markets. Other factors, such as the availability of favorable government incentives, energy costs, and the utility of existing infrastructure
were also mentioned. However, no data on this question from the cellulosic bio-butanol producers were available because of confidentiality issues. Fig. 5.8 shows the distribution of the factors for choosing the production plant location.

![Fig. 5.8 Factors for choosing the location of bio-fuel production site](image)

### 5.2.9 The weights of economy and environmental issues

For the question about environmental protection, the mean of the weights of economic and environmental importance were calculated for each type of secondary bio-fuel producer. Table 5.3 shows the results of the calculation. The economic and environmental weights were used as the quantitative indicators to measure the preference between environmental or economic issues. The results indicated that economic issues have a very heavy weight, which was 75% for cellulosic bio-ethanol producers and 80% for advanced bio-ethanol producers with environmental issues being viewed as controversial. The cellulosic bio-ethanol producers gave minimal consideration to environmental issues but the advanced producers did not consider them as primary issues. The cellulosic bio-butanol responder indicated that there was not relationship between economic and environmental issues, but they also implied that the environmental aspects were considered.

### Table 5.3 weight of economy and environmental issue for each type of bio-fuel producer

<table>
<thead>
<tr>
<th>Producer type</th>
<th>Economy weight</th>
<th>Environmental weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulosic Bio-ethanol Producer</td>
<td>75%</td>
<td>40%</td>
</tr>
</tbody>
</table>

97
<table>
<thead>
<tr>
<th>Advanced Bio-ethanol Producer</th>
<th>80%</th>
<th>0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>mean</td>
<td>77.5%</td>
<td>20%</td>
</tr>
</tbody>
</table>

5.2.10 Summary of results for objective 2

The logistical activities of cellulosic bio-butanol production are summarized in
Table 5.4. The bio-butanol producers contract with third-party feedstock suppliers to acquire their feedstock. The third-party feedstock aggregators deliver the feedstock to the producer by truck for free. After the feedstock arrives at the production plant, the feedstock is stored on-site and awaits further processing. After the completion of the production process, bio-butanol is stored inside the ASTs at the production plant and then delivered to the customers by the third-party distribution companies. In addition, when choosing the location of the bio-butanol production plant, two factors were critical: feedstock availability and market availability.
Table 5.4 Summary of results for objective 2

<table>
<thead>
<tr>
<th>Expected outcomes</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>The annual cellulosic biomass-to-bio-butanol yield</td>
<td>As shown in Table 5.2</td>
</tr>
<tr>
<td>The method and frequency of acquiring the feedstock</td>
<td>Contract with third-party aggregator to deliver the feedstock with a regular basis</td>
</tr>
<tr>
<td>The method of feedstock transportation</td>
<td>Suppliers deliver the feedstock to the producer through truck</td>
</tr>
<tr>
<td>The location of feedstock storage</td>
<td>Inside the bio-fuel production site</td>
</tr>
<tr>
<td>The location of feedstock pre-processing</td>
<td>Inside the bio-fuel production site</td>
</tr>
<tr>
<td>The location of bio-butanol storage</td>
<td>In the ASTs inside the bio-refinery</td>
</tr>
<tr>
<td>The method of bio-butanol transportation</td>
<td>The bio-butanol is transported to the customer by railway or truck</td>
</tr>
<tr>
<td>The factors for choosing the location of production site</td>
<td>Feedstock availability and market availability</td>
</tr>
<tr>
<td>The relative weights of economy and environmental issues</td>
<td>Economy: 77.5%  Environmental: 20%</td>
</tr>
</tbody>
</table>
5.3 Results of objective 3

In the cellulosic biofuel supply chain, three major segments are identified: upstream, midstream, and downstream segments. The upstream segment includes the operations of biomass production, specifically harvesting, collection, pre-processing, storage, and distribution. The midstream segment refers to the conversion of biomass to bio-fuel. The downstream segment is the bio-fuel storage and bio-fuel distribution (Meyer et al 2014). Objective 3 was to identify the physical infrastructure of a bio-butanol supply chain. From the results of literature review, case study and survey, the participants of the cellulosic bio-butanol supply chain were identified and the construction of a cellulosic bio-butanol supply chain network was completed.

5.3.1 Physical infrastructure of the cellulosic bio-butanol supply chain

The physical infrastructure of the cellulosic bio-butanol supply chain includes the biomass supply site, the biomass storage site, the bio-butanol production site, the bio-butanol storage site, the bio-butanol customers, and the transportation within the supply chain. The following sections discuss the basic introduction of the physical infrastructure. The main details and characteristics of the infrastructures are shown in the results of the survey.

5.3.1.1 Biomass supply site

The biomass supply site is the beginning of this supply chain network because the whole supply chain activities begin here. There is no upper-level activity beyond that. The biomass supply site usually refers to the place for growing and harvesting the biomass. In some cases, it only refers to the place for biomass purchasing. In practice, the wet biomass cannot be used to produce bio-fuel directly, so the biomass needs to be stored and dried on-site after it is harvested (EPA 2010). In addition, biomass deteriorates over the time of drying. This reduces the volume and moisture of biomass and also reduces the biomass transportation logistical costs (EPA 2010). The main details about biomass supply site are discussed in section 5.3.2.1.1.

5.3.1.2 Biomass storage site

Biomass for cellulosic bio-butanol production is seasonally available. Most are harvested annually or semi-annually (EPA 2010). However, the demand of bio-butanol is continuous since the bio-butanol needs to keep producing continuously. Therefore, a biomass storage site is necessary to support the continuous production of cellulosic bio-butanol. The biomass storage site can be used to store and preprocess the biomass. Therefore, the biomass storage site is equipped with millers or grinders to pre-process the biomass. The biomass storage site can be located at the secondary storage warehouse and the bio-butanol production plant. The characteristics of the biomass storage site are shown in section 5.3.2.2.1.
5.3.1.3 Bio-butanol production plant

The bio-butanol production plant is the major infrastructure piece of the supply chain network. It is equipped with a biomass storage site, a bio-butanol production system, and a bio-butanol storage site. The biomass storage site can store the biomass and support a continuous biofuel production. The bio-butanol production system includes the facilities for biomass pre-treatment, enzymatic hydrolysis, fermentation, distillation and purification. The bio-butanol storage site can be used for bio-butanol storage. The details of the bio-butanol production plant are discussed in section 5.3.2.2.

5.3.1.4 Bio-butanol storage site

The bio-butanol storage site refers to bio-butanol aboveground storage tanks (ASTs). The ASTs are large concrete tanks used for fuel storage. The bio-butanol storage site is located inside the bio-butanol production plant. After bio-butanol is produced from the production facilities, it needs to be stored in a safe place for a period of time before being transported to the next place. The details of bio-butanol storage are discussed in section 5.3.2.2.4 bio-butanol storage.

5.3.1.5 Bio-butanol customers

The bio-butanol can be used as a solvent, a gasoline additive, and a fuel. So the customers for bio-butanol can be chemical factories as well as fuel distributors, and must be equipped with warehouses or ASTs to store the bio-butanol. The main characteristics of the bio-butanol customers are discussed in section 5.3.2.4.

5.3.1.6 Transportations within the network

The biomass is transported from the biomass supply site to the bio-butanol storage site by truck. The details about biomass transportation are discussed in section 5.3.2.1.2. The bio-butanol is transported from the bio-butanol storage site to the bio-butanol customer by railway or tanker truck. The details about bio-butanol transportation are discussed in section 5.3.2.3.1.

5.3.2 Participants of the cellulosic bio-butanol supply chain network

From the aforementioned physical infrastructure of the cellulosic bio-butanol supply chain, the participants of the cellulosic bio-butanol supply chain were identified. Supply chain networks are complex because they involve many companies and attendant activities. It is difficult to track all the suppliers of a supply chain, because each supplier has their own sub-suppliers. Therefore, it is appropriate to distinguish between primary and supporting members. The primary members are defined as the “companies or organizations who carry out value-adding activities in the business processes designed to produce a specific output for a particular customer or market”. In other words, primary members refer to the companies who directly participate in the supply chain of a product, while the supporting members refer to the companies that provide support and resources to the primary members. Identifying the primary members simplifies
understanding the management processes and capture the essential aspects of the supply chain (Lambert et al 2000).

Four major participants (suppliers, producers, distributors and customers) were identified by analyzing the literature review, results of the case study, and results of the survey. From the literature review and the results of the case study, the physical infrastructure needed for cellulosic bio-butanol supply chain were determined. From the results of the case study and the survey, the locations of each physical infrastructure were identified. By analyzing the location of each physical infrastructure, the participants of the supply chain were identified. The main characteristics and details of each supply chain participant are discussed in the following sections.

5.3.2.1 Suppliers

The suppliers in a cellulosic bio-butanol supply chain network are the agents who sell the cellulosic biomass to the bio-butanol producers. The major cellulosic biomass in this supply chain are agricultural and forestry. The agents typically refer to local farmers and third-party feedstock aggregators. Some of the suppliers, especially the local farmers, need to harvest the biomass feedstock from the field. According to the results of objective 2, suppliers are responsible for feedstock delivery. So the function of suppliers includes feedstock harvesting and feedstock delivery.

5.3.2.1.1 Biomass harvest

Biomass harvesting includes all necessary steps performed before the biomass is ready to be delivered and stored. Cellulosic bio-butanol can be produced from various types of feedstock, such as various agricultural residues (corn stover, sorghum stalks, wheat straws, among others), different wood residues (mill residue, forest residue, and forest thinning), and some herbaceous energy crops (switchgrass and miscanthus) (EPA 2010). Different types of feedstock require different harvesting methods. For this research, sorghum stalks are the proposed feedstock. Since the sorghum stalks are agricultural residues, its harvesting method is the same as the other agricultural residues. Fig. 5.9 displays the harvesting method for agricultural residues.

![Fig. 5.9 agricultural residue harvesting process](image)

The first step in harvesting agricultural residues is to shred the standing stalk; the shredded stalks are raked together before baling; raked stalks are baled into round or square shapes; and then picked up from the field. During the baling process, the stalks
need to be picked up high enough to avoid being mixed with dirt. The baled stalks are moved to the roadside and get ready to be transported (EPA 2010).

The equipment needed to complete these steps includes combines, shredders, rakes, balers, bale wagons, and trailers. After the plants are harvested by the combines, the shredded stalks are used to cut the standing stalks. The rakes are used to rake all of the shredded stalks together before baling. The baling process is completed by balers and bale wagons. After baling, the stalks are moved to the roadside by the trailers (EPA 2010).

5.3.2.1.2 Biomass delivery

According to the results of the survey, suppliers not only provide raw materials to the producers but also transport the raw materials to the production site. Generally, the producer chooses some potential suppliers and contracts them. The raw material is delivered to the producer on a periodic basis according to the contract agreements. After the feedstock baling process, the based cellulosic feedstock is transported from field to the roadside. Later, the feedstock is loaded onto the wagons that are pulled by high-speed tractors and then shipped to the storage site. At last, the feedstock is transported from the storage site to production plant by trucks and trailers. Fig. 5.10 describes the transportation flow of cellulosic feedstock from field to production plant (EPA 2010).

![Cellulosic Feedstock transportation flow](image)

Under the default assumption of the GREET model, the cellulosic bio-fuel feedstock transportation distances from site of production to production plant vary according to feedstock type. Table 5.5 shows the one-way transportation distances of agriculture residues, switchgrass and forest wastes (EPA 2010).

<table>
<thead>
<tr>
<th>Feedstock Type</th>
<th>Agriculture residues</th>
<th>Switchgrass</th>
<th>Forest Wastes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transportation distances</td>
<td>30 miles</td>
<td>40 miles</td>
<td>75 miles</td>
</tr>
</tbody>
</table>
5.3.2.1.3 Suppliers associated costs

The suppliers in the cellulosic bio-butanol supply chain are responsible for harvesting and delivering biomass. So the costs associated with suppliers include feedstock harvesting and transportation costs.

In the document, “Renewable Fuel Standard Program 2” (EPA 2010), the cost of different types of cellulosic ethanol feedstock is estimated based on the Forest and Agriculture Sector Optimization Model (FASOM). Based on the similarity of upstream supply chain processes between the cellulosic ethanol and cellulosic bio-butanol, the cellulosic ethanol feedstock cost can be used to estimate the cellulosic bio-butanol feedstock. Table 5.6 shows cellulosic biomass cost. The harvesting cost in Table 5.6 includes the cost of farmer payments, nutrients, mowing, raking, baling, and hauling to roadside. The hauling cost is cost of hauling the biomass from roadside to secondary storage sites and further to the production plant. The grinding cost is the same for three types of cellulosic feedstock. Although the agriculture cost predicted by FASOM is significantly lower than the cost calculated by the RFSP researchers (ranging from $44.97 to $46.20/dry ton), the costs outlined by FASOM are preferred because the harvesting technology of FASOM is more advanced. In addition, the document also estimates the agriculture residue harvesting cost in detail. This information is summarized in Table 5.7 (EPA 2010).

<table>
<thead>
<tr>
<th>Feedstock type</th>
<th>Agriculture Residue</th>
<th>Switchgrass</th>
<th>Forest Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>Harvesting cost</td>
<td>$34.49/dry ton</td>
<td>$40.85/dry ton</td>
<td>$20.79/dry ton</td>
</tr>
<tr>
<td>Hauling cost</td>
<td>$21.53/ton on average or $ 17.91/ton on average</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Grinding cost</td>
<td></td>
<td>$11.00/ton</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.7 Agriculture residues cost

<table>
<thead>
<tr>
<th>Operations</th>
<th>Farmer</th>
<th>Nutrients</th>
<th>Shred</th>
<th>Rake</th>
<th>Bale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Costs $/ton</td>
<td>10.00</td>
<td>11.81</td>
<td>4.80</td>
<td>4.70</td>
<td>10.84</td>
</tr>
</tbody>
</table>

In the RFSP 2, the estimated transportation costs of agriculture residues from farm to secondary storage site, and from storage site to the production plant are outlined. To estimate the costs of hauling cellulosic feedstock from farm to secondary storage site, the total costs of farm tractor, trailer, fuel, and lube are considered. The total cost here is $6.14/ton. The farm tractor is assumed to haul 12 tons of cellulosic feedstock at an average speed of 22 m.p.h., which results in a unit transportation cost of $0.64/ton/mile.
Therefore, the cellulosic feedstock transportation cost from farm to storage site is 
(\$6.14+0.64*D1)/ton, where D1 denotes the transportation distances from the farm to 
secondary storage site. The way to estimate the cost of shipping cellulosic feedstock fr 
om storage site to production plant is similarly determined. The total costs for the truck, 
flatbed trailer, and fuel are calculated, for a total of $6.90/ton. The truck is assumed to 
ship 24 tons of cellulosic feedstock at an average speed of 30 m.p.h., which results in a 
unit transportation cost of $0.17/ton-mile. Therefore, the cellulosic feedstock 
transportation cost from storage site to production plant is ($6.90+0.17*D2)/ton, where 
D2 denotes the transportation distances from storage site to production plant (EPA 
2010). Table 5.8 summarizes the cellulosic transportation costs mentioned here.

<table>
<thead>
<tr>
<th>Transportation Cost ($/ton)</th>
<th>Farm to storage site</th>
<th>Storage site to production plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.14+0.64*D1</td>
<td></td>
<td>6.90+0.17*D2</td>
</tr>
</tbody>
</table>

5.3.2.2 Producers

The producer here indicates the agent who produces cellulosic bio-butanol, responsible 
for several functions. Producing cellulosic bio-butanol is not the only function of the 
producers in this supply chain network. According to the results of objective 1 and 
objective 2, cellulosic bio-fuel producers prefer to store and pre-process the biomass 
feedstock at the production site. In addition, based on the results of objective 2, setting 
up the storage sites of the bio-fuel in the ASTs inside the production site is very common 
in the second-generation bio-fuel industry. Therefore, the functions of the producer in 
the cellulosic bio-butanol supply chain network include feedstock storage, feedstock 
pre-processing, bio-butanol production, and bio-butanol storage. More detailed 
information for these four functions is reviewed in the next section.

5.3.2.2.1 Feedstock storage

Outdoor storage causes an average of 15% dry matter loss (EPA 2010). Feedstock 
wrapped with dry bales in net or plastic wrap and stored on a well-drained surface has 
significantly lower dry matter loss compared to that of wrapped dry bales laying on the 
ground (EPA 2010). So the biomass should be baled and stored indoor (EPA 2010). 
Indoor storage involves a concrete slab with a roof, supported by poles, with open sides 
(pole-barn). Depending on the amount of baled biomass to be stored, the slab must be 
sized to include aprons around all four edges with aisles between biomass stacks to 
accommodate stacking and hauling equipment, as well as for fire safety (EPA 2010). In 
addition to this pole-barn storage, other indoor storage methods are also be considered. 
For objective 1, the biomass feedstock is baled in plastic bags and stored in the 
basement. In addition, according to the interview with one of the secondary bio-fuel
companies from objective 2, the grain bins can also be used as the feedstock storage facilities.

5.3.2.2.2 Feedstock preprocess

Feedstock pre-processing for cellulosic bio-butanol include physical pre-treatment and chemical pre-treatment of the biomass. Generally, physical pre-treatment precedes the chemical pre-treatment. Physical pre-treatment includes size reduction and dirt removal. To complete the physical pre-treatment, millers or grinders are used to chop the biomass into smaller pieces and a cyclone separator is then used to clean the tar and char. To complete the chemical pre-treatment, different types of pre-treatment reactor systems are used. In addition to the pre-treatment reactor systems, different pre-treatment chemicals are also needed based on different pre-treatment methods. There are six methods to pre-treat biomass: low pH method, neutral pH method, high pH method, an organic solvation process, an ionic liquid method, and biological retreatment (Dutton, 2017). The low pH method requires acids to accelerate the reaction time. The acids include dilute sulfuric acid (H$_2$SO$_4$), gaseous sulfur dioxide (SO$_2$), hydrochloric acid (HCl), phosphoric acid (H$_3$PO$_4$), and oxalic acid (C$_2$H$_2$O$_4$). The high pH method requires liquid ammonia or lime. The organic solvation process needs acetone, ethanol, methanol, etc. Ionic liquid pre-treatment requires salt to make ionic liquids (Dutton 2017). Cellulosic bio-butanol producers also need several solution tanks to store these pre-treatment chemicals.

5.3.2.2.3 Bio-butanol production

After the chemical pre-treatment, there are three steps to produce bio-butanol. At first, an enzymatic hydrolysis process is conducted to hydrolyze the cellulosic biomass into monosaccharides. After that, an anaerobic fermentation process proceeds to convert the sugars into iso-butanol by using certain microorganisms (Wang et al 2015). Finally, a purification or recovery process is used in order to recover the iso-butanol from the fermentation broth. The reason is that the fermentation process not only produces iso-butanol but also generates other byproducts such as acetone and ethanol. To complete these three processes, different equipment is required (IBRF 2017). The enzymatic hydrolysis is completed in high solids enzymatic hydrolysis reactors. To complete this process, enzymes are needed to accelerate the process. So coolers are needed to store the enzymes, which prefer low temperatures. The fermentation process are completed in fermentation reactor systems. Both distillation recovery and membrane recovery separates bio-butanol from the fermentation broth. The distillation recovery is completed in the distillation column. The membrane recovery is completed in membrane filtration system. Besides, if a dynamic impregnator reactor system is used to produce bio-butanol, enzymatic hydrolysis, fermentation, and bio-butanol recovery, it can be completed in one single vessel.
5.3.2.2.4 Bio-butanol storage

At the cellulosic bio-butanol production plant, the refined fuel-grade bio-butanol is generally stored in a few large aboveground storage tanks (AST), specifically the iso-butanol ASTs. In addition to the fuel storage equipment, there are some additional requirements for bio-butanol storage (Butamax et al 2010). The bio-butanol should be stored in isolated and approved areas. The areas must avoid excessive heat, highly reactive ingredients, and any potential sources of ignition. Static electrical discharges and any other source of ignition must be avoided when pumping and sampling. Finally, welding and soldering must be avoided since the tanks may still contain some flammable residues or vapors (Butamax et al 2010).

5.3.2.2.5 Locations of the producers

Because the production sites need to be connected with both suppliers and retailers, several aspects need to be considered when choosing the location for a production site. According to the results from objective 2, the major factors of deciding the plant location include the availability of feedstock, availability of fuel and co-product markets, energy costs, and government incentives. The distance between the production site and the raw material harvesting site must be less than 75 miles (EPA 2010), otherwise the feedstock logistical cost is too high and the profits reduced. Similarly, it is better to locate the production plant near the fuel and co-product markets, so that the logistical costs could also be reduced. Besides, according to the results of objective 1, producing biofuel requires hot water. So the location of the bio-butanol production plant must have access to sufficient water resources.

5.3.2.2.6 Producers’ associated costs

The detailed costs associated with the producers are summarized in Table 5.9. The costs are estimated from a retrofitted production plant for producing bio-butanol from agricultural residue (wheat straw) over a five year period. It is also necessary to note that the associated costs are based on the production processes of biomass milling, low pH pre-treatment, enzymatic hydrolysis, fermentation, and distillation recovery. The cost of producing one kg of bio-butanol from wheat straw by distillated recovery method is $1.37. In addition, if expanding an existing plant, the cost of producing one kg of bio-butanol from wheat straw by membrane recovery method is $0.82. And the cost of producing one kg of bio-butanol from wheat straw by distillation recovery method is $1.07 (Dutton 2017).
Table 5.9 Production costs for bio-butanol from wheat straw

<table>
<thead>
<tr>
<th>Description</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual bio-butanol yield: 150<em>10^6 kg or 48</em>10^6 gal</td>
<td></td>
</tr>
<tr>
<td>Equipment Purchase Cost</td>
<td>$27.66*10^6</td>
</tr>
<tr>
<td>Total Plant Direct Cost</td>
<td>$88.08*10^6</td>
</tr>
<tr>
<td>Total Plant Indirect Cost</td>
<td>$52.85*10^6</td>
</tr>
<tr>
<td>Total Plant Cost</td>
<td>$140.93*10^6</td>
</tr>
<tr>
<td>Contractor’s Fee &amp; Contingency</td>
<td>$21.14*10^6</td>
</tr>
<tr>
<td>Direct Fixed Capital Cost</td>
<td>$162.06*10^6</td>
</tr>
<tr>
<td>Production costs for bio-butanol from wheat straw</td>
<td>$1.37/kg or $4.28/gal</td>
</tr>
</tbody>
</table>

5.3.2.3 Distributors

The distributors here are the agents who deliver the materials or products from suppliers to producers or from producers to customers. These agents typically refer to the third-party logistical companies who deliver the bio-butanol from producers to customers. In this supply chain, in addition to third-party companies, suppliers can also act as distributors, because they take the responsibility for delivering the raw material to the producer. In practice, distributors contract with the producers to deliver the bio-fuel by fuel tanker truck or by railway, based on the distances between producers and customers. The function of distributors includes biomass and bio-fuel delivery. The function of biomass delivery was previously described in section 5.3.2.1.2. The following section contains a description of bio-butanol delivery.
5.3.2.3.1 Bio-butanol distribution

**Route of Bio-butanol Transportation: Blended in Gasoline Refinery**

![Diagram of Bio-butanol Transportation: Blended in Gasoline Refinery]

**Route of Bio-butanol Transportation: Blended in Fuel Terminal**

![Diagram of Bio-butanol Transportation: Blended in Fuel Terminal]

**Route of Bio-butanol Transportation: Deliver to Customers Directly**

![Diagram of Bio-butanol Transportation: Deliver to Customers Directly]

**Fig. 5.11 Possible routes for bio-butanol transportation**

According to the literature review, there are two routes for transporting bio-butanol based on different blending locations of bio-butanol. For the route where blending takes place at gasoline refineries, the bio-butanol is first transported from bulk bio-butanol ASTs to refineries by marine cargo, railway tanker cars and tanker trucks. After being blended with gasoline in the refineries, the blended fuel is distributed by pipeline to the fuel terminals and is then shipped to retail sites by tanker trucks (Butamax et al 2010). For the other route, the blending is done at the fuel terminals. The bio-butanol is transported from the bulk bio-butanol ASTs to the fuel terminals by marine cargo, railway tanker cars and tanker trucks, and finally blended with the gasoline that is transported from the refineries to the same terminals via pipeline. After blending both in a certain proportion, the blended fuel is shipped to retail sites by tanker trucks (Butamax et al 2010). Besides these two routes, there is a third choice. According to the results of objective 2, bio-butanol producers deliver bio-butanol directly to their customers by railway or tanker trucks. These three possible routes of bio-butanol transportation are displayed in Fig. 5.10.

5.3.2.3.2 Distributors’ associated costs

The major cost for distributors is the bio-butanol’s delivery. The delivery costs can be vary based on different transportation modes. The costs of delivering bio-butanol by tanker truck and railway are summarized in Table 5.10.

**Table 5.10 Transportation costs of bio-butanol**

<table>
<thead>
<tr>
<th>Mode</th>
<th>Costs</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Truck</td>
<td>$0.05 t/km</td>
<td>Searcy et al 2007</td>
</tr>
<tr>
<td>Pipeline</td>
<td>$0.062 E^{-0.5885} L/km</td>
<td></td>
</tr>
</tbody>
</table>
5.3.2.4 Customers

The customers in the cellulosic bio-butanol supply chain indicate the agents who purchase bio-butanol from the producer. Cellulosic bio-butanol can be used in solvents, jet fuel, off-road gasoline blending (ship), and on-road gasoline blending (Gevo, available online). Therefore, the bio-butanol customers refer to but are not limited to the fuel distribution companies. In practice, after the fuel distributors receive the bio-butanol from the producer, it is stored in ASTs, and then blended with gasoline in certain percentages when delivery to their customers is imminent.

5.3.2.4.1 Customers’ associated costs

The cost for bio-butanol customers refers to the cost of purchasing bio-butanol from producers. The bio-butanol purchasing price is hard to estimate. It can be affected by different factors, including production costs and results of price negotiations between customers and producers. The production costs of bio-butanol are different based on different feedstock used, different pre-treatment processes, different recovery methods, and more. In addition, the results of price negotiations are hard to predict.

5.3.3 Cellulosic bio-butanol supply chain network

From the secondary data presented and the results of case study and survey, the supply chain network structure of cellulosic bio-butanol was developed. The three primary aspects of the supply chain network structure are the structural dimension, supply chain business processes links, and participants in supply chain. The network structure of the cellulosic bio-butanol supply chain network can therefore be constructed. The details of the cellulosic bio-butanol supply chain network will now be examined. In a cellulosic bio-butanol physical supply chain network, the bio-butanol producer receives raw material from both local farmers and feedstock aggregators, and then delivers the bio-butanol to the customer through third-party logistics companies. These members, especially the producers, use contracts to link themselves with the other members. Producers contract with suppliers to obtain biomass feedstock. Producers also contract with distributors to deliver their bio-butanol. And customers contract with producers to purchase bio-butanol. The associated costs, functions, equipment and facilities of each participator in this supply chain network are summarized in

<table>
<thead>
<tr>
<th>Railway</th>
<th>$0.03t/km</th>
</tr>
</thead>
<tbody>
<tr>
<td>Available on:</td>
<td><a href="https://ppiaf.org/sites/ppiaf.org/files/documents/tools/railways_toolkit/ch1_1_4.html">link</a></td>
</tr>
</tbody>
</table>
Table 5.11. The overview of cellulosic bio-butanol supply chain network is shown in Fig. 5.12 Cellulosic Bio-butanol Supply chain network.

Fig. 5.12 Cellulosic Bio-butanol Supply chain network
Table 5.11 Detailed information for each participant in the cellulosic bio-butanol supply chain network

<table>
<thead>
<tr>
<th>Role</th>
<th>Agent</th>
<th>Function</th>
<th>Associated costs and earnings</th>
<th>Equipment/ facilities</th>
</tr>
</thead>
</table>
| Supplier              | • Local farmer  
                      • Feedstock aggregator  | Provide and deliver raw material to producer | • Raw material harvest costs  
                      • Raw material delivery costs  
                      • Raw material selling profit | • Millers  
                      • Millers/grinders  
                      • Biomass harvest tools  
                      • Trucks |
| Producer              | • Bio-butanol production company                | Store and pre-process raw materials, produce and store bio-butanol | • Raw material purchase cost  
                      • Bio-refinery capital cost  
                      • Bio-butanol production cost  
                      • Third party logistics contract cost  
                      • Bio-butanol selling profit | • Grain bins  
                      • Grinds/millers  
                      • Pre-processing facilities  
                      • Hydrolysis facilities  
                      • Fermentation facilities  
                      • Recover facilities  
                      • ASTs |
| Distributor           | • Third-party logistics company                | Deliver bio-butanol from producer to retailers | • Bio-butanol producer contract income  
                      • Bio-butanol delivery cost | • Tanker trucks  
                      • Railways |
| Customer              | • Fuel distributor                              | Purchase bio-butanol from producer            | • Bio-butanol purchase cost  
                      • Selling of bio-butanol products | • ASTs |
5.4 Results of objective 4

The following sections present the mathematical model and resulting optimized solutions of the cellulosic bio-butanol supply chain.

5.4.1 LCA integration

To integrate the life cycle assessment into a mathematical model, the environmental impact of each process of this supply chain was considered. Therefore, the scope of this life cycle assessment included sorghum stem cultivation and harvest, sorghum stem transportation, bio-butanol production, bio-butanol transportation. The GHG emissions were used as the environmental impact indicators. In order to simplify the calculation, the majority of GHG emissions were aggregated into one single indicator called “Carbon Dioxide Equivalent Emissions” through the method PICC 2007 GWP 100a V1.02, available in SimaPro 8.2.3.0. However, the data of iso-butanol production was gathered from GREET 2015, the calculation method was different from SimaPro. Hence, the GHG emissions were aggregated into a CO₂ equivalent indicator, and the GHG emissions of iso-butanol production were represented by the total GHG emissions. Table 5.12 shows the input parameters of each process:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Source</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_B )</td>
<td>The GHG emission of cultivating and harvesting 1kg of sorghum stem</td>
<td>SimaPro: Sweet sorghum stem {Row}</td>
<td>0.0325 kg CO₂ eq /kg</td>
</tr>
<tr>
<td>( E_{TB} )</td>
<td>The GHG emission of transporting 1 kg of feedstock by tractor and trailer from farm to bio-refinery</td>
<td>SimaPro: Transport, tractor and trailer, agricultural {GLO}</td>
<td>0.000392 kg CO₂ eq / (kg*km)</td>
</tr>
<tr>
<td>( E_F )</td>
<td>The GHG emission of producing 1kg of iso-butanol</td>
<td>GREET 2015: Iso-butanol bio product from sugar (Corn Stover)</td>
<td>2.68 kg GHG / kg</td>
</tr>
<tr>
<td>( E_{TUF} )</td>
<td>The GHG emission of transporting bio-butanol by truck</td>
<td>SimaPro: Transport, combination truck, gasoline powered/ US</td>
<td>7.35E-5 kg CO₂ eq / (kg *km)</td>
</tr>
<tr>
<td>( E_{TRF} )</td>
<td>The GHG emission of transporting bio-butanol through railway</td>
<td>SimaPro: Transport, train, diesel powered/ US</td>
<td>2.2E-5 kg CO₂ eq / (kg*km)</td>
</tr>
</tbody>
</table>
5.4.2 Notations for the mathematical model

The definitions and relevant notations that were used in the mathematical model are summarized in Table 5.13.

<table>
<thead>
<tr>
<th>Notation</th>
<th>definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>Set of cellulosic biomass suppliers, indexed by $i$</td>
</tr>
<tr>
<td>$J$</td>
<td>Set of bio-butanol production plant candidate, indexed by $j$</td>
</tr>
<tr>
<td>$K$</td>
<td>Set of bio-butanol customers, indexed by $k$</td>
</tr>
<tr>
<td>$B$</td>
<td>Set of biomass type, indexed by $b$</td>
</tr>
<tr>
<td>$F$</td>
<td>Bio-butanol</td>
</tr>
<tr>
<td>$L$</td>
<td>Distributor</td>
</tr>
<tr>
<td>$P$</td>
<td>The time period of project, indexed by $p$ (yr.)</td>
</tr>
<tr>
<td>$R$</td>
<td>Discount rate</td>
</tr>
<tr>
<td>$D_k$</td>
<td>The demand of customer $k$</td>
</tr>
<tr>
<td>$u_{Bi}$</td>
<td>The maximum harvest limit of biomass $b$ from supplier $i$ (kg)</td>
</tr>
<tr>
<td>$x_{Bi}$</td>
<td>The amount of biomass $b$ needed from supplier $i$ (kg)</td>
</tr>
<tr>
<td>$x_{Bi j}$</td>
<td>The amount of biomass $b$ transported from supplier $i$ to bio-refinery $j$ (kg)</td>
</tr>
<tr>
<td>$x_{Fj}$</td>
<td>The amount of bio-butanol produced from production plant $j$ (kg)</td>
</tr>
<tr>
<td>$x_{FU j k}$</td>
<td>The amount of bio-butanol transported from production $j$ to customer $k$ by truck (kg)</td>
</tr>
<tr>
<td>$x_{F R j k}$</td>
<td>The amount of bio-butanol transported from production $j$ to customer $k$ by railway (kg)</td>
</tr>
<tr>
<td>$x_{F k}$</td>
<td>The amount of bio-butanol delivered to customer $k$ (kg)</td>
</tr>
</tbody>
</table>
| $y_j$    | Is 1, if the production plant $j$ is open  
|          | Is 0, otherwise |
| $y_{U k}$ | Is 1, if the bio-butanol delivered from bio-refinery $j$ to customer $k$ by truck  
|          | Is 0, otherwise |
| $y_{R k}$ | Is 1, if the bio-butanol delivered from bio-refinery $j$ to customer $k$ through railway  
<p>|          | Is 0, otherwise |
| $T_{i j}$ | The amount of money exchange between supplier $i$ and producer $j$ |</p>
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{jL}$</td>
<td>The amount of money exchange between producer i and distributor L</td>
</tr>
<tr>
<td>$T_{jk}$</td>
<td>The amount of money exchange between producer i and customer k</td>
</tr>
<tr>
<td>$\Pi_i$</td>
<td>The profit for supplier i</td>
</tr>
<tr>
<td>$\Pi_j$</td>
<td>The profit for producer j</td>
</tr>
<tr>
<td>$\Pi_L$</td>
<td>The profit for distributor</td>
</tr>
<tr>
<td>$\Pi_k$</td>
<td>The profit for customer k</td>
</tr>
<tr>
<td>$E_{Bi}$</td>
<td>The GHG emissions of cultivating and harvesting raw material B from harvesting site I (kg CO2-eq/kg)</td>
</tr>
<tr>
<td>$E_{Tb}$</td>
<td>The GHG emissions of transporting biomass B from harvesting site I to the bio-refinery j (kg CO2-eq/kg*mile)</td>
</tr>
<tr>
<td>$E_{TUF}$</td>
<td>The GHG emissions of transporting bio-butanol F from bio-refinery j to the customer k (kg CO2-eq/kg*mile) by truck</td>
</tr>
<tr>
<td>$E_{TRF}$</td>
<td>The GHG emissions of transporting bio-butanol F from bio-refinery j to the customer k (kg CO2-eq/kg*mile) by railway</td>
</tr>
<tr>
<td>$E_{Fj}$</td>
<td>The GHG emissions of producing bio-butanol in the bio-refinery j (kg CO2-eq/kg)</td>
</tr>
<tr>
<td>$C_{Bi}$</td>
<td>The unit cost of harvesting biomass b from producer i ($/kg)</td>
</tr>
<tr>
<td>$C_{TB}$</td>
<td>The unit cost of transporting biomass b from supplier i to the bio-refinery j ($/kg*mile)</td>
</tr>
<tr>
<td>$C_{TUF}$</td>
<td>The unit cost of transporting bio-butanol F from bio-refinery j to customer k by truck ($/kg*mile)</td>
</tr>
<tr>
<td>$C_{TRF}$</td>
<td>The unit cost of transporting bio-butanol F from bio-refinery j to customer k through railway ($/kg*mile)</td>
</tr>
<tr>
<td>$C_j$</td>
<td>The capital cost of building the bio-refinery j ($)</td>
</tr>
<tr>
<td>$C_{Fj}$</td>
<td>The unit cost of producing 1 kg of bio-butanol from production plan j ($/kg)</td>
</tr>
<tr>
<td>$C_{Fk}$</td>
<td>The selling price of bio-butanol F in the customer k ($/kg)</td>
</tr>
<tr>
<td>$\lambda_{ij}$</td>
<td>The transportation distance from harvest site I to the bio-refinery j (mile)</td>
</tr>
<tr>
<td>$\lambda_{jk}$</td>
<td>The transportation distance from bio-refinery j to distribution center k (mile)</td>
</tr>
<tr>
<td>$\alpha_{Bj}$</td>
<td>The bio-butanol F yield from biomass b in the bio-refinery j (kg/kg)</td>
</tr>
</tbody>
</table>
5.4.3 Environmental objective function

To integrate these LCA input parameters into the mathematic model, the following environmental objective function are developed:

$$\text{Min } e_l = P \times (E_{\text{feedstock cultivation and harvest}} + E_{\text{feedstock transportation}} + E_{\text{bio-butanol production}} + E_{\text{bio-butanol transportation}})$$

where $E_{\text{feedstock cultivation and harvest}}$ is the GHG emissions of sorghum stem cultivation and harvest (kg CO$_2$ eq). $E_{\text{feedstock stem transportation}}$ is the GHG emissions of feedstock transportation (kg CO$_2$ eq). $E_{\text{bio-butanol production}}$ is the GHG emissions of bio-butanol production (kg CO$_2$ eq). And $E_{\text{bio-butanol transportation}}$ is the GHG emissions of bio-butanol transportation (kg CO$_2$ eq).

The GHG emissions of feedstock cultivation and harvest is:

$$E_{\text{feedstock cultivation and harvest}} = E_B \times \sum_{i=1}^{I} x_{Bi} \quad \forall \ i \in I$$

The GHG emissions of feedstock transportation (from farm site to production site) is:

$$E_{\text{feedstock transportation}} = E_{TB} \sum_{l=1}^{L} \sum_{j=1}^{J} x_{bij} (\lambda_{ij}) y_j \quad \forall \ l \ j \ i \in I$$

The GHG emissions of biofuel transportation (from production site to customers) is:

$$E_{\text{bio-butanol transportation}} = \sum_{k=1}^{K} \sum_{j=1}^{J} E_{TU} (x_{FUj}) (\lambda_{jk}) y_{Uk} + \sum_{k=1}^{K} \sum_{j=1}^{J} E_{TR} (x_{FRjk}) (\lambda_{jk}) y_{Rk}$$

$$\forall \ l \ j \ i \in I, k \in K$$

The GHG emissions of bio-butanol production is:

$$E_{\text{bio-butanol production}} = \sum_{j=1}^{J} E_F (x_{Fj}) y_j \quad \forall \ j \in J$$

To generate the economic objective function, the profit function of each participant is introduced first. Then the global profit function is created by summing the profit functions of each participant.

5.4.4 Economic objective function

The economic objective function is indicated in the following equation:

$$\text{Max } ec = \sum_{p=1}^{P} \frac{1}{(1 + R)^p} \times (C_{\text{bio-butanol selling}} - C_{\text{feedstock harvest}}$$

$$- C_{\text{feedstock transportation}} - C_{\text{bio-butanol production}} - C_{\text{bio-butanol transportation}})$$

$$- C_{\text{production plant set up}}$$

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where \( C_{\text{bio-butanol selling}} \) is earnings of selling bio-butanol ($), \( C_{\text{feedstock harvest}} \) is the cost of sorghum stem harvest ($), \( C_{\text{feedstock transportation}} \) is the cost of sorghum stem transportation ($), \( C_{\text{bio-butanol production}} \) is the cost of bio-butanol production ($), \( C_{\text{bio-butanol transportation}} \) is the cost of bio-butanol transportation ($), and \( C_{\text{production plant set up}} \) is the cost of building a bio-butanol production plant ($).

The earnings of selling bio-butanol is:

\[
C_{\text{Bio-butanol selling}} = \sum_{k=1}^{K} C_{Fk}(x_{Fk}) \quad \forall \ k \in K
\]

The cost of feedstock harvest is:

\[
C_{\text{feedstock harvest}} = \sum_{i=1}^{I} C_{Bi}(x_{Bi}) \quad \forall \ i \in I
\]

The cost of feedstock transportation is:

\[
C_{\text{feedstock transportation}} = \sum_{j=1}^{J} \sum_{i=1}^{I} C_{TB}(x_{Bij})(\lambda_{ij})y_j \quad \forall j \in J, i \in I
\]

The cost of bio-butanol production is:

\[
C_{\text{bio-butanol production}} = \sum_{j=1}^{J} C_{Fj}(x_{Fj})y_j \quad \forall j \in J
\]

The cost of building a bio-butanol production plant is:

\[
C_{\text{production plant set up}} = \sum_{j=1}^{J} C_{j}(y_j) \quad \forall j \in J
\]

The cost of bio-butanol transportation is:

\[
C_{\text{bio-butanol transportation}} = \sum_{j=1}^{J} \sum_{k=1}^{K} C_{TFU}(x_{FUjk})(\lambda_{jk})y_{lk} - \sum_{j=1}^{J} \sum_{k=1}^{K} C_{TRF}(x_{FRjk})(\lambda_{jk})y_{Rk} \quad \forall l \ j \in J, k \in K
\]

The proof of the above economic objective function is shown below.

The profit for each supplier is the earnings of selling biomass minus the sum of biomass harvest costs and biomass delivery cost:

\[
\Pi_i = \sum_{j=1}^{J} T_{ij}(y_j) - C_{Bi}(x_{Bi}) - \sum_{j=1}^{J} C_{TB}(x_{Bij})(\lambda_{ij})y_j
\]

The profit for each producer candidate is the selling price of cellulosic bio-butanol minus the bio-butanol production cost, the fixed bio-refinery set-up cost, the 3rd party logistic contract cost, and the biomass purchased cost:

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\( \Pi_j = y_j \times \left( \sum_{k=1}^{K} T_{jk} - \sum_{i=1}^{I} T_{ij} - C_{Fj} \times x_{Fj} - T_{jL} \right) \)

The profit for the distributor is the earnings from the producer’s contract minus the cost of bio-butanol delivery:

\[
\Pi_L = \sum_{j=1}^{J} T_{jL} y_j - \sum_{j=1}^{J} \sum_{k=1}^{K} C_{TU}^F (x_{FU,j,k}) (\lambda_{j,k}) y_{Uk} \\
- \sum_{j=1}^{J} \sum_{k=1}^{K} C_{TR}^F (x_{FR,j,k}) (\lambda_{j,k}) y_{Rk}
\]

The profit for the customer is the selling price of bio-butanol minus the cost of the bio-butanol purchase:

\[ \Pi_k = C_{FK} (x_{FK}) - \sum_{j=1}^{J} T_{jk} (y_j) \]

Therefore, the economic objective function is the sum of these profit functions:

\[
e c = \sum_{p=1}^{P} \frac{1}{(1 + R)^p} \times \left( \sum_{l=1}^{I} \Pi_l + \sum_{j=1}^{J} \Pi_j + \Pi_L + \sum_{k=1}^{K} \Pi_k \right) - C_{production \ plant \ set \ up}
\]
\[
= \sum_{p=1}^{P} \frac{1}{(1 + R)^p} \\
\times \left( \sum_{j=1}^{J} \sum_{i=1}^{I} T_{ij} (y_j) - \sum_{i=1}^{I} C_{Bi} (x_{Bi}) - \sum_{j=1}^{J} \sum_{i=1}^{I} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j + \sum_{k=1}^{K} \sum_{j=1}^{J} (T_{jk}) y_j \right) \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j + \sum_{k=1}^{K} \sum_{j=1}^{J} (T_{jk}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{ij}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} C_{Fj} (x_{Fj}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j \\
+ \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TUf} (x_{TuLj}) (\lambda_{Lj}) y_{uk} \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{k=1}^{K} C_{TRF} (x_{FRjk}) (\lambda_{jk}) y_{rk} + \sum_{k=1}^{K} \sum_{j=1}^{J} \sum_{k=1}^{K} C_{Fk} (x_{Fk}) - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} \sum_{k=1}^{K} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j + \sum_{k=1}^{K} \sum_{j=1}^{J} (T_{jk}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{ij}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} C_{Fj} (x_{Fj}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j \\
+ \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TUf} (x_{TuLj}) (\lambda_{Lj}) y_{uk} \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{k=1}^{K} C_{TRF} (x_{FRjk}) (\lambda_{jk}) y_{rk} + \sum_{k=1}^{K} \sum_{j=1}^{J} \sum_{k=1}^{K} C_{Fk} (x_{Fk}) - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} \sum_{k=1}^{K} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j + \sum_{k=1}^{K} \sum_{j=1}^{J} (T_{jk}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{ij}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} C_{Fj} (x_{Fj}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j \\
+ \sum_{j=1}^{J} \sum_{i=1}^{I} (T_{jL}) y_j - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TUf} (x_{TuLj}) (\lambda_{Lj}) y_{uk} \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{k=1}^{K} C_{TRF} (x_{FRjk}) (\lambda_{jk}) y_{rk} + \sum_{k=1}^{K} \sum_{j=1}^{J} \sum_{k=1}^{K} C_{Fk} (x_{Fk}) - \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} \sum_{k=1}^{K} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j \\
- \sum_{j=1}^{J} \sum_{i=1}^{I} \sum_{L=1}^{L} C_{TB} (x_{Bi}) (\lambda_{ij}) y_j + \sum_{k=1}^{K} \sum_{j=1}^{J} (T_{jk}) y_j \right)
\]
\[
\sum_{p=1}^{P} \frac{1}{(1 + R)^p} \times (C_{\text{Biobutanol selling}} - C_{\text{Feedstock harvest}} - C_{\text{Feedstock transportation}} - C_{\text{Biobutanol production}} - C_{\text{Biobutanol transportation}})
\]

5.4.5 Constraints
The feedstock \( B \) harvested from the supplier should not exceed its upper harvesting limit of feedstock \( b \):

\[
x_{Bi} \leq u_{Bi} \quad \forall \ i \in I
\]

(1)

The total amount of biomass \( B \) delivered to different bio-refineries from supplier \( i \) should be equal to the amount of feedstock harvested from supplier \( i \):

\[
\sum_{j=1}^{J} x_{Bij} \times y_j = x_{Bi} \quad \forall \ i \in I, j \in J
\]

(2)

The amount of feedstock \( B \) in each bio-refinery \( j \) should be:

\[
\sum_{i=1}^{I} x_{Bij} = x_{Bj} \quad \forall \ i \in I, j \in J
\]

(3)

The amount of bio-butanol produced in bio-refinery \( j \) should be equal to the amount of feedstock \( b \) in the bio-refinery times the conversion rate.

\[
\alpha_{Bj}(x_{Bj})y_j = x_{Fj} \quad \forall \ i \in I, j \in J
\]

(4)

The amount of bio-butanol delivered from bio-refinery \( j \) to different customer should not exceed the amount of bio-butanol produced from bio-refinery \( j \)

\[
\sum_{k=1}^{K} x_{FUjk}y_{uk} + \sum_{k=1}^{K} x_{Fjk}y_{rk} \leq x_{Fj} \quad \forall \ j \in J, k \in K
\]

(5)

The amount of bio-butanol delivered to each customer \( k \) should be:

\[
\sum_{j=1}^{J} x_{FUjk}y_{uk}y_j + \sum_{j=1}^{J} x_{Fjk}y_{rk}y_j = x_{Fk} \quad \forall \ j \in J, k \in K
\]

(6)

The amount of bio-butanol delivered from the bio-refinery to each customer \( k \) should not exceed the demand of customer \( k \):

\[
D_k \geq x_{Fk} \quad \forall \ k \in K
\]

(7)

Introduce a binary variable to model the selection of bio-refineries:

\[
y_j \leq 1, \ y_j \in N^+ \quad \forall \ j \in J
\]

(8)
Introduce a binary variable to model the selection of the bio-butanol transportation mode:
\[ y_{UK} \leq 1, \; y_{UK} \in N^+ \quad \forall \; k \in K \] (9)

Introduce a binary variable to model the selection of the bio-butanol transportation mode:
\[ y_{RK} \leq 1, \; y_{RK} \in N^+ \quad \forall \; k \in K \] (10)

5.4.6 Implementation of Mathematical Model: Case study in Missouri

The state of Missouri (MO) is ranked as one of the top ten states in sorghum production (USDA 2017). Its major sorghum producers are located in the southeastern part of MO while its major fuel distributors are located in central MO. So the two important factors for bio-butanol production plant selection (feedstock stock availability and market availability) cannot be achieved at the same time. But this is a good opportunity to investigate the priority between the market availability and feedstock availability in the selection of the cellulosic bio-butanol production plant. The details of this case are illustrated below.

According to the USDA’s National Agriculture Statistic Service of 2015, MO has a total of 155,000 acres of planted sorghum (as indicated in Table 5.14). There are 88,900 acres of planted sorghum farmland in the southeast of MO, which represents 57.35% of the total sorghum planted farmland of MO (USDA 2015). Therefore, compared to other regions in MO, the southeast region of Missouri is a better location to source feedstock for the sorghum stem bio-butanol supply chain.

<table>
<thead>
<tr>
<th>Region in MO</th>
<th>Area Planted (Acres)</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Northeast</td>
<td>6,900</td>
<td>4.45%</td>
</tr>
<tr>
<td>Central</td>
<td>9,500</td>
<td>6.13%</td>
</tr>
<tr>
<td>Southwest</td>
<td>3,600</td>
<td>2.32%</td>
</tr>
<tr>
<td>South Central</td>
<td>3,500</td>
<td>2.26%</td>
</tr>
<tr>
<td>Southeast</td>
<td>88,900</td>
<td>57.35%</td>
</tr>
<tr>
<td>Other Districts</td>
<td>42,600</td>
<td>27.48%</td>
</tr>
<tr>
<td>Missouri</td>
<td>155,000</td>
<td>100%</td>
</tr>
</tbody>
</table>
However, fewer potential customers (fuel distributors) can be found in the southeast of MO. Major fuel distributors are located in the central region of MO.

Fig. 5.13 was created through a map tool called Zee Map, with the red markers on the map representing the fuel distributors in and around MO. According to this map, many fuel distributors were located around the city of St. Louis, with just a few customers located within the southeast region. That means that the central region of MO has a larger market. In the central region of MO, there were fewer sorghum stems available as feedstock but larger market potential, while the southeastern region of MO has more sorghum stems but less market potential. In other words, an important tradeoff exists between feedstock availability and market availability. Therefore, two scenarios were used to compare the priority between feedstock availability and market availability. In order to address this tradeoff, the developed MOLP model was used. The model was applied in two scenarios, central region of Missouri and southeast region of Missouri. In each scenario, a potential location of the bio-butanol production plant, the locations of a few possible suppliers, and the locations of possible customers were given. The model was applied and the optimal solutions of each scenario were compared. The supply chain profits of each scenario were compared under the same GHG emissions and production capacities. The scenario with maximum supply chain profits was selected and the optimal location of the sorghum stem bio-butanol production plant was thus determined.

Fig. 5.13 Fuel Distributors near the major sorghum supply county
Scenario 1: Central MO

In this scenario, three counties (Callaway, Boone, and Osage) were selected as the suppliers due to their larger sorghum planted areas. The sorghum planted area of each selected county is shown in Table 5.15. The planted area of each county was obtained from USDA NASS data (2014), and the sorghum stem production was calculated through a sorghum stem yield of 21.5 t/ac (Almodares et al. 2008).

Table 5.15 Related information of selected suppliers in Central MO (USDA 2014, Almodares et al. 2008)

<table>
<thead>
<tr>
<th>County Name</th>
<th>Area Planted (ac.)</th>
<th>Sorghum Stem Production (t.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Callaway</td>
<td>1,700</td>
<td>36,550</td>
</tr>
<tr>
<td>Boone</td>
<td>2,000</td>
<td>43,000</td>
</tr>
<tr>
<td>Osage</td>
<td>1,200</td>
<td>25,800</td>
</tr>
</tbody>
</table>

In order to lower the feedstock transportation cost, the geographical middle point of these three counties was selected as the location of the bio-butanol production plant. Therefore, the county of Callaway was selected as the site of the bio-butanol production plant.
production plant in central MO, as shown in Fig. 5.14 Central MO scenario. In Fig. 5.14, the state boundary of MO was highlighted in purple, and the three selected suppliers were highlighted in pink. The yellow marker represented the location of the bio-butanol producer. The red markers represented the possible customers. In addition, because the agriculture residue biomass feedstock has a transportation distance limit of 30 miles, a blue circle was used to represent this 30-mile-radius limitation. The bio-butanol production plant was located at the center of the blue circle, and light blue shade was the possible sourcing area. Since all of the suppliers were covered or almost covered by the blue circle, a worst-case scenario was used to calculate the distances between producer and suppliers. Therefore, the distances between producers and suppliers were assumed to be 30 miles. There were eight possible customers (fuel wholesale companies and fuel companies) in the central region, with a minimum distance of 36 miles and a maximum distance of 127 miles. The respective demands of each customer and the travel distances between the producer and customers are in Table 5.16. The travel distances between the producer and each customer were estimated by using the shortest travel distance in Google Map.

<table>
<thead>
<tr>
<th>Customer</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distances (miles)</td>
<td>36.66</td>
<td>82.64</td>
<td>110.6</td>
<td>111.85</td>
<td>126.76</td>
<td>108.74</td>
<td>104.4</td>
<td>113.1</td>
</tr>
<tr>
<td>Demand (thousand tons)</td>
<td>1,000</td>
<td>800</td>
<td>1,500</td>
<td>1,000</td>
<td>1,300</td>
<td>1,500</td>
<td>2,000</td>
<td>2,000</td>
</tr>
</tbody>
</table>

Scenario 2: Southeastern MO

In this scenario, three counties (Dunklin, Pemiscot, and New Madrid) were selected as the suppliers due to their larger sorghum planted areas. The sorghum planted area of each selected counties are shown in Table 5.17. Similar to scenario 1, the sorghum stem productions were calculated through a sorghum stem yield of 21.5 t/ac.

<table>
<thead>
<tr>
<th>County Name</th>
<th>Area Planted (ac.)</th>
<th>Sorghum Stem Production (t.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dunklin</td>
<td>4,000</td>
<td>86,000</td>
</tr>
<tr>
<td>Pemiscot</td>
<td>3,700</td>
<td>79,550</td>
</tr>
</tbody>
</table>
In order to lower the feedstock transportation cost, the geographical middle point of these three counties was selected as location of bio-butanol production plant. Therefore, the bio-butanol production plant in the Southeastern MO was selected to be in the county of New Madrid, as indicated in Fig. 5.15. In Fig. 5.15, the boundary of MO was highlighted with purple, and the three selected suppliers were highlighted in pink. The yellow marker represented the location of the bio-butanol producer. The blue circle was the possible sourcing area. Just as in the first scenario, all of the suppliers were covered or almost covered by the blue circle, therefore the distances between producers and suppliers were assumed to be 30 miles. In addition, the red markers in Fig. 5.15 represented the fuel terminals near the southeastern region of MO. There were six possible customers (fuel wholesale companies and fuel companies) in the southeastern region. In order to better compare these two scenarios, the number of possible customers should be the same. So two more fuel companies near the southeastern region were also selected as the possible customers. The respective demands of each customer and the travel distances between producer and suppliers are in Table 5.18. Similar as in the first scenario, the travel distances were identified by Google Map.
5.4.6.1 Input parameters

Before implementing the model, the input parameters should be determined first.

Table 5.19 shows the input parameters of each process of sorghum stem bio-butanol supply chain.

Table 5.19 Values of input parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{Bi}$</td>
<td>Table 5.15 and Table 5.17</td>
<td>USDA 2014</td>
</tr>
</tbody>
</table>
### Table 5.16 and Table 5.18

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{Bi}$</td>
<td>$34.5/ton or $0.038/kg</td>
<td>EPA 2010</td>
</tr>
<tr>
<td>$C_{Bi,j}$</td>
<td>$6.14/ton + 0.64/ton<em>mile or $ 0.0068/kg + 0.0007/kg</em>mile</td>
<td>Searcy et al. 2007</td>
</tr>
<tr>
<td>$C_{FU,jk}$</td>
<td>$0.06/ton<em>km or $0.00009/kg</em>mile</td>
<td>Available on: <a href="https://ppiaf.org/sites/ppiaf.org/files/documents/toolkits/railways_toolkit/ch1_1_4.html">https://ppiaf.org/sites/ppiaf.org/files/documents/toolkits/railways_toolkit/ch1_1_4.html</a></td>
</tr>
<tr>
<td>$C_{FR,jk}$</td>
<td>$0.03/ton<em>km or $0.00005/kg</em>mile</td>
<td>Dutton 2017</td>
</tr>
<tr>
<td>$C_j$</td>
<td>$140,930,000</td>
<td></td>
</tr>
<tr>
<td>$C_{Fj}$</td>
<td>$0.72/kg</td>
<td></td>
</tr>
<tr>
<td>$\alpha_b$</td>
<td>8.5g/L or</td>
<td></td>
</tr>
<tr>
<td>$\lambda_{ij}$</td>
<td>30 miles</td>
<td>EPA 2010</td>
</tr>
<tr>
<td>$\lambda_{jk}$</td>
<td>Table 5.16 and Table 5.18</td>
<td>Google map</td>
</tr>
<tr>
<td>$C_{FR}$</td>
<td>$3.00/gallon</td>
<td>Yang 2017</td>
</tr>
<tr>
<td>$D_k$</td>
<td>Table 5.16 and Table 5.18</td>
<td>Monte Carlo simulation in excel</td>
</tr>
</tbody>
</table>

### 5.4.6.2 General assumptions

In order to better understand the tradeoff between feedstock availability and market availability, some irrelevant variables should be controlled for. Therefore, for both scenarios, it is assumed that:

- The time period of this project is five years.
- The discount rate is 10%.
- The unit sorghum stem harvest cost is the same for all the suppliers.
- The unit sorghum stem transportation cost is the same and the transportation distance between suppliers and producer are all held equal at 30 miles.
- The bio-butanol selling price is $3.00 per gallon for all customers.
- Both bio-butanol transportation methods are acceptable to all customers.
- The conversion rate of bio-butanol is the same for all producers.
- When applying the $E$-constraint method, 600 grid points are used to divide the feasible range of the model.

### 5.4.7 Results of the model application

#### 5.4.7.1 Results for central MO scenario

In the first case scenario, the limitation of feedstock availability does not allow the producer to serve all eight possible customers. Customer #5, located 126.76 miles from the producer, could not be served. In other words, instead of having eight customers,
the producer in central MO only has seven. In addition, the optimal bio-butanol transportation method is railcar, due to its low delivery cost and relatively low GHG emissions. The maximum supply chain profits for five years are $3,050,577,573, with GHG emissions of 116.56 million tons of CO₂ eq for five years and an annual production amount of 9,577,273 tons of bio-butanol. The minimum GHG emissions are zero with a profit of zero. The ε-constraint method is used to solve the multi-objective model. The tradeoff between economic objective and environmental objective can be seen in Fig. 5.16.

![Fig. 5.16 Relationship between total profits and GHG emissions in the first case scenario](image)

In Fig. 5.16, 20 grid points are selected to show the tradeoff between the economic objective and the environmental objective. The relationship between total profits and the GHG emissions is positive-linear. If the GHG emissions decrease by 194.27 thousand tons CO₂ eq, the total profits of bio-butanol supply chain will decrease by $5.3 million. In other words, to reduce GHG emissions by 1 ton CO₂ eq, the total supply chain profits decrease by $27.2.

5.4.7.2 Results for southeastern MO scenario

In the second scenario, by taking advantage of locating the plant near the feedstock sources, all of the customers’ demands are fully satisfied. However, the eight nearby customers would not consume all of the feedstock resources. Actually, according to the results, the nearby customers would only consume half of the total feedstock resources. Therefore, producers need to explore the possibility of reaching more distant customers to consume the remaining amount of feedstock. According to an additional analysis, customers within 544 miles could feasibly be served by railcar and customers within
272 miles could feasibly be served by truck. Serving the customers under these distances would still make profits for the whole bio-butanol supply chain.

Additionally, in this scenario the optimal bio-butanol transportation method is railcar, based on its low delivery cost and low GHG emissions. The maximum profits for five years are $3,403.16 million, with total GHG emissions of 128.995 million tons of CO\textsubscript{2} eq produced within five years, and an annual production yield of 10,600,000 tons of bio-butanol. The minimum GHG emissions are zero with a profit of 0. In order to solve the MOLP problem, the $\varepsilon$-constraint method was used.

In Fig. 5.17, 20 grid points are selected to show the tradeoff between the economic objective and environmental objective. The relationship between total profits and GHG emissions is positively linear. If the GHG emissions decrease by 214.99 thousand tons of CO\textsubscript{2} eq, the total profits of bio-butanol supply chain would decrease by $5.7$ million. In other words, to reduce the GHG emissions for one ton of CO\textsubscript{2} eq, the supply chain profits will decrease by $26.5$.

5.4.7.3 Comparing the results of both scenarios

The producer in the southeastern MO case pays less to reduce one ton CO\textsubscript{2} eq than the producer in the central MO case. In addition, the maximum profits for five years of bio-butanol supply chain in southeastern MO are $352.580$ million higher than the profits from the Central MO case. However, the associated GHG emissions of the southeastern MO case are 12.44 million tons CO\textsubscript{2} eq higher than that of the central MO case. Therefore, in order to better compare both cases, an additional analysis is conducted to estimate the economic differences between the two cases under the same GHG emissions. The results of this analysis are shown in Fig. 5.18.
Fig. 5.18 Compare the total supply chain profits of two cases under the same GHG emissions

From Fig. 5.18, it is obvious that the total supply chain profits from the southeastern MO plant are still higher than the profits of the central MO plant even under the same GHG emissions. Therefore, the performance of the southeastern MO scenario is better than the performance of the central MO scenario. That means, under the assumptions made in this research, the feedstock availability is much more important than the market availability when designing a sorghum stem bio-butanol supply chain network in MO.

5.4.7.4 Determining the production size of the bio-butanol supply chain

According to the previous analysis, if the production plant in the southeastern region only serves the eight nearby customers, it would consume a relatively low amount of sorghum stalks in the region. Since the feedstock supply is not exhausted, more customers would be needed to consume it, and therefore increase the production size and total profits. So, a further analysis is conducted to see if exploring the potential for more customers would improve the performance of the supply chain network.

In addition to the eight nearby customers, this analysis includes the other six customers from the central MO region to see if the production size and total profits could be increased simultaneously. The results of this analysis are shown in Fig. 5.19.

Fig. 5.19, indicated a positively linear relationship between total profits and GHG emissions. To reduce the GHG emissions for one ton of CO₂ eq, the supply chain profits were decrease by $24.4, which was less than the costs of previous two cases.
To decide on the ideal size of the bio-butanol production plant, the tradeoff between economic objective and environmental objective needs to be considered. In this case, an additional analysis is conducted to compare the production sizes under the different possible weights between economic and environmental objectives. The results of this analysis are shown in Table 5.20. For example, if 5% of the total supply chain profits are used to reduce GHG emissions, the production yield is decreased from 18,900,000 tons to 17,953,331 tons. If more profits are used to decrease GHG emissions, the production yield will decrease to a lower value.

<table>
<thead>
<tr>
<th>Economic weight (%)</th>
<th>Total profits under this weight (million dollars)</th>
<th>GHG emissions under this weight (million tons CO₂ eq)</th>
<th>Production size (million tons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>6,026.16</td>
<td>230.15</td>
<td>18.9</td>
</tr>
<tr>
<td>95</td>
<td>5,724.85</td>
<td>217.80</td>
<td>17.95</td>
</tr>
<tr>
<td>90</td>
<td>5,423.54</td>
<td>205.45</td>
<td>17.01</td>
</tr>
<tr>
<td>85</td>
<td>51,22.24</td>
<td>193.10</td>
<td>16.06</td>
</tr>
<tr>
<td>80</td>
<td>4,820.93</td>
<td>180.75</td>
<td>15.11</td>
</tr>
<tr>
<td>75</td>
<td>4,519.62</td>
<td>168.41</td>
<td>14.17</td>
</tr>
</tbody>
</table>
5.4.7.5 Sensitivity Analysis

In order to provide more insights of the modelling results, a sensitivity analysis was conducted. In this section, the values of some important input parameters were changed to study the effects of these parameters into the objective functions. To illustrate how these parameters affect the optimal solutions, the values of demand, biomass harvest unit cost, bio-fuel production unit costs, bio-fuel transportation unit cost, and bio-fuel unit price are changed in the range of [-50%, 50%]. The total supply chain profits and the GHG emissions were calculated based on the changes of each input parameters. The following presents the results of the sensitivity analysis.

![Graph showing NPV against percentage change in cost parameters](image)

**Fig. 20 The NPV against the percentage change in the costs parameters.**

Fig. 20 indicated the changes of some costs and their effects in the total supply chain profits. The changes in sorghum stalk harvest costs and bio-butanol transportation costs caused very limited changes in the total supply chain profits. Changes of bio-butanol
production costs and bio-butanol sale prices affect the total supply chain profit the most. By decreasing the bio-butanol production costs by 50%, the total profits increased 388.12%. While the bio-butanol supply chain was non-profitable when increasing the production costs by more than 10%. The total supply chain profits increased by 443.63% by increasing the bio-butanol sale price by 50%. While the bio-butanol supply chain was non-profitable when decreasing the bio-butanol sale price by more than 10%.

Fig. 21 The objective functions against the percentage change in demand

Fig. 21 indicated the change in demand and the effects on the total supply chain profits and GHG emissions. The GHG emissions has a decreasing and linear trend as the demand decreasing. Decreasing the current demand for 10% caused a 10% decrease in GHG emissions. The GHG emissions increased as the demand increased, though the effects were very limited. Increasing the demand by 10% only caused a 3.37% increase in GHG emissions. However, after increasing the current demand for more than 10%, the GHG emissions began to decrease. Increasing the current demand for 10% caused a 0.01% decrease in GHG emissions. The total supply chain profits also has the similar changing pattern when the demand was decreased. However, the supply chain profits increased as the demand increased, though the changings were very limited. The supply chain profits only increased by 4.35% when the demand increased by 50%. It is necessary to point out the after increasing the demand by 10%, the supply chain profits increased but the GHG emissions decreased.
6 Discussion

6.1 The production processes of bio-butanol industry

The Integrated Biorefinery Research Facility (IBRF) at the National Renewable Energy Laboratory (NREL) can produce a variety of fuels and chemicals from cellulosic biomass (IBRF, 2017; NREL 2012) including bio-butanol. Therefore, the production process and production equipment at the IBRF can be used to study the production process of cellulosic bio-butanol specifically.

The reorder frequency and inventory level of IBRF can be used as the reference to calculate the feedstock inventory level. If the demand is stable and the feedstock supply is continuous, adopting short-periodical reviews of inventory and small quantity fulfillment of feedstock is a reasonable step. However, if the demand fluctuates and the feedstock cannot deliver continuously, the lead-time of the feedstock fulfillment will be longer and the inventory level will increase. In this case, the data from IBRF should not be used. The inventory-handling plan should therefore be determined based on demand, feedstock availability, and production capacity.

There are seven chemical pretreatment methods for cellulosic biomass (Dutton 2017). However, this research did not review the comparative advantages and disadvantages of each pretreatment method. The details of each chemical pretreatment method can be found in Dutton (2017). The selection of a specific chemical pretreatment method should be based on the requirements of bio-butanol production, the price of pretreatment chemicals, the pretreatment reaction time, and the required energy consumption.

In order to identify the criteria for selecting the location of bio-butanol production plant, an observation of the bio-butanol production plant’s surroundings was conducted. However, since the IBRF is a research facility of the NREL, the criteria for its location selection is different from those of a commercial company. Therefore, the results of IBRF surroundings should not be used as a reference for commercial companies to select the location of their production plant. However, the production of cellulosic bio-fuel requires a lot of water (National Research Council 2008). The location of a cellulosic bio-butanol production plant should have access to sufficient water sources.

There are two major types of bio-butanol production: direct microbial conversion (DMC) and simultaneous saccharification and fermentation (SSF). Although they are different production methods, both of them include the same production process as the INRF. In other words, both literatures and the IBRF share the production processes of size reduction, pretreatment, enzymatic hydrolysis, fermentation, and bio-butanol recovery. Therefore, the processes of bio-butanol production for this objective also include these five major steps. For more details about the optimization of these bio-

The structural dimensions of a cellulosic bio-butanol supply chain network can be identified in objective 1. The structural dimension comprises a horizontal structure, a vertical structure, and a horizontal position of the specific company. There are four supply chain tiers in the horizontal structure of the cellulosic bio-butanol supply chain, cellulosic biomass supplier, bio-butanol producer, bio-butanol distributor, and bio-butanol customer. From this horizontal structure, it is obvious that the horizontal position of cellulosic bio-butanol companies (the specific company) is located in the middle of the supply chain. The vertical structure of cellulosic bio-butanol can be varied, because of the different types of biomass feedstock and the different uses of cellulosic bio-butanol.

6.2 The logistic activities in bio-butanol supply chain

There are 7 responses out of 17 research sample were collected in this survey. One of 7 responses were bio-butanol producers and the rest are cellulosic bioethanol producers. According to Morone and Pandey (2014), although the transportation route and method of bio-butanol is different from the bioethanol, they can use similar feedstock and production facilities. That means that the cellulosic bio-butanol supply chain can share similar upstream and middle-stream logistic activities with the cellulosic bioethanol supply chain. Therefore, the sample population of this survey can be expanded to second generation bioethanol companies in the U.S. Hence, it is reasonable to use the data from bioethanol companies to map the logistical activities in bio-butanol supply chain.

From the results of objective 2, contracting with third-party aggregators for feedstock sourcing is the most popular answer in the responses. The seasonal availability of cellulosic biomass requires storing a large amount of biomass to ensure continuous production. Contracting with third-party aggregators would achieve a continuous supply of biomass feedstock. However, it also increases the feedstock purchasing costs. Therefore, it is better to use a hybrid-sourcing method. Producers can source from both farmers and third party aggregators. During the harvest season, producers can source feedstock from farmers to achieve a lower price. During the other seasons, producers can source feedstock from third-party aggregators to achieve a continuous supply of biomass feedstock.

Based on the results of objective 2, suppliers deliver the biomass feedstock to producers. Although there is a company that chose to contact third-party distribution centers to deliver their biomass feedstock, this company also indicated that part of their biomass feedstock was delivered directly by suppliers.
According to the literature review, using secondary storage sites to store feedstock is better than storing the biomass in the harvesting or production sites (EPA 2010). However, according to the results of objective 2, responders seldom use secondary storage sites. More responders prefer to store the feedstock at the production site. Unfortunately, the reasons behind the selection of their biomass storage location are not investigated in this research. Therefore, further analysis can focus on investigating the pro and cons of using different biomass storage locations.

According to the survey results, all of the responders choose to pre-process the feedstock at the production site. However, this is an unwise choice because the unprocessed biomass contains higher moisture content and contaminants and this in turn can greatly increase the long-term transportation costs (Holm-Nielsen and Ehimen 2016). According to the literature review, the secondary storage site is a good location at which to pre-process biomass. By pre-processing the harvested raw material in secondary storage site, the raw material can be harvested by using only two machines before it is loaded onto the roadside. In this way, the raw material does not hit the ground, which can significantly reduce loss of dry matter. Furthermore, since the feedstock is milled at the secondary storage site to achieve a higher bulk-density, transportation costs can be lower when it is transported from the storage site to the biofuel production plant (EPA 2010). However, responders in this survey seldom use secondary biomass storage sites for biomass pre-processing. Instead, they prefer to pre-process biomass at the production sites. The reason could be that the literature does not consider the additional transportation costs of delivering biomass to secondary storage sites. Another reason could be that the distances between suppliers and producers are usually less than 75 miles (EPA 2010) whereas other results in the literature only apply to cases with longer transportation distances. In order to obtain guidelines on how to choose the feedstock preprocessing location, more data need to be gathered and analyzed.

From the results of the survey, bio-fuel producers contract with third-party distribution companies to deliver the bio-fuel by truck or railway. It was found that 40% of responders prefer to use railway only and 40% of responders prefer to use a fuel-tanker truck only. In addition, 20% of responders prefer to use both modes. Although the unit price of transporting biofuel by railway is lower than a tanker-truck, it does not guarantee that railway is always the better choice over the tanker-truck. For example, in the case of small quantities and short-distance transportation, the tanker truck is a more flexible option than railway. Therefore, the selection of transportation methods depends on different circumstances.

From the data collected by the survey, feedstock availability and market availability are two major factors for choosing a bio-butanol production location. A production site located close to both suppliers and customers can largely lower the transportation costs but in practice it is difficult to achieve both at the same time. In many cases, producers
can only achieve one of these two major factors. Therefore, further research can focus on dealing with the tradeoff between feedstock availability and market availability. In this dissertation, the priority between these two factors were compared by applying the mathematical model in two cases. One case with a production plant locates near to the suppliers. Another case with a production plant locates near to the customers. The priority between these two factors can be determined by selecting the case with the higher supply chain profits under the same GHG emissions.

Developing the supply chain for cellulosic bio-butanol must consider environmental impacts since it is a renewable fuel. However, according to the results of objective 2, second-generation bio-fuel producers are reluctant to pay sufficient attention to environmental issues. Future research can investigate the reasons behind this current industry behavior.

6.3 The physical infrastructure of bio-butanol supply chain

In objective 3, the physical infrastructure and the participants of cellulosic bio-butanol supply chain are identified. Through this objective, the supply chain network structure of cellulosic bio-butanol is constructed. The reviewed and published research in the topic does not discuss how to design a supply chain network for cellulosic bio-butanol and the previous research only discusses the supply chain network design of cellulosic bioethanol. Although the supply chain network of cellulosic bio-butanol shares some similarities with that of cellulosic bio-ethanol, they still have their own characteristics. Since both cellulosic bio-butanol and cellulosic bio-ethanol use cellulosic biomass as their feedstock, both of them have similar suppliers and similar upstream supply chain activities. In addition, the production process of cellulosic bioethanol and cellulosic bio-butanol can also be similar. They both have the processes of pretreatment, saccharification, fermentation, and recovery (Morales et al 2015, Brown et al 2012). However, their downstream supply chain activities are different. Cellulosic bio-butanol is less corrosive and water immiscible (Dürre 2007), allowing it to be transported by pipeline; while cellulosic bio-ethanol is corrosive and can completely miscible with water, prohibiting it from being transported by pipeline. Therefore, bio-butanol can be transported to a nearby gasoline refinery, then blended with gasoline and delivered to the fuel distributors by pipeline. Instead, cellulosic bio-ethanol can only be directly transported to the fuel distributors. This difference allows bio-butanol production plant to have a wider selection of locations and lower bio-fuel logistic costs.

Many cellulosic bio-fuel supply chain networks include a few secondary biomass storage sites (Gunnarsson et al. 2004, You et al. 2011, Poudel et al. 2016). However, in the proposed supply chain network, the biomass storage site is located at the bio-butanol production site. This decision is supported by the survey results of current cellulosic bio-fuel companies in the U.S. In addition, for agriculture residue feedstock, the
transportation distance should be less than 30 miles. So it is not necessary to set up a secondary biomass storage site.

The seasonal availability of cellulosic biomass is one of the major characteristics of a cellulosic bio-butanol supply chain. It requires storing a large amount of biomass for continuous production of cellulosic bio-butanol. Purchasing feedstock from local farmers is cheap but requires large storage space. Contracting with third-party feedstock aggregators would achieve a continuous supply of cellulosic feedstock and a low inventory level, but also increase the feedstock purchase cost. Therefore, this tradeoff needs to be considered when choosing a purchasing policy.

6.4 The mathematical model for a green bio-butanol supply chain network design

Unlike other models for bio-fuel supply chain network design (Marvin et al 2011, Poudel et al 2016), the model proposed in this dissertation considers environmental impacts. In the proposed model, two objective functions (environmental and economic) were used to maximize the global supply chain profits and to minimize GHG emissions. LCA was used to evaluate the GHG emissions of each activity in the cellulosic bio-butanol supply chain.

The models discussed in literature have biomass secondary storage sites (You et al 2011) but these cannot be directly applied to the supply chain network design of cellulosic bio-butanol since the storage sites in the literature are located at the secondary storage sites. Compared with a cellulosic bio-fuel supply chain network that has the storage site inside the production plant, adopting a secondary storage site will introduce additional renting and transportation costs. To solve this problem, a model is proposed in this dissertation based on the specific network structure of a cellulosic bio-fuel supply chain. Therefore, feedstock storage costs were not considered in the economic objective function of the proposed model.

The developed mathematical model can be used to select the potential locations for a bio-butanol production site. It can select the optimal bio-butanol production location(s) from several candidates of bio-butanol production locations. In this research, in order to analyze the impact of feedstock availability and market availability on location selection of production plant, the proposed model is applied twice: the first run is for feedstock availability and the second run is for market availability. The result showed that feedstock availability has a higher priority in the location selection process.

The results of model application showed a positively linear relation between economic and environmental objectives. This could be caused by the same bio-butanol selling price of all customers and the single location of possible production plant. In addition, the assumption that both railway and tanker truck delivery are acceptable for all
customers may also lead to this conclusion. However, in practice, the selling price of each customer can be varied, there can be multiple possible locations of the production plants, and the railway deliver may not be the acceptable choice for all customers.

From the model application, the results indicated a total supply chain profit of 6,026.16 million dollars, a total GHG emissions of 230.15 million tons of CO2, and a production capacity of 18.9 million tons. In order to see whether these number is reasonable, supply chain network design modelling results from other researches were used to compare with the modeling results from this research. Table 21 shows that the results from this research is reasonable.

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>Maximum Profits (million dollars)</th>
<th>GHG emissions (million tons of CO\textsubscript{2} eq)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass-Bio-ethanol</td>
<td>7070 for 20 years</td>
<td>--</td>
<td>Marvin et al (2011)</td>
</tr>
<tr>
<td>Biomass-Biofuel</td>
<td></td>
<td>27 for 1 year</td>
<td>Zhang (2011)</td>
</tr>
<tr>
<td>Sorghum stalk-Biobutanol</td>
<td>6026 for 5 years</td>
<td>230 for 5 years</td>
<td>In this research</td>
</tr>
</tbody>
</table>

Table 21 Modelling results comparisons
7 Summary and Conclusions

In this research, an ideal supply chain network for cellulosic bio-butanol was constructed and optimized. The network was constructed by identifying three important aspects of a supply chain network structure: structural dimension, participants within the supply chain, and the supply chain’s business process links. The structural dimension was identified by examining the production processes of the bio-butanol industry. The supply chain business process links were identified by studying the logistical activities in the bio-butanol supply chain. The participants of were identified by determining the physical infrastructure of the supply chain network. The cellulosic bio-butanol supply chain network was optimized by developing a multi-objective linear integer programming model.

A case study was conducted to understand the production processes of the cellulosic bio-butanol industry. The proposed activity for the case study was to visit the integrated Bio-Refinery Research Laboratory of the National Renewable Energy Laboratory in Denver, Colorado. During the visit, the production processes of cellulosic bio-butanol and the necessary equipment were explored and documented.

To map out the logistical activities of the cellulosic bio-butanol supply chain, a survey was conducted. The survey consisted of sending a questionnaire to operating cellulosic bio-ethanol and bio-butanol producers in the U.S. The questionnaire included questions related to supply chain logistical activities and attitudes about environmental impacts.

The necessary components of the physical infrastructure of a cellulosic bio-butanol supply chain network were identified by analyzing secondary sources in the literature, the results of the case study, and the results of the survey. By analyzing these data sources, the physical infrastructure of cellulosic bio-butanol supply chain network, the participants of the bio-butanol supply chain network, and the associated functions and costs of each participant were determined.

The green cellulosic bio-butanol supply chain network was constructed by developing a mathematical model with two objective functions. The life cycle analysis technique was used to formulate the environmental objective function and the net present value was used to formulate the economic objective function. The $\varepsilon$-constrain method was used to solve the two conflicting objectives. The model was applied using data from the state of Missouri to determine the ideal locations for a sorghum stalk bio-butanol production plant, the annual production yield of sorghum stalk bio-butanol, and the transportation methods required by the supply chain network.

The major conclusions of this dissertation are as follow:
The equipment inside the bio-butanol production plant includes knife mills, pretreatment reactors, enzymatic hydrolysis reactors, fermentation reactors, and membrane filtration systems.

The production processes of bio-butanol include biomass milling, chemical pretreatment, enzymatic hydrolysis, fermentation, and bio-butanol recovery.

The structural dimension of the bio-butanol supply chain contains four tiers of a horizontal structure: supplier, manufacturer, distributor, and customer. The bio-butanol companies are located in the middle of the horizontal structure. The vertical structure of bio-butanol supply chains is varied, depending on the number and types of biomass feedstock produced and the number and types of bio-butanol purchasers.

The logistical activities of the cellulosic bio-butanol supply chain include feedstock sourcing, feedstock delivery, feedstock storage, feedstock preprocessing, bio-butanol production, bio-butanol storage, bio-butanol delivery, and bio-butanol sale.

The cellulosic bio-fuel producers indicated that environmental issues were considered during the operation of the companies. They are willing to sacrifice up to 20% of their profits to improve their respective plant’s environmental performance.

Biomass feedstock availability and biofuel market availability are the two primary factors for choosing the ideal locations of a cellulosic bio-butanol production plant.

The business processes links among the suppliers, producers, distributors, and customers are managed processes links. Producers use contracts to link themselves with potential suppliers, distributors, and customers.

The physical infrastructure of a cellulosic bio-butanol supply chain network includes a biomass supply site, a biomass storage site, a bio-butanol production plant, a bio-butanol storage site, a bio-butanol customer, and a transportation mode within the network.

The participants in the cellulosic bio-butanol supply chain network include a biomass supplier, a bio-butanol manufacturer, a bio-butanol distributor, and a bio-butanol customer. The biomass supplier refers to third-party biomass aggregators and biomass farmers. The bio-butanol manufacturer refers to the cellulosic bio-butanol production companies. The bio-butanol distributor refers to the third-party logistics company. The bio-butanol customer refers to gasoline or fuel companies.

The model was applied in two cases within Missouri (MO) to compare the respective impact of feedstock availability and market availability on location selection. Under the assumptions made in this research, feedstock availability is much more important than the market availability when designing a sorghum stem bio-butanol supply chain network in MO. Under the same
estimated GHG emissions, the supply chain profits with ideal feedstock availability are at least $14,330,579 higher than the supply chain profits with ideal market availability.

- According to the analysis of two case scenarios in MO, the optimal location for the bio-butanol production plant is located in the southeastern region of MO where there are abundant sorghum stem resources. The optimal location of cellulosic bio-butanol production can achieve a maximum profit of $3,403.16 million within five years, a total GHG emission of 128.995 million tons of CO2 eq within five years, and an annual production yield of 10,600,000 tons of bio-butanol.

- The production size of bio-butanol production plant is based on the tradeoff between the economic and environmental objectives. If 5% of the total supply chain profits are used to reduce GHG emissions, the production yield is decreased from 18,900,000 tons to 17,953,331 tons. The lower GHG emissions results in a smaller sized production plant.
Appendix A: Questionnaire

Sustainable design of a cellulosic bio-butanol supply chain network with life cycle assignment

The purpose of this survey is to know the logistics activities of renewable bio-fuel supply chain from the aspects of economy and environmental protection then further provide more valuable information for the future supply chain network analysis and help to construct constrains in the mathematical model.

The collected data, following analysis and results will remain confidence and will only be used for this study (including related reports).

The identity of the respondents and respondents’ firm will remain undisclosed in any publication resulting from this study. The research is being conducted by Li Liang, Graduate Research assistant and PhD student in the Department of Sustainable Biomaterials at Virginia Polytechnic Institute and State University (Virginia, United States).

If you have any questions, please contact Li Liang by email at lli91@vt.edu.

Section 1: Basic information collected

1. Which kind of the following biofuel dose your company produce?
   - [ ] Cellulosic bio-butanol fuel (Continue to the second question)
   - [ ] Cellulosic bioethanol fuel (Continue to the third question)
   - [ ] None of above (Continue to section 2)

2. What’s the price of your cellulosic bio-butanol per gallon?

3. What’s the annual cellulosic biofuel yield of your production plant?

4. What’s the biomass to fuel yield of your production plant?
   - [ ] Under 20%
   - [ ] 21%-40%
   - [ ] 41%-60%
   - [ ] 61%-80%
   - [ ] 81%-100%
   - [ ] No Responses

Section 2: Supply chain management:

1. How do you acquire the feedstock?
☐ Contracting in-house with growers or land owners
☐ Using third party feedstock aggregator?
☐ Directly buy on the spot market or from recognized merchants
☐ Others_________
☐ No responses

2. Are you purchase the feedstock only one time in a year or you need to backorder feedstock several times?
☐ Purchase only once a year without backorder
☐ Purchase once a certain amount a year but need backorder several times
☐ It depends on the demand fluctuation by the year
☐ Others________________
☐ No responses

3. How do you acquire the vehicle for feedstock transportation?
☐ Contract with third party distribution center
☐ Directly purchase vehicles from merchants
☐ Suppliers have vehicles and deliver biomass for free
☐ Others___________
☐ No responses

4. Where will feedstock be stored?
☐ Storing the biomass in the production plant without storing at the harvest site.
☐ Storing the biomass at the harvest site and then transport to the bio-refinery as needed.
☐ Storing the biomass at a collective storage facility and then transport to the production plant from the intermediate storage location as needed
☐ Others________
☐ No responses

5. Where will feedstock be preprocessed?
☐ At the harvest site.
☐ In the secondary storage site.
☐ In the production plant.
☐ Others________
☐ No responses

6. Where do you store the biofuel?
☐ In ASTs inside the production plant
In ASTs near the production plant, ______ miles away from the production plant

Underground storage tank near the production plant, ______ miles away from the production plant

Others__________

No responses

7. Which kind(s) of vehicle are you using to ship the biofuel from ASTs to fossil fuel refineries/terminals?

- Railway
- Fuel tanker
- Underground pipeline
- Marine oil tanker
- Others__________
- No responses

8. How do you acquire the vehicle for fuel transportation?

- Contract with third party distribution center
- Directly purchase vehicles from merchants
- Others__________
- No responses

9. Where will bio-fuel be shipped to from the production plant?

- To the fuel terminal.
- To the local gas station.
- Others__________
- No responses

10. What factors would you consider when choosing the location your production plant, please list three factors

- ________
- ________
- ________

Section 3: Environmental issue:

What do you think is the best to balance the weight between economy and environmental issue?

Your choice economy environmental

- 40% 60%
End of Survey

Thank you for your help. Again, this information will be kept confidential. If you any questions, please contact Li Liang by email at lli91@vt.edu.
Appendix B: Mathematical Model

The raw materials $b$ harvested from the harvesting site $i$ should not exceed its upper harvesting limit of raw material $b$ at $i$.

$$x_{bi} \leq u_{bi} \quad \forall i \in I, b \in B$$

(1)

The amount of biomass shipped to the storage sites $l$ is less than or equal to the raw material harvested from the harvesting site

$$\sum_{l=1}^{L} x_{bl} \times y_{l} \leq x_{bi} \times y_{l} \quad \forall l \in L, i \in I, b \in B$$

(2)

The biomass shipped to the storage site $l$ should not exceed its upper storage limit of.

$$\sum_{b=1}^{B} x_{bi} \times y_{l} \leq u_{bi} \times y_{l} \quad \forall i \in I, b \in B$$

(3)

The amount of biomass shipped to the bio-refinery $j$ is less than or equal to the biomass stored in the storage site

$$\sum_{j=1}^{J} x_{bij} \times y_{j} \leq x_{bi} \times y_{l} \quad \forall l \in L, i \in I, b \in B$$

(4)

The biomass in the bio-refinery should be less than or equal to the transporting biomass from storage site to bio-refinery

$$x_{bj} \times y_{j} \leq \sum_{l=1}^{L} x_{blj} \times y_{l} \times y_{j} \quad \forall l \in L, i \in I, b \in B$$

(5)

The amount of bio-butanol produced is less than or equal to the yield of bio-butanol from biomass in the bio-refinery times the amount of biomass stored in the bio-refinery.

$$x_{Fj} \times y_{j} \leq R_{bj} \times x_{bj} \times y_{j} \quad \forall j \in J$$

(6)

The amount of bio-butanol produced in the bio-refinery should not exceed the production capacity of bio-butanol in the bio-refinery

$$x_{Fj} \times y_{j} \leq u_{pFj} \times y_{j} \quad \forall j \in J$$

(7)

The amount of bio-butanol shipped from the bio-refinery to the distribution center should not exceed the amount of bio-butanol produced from bio-refinery

$$\sum_{k=1}^{K} x_{Fjk} \times y_{j} \times y_{k} \leq x_{Fj} \times y_{j} \quad \forall j \in J, k \in K$$

(8)

The volume of bio-butanol shipped from the bio-refinery to the demand zone should not exceed the storage capacity of bio-butanol in the distribution center

$$\sum_{j=1}^{J} x_{Fjk} \times y_{j} \times y_{k} \leq u_{sFk} \times y_{k} \quad \forall j \in J, k \in K$$

(9)

The amount of bio-fuel shipped to the distribution center should be greater than the demand of distributed center

$$x_{Fjk} \times y_{j} \times y_{k} \geq \sum_{j=1}^{J} x_{Fjk} \times y_{j} \times y_{k} \quad \forall j \in J, k \in K$$

(10)
\[ \sum_{j=1}^{J} x_{Fjk} \times y_j y_k \leq D_{Fk} \times y_k \quad \forall j \in J, k \in K \tag{11} \]

Introduce a binary variable to model the selection of bio-refineries:
\[ y_j \leq 1, y_j \in N^+ \quad \forall j \in J \tag{12} \]

Introduce a binary variable to model the selection of storage site:
\[ y_l \leq 1, y_l \in N^+ \quad \forall l \in L \tag{13} \]

Introduce a binary variable to model the selection of demand zones:
\[ y_k \leq 1, y_k \in N^+ \quad \forall k \in K \tag{14} \]

The amount of byproduct produced in the bio-refinery less than or equal to the amount of pretreated biomass being converted in the bio-refinery through a mass balance coefficient
\[ x_{gj} \leq \eta_{gj} x_{bj} \quad \forall j \in J, b \in B, g \in G \tag{15} \]

Economic objective function:
\[ \max ec = C_{\text{butanol selling}} + C_{\text{byproduct sell}} - C_{\text{raw materials purchase}} - C_{\text{raw material storage}} - C_{\text{biomass transportation}} - C_{\text{biorefinery setup}} - C_{\text{bio-butanol production}} - C_{\text{butanol transportation}} \]

The benefit of selling bio-butanol is:
\[ C_{\text{butanol}} = \sum_{j=1}^{J} \sum_{k=1}^{K} C_{Fjk} x_{Fjk} \times y_j y_k \quad \forall j \in J, k \in K \]

The cost of harvesting raw materials is:
\[ C_{\text{raw materials purchase}} = \sum_{b=1}^{B} \sum_{i=1}^{I} C_{bli} x_{bli} \quad \forall b \in B, i \in I \]

The cost of storing raw materials is:
\[ C_{\text{raw materials storage}} = \sum_{i=1}^{I} \sum_{b=1}^{B} C_{bli} x_{bli} \times y_l \quad \forall b \in B, l \in L \]

The cost of biomass transportation (from harvesting site to storage site, and from storage site to bio-refinery) is:
\[ C_{\text{biomass transportation}} = \sum_{l=1}^{L} \sum_{i=1}^{I} \sum_{b=1}^{B} C_{lit} x_{bli} \lambda_{il} \times y_l y_j + \sum_{l=1}^{L} \sum_{j=1}^{J} \sum_{b=1}^{B} C_{ljq} x_{bjq} \lambda_{lj} \times y_l y_j \quad \forall l \in L, j \in J, i \in I, b \in B \]

The cost of biofuel transportation is:
\[ C_{\text{biofuel transportation}} = \sum_{k=1}^{K} \sum_{j=1}^{J} C_{Fjk} x_{Fjk} \lambda_{jk} \times y_j y_k \]
The costs of installing bio-refineries is:

\[ C_{\text{setup}} = \sum_{j=1}^{J} c_j y_j \quad \forall j \in J \]

The cost of butanol production is:

\[ C_{\text{production}} = \sum_{j=1}^{J} \sum_{b=1}^{B} C_{b,j} x_{b,j} \times y_j \quad \forall k \in K, b \in B \]

The benefit of selling byproducts is:

\[ C_{\text{byproduct}} = \sum_{j=1}^{J} \sum_{g=1}^{G} C_{g,j} x_{g,j} \times y_j \quad \forall k \in K, g \in G \]

Environment objective function:

\[ \text{Min } e_i = E_{\text{raw material transportation}} + E_{\text{harvest}} + E_{\text{feedstock storage}} + E_{\text{biorefinery operation}} - E_{\text{butanol transportation}} \]

The GHG emissions of raw material harvest activity is:

\[ E_{\text{raw materials harvest}} = \sum_{b=1}^{B} \sum_{i=1}^{I} E_{b,i} x_{b,i} \quad \forall b \in B, i \in I \]

The GHG emissions of biomass transportation (from harvesting site to storage site, and from storage site to bio-refinery) is:

\[ E_{\text{biomass transportation}} = \sum_{l=1}^{L} \sum_{i=1}^{I} \sum_{b=1}^{B} E_{T1} x_{b,i} \lambda_{i,l} \times y_l y_j + \sum_{l=1}^{L} \sum_{j=1}^{J} \sum_{b=1}^{B} E_{T2} x_{b,j} \lambda_{i,l} \times y_l y_j \]

\[ \forall l \in L, j \in J, i \in I, b \in B \]

The GHG emissions of biofuel transportation is:

\[ E_{\text{biofuel transportation}} = \sum_{k=1}^{K} \sum_{j=1}^{J} E_{T3} x_{F,j} \lambda_{j,k} \times y_j y_k \]

The GHG emissions of storing raw materials is:

\[ E_{\text{raw materials storage}} = \sum_{l=1}^{L} E_{l} \sum_{b=1}^{B} x_{b,l} \times y_l \quad \forall b \in B, l \in L \]

The GHG emissions of butanol production is:

\[ E_{\text{production}} = \sum_{b=1}^{B} E_{B,b} x_{B,b} \times y_j \quad \forall k \in K, b \in B \]
## Appendix C: Input Data Sources

<table>
<thead>
<tr>
<th>Parameter</th>
<th>definition</th>
<th>sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_{Bl}$</td>
<td>The upper harvesting limit of raw material $B$ harvested from harvesting site $I$ (kg)</td>
<td>The result from questionnaire survey</td>
</tr>
<tr>
<td>$u_{wBlj}$</td>
<td>The transportation capacity of biomass $B$ shipped from harvesting site $I$ to the bio-refinery $j$ during period $t$ in terms of weight (kg)</td>
<td>Based on the selected transportation mode</td>
</tr>
<tr>
<td>$u_{vBlj}$</td>
<td>The transportation capacity of biomass $B$ shipped from harvesting site $I$ to the bio-refinery $j$ in terms of volume ($m^3$)</td>
<td>Based on the selected transportation mode</td>
</tr>
<tr>
<td>$u_{sBj}$</td>
<td>The storage capacity of biomass $B$ in the bio-refinery $j$ ($m^3$)</td>
<td>Based on the size of the storage site</td>
</tr>
<tr>
<td>$u_{pFj}$</td>
<td>The production capacity of bio-butanol $F$ in the bio-refinery $j$ (gal)</td>
<td>Based on the result from case study</td>
</tr>
<tr>
<td>$u_{sFj}$</td>
<td>The storage capacity of bio-butanol $F$ in the bio-refinery $j$ (gal)</td>
<td>From objective 1</td>
</tr>
<tr>
<td>$u_{wFjk}$</td>
<td>The transportation capacity of bio-butanol $F$ shipped from bio-refinery $j$ to the distribution center $k$ in terms of weight (kg)</td>
<td>Refer to Wikipedia: <a href="https://en.wikipedia.org/wiki/Tank_truck">https://en.wikipedia.org/wiki/Tank_truck</a></td>
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<tr>
<td>$u_{vFjk}$</td>
<td>The transportation capacity of bio-butanol $F$ shipped from bio-refinery $j$ to the distribution center $k$ in terms of volume (gal)</td>
<td>Refer to Wikipedia: <a href="https://en.wikipedia.org/wiki/Tank_truck">https://en.wikipedia.org/wiki/Tank_truck</a></td>
</tr>
<tr>
<td>$u_{sFk}$</td>
<td>The storage capacity of bio-butanol $F$ in the distribution center $k$ (gal)</td>
<td>Based on the result from case study</td>
</tr>
<tr>
<td>$E_{Bl}$</td>
<td>The GHG emission of cultivating and harvesting raw material $B$ from harvesting site $I$ (kg CO2-eq/kg)</td>
<td>SimaPro</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Source/Method</td>
</tr>
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<tr>
<td>$E_{Blj}$</td>
<td>The GHG emission of transporting biomass $B$ from harvesting site $I$ to the bio-refinery $j$ ($\text{kg CO}_2\text{-eq/kg*mile}$)</td>
<td>GREET Model</td>
</tr>
<tr>
<td>$E_{Fjk}$</td>
<td>The GHG emission of transporting bio-butanol $F$ from bio-refinery $j$ to the distribution center $k$ ($\text{kg CO}_2\text{-eq/kg*mile}$)</td>
<td>GREET Model</td>
</tr>
<tr>
<td>$E_{sBj}$</td>
<td>The GHG emission of storing biomass $B$ in the bio-refinery $j$ ($\text{kg CO}_2\text{-eq/kg}$)</td>
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</tr>
<tr>
<td>$E_{sFj}$</td>
<td>The GHG emission of storing bio-butanol $F$ in the bio-refinery $j$ ($\text{kg CO}_2\text{-eq/gal}$)</td>
<td>GREET Model</td>
</tr>
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<td>$E_{Bj}$</td>
<td>The GHG emission of converting biomass $B$ in the bio-refinery $j$ ($\text{kg CO}_2\text{-eq/kg}$)</td>
<td>GREET Model</td>
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<td>$C_{Bl}$</td>
<td>The unit cost of harvesting raw material $B$ from harvesting site $I$ ($$/kg)</td>
<td>Based on the result from questionnaire survey</td>
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<td>$C_{Blj}$</td>
<td>The unit cost of transporting biomass $B$ from harvesting site $I$ to the bio-refinery $j$ ($$/kg*mile)</td>
<td>Searcy et al 2007</td>
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<tr>
<td>$C_{Fjk}$</td>
<td>The unit cost of transporting bio-butanol $F$ from bio-refinery $j$ to distribution center $k$ ($$/kg*mile)</td>
<td>Literature review</td>
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<tr>
<td>$C_{j}$</td>
<td>The capital cost of building the bio-refinery $j$ ($$)</td>
<td>Literature review</td>
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<tr>
<td>$C_{Bj}$</td>
<td>The unit cost of converting biomass $B$ in the bio-refinery $j$ ($$/kg)</td>
<td>Bharadwaj 2015</td>
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<td>$C_{gj}$</td>
<td>The selling price of byproduct $g$ produced in the bio-refinery $j$ ($$/kg)</td>
<td>Literature review</td>
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<tr>
<td>$C_{Fk}$</td>
<td>The selling price of bio-butanol $F$ in the distribution center $k$ ($$/gal)</td>
<td>Based on Questionnaire survey result</td>
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<td>$H_{Bj}$</td>
<td>The holding cost of biomass $B$ stored in the bio-refinery $j$ ($$/m^3)</td>
<td>Objective 1</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Source</td>
</tr>
<tr>
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<tr>
<td>$H_{Fj}$</td>
<td>The holding cost of bio-butanol $F$ stored in the bio-refinery $j$ ($/\text{gal}$)</td>
<td>Objective 1</td>
</tr>
<tr>
<td>$\rho_B$</td>
<td>The density of biomass $B$ ($\text{kg/m}^3$)</td>
<td>Literature review</td>
</tr>
<tr>
<td>$\rho_F$</td>
<td>The density of bio-butanol $F$ ($\text{kg/gal}$)</td>
<td>Literature review</td>
</tr>
<tr>
<td>$\lambda_{ij}$</td>
<td>The transportation distance from harvesting site $I$ to the bio-refinery $j$ (mile)</td>
<td>Google Map</td>
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<tr>
<td>$\lambda_{jk}$</td>
<td>The transportation distance from bio-refinery $j$ to distribution center $k$ (mile)</td>
<td>Google Map</td>
</tr>
<tr>
<td>$R_{FBj}$</td>
<td>The bio-butanol $F$ yield from biomass $B$ in the bio-refinery $j$ (gal/kg)</td>
<td>Based on results from Objective 1 and 2</td>
</tr>
<tr>
<td>$\eta_{gBj}$</td>
<td>The byproduct production $g$ yield from biomass $B$ in the bio-refinery $j$ (%)</td>
<td>Literature review</td>
</tr>
</tbody>
</table>
Appendix D: Worldwide Bio-ethanol and Bio-butanol Companies

<table>
<thead>
<tr>
<th>No.</th>
<th>Name</th>
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<td>Gevo</td>
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<td>Aemetis, Inc</td>
<td>Bioethanol</td>
<td>(408) 213-0940</td>
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<td>Bioethanol</td>
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<td><a href="mailto:info@cathaybiotech.com">info@cathaybiotech.com</a></td>
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<td>33</td>
<td>China New Energy</td>
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<td><a href="mailto:secretary@zkty.com.cn">secretary@zkty.com.cn</a></td>
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<td>GranBio</td>
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<td>Petrobras</td>
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<td><a href="mailto:municacao@ctc.com.br">municacao@ctc.com.br</a></td>
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<td><a href="mailto:media@lanzatech.com">media@lanzatech.com</a></td>
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<td>Chemistry and Industrial Development Org</td>
<td>woody Bioethanol</td>
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<td><a href="mailto:empolis@chempolis.co.uk">empolis@chempolis.co.uk</a></td>
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<td>St1 Biofuels</td>
<td>Waste based Bioethanol</td>
<td><a href="mailto:Risto.Savolainen@st1.com">Risto.Savolainen@st1.com</a></td>
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<td>Beta Renewables</td>
<td>Corn Ethanol</td>
<td><a href="mailto:o@betarenewables.com">o@betarenewables.com</a></td>
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<td>Butalco GmBH</td>
<td>Bioethanol &amp; Bio-butanol</td>
<td><a href="mailto:leaf@lesaffre.fr">leaf@lesaffre.fr</a></td>
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<td>51</td>
<td>SEKAB</td>
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<td><a href="mailto:info@sekab.com">info@sekab.com</a></td>
<td>Sweden</td>
</tr>
</tbody>
</table>
Appendix E: Code of mathematical model in CPLEX

/ parameters
int i = ...; // # of harvesting site
int j = ...; // # of butanol production plant
int k = ...; // # of distribution center
int p = ...; // # of year of this project
range I = 1..i;
range J = 1..j;
range K = 1..k;
range P = 1..p;

float UB[I] = ...; // The maximum harvest limit of sorghum stem from supplier i
float D[K] = ...; // Demand of customer k
float CB = ...; // The unit cost of harvesting sorghum stem from supplier i
float R = ...; // The interest rate of each year
float CTB1 = ...; // The unit cost of transporting sorghum stem without distance
float CTB2 = ...; // The unit cost of transporting sorghum stem with distances
float CTFU = ...; // The unit cost of transporting bio-butanol by truck
float CTFR = ...; // The unit cost of transporting bio-butanol by railway
float CJ[J] = ...; // The capital cost of building bio-refinery j
float CFJ[J] = ...; // The unit cost of producing biobutanol from bio-refinery j
float SFK[K] = ...; // The selling price biobutanol in customer k
float VB[I][J] = ...; // The transportation distance from harvest site i to bio-refinery j
float VF[J][K] = ...; // The transportation distance from bio-refinery j to customer k
float AB = ...; // The bio-butanol yield from sorghum stem
float EB = ...; // The GHG emission of cultivating and harvesting sorghum stem from supplier i
float ETB = ...; // The GHG emission of transporting sorghum stem
float ETFU = ...; // The GHG emission of transporting bio-butanol by truck
\( \text{float } \text{ETF} = \ldots; \quad \text{// The GHG emission of transporting bio-butanol by railway} \)

\( \text{float } \text{EF} = \ldots; \quad \text{// The GHG emission of producing bio-butanol} \)

\text{// Variables}
\[
\begin{align*}
\text{dvar float} & \text{+ XB}[I]; & \quad \text{// The amount of sorghum stem harvested from harvesting site } i \\
\text{dvar float} & \text{+ XFJ}[J]; & \quad \text{// The amount of bio-butanol produced in bio-refinery } j \\
\text{dvar float} & \text{+ XTB}[I][J]; & \quad \text{// The amount of transporting sorghum stem} \\
\text{dvar float} & \text{+ XTFU}[J][K]; & \quad \text{// The amount of transporting bio-butanol by truck} \\
\text{dvar float} & \text{+ XTFR}[J][K]; & \quad \text{// The amount of transporting bio-butanol by railway} \\
\text{dvar float} & \text{+ XFK}[K]; & \quad \text{// The amount of bio-butanol delivered to } k \\
\end{align*}
\]

\text{// Binary Variables}
\[
\begin{align*}
\text{dvar boolean } Y[J]; & \quad \text{// Determine whether bio-refinery } j \text{ is built} \\
\text{dvar boolean } YR[K]; & \quad \text{// Determine whether bio-butanol is delivered by truck} \\
\text{dvar boolean } YU[K]; & \quad \text{// Determine whether bio-butanol is delivered by railcar} \\
\end{align*}
\]

\text{// Epsilon constrain method}
\[
\begin{align*}
\text{float } f2\text{MAX} = \ldots; & \quad \text{// The maximum value of environmental objective function} \\
\text{float } f2\text{MIN} = \ldots; & \quad \text{// The minimum value of environmental objective function} \\
\text{float } f1\text{MAX} = \ldots; & \quad \text{// The maximum value of economic objective function} \\
\text{float } f1\text{MIN} = \ldots; & \quad \text{// The minimum value of economic objective function} \\
\text{float } P2 = \ldots; & \quad \text{// The number of grid point of the environmental objective} \\
\text{float } \text{eps} = \ldots; & \quad \text{// An adequately small number} \\
\text{float } z = \ldots; & \quad \text{// The number of times to solve the model} \\
\text{dvar float} & \text{+ } f1; \\
\text{dvar float} & \text{+ } f2; & \quad \text{// The environmental objective function} \\
\text{dvar float} & \text{+ } C2; & \quad \text{// Slack variables of the environmental objective function} \\
\end{align*}
\]

\text{// Objective function}
maximize f1 + eps*C2;
//introduce epsilon constrain method

//Constrain
subject to
{
    forall (i in I, j in J, k in K, p in P)
        sum(p in P) 1/(1+R)^p *
            (sum(k in K) SFK*XFK[k] -
                sum(j in J) VB[i][j]*XTB[i][j]*Y[j] -
                VB[i][j]*XTB[i][j]*Y[j] -
                CTB1 * sum(i in I, j in J) XTB[i][j]*Y[j] -
                CTB2 * sum(i in I, j in J) VB[i][j]*XTB[i][j]*Y[j] -
                //sorghum stem transportation cost
                CFJ[j]*XFJ[j]*Y[j] -
                //biobutanol production cost
                CTFR * sum(j in J, k in K) VF[j][k]*XTFR[j][k]*YR[k]
            )
        -CJ[j]*Y[j] == f1;
//bio-butanol production plant set up cost

    forall (i in I, k in K)
        sum(i in I) XB[i] * EB +
//GHG emission of harvesting sorghum stem
                ETB * sum(i in I, j in J) VB[i][j]*XTB[i][j]*Y[j] +
//GHG emission of transporting sorghum stem

}
EF * XFJ[j]*Y[j] +  //GHG
emission of producing bio-butanol

\[ \sum_{j \in J, k \in K} VF[j][k]*XTFU[j][k]*ETFU YU[k] + \]  //GHG
emission of transporting bio-butanol by truck

\[ \sum_{j \in J, k \in K} VF[j][k]*XTFR[k]*ETF*YR[k] == f2; \]  //GHG
emission of transporting bio-butanol by railway

\[ f2 + C2 == f2MIN + z*(f2MAX-f2MIN)/P2; \]

forall (i in I)  //The sorghum stem harvested from
//supplier i should not exceed its upper harvesting limit of raw material b at i.
\[ XB[i] <= UB[i]; \]

forall (i in I)  //The total amount of biomass b deliver to
different bio-refineries from supplier i should be equal to the amount of feedstock
harvested from supplier i
\[ \sum_{j \in J} XTB[i][j] == XB[i]; \]

forall (j in J)  //The amount of bio-butanol produced in
//bio-refinery j should be equal to the amount of feedstock b in the bio-refinery times
//the conversion rate.
\[ \sum_{i \in I} XTB[i][j]/AB*Y[j] == XFJ[j]; \]

forall (j in J)  //The amount of bio-butanol delivered from
//bio-refinery j to different customer should not exceed the amount of bio-butanol
produced from bio-refinery j
\[ \sum_{k \in K} XTR[j][k]*YR[k] + \sum_{k \in K} XTFU[k]*YU[k] <= XFK[j]; \]

forall (k in K)  //The amount of bio-butanol delivered to
each customer k
\[ \sum_{j \in J} XTR[j][k]*YR[k] + \sum_{j \in J} XTRU*YU[k] == XFK[k]; \]
forall (k in K) //The amount of bio-butanol delivered from bio-refinery to each customer k should not exceed the demand of customer k.
    D[k] >= XFK[k];
}
Appendix F: Invitation Letter for the Questionnaire Survey

Hello Dear Renewable Bio-fuel Producer:

Renewable bio-fuel has a great potential in the future. However paradoxically, various internal and external barriers, such as strategic issues, suppliers and third party issues, hampered the commercialization of renewable biofuel. In order to remove some of these barriers, renewable bio-fuel supply chain should be optimized. In this case, understanding the logistics activities in the renewable bio-fuel supply chain is very necessary.

The Sustainable Innovation Management Team from Virginia Tech would like to invite you to participate in a 15 min questionnaire survey and help us to understand the logistics activities in the renewable bio-fuel supply chain and further remove the barriers of renewable bio-fuel commercialization.

The collected data, following analysis and results will remain confidence and will only be used for this study (including a dissertation and publication).

The questionnaire survey only includes 15 questions and can be completed in 10 minutes.

Follow this link to the Survey:
Take the survey
Or copy and paste the URL below into your internet browser:

We would appreciate it if you would spend your valuable time to complete this survey.
Thank you so much for your reading.

Best Regards,

Li Liang
Ph.D. student
Sustainable Biomaterials, Virginia Tech
Email: lli91@vt.edu
Phone: (540) 808-5755
Sustainable Innovation Management Team:
www.sim.sbio.vt.edu
Appendix G: Implementation of the cellulosic bio-butanol supply chain network design model

The mathematical model was formulated and its feasibility was shown by the model application. The green cellulosic bio-butanol supply chain network design requires investors to apply this model in their own cases. This chapter introduces a procedure to implement this green supply chain network model. From this chapter, readers can learn how to use the model to design a cellulosic bio-butanol supply chain network with the maximum profitability and minimum GHG emissions. The steps of the model’s implementation are shown in Fig. 0.1. Each step is explained in detail in the following paragraphs.

---

**Fig. 0.1 Steps to implement the supply chain network design model**

**Step 1. To identify potential suppliers, distributors, and customers within the supply chain**

The participants in a cellulosic bio-butanol supply chain include suppliers, producers, distributors, and customers. Identifying potential suppliers and customers is an important step because they will impact the location of the bio-butanol production plant. To identify potential suppliers, users need to first determine which cellulosic biomass is used to produce bio-butanol. Different types of biomass have different conversion rates and different harvest costs. Users can use Table 5.2 on page 99 and Table 5.6 on page 109 of this dissertation as references to select the ideal type of biomass. The
identification of possible suppliers must also include a consideration of biomass quality, price, supplier’s aggregation, and customer services. To identify potential customers, users need to consider the customer demands from different usages of cellulosic bio-butanol. Users can use section 3.1.4 as reference for bio-butanol usage. Besides that, users can also take the co-products purchasers as the possible customers. The identification of potential distributors should take into consideration the price, speed, and the routes of bio-butanol transportation modes.

Step 2. To determine the production method of cellulosic bio-butanol

The two production methods for cellulosic bio-butanol are direct microbial conversion (DMC) and simultaneous saccharification and fermentation (SSF). These two major production methods can further evolve into several segmentations, such as catalytic pyrolysis and hydro-treating, to hydrocarbons, dilute acid hydrolysis, fermentation to acetic acid, chemical synthesis, enzymatic hydrolysis and consolidated bioprocessing (Brown et al 2012). Among these particular segmentations, the most economical one is consolidated bioprocessing (CBP) (Lynd et al 2005), since it can simultaneously complete the enzyme production, hydrolysis and fermentation in one single step and save more than 50% of the production cost comparing with the other production configurations such as SSF (Olson et al 2011). However, the determination of the production method should also consider the potential GHG emissions.

Step 3. To select the possible locations of cellulosic bio-butanol production plant

The users must select several potential locations which could be used to set up the bio-butanol production plant. To select the possible locations, several factors need to be considered. These factors include feedstock availability, market availability, energy costs, availability of favorable government incentives, and the utility of existing infrastructure networks. Among them, feedstock availability should be considered first. After selecting a few potential locations, the optimal location can be determined by the proposed mathematical model.

Step 4. To collect the related data about each production location

To apply the model, some input parameters are needed. The input parameters include:

- The maximum harvest quantity of biomass feedstock from each potential supplier
- The distances between each potential production plant and each potential feedstock supplier
- The capital investment required for setting up a bio-butanol production plant in each potential location
- The production costs of bio-butanol
- The distances between each potential production plant and potential customers
- The demands of each customer

Besides the above data, several additional input parameters are required. These parameters include the unit harvest costs of each supplier, the unit transportation costs of the particular biomass, the unit transportation costs of bio-butanol, the unit production costs of bio-butanol, and the GHG emissions for each activity in the supply chain network. The economic costs can be found in Table 5.19. And the data for GHG emissions can be found in Table 5.12. After the data was collected, users can input these data into an MS Excel work sheet, access database or other database software. Error! Reference source not found. provides an example of data entered into the excel work sheet.

![Fig. 0.2 Data in Excel worksheet](image)

**Step 5. To calculate the payoff table**

The payoff table is used to estimate the feasible solution range for the multi-objective mixed-integer linear programing model. The payoff table is obtained by lexicographic optimization. The payoff table for this model is shown in Error! Reference source not found.. The process to obtain the payoff table is not difficult. The \( f_1(x_1^*) \) can be obtained by maximizing the economic objective function only. The \( f_2(x_1^*) \) can be obtained by calculating the environmental objective function by using the variables from \( f_1(x_1^*) \). The \( f_2(x_2^*) \) can be obtained by minimizing the environmental objective function only. The \( f_1(x_2^*) \) can be obtained by calculating the economic objective function by using the variables from \( f_2(x_2^*) \). The optimization of each objective function can be completed with Excel, Lingo or other mathematical programming software.
Table 0.1 payoff table for the model implementation

<table>
<thead>
<tr>
<th></th>
<th>$f_1(x)$</th>
<th>$f_2(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max $f_1(x)$</td>
<td>$f_1(x_1^*)$</td>
<td>$f_2(x_1^*)$</td>
</tr>
<tr>
<td>Min $f_2(x)$</td>
<td>$f_1(x_2^*)$</td>
<td>$f_2(x_2^*)$</td>
</tr>
</tbody>
</table>

Where $f_1(x)$ refers to the economic objective function and $f_2(x)$ refers to the environmental objective function.

In order to better illustrate the method of calculating the payoff table, a simple example is shown here:

\[
\begin{align*}
\text{Max} & \quad 3x + 2y \\
\text{Min} & \quad 2x + 3y \\
\text{St}: & \quad x + y \leq 8 \\
& \quad 2x + y \geq 4
\end{align*}
\]

To calculate the payoff table, the following program needs to be solved for:

\[
\begin{align*}
\text{Max} & \quad 3x + 2y \\
\text{Min} & \quad 2x + 3y \\
\text{St}: & \quad x + y \leq 8 \\
& \quad 2x + y \geq 4
\end{align*}
\]

After solving for the above program, we get an optimal value of 24, with $x$ equal to eight (8) and $y$ equals to zero (0). We use these $x$ and $y$ values to calculate the other objective function, and get a value of 16.

To obtain the other values, the following program is solved for:

\[
\begin{align*}
\text{Min} & \quad 2x + 3y \\
\text{St}: & \quad x + y \leq 8 \\
& \quad 2x + y \geq 4
\end{align*}
\]

After solving this program, we get an optimal value of eight (8), with $x$ equal to four (4) and $y$ equal to zero (0). We use these $x$ and $y$ values to calculate the other objective function, and get a value of 12. Therefore, the payoff table is shown as follows.

Table 0.2 example of payoff table

<table>
<thead>
<tr>
<th></th>
<th>$f_1(x)$</th>
<th>$f_2(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max $f_1(x)$</td>
<td>24</td>
<td>16</td>
</tr>
<tr>
<td>Min $f_2(x)$</td>
<td>12</td>
<td>8</td>
</tr>
</tbody>
</table>
Step 6. To solve the model into optimization software

In order to solve the model, mathematical optimization software is used. Table 3.6 in provides detailed information for six popular optimization software packages. Any of them can be used to solve this model. In this research, optimization software CPLEX was used to solve the model. The code in CPLEX for this model is shown in Appendix E. If using CPLEX as the optimization software, users can make some changes to the provided code based on their particular situations.

Step 7. To calculate the model with the \( \varepsilon \)-constraint method

The \( \varepsilon \)-constraint method is used to optimize one of the objective functions by putting other objectives as constraints. Equation 1 is the original optimization program, and Equation 2 is the transferred optimization program. Through this transformation, the original multi-objective problem can be transferred into a single objective problem. The right hand side (RHS) of each constraint is determined by the payoff table. The payoff table shows the results coming from the individual optimization of each objective function, with these results obtainable through a conventional linear programming (LP) optimizer (Mavrotas 2009).

\[
\begin{align*}
\text{Max } f_1(x) \\
\text{Min } f_2(x) \\
\text{st } \\
x \in S,
\end{align*}
\]

\[
\begin{align*}
\text{Max } (f_1(x) + \text{eps} \times s_2) \\
\text{st } \\
f_2(x) - s_2 = e_2, \\
x \in S \text{ and } s_2 \in \mathbb{R}^+,
\end{align*}
\]

Where \( x \) is the vector of decision variables; \( f_1(x) \) is the economic objective function; \( f_2(x) \) is the environmental objective function; \( S \) is the feasible region; \( \text{eps} \) is a very small number (usually from \( 10^{-3} \) to \( 10^{-6} \)); \( e_2 \) is obtained by dividing the range of feasible solutions into evenly distributed intervals; and \( s_2 \) is the slack or surplus variable of the environmental objective function.

If using CPLEX as the optimization software, users can use Appendix E as a reference to apply the \( \varepsilon \)-constraint method. The user needs to decide how many grid points or intervals should be used to divide the range of feasible solutions. The number of grid points or intervals is indexed by P2 in the model’s code. By changing the number of \( z \) from 1 to P2, and calculating the model each time the number changes, the users can get a few feasible solutions.
Step 8. To select the optimal solutions from the Pareto curve

The Pareto curve can be obtained by plotting the feasible solutions from Step 5. The optimal solution can be found on the turning point of the curve. If the plot shows a linear relationship between two objectives (just like the model application in this research), users need to determine the optimal solution for themselves. In this case, users need to decide how much profit should be sacrificed to reduce GHG emissions.
Reference


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