EXPLORING BIOMASS QUALITY

WITHIN THE BIOMASS-TO-BIOFUEL SUPPLY CHAIN

USING PRINCIPAL COMPONENT ANALYSIS

by

AMANDA HYDAR, B.S.

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COMMITTEE MEMBERS: Krystel Castillo, Ph.D., Chair Frank Chen, Ph.D. Hungda Wan, Ph.D.

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DEDICATION

Alhamdulillah for everything.

To my fiancé, thank you for being my support system and best friend; sharing my success and happiness with you means the world to me.

To my family, I am so blessed to have you and forever grateful for your unwavering confidence in me.

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Amanda Hydar, M.S. The University of Texas at San Antonio, 2019

Supervising Professor: Krystel Castillo, Ph.D.

With a large effort to replace petroleum-based fuels and chemicals with a more sustainable source of energy, research in biofuel has become a topic of interest. The goal of this thesis is to first establish an important gap in the literature through an in-depth review of current biomass-to-biofuel research, followed by an analysis of biomass preprocessing data. The data obtained from pre-processing two types of biomass, with varying moisture content, are used to develop conclusions on how variables such as throughput, grinding energy, and logistics costs are related to the aforementioned factors, as well as to each other. Test data from Idaho National Laboratory was obtained and Principal Component Analysis (PCA) was used to investigate the correlation between selected factors and the overall performance of the system. The following factors were used for this study: corn stover versus switchgrass and incoming moisture percentage from each stage of grinding. The principal components were analyzed, and it was found that principal component 1, which was a value derived from measured throughput, measured energy consumption, and preprocessing cost, was the source of the most significant variance. Results from PCA also indicate that the type of biomass had a significant effect on the system's performance; ideal setup, which returned the largest throughput while minimizing energy consumption, was found to be preprocessing switchgrass with moisture content around 10%.

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CHAPTER ONE: INTRODUCTION

Biomass is an alternative energy source used to produce biofuels, which can help alleviate our reliance on fossil fuels and promote energy assurance and independence. Fossil fuels such as coal, oil, and natural gas contribute to greenhouse gas emissions [1]. In order to reduce emissions, many researchers have stepped forward to develop knowledge of logistics for sources of renewable energies such as biomass-to-biofuel applications.

Biomass is, by definition, organic matter, especially plant matter, and it can be converted to fuel. Biomass for the production of bioenergy can be classified in three generations. The *first generation* includes edible crops such as sorghum and corn. *Second generation* biofuels have been developed from non-edible crops such as wood chips, switchgrass, Miscanthus, organic waste, and food crop waste (e.g., corn stover). The *third generation* of biomass utilizes algae, a low cost, high energy, and entirely renewable source of energy. Following the debate of food versus fuel, research efforts are focused on the development of second and third generation biofuels.

Among the many reasons biomass has been a fruitful topic of research, energy assurance is one to be noted. With the ability to yield biomass in significant quantities every year, the amount of energy able to be produced is abundant; according to data presented in the 2016 Billion-Ton Report, total biomass energy consumption reached nearly 5,000 Trillion Btu in 2014 [2]. Moreover, biofuel offers a better alternative for environmental health since biofuels produce fewer greenhouse gas emissions than petroleum-based fuels [2]. In addition, biomass is a sustainable energy source with net zero emissions [3].

While biofuels are a suitable alternative to fossil fuel consumption, it is critical to design efficient feedstock logistics to allow biofuels to compete with fossil fuels. The design of

networks that define the flow of biomass from the land to the biorefinery is referred in the literature as the study of biomass-to-biorefinery supply chains. Modeling and optimization of this supply chain is a focused area of research that aims to develop solutions to make bioenergy systems cost-effective. The main objectives of biomass-to-biorefinery supply chain optimization are typically focused on reducing overall costs, reducing emissions, and increasing sustainability.

Many characteristics of biomass come into play when considering how to efficiently utilize biomass as an alternative form of energy generation. Operations such as handling, storage, transportation, and conversion are all effected by the physical and chemical properties of the given biomass; these properties include, but are not limited to, chemical composition, density, particle size, moisture content, calorific value, and ash content [4]. Lam and Sokhansanj [4] go into further detail as to how each engineering property of biomass is calculated/determined and how operators control the way biomass is prepared for either its handling or its conversion to other forms; they conclude that a deep understanding of biomass physical and chemical properties, and the ability to characterize these properties, are required for design and safe operation of processing facilities.

Throughout this thesis, *biomass quality* is an underlying topic. Quality of the biomass mainly determines its value for specific conversion systems. Biomass quality is largely dependent on the aforementioned properties of biomass. For example, parameters on characteristics such as chlorine, ash content, and ash melting point are vital for thermal conversion [5]. In addition, biological conversion relates to carbohydrates and lignin content, while anaerobic digestion has criteria for digestibility and bio-gas yield [4]. While some fundamental properties are unable to be changed, others may be optimized with pretreatment processes such as drying, compacting, or size reduction; these processes may adjust particle size,

moisture content, and bulk density [4]. Furthermore, characteristics developed along the supply chain as a result of contamination and various influencing factors will negatively affect biomass quality and create problems along the supply chain.

Biomass Physical and Chemical Properties

Lignocellulosic biomass is made up primarily of lignin, cellulose, and hemicellulose, as well as various plant components such as sugars, starch, acids, fats, and oils, water (moisture) and ash [6]. A clear understanding of the physical and chemical composition of biomass is increasingly important because these characteristics impact the quality.

Lignin content, for example, can hinder bioconversion through formation of anti-quality compounds or inhibitors, such as polyphenols [6]. Additionally, lignin is considered a fundamental biomass characteristic, meaning it is not easily changed or broken down by enzymes or microorganisms. Therefore, a higher percentage of lignin content will result in problems along the conversion process; biomass becomes more suitable for biochemical conversion when cellulose and hemicellulose are higher in content [6].

Another example of a fundamental property of biomass is the *ash content*, which may be increased from soil contamination. Ash content relates to the operational problems that occur during processing and combustion such as slagging and fouling and is, therefore, a critical consideration when designing the processes required for preparation and conversion [7].

Moisture content is an important physical property when designing a drying process due to the desire to minimize mold formation [8] and off-gassing issues [9].

Biomass density is often categorized as bulk density and particle density. *Bulk density* is the received kg/m³ value and essentially determines the ease of handling as well as the cost of transport [6]. *Particle density* is the mass of a single particle over its volume. Both bulk density

and particle density largely affect supply logistics, transportation, and storage of biomass and as a result, the overall cost [7]. *Particle size* is summarized into three dimensions: length, width, and thickness. The size of particle is important for handling, storage, and efficient downstream conversion [10]. Understanding these properties and ensuring the correct biomass type and quality is used can play a major role in costs, yield, and end product quality.

Standardization of biomass quality, while critical for the growth of the bioenergy industry, is extremely underdeveloped. The International Organization for Standardization recently released ISO 17225 series, which includes definition and classification standards, as well as standards for chemical and mechanical testing relating to biomass quality [11]. Additional guidelines for determining and characterizing properties of biomass are available through standards such as the ASABE Book of Standards [12], ASTM Standards [13], and CEN Standards [14].

Processes within the Biomass to Biofuel Supply Chain

While processes along the biomass-to-biofuel supply chain (BSC) may vary depending on biomass type, preparation, and conversion techniques, the supply chain generally includes the following major elements: (1) farms, (2) storage facilities, (3) biorefinery plants, (4) blending facilities, (5) retail outlets, and (6) transportation [15]. Further, these elements may be categorized according to two interdependent and interconnected processes: the production planning and control processes, and the distribution and logistical processes [16]. The production planning of biomass. The distribution and logistical processes consists of storage, transportation, and transshipment of biomass [17]. Figure 1, for example, illustrates an example of the stages and processes for corn stover in preparation for biochemical conversion [18].



Figure 1. Flow Diagram of the 2012 Baseline Design Case to Supply Biochemical Conversion

The BSC is complex, with many variables to consider along with uncertainty and variability involved within each stage. Dealing with biomass quality uncertainty, biomass availability, and demand uncertainty can be a daunting task, but are important aspects when determining the most efficient chain structure. This challenge has led researchers to focus on the development of optimization models with the objective of minimizing costs associated with production, logistics, and operation of different sites [19]. Extensive literature focusing on the modeling and optimization of the BSC is available and will be discussed in further detail in Chapter 2.

Considering Biomass Quality in Supply Chain Optimization

Biomass quality is a relevant aspect to consider when optimizing supply chain operations. Uncertainty in biomass quality is often present along the supply chain and can ultimately lead to unexpected variability when analyzing profitability of bioenergy investments. Many variables affect biomass quality throughout the supply chain. For example, during storage, the biomass quality may change due to weather fluctuations and even to microbial activity [20]. The moisture content of biomass is often a decision variable considering it affects the energy availability, boiler efficiency and combustion stability, yet it is not realistic to account for moisture content as one static value when it varies throughout the supply chain processes. Ignoring the uncertainty and variability of these variables could lead to inaccurate results and therefore discrepancies in supply chain logistics, which can be a costly mistake.

Aside from considering variability and uncertainty of these characteristics, it is important to consider multiple biomass properties, as opposed to singling out a single variable, as they may be interconnected. For example, a recent study aimed to optimize all the steps directly effecting biomass quality in the biomass supply chain to improve the cost-benefit balance [20]. Four methodologies were presented in this study, which considered the effects of moisture content, ash content, and, finally, the origin, handling, and harvesting season of biomass; all variables analyzed were shown to directly affect the quality of biomass. Results from economic analysis concluded that the highest differences between the heating value and the best possible estimation of the biomass received in the power plant have been obtained when the ash content varies from the reference value (e.g., differences up to 760 kJ/kg have been observed for an ash content of 6%). For the rest of the parameters studied (harvesting season and biomass origin), the maximum heating value differences are always below 575 kJ/kg, but there is a difference nonetheless [20]. These findings illuminate the fact that, although one may focus on a single variable to analyze general effects, other factors which effect the overall supply chain must not be ignored.

Based on previous works' findings, it can be concluded that quality control methods for biomass are necessary and beneficial to minimize supply chain costs. One recent publication, which integrated biomass quality variability in a stochastic supply chain optimization model, concluded that supply chain cost could increase as much as 27%-31% when biomass quality (defined as moisture and ash content) is poor [21]. Therefore, this thesis focuses on reviewing

biomass supply chain optimization methods and building upon this research while including biomass quality as a main consideration.

The goal of this thesis is to investigate how biomass physical and chemical composition effects supply chain logistics. This thesis aims to provide both theoretical and practical insights on the impact of biomass variability on the performance of the preprocessing systems through the use of statistical techniques applied to a realistic case study.

This paper is organized as follows: Chapter 2 provides and in-depth literature review on existing published works that address quality characteristics of biomass and challenges when building decision support systems for the design and planning of biomass logistics; this includes a discussion regarding the categorization of papers found and their approach to quality consideration within BSCs through varying optimization techniques. Chapter 3 describes the methodology, which was used to analyze data and develop conclusions for further investigation as well as a brief explanation on how this thesis expands on previous works. Chapter 4 provides insight as to how data was collected and applies the Principal Component Analysis technique to a realistic case study. Chapter 5 summarizes outcomes and reviews the significance of findings. Finally, Chapter 6 highlights fruitful areas of future research.

CHAPTER TWO: LITERATURE REVIEW

Each paper reviewed considers the modeling and quantification of quality of biomass as an important factor in optimizing supply chain operations. Eighty-eight scientific publications identified as significant references in terms of modeling and optimization have been reviewed. The publications range from 2002-2018. The intention of this review is to begin exploring how current published works have addressed biomass quality, which has a significant influence on supply chain logistics. In doing so, this review illuminates an important gap in literature by discussing under met topics in recent research efforts and defining a future research agenda.

With a multitude of methods used, it was necessary to classify all articles for purpose of clarity and organization of material. Generally, operational research (OR) models involve an objective function, decision variables, and specified constraints, all of which are modeled using a specific optimization technique. Thus, each publication was evaluated and categorized based on its classification within two categories: (1) optimization method utilized, and (2) quality aspect considered. Keywords inputted into databases included the following: (Modeling Or Optimization) and (bio*) and (Supply chain) and (Quality). Multiple databases were used including, but not limited to, Google Scholar, ScienceDirect, Scopus, IEEE Xplore, and Wiley Online Library. All material that was not considered academic or published in a scientific journal was excluded from reviewed literature. Figure 2 shows a summary of the distribution of papers gathered based on scientific journal. The aims and scope of the majority of the journals are related to broad topics in energy and sustainability; a few journals are specialized such as the Biomass and Bioenergy journal. Noteworthy, only eight published works in modeling and optimization of biomass quality variability were found from journals in the industrial and systems engineering and/or computer optimization community.



Figure 2. Scientific Journal Distribution

Following assessment and categorization, Figures 3 and 4 were developed to summarize the array of articles. The first level of classification being the optimization method used; each paper was determined to use mathematical programming or computer simulation and further characterized according to sub-categories described in section 3. In addition, the quality characteristics discussed in each paper is noted in the far right column.

	Mathematical Modeling									
Year, Author/		Determ	ninistic	Stock	nastic	Heu	ristic	Non-	Linear	Quality Characteristic Considered
Optin	nization Method	tion Method Single Mul Objective Object		Single Objective	Multi- Objective	Single Objective	Multi- Objective	Single Objective	Multi- Objective	
2017	Belart	x								Moisture Content
2016	Castillo	х								Ash, Moisture Content
2014	Hartley	х								Density, Seasonality
2010	Huang	х								Moisture Content
2014	Lin	х								Moisture Content, Density
2012	Marvin	х								Moisture Content
2014	Sosa	х								Moisture Content, Density
2018	Hernandez	х								Moisture Conent, Ash Content, Seasonality
2017	Giuliano	х								Lignin Conent, Seasonality
2012	Acuna	х								Moisture Content
2014	Khorshidi	х								Moisture Conent
2012	Alam	х								Seasonality
2018	Malladi	х								Seasonality
2015	Taskhiri	х								Moisture Conent
2011	Van Dyken	х								Moisture Content, Density
2009	Alfonso		х							Moisture Content, Ash Content, Seasonality
2017	Arora		х							Moisture Content, Ash Content
2015	Cambero		х							Moisture Content, Ash Content, Density
2016	Cambero		x							Moisture Content, Ash Content, Density
2012	Cucek		x							Moisture Content, Density
2013	Kanzian		х							Drv Matter Loss
2014	Perez-Fortes		х							Moisture Content, Ash Content, Density, Seasonality, Dry Matter Losses
2017	Tan		х							Moisture Conent, Seasonality
2012	You		х							Moisture Content, Ash Content, Density, Seasonality
2016	Azadeh			х						Moisture Conent
2014	Azadeh			х						Moisture Conent
2017	Castillo			x						Moisture Content, Ash Content, Seasonality
2012	Chen			х						Moisture Conent
2014	Gonzalez-Salazar			х						Moisture Content, Density
2016	Lopez-Diaz			х						Density
2014	U			х						Moisture Content
2015	Shabani			х						Moisture Content, Ash Content
2015	Zamar			x						Moisture Content
2012	Chen				х					Moisture Conent
2017	Cobuloglu				х					Seasonality
2012	Gebreslassie				х					Moisture Conent, Density, Seasonality,
2002	Gigler				х					Moisture Conent, Particle Size
2014	Marufuzzman				х					Energy Loss
2018	Xie				х					Moisture Content, Density
2007	Gronalt					х				Moisture Content, Seasonality
2008	Reche-Lopez					х				Density
2015	Poudel					х				Density
2016	Poudel					х				Seasonality
2017	Quddus					х				Moisture Content, Density, Seasonality
2013	Gomez-Gonzalez					x				Density
2010	Vera					x				Density
2017	Yang					x				Composition. Quality Control
2012	You						х			Moisture Content, Ash Content, Density, Seasonality
2016	Hernandez-Calderon							х		Density
2012	Shabani							х		Moisture Content, Ash Content, Density
2017	Tan								х	Moisture Content, Density

Figure 3. Matrix of Mathematical Programming Papers Reviewed

				Simu	Quality Characteristic Considered			
Year, Author/ Optimization Method		Discrete Event Simulation		Continuous		Agent-based	Simulation-based Optimization Approach	
		Single	Multi-	Simulation	Simulation	Single	Multi-	
		Objective	Objective			Objective	Objective	
2013	Amundson	Х						Moisture Content, Density
2017	Kishita	х						Moisture Content
2016	Pinho	х	х					Moisture Content
2011	Mobini	х						Moisture Conent
2015	Windisch	х						Moisture Content
2012	Woli		х					Moisture Content, Seasonality
2015	Bai			х				Density
2014	Mobini			х				Moisture Content, Density
2017	Sándor			х				Moisture Content, Dry Matter Loss
2017	Shu				х			Density
2014	Singh				х			Seasonality
2013	Ebadian					х		Moisture Content, Seasonality, Dry Matter Loss
2011	Faulkner					х		Density, Seasonality
2013	Sharma				X Moisture Content, Seasonalit		Moisture Content, Seasonality	
2017	Chavez					Х		Moisture Content, Ash Content, Dry Matter Loss

Figure 4. Matrix of Computer Simulation Papers Reviewed

To efficiently incorporate biomass quality into supply chain optimization, both aspects of biomass physical and chemical characteristics, as well as outside factors affecting these characteristics are used as parameters to optimize the objective function(s). A large reason behind the lack of implementation of quality considerations into optimization models is the fact that many biomass quality characteristics involve uncertainty due to the variability associated with various types of biomass as well as preprocessing conditions. Uncertainty is often difficult to model, but is nevertheless germane to accurately make design and management decisions within the supply chain. Variability arises from production and harvest conditions, collection and storage practices, and species variation [22]. If biomass quality variations are ignored, the costs, which are associated with such variability, will have a detrimental impact when in the operational stage. Castillo-Villar et al. [21] quantify and control the impact of biomass quality variability on supply chain related decisions and technology selections in a recent article. The results show that high moisture and ash contents negatively affect the delivery cost and supply chain cost could increase as much as 27%-31% when biomass quality is poor. Another article, which focuses on minimizing cost through a robust optimization model, included both uncertainties in biomass quality and biomass availability. The model finds a major trade-off between profit and variability of biomass quality; results reveal that profit decreases by up to 23% when there is a $\pm 13\%$ variation in moisture content and $\pm 5\%$ change in higher heating value [23]. Khorshidi et al. [24] investigate quality and quantity impacts on both economic and performance objectives through considering three biomass feedstocks with varying co-firing levels; results show that increasing biomass quality improved plant performance with a moderate increase in electricity costs. Including characteristics such as chemical composition, ash and moisture content, seasonality, dry matter loss, and density and their inherent variability is an

important and largely overlooked necessity in modeling and optimizing biomass-to-biofuel supply chain operations.

Current Research Considering Biomass Quality

Lignocellulosic biomass is comprised primarily of cellulose, hemicellulose, and lignin. Giuliano et al. [25] conclude that composition of the biomass feedstock in terms of cellulose, hemicellulose and lignin content has a significant role in biomass allocation to the three product production processes considered for levulinic acid, succinic acid, and ethanol. Further, the authors suggest considering the quality of composition while still in the conceptual design phase should mitigate the negative effect of the change of biomass composition on the plant performance. One reason for this is lignin's inability to be degraded by enzymes and microorganisms; with this effect, the biomass tends to be difficult to utilize in biochemical conversions [6]. Biomass with lower lignin content could help reduce the heavier molecular weight compounds present in pyrolysis oil and produce a more homogenous liquid [26]. Fahmi et al. [27] gather that total liquid yield, increases as lignin increases, while the ash and alkali metal content decreases. Unfortunately, the process of minimizing lignin content involves costly pre-treatment processes, which involve solvents, acids and bases, or high temperature methods to remove hemicelluloses and lignin from cellulose [28]. These processes are often costly and the development of new cost-effective methods is a growing issue associated with biochemical conversion. For these reasons, it is important to consider the chemical composition of biomass feedstock when aiming towards cost reduction and overall process optimization.

Ash, a noncarbohydrate component of biomass, has a negative impact on feedstock value for bio-chemical conversion; it displaces valuable carbohydrate content and decreases pretreatment efficacy [29]. Soil found in biomass, for example, will decrease the amount of

convertible biomass content and will increase the neutralization capacity of corn stover during dilute-acid pre-treatment, which reduces the conversion yield [30]. Because of these negative effects on overall value and yields, high quality biomass is considered to have low ash content among its characteristics, and there is often a threshold of maximum ash content on a dry basis for conversion efficiency [31]. Alfonso et al. [31] present a methodology to assess optimal management and energy use of distributed biomass resources while including biomass quality as a consideration; within this methodology's quantification, three generation ratios and characterization of produced waste biomass are used, including ash content as well as maximum ash content restrictions. Specifically, this study takes into account that ash content should be lower than 3% and 5% for both plant types BP1 and BP2. It is found that low average ash content (<3%) and high potential for self-consumption of biomass formulated the ideal situation for the installation of a pellet plant. From another standpoint considering ash content, Arora et al. [32] offer a Multi-Objective Optimization (MOO) approach which is used to minimize the manufacturing costs and the environmental impacts of the biomass-to-ammonia process specific to each feedstock and country; the authors note that the incineration of fly ash from the gasifier is a major contributor to human toxicity. Shabani et al. [33] developed a mathematical model to optimize the supply chain of a forest biomass power plant while considering supply, storage, production and ash management. Investment in a new ash recovery system is analyzed and the model shows that this new system has significant economical and environmental benefits. It is evident from these studies that the ash content of biomass has a significant impact on multiple levels of the biomass-to-biorefinery supply chain.

Zamar et al. [34] define moisture content within their model as the percentage equivalent of the ratio of the weight of water to the total weight of the biomass and describes that when it

comes to biomass, the higher the moisture content, the lower the net energy content. According to Acuna et al. [35], the single most important quality attribute is the moisture content of chips or raw material delivered to energy plants. Acuna et al. [35] find that both the proportion and volume of the biomass material delivered to the plant are very sensitive to specifications on moisture content range limits and the length of the storage (drying) period. It is found that when comparing a scenario with no storage, to that of implemented drying methods before chipping and delivery of biomass, a reduction in volume harvested of up to 33% could be achieved to meet monthly energy demand. Drying and storage methods are a large area of study among researchers who aim to decrease moisture content in biomass. One example comes from Windisch [36], who developed an alternative, information-based process using data on transportation distance, drying models for forecasting the moisture content, and data on the volume of the storages. Through investigation of their effects using discrete-event simulation and a cost-benefit analysis, it is concluded that decreasing the moisture content increases the energy density of the material, as well as improves the mass per volume ratio. More specifically, average moisture content of 4.38% in the peak period of moisture content scenario increased the average energy density per truckload by 12.16% [36]. An optimization model presented by Van Dyken et al. [37] focuses on the relationship between moisture and energy content in a discretized framework and long-term processes such as storage with passive drying effects. Similar to this methodology, many optimization approaches consider moisture content as a significant variable, and present models analyze drying techniques to lower biomass moisture content. For example, Belart et al. [38] present a mixed integer model to optimize residue delivery while considering energy content of drier residues; findings point that shifting to a material with lower moisture content decreases the overall production costs by 20.4%. Moisture

content considerations are also important for the equipment used to process biomass at various stages. Tan et al. [39] discuss how biomass power plants restrict the moisture content on each variant of biofuel to guarantee the normal running of the generator settings and accounted for these restrictions while optimizing profit margins, environmental factors, and electricity generation. Similarly, optimal locations and capacities of biorefineries are determined simultaneously with biomass harvest and distribution by Marvin et al. [40] and a 15% moisture content restriction is implemented. It is found that moisture content is an important parameter to consider when minimizing cost throughout the biomass supply chain [41]–[44].

A specific source of variability in biomass quality lies in the feedstock seasonality. Considering seasonality when attempting to model biomass supply chain operations provides a more adaptive and accurate model. An illustration of this is found in Xie et al.'s [45] multistage, mixed integer programming model which integrates multimodal transport into the cellulosic biofuel supply chain design under feedstock seasonality; through creating a model which adapted to feedstock seasonality, more cost effective and capable handling policies on distance limits for biomass truck deliveries are able to be made. Another demonstration of how season-to-season variations in biomass quality affects supply chain configuration is revealed by Lin et al. [46] while considering that Miscanthus yield is highly dependent on moisture stress; Lin et al. developed a model which could quantify how the resulting change of biomass yield from seasonality would affect farmers' tactical operating decisions. With moisture content being a significant biomass quality variable, understanding the impact and causes (such as seasonality) of moisture variability is imperative. Sosa et al. [47] developed a linear programming tool in which seasonally varying moisture content is a driving factor for cost optimization. Although the constraint on moisture content increases both transport and overall supply chain costs, optimal

truckloads are achieved by controlling wood moisture content. Sharma et al. [48] account for seasonality through a yield adjustment factor which varied between 0 and 1 and adjusted the biomass yield change with progressing harvest season. These variations, resulting from biomass seasonality, play a large role in risk management. Expanding on risk management, Gebresslassi et al. [49] analyze the risk associated with uncertainty in feedstock supply through comparison of both deterministic and stochastic solutions and their effects on annual cost and financial risk. Due to the consideration of uncertainty, it was concluded that the stochastic model had a better performance under variations due to seasonality. Accounting for the variability and uncertainty of biomass quality associated with seasonality provides a more accurate solution.

While the storage of biomass is necessary to compensate for seasonal variability in production and consumption, dry matter and energy losses often occur during this process due to microbial activity. A recent study in Germany conducted extensive field trials, which indicate that five months of storage results in dry matter loss of 11.1% and energy losses of up to 11.3% [50]. These storage and seasonal effects on dry matter and energy losses have become an important consideration within biomass supply chain optimization; Sokhansanj et al. [30] include dry matter loss of biomass in a simulation of collection, storage, and transportation operations for supplying agricultural biomass to a biorefinery. This simulation concludes that moisture content and the dry matter loss of biomass through the supply chain is heavily influenced by weather conditions, including rain and snow. This type of weather uncertainty in the biomass supply chain is addressed by Sharma et al. [48], in which a scenario optimization model is developed with the intent to minimize the cost of biomass supply to biorefineries over a one-year planning period under various weather scenarios. The results indicate that available harvest work hours affected cost related decisions and biomass storage method selected should dependent on the cost

and dry matter loss during storage. A consideration to mitigate these losses is the implementation of pre-treatment processes. Perez-Fortes et al. [51] present an optimization of pre-treatment selection for the use of woody waste in co-combustion plants in which biomass transportation, storage, and change of properties such as dry matter and energy density were studied under varying pre-treatment conditions. This study proposed location-allocation decisions with selection of pre-treatment technologies and summarized biomass property changes according to each pre-treatment; chipping, torrefaction, pelletization, and storage are all found to have an effect on matter loss percentage [51]. Further, several collected articles take into account dry matter and energy losses through various approaches including CO₂ emission minimization [52], storage systems in agricultural biomass supply chain for cellulosic ethanol production [53], truck configuration [47], and analysis of upland and lowland varieties [54]. Dry matter loss has been proven to be difficult to model due to continuous changes in moisture content, which impacts the amount of dry matter and energy losses. Prediction models, which can be used within optimization models, are essential to account for such variation.

Bulk and unit density of biomass are important properties to keep consistent through the supply chain because they significantly influence storage, transportation, and handling characteristics and, by extension, feedstock cost and quality [18]. For example, the spatial distribution and low bulk density characteristics of woody biomass tend to make collection and transportation difficult, as compared to traditional energy sources [55]. Because density is a fundamental characteristic of biomass, and affects operations along the supply chain, it is often a measurement used to quantify the quality of biomass. An example of this is explained by Reche-Lopez et al. [56], in which they define the theoretical biomass potential from the net density of dry biomass, while optimizing technology decisions. Similar techniques have been applied which

include biomass density as a parameter to better define biomass properties among many optimization models [49], [51], [57]–[59]. Further, the study of biomass density has been applied to pre-processing techniques such as densification. Quddus et al. [60] propose an optimization model to help minimize cost and mitigate emissions along the supply chain. Three technologies are presented, namely conventional pellet processing, high moisture pellet processing, and ammonia fiber expansion. These methods are used with various types of biomass for pre-processing/pre-treatment and densification. Densification is found to overcome issues related to physical and chemical composition, storage, and logistics to successfully co-fire higher percentages of biomass with coal [61].

Figure 5 depicts a summary of the distribution of research papers by quality characteristics addressed. It is observed, that moisture content is the most studied biomass quality feature (40.5%), followed by density (21.6%), then seasonality, ash content, dry matter loss and overall composition have received less attention in the literature. Filling in these gaps to provide further research as to how these biomass properties effect the handling, transportation, and conversion of biomass is vital to designing and planning an optimized supply chain. It is also worth noting that there were several papers that included two or more biomass quality aspects (refer to Figures 2 and 3 for details). This approach is ideal for obtaining the most realistic solutions. Each biomass property plays an important role in the biomass-to-biorefinery supply chain and encompassing several considerations into one model enables the research to develop stronger conclusions regarding optimal supply chain design. For example, a recent work by Castillo et al. [62] proposes a Biomass Supply Chain Cost of Quality (BioSC-COQ) which considers both moisture and ash content and is able to select the optimal levels for each property to minimize overall cost. In another article, You et al. [57] take an in-depth approach for design

and operations of cellulosic ethanol supply chains under economic, environmental, and social criteria and take into account several quality characteristics such as density, moisture content, ash content, and seasonality. This allowed results to reveal significant trade-offs and simultaneous prediction of the optimal network design, facility location, technology selection, capital investment, and logistics management decisions, among others. Although the complexity of these studies increases, as more considerations are included, the development of more comprehensive models aims to more accurately quantify feedstock quality implications.



Figure 5. Pie Chart of Quality Characteristic Distribution

Modeling Approaches

As the most prevalently used method for Operations Research problems, *mathematical programming* serves as a versatile tool for optimizing a function of several variables within specific constraints. In other words, each mathematical program takes an objective function to maximize or minimize while taking into account all decision variables and establishing constraint relationships linking said variables. Mathematical programming may be further broken

down into either a *deterministic, stochastic, or heuristic approach*. Further, the approach may either seek to optimize a single variable or multiple variables, referred to as *single-objective or multi-objective*, respectively. Summarizing, the modeling approaches used by researchers to study the uncertainty of biomass quality and its impact on logistics and operations are presented in Figure 6, with more details on all references in Figure 3.



Distribution of Modeling Approaches

Figure 6. Modeling Approaches used Throughout Literature

Deterministic models assume certainty in all input parameters and are the more commonly used approach in biomass supply chain modeling. This is largely due to the fact that a deterministic approach is not as computationally challenging as stochastic approaches. The deterministic mathematical modeling with a single objective or multiple objectives is by far the most used approach with 35% of the reviewed manuscripts [20], [24], [25], [31], [32], [35], [37]–[39], [41], [42], [46], [47], [51], [52], [55], [57], [59], [62]–[67].

A *stochastic approach* allows for random variation through developing probabilistic models for real-life systems, which have an element of uncertainty. Although stochastic

modeling is desired due to uncertainties within the supply chain, this method of optimization requires a considerable amount of computational effort to solve real-life size problems and the algorithm development tends to be convoluted. Common methods used in stochastic optimization are Monte Carlo Simulation, Stochastic Mixed Integer Linear Programs (SMILP), Integer Stochastic Programming (ISP), Stochastic Mixed Integer Non-Linear Programs (SMINLP), Markov Decision Process (MDP), and Linear Programs (LP) with Scenario Generation (SG). Generally, from the modeling perspective, the multistage stochastic programming method results in more cost-effective but computationally expensive solutions than values obtained from deterministic and two-stage stochastic solutions [68]. In regards to biomass quality specifically, stochastic programming allows models to incorporate the uncertainty in weather conditions, seasonality, and ultimately quality uncertainties. The stochastic modeling approach with a single objective follows with 15% of the papers [21], [23], [34], [44], [49], [68]– [76].

Moreover, *heuristic approaches* account for 12% of the studies [56], [57], [60], [77]– [82]. Heuristic approaches differ from other mathematical programming approaches in the sense that they will not necessarily look for optimal solutions, but will evaluate a problem in a shorter period of time and obtain near-optimal solutions. This approach is taken when optimization problems are NP-hard, no polynomial time algorithm exists, and computation times are too high for practical purposes [83].

Non-Linear Programming (NLP), mixed integer non-linear programming (MINLP), and Stochastic Mixed Integer Non-Linear Programming models have non-linear constraints and/or objective functions. Non-linear programs may become extremely complex and are, therefore, less commonly used than LP methods. However, some aspects of real world problems should not

be modeled with the simplicity of linearity and require NLP, MINLP, or SMINLP models. The complexity of this approach contributes to the lower percentage of contribution to the literature at less than 5% of collected papers falling into this category [33], [39], [84].

Hybrid approaches have also been taken in recent studies. Gómez-González et al. [80] introduce a hybrid method employing discrete particle swarm optimization and optimal power flow to find the best location and sizing of biomass fueled micro-scale energy systems and considered biomass density and other chemical and physical characteristics of biomass in the cost function. A heuristic approach allows the decomposition of the problem into a series of small sub problems, each of which include few consecutive time periods, which are drawn from the overall planning horizon. Poudel et al. [79] demonstrate this technique in a hybrid decomposition algorithm in combination with Rolling Horizons (RH) heuristics for designing a multi-modal transportation network under biomass supply uncertainty. Quddus et al. [60] take a similar approach using Rolling Horizon heuristics to enhance the Progressive Hedging algorithm used to solve a two-stage stochastic mixed-integer programming model. The model assumes the biomass to be densified within the objective function and aims to manage multi-purpose pellet processing depots under feedstock supply uncertainty.

Simulation is used widely in biomass supply chain management due to its ability to study complex systems. Simulation differs from mathematical programming in that it allows fine-gain modeling and can cope easily with random events [29]. Simulation modeling is a prominent approach that is used when either the system is too complex to be modeled by mathematical models, or when the degree of uncertainty in the model is to the extent that ignoring it leads to biased results [85]. However, drawbacks to simulation include that scenarios often require multiple runs, which can be time consuming and these scenarios are user-defined; thus, the

solution depends on the scenarios explored. Moreover, traditional simulation models do not optimize the system but rather capture the uncertainty in scenarios or case studies. Simulation techniques are further classified into *discrete event*, *continuous*, or *agent-based simulation*.

Discrete Event Simulation (DES) has been widely used to model supply chains. With the ability to model supply chain performance under significant levels of operational uncertainty, it is a useful alternative to analytical modeling. Integrated Biomass Supply Analysis Logistics model, commonly referred to as IBSAL, is one of the more commonly used DES models and has the ability to consider the impact of weather, moisture content, and dry matter loss through detailed DES [30]. DES accounts for 10% of gathered articles with 6 papers reviewed [36], [54], [85]–[88].

Continuous Simulations tracks responses continuously based on specified differential equations. As opposed to countable phenomena used in DES, Continuous Simulation reflects a dynamic system; this is useful for systems that are continuously changing over time. Five percent of papers found used continuous simulation [89]–[91].

Agent-Based Simulation, also referred to as Individual-Based Modeling, is used to simulate the interactions of autonomous agents while assessing the individual or collective entity's effects on the entire system. Agent-based modeling offers ways to more easily model individual behaviors and how behaviors affect others in ways that have not been available before [92]. This is an extremely useful tool for modeling agent behavior within supply chains due to its ability to explicitly incorporate the complexity arising from individual behaviors and interactions, which mimic real-world scenarios. Agent-based simulation was only discussed in two papers and therefore account for about 3% of the distribution [93], [94].

Simulation-based Optimization approaches are considered an entirely different category and are used to solve optimization problems, which are subject to a certain level of uncertainty. This technique differs from the aforementioned simulation approaches because it optimizes the output, rather than mimicking the real system. First, mathematical modeling is used to develop and optimize a system and computer-based simulation follows to gather information about the system's behavior. Although this technique allows for a more realistic and in-depth approach, the complexity of the simulation makes it subject to various levels of noise, not necessarily differentiable, and computationally expensive to evaluate [95]. All simulation-based optimization based papers were found to be single objective and make up 5% of the collected literature [16], [53], [96], [97].

Remarkably, simulation approaches are not the preferred modeling choice in the literature. Furthermore, multi-criteria stochastic as well as non-liner modeling are not popular approached due to their computational complexity and sophistication. The Operations Research community can make relevant advances on these fields.

Challenges and Gaps in the Literature

This review of literature suggests that, while biomass quality is becoming increasingly relevant in recent research, there is room for development and expansion. For example, from the 88 papers discussed, only 14 papers considered the ash content of biomass within the model, 7 include dry matter loss, and a mere 3 papers discussed chemical composition such as lignin content. In addition, the majority of literature took a deterministic approach, when, in practice, real-world systems are subject to uncertainties that come into play when quantifying and modeling biomass quality characteristics and have a large impact on the overall logistics network. Furthermore, a large number of articles relating to the optimization of biomass-to-

biorefineries supply chains did not include quality and unrealistically assume pristine dry biomass supply; this finding was interesting because, as previously mentioned, these characteristics affect multiple aspects of the biomass supply chain from conversion processes to storage and transportation. The main conclusions from this literature review can be summarized as follows:

- Biomass quality characteristics including composition, moisture and ash content, bulk density, dry matter and energy losses, and variability and seasonality of quality have shown a considerable impact on performance and costs of using biomass as an alternative energy source. Cost reductions along supply chain operations ranging from 6%-31% were found through several studies quantifying biomass quality effects [21], [36], [38], [47]. Further, it is important to account for the uncertainties and variability inherent to biomass quality during both design and management phases of the supply chain [22].
- A deeper exploration into the quantification and control of the impacts of ash, biomass composition, and quality variability on the biomass supply chain is needed; these specific characteristics were not addressed in the literature as much as moisture content, bulk density, and seasonality were.

Through expansion of these existing models and incorporating uncertainty, quality considerations such as dry matter loss and composition, and inclusion of multiple objectives, it is the hope that a more realistic long-term plan towards sustainability is within reach. It is the aim of this thesis to further justify these conclusions through establishing relationships between biomass quality and preprocessing logistics using a multivariate analysis.

CHAPTER THREE: METHODOLOGY

The multivariate analysis selected to analyze the impact of multiple biomass factors on performance metrics such as throughput, energy consumption, logistics, and preprocessing costs is the Principal Component Analysis (PCA). In this chapter, a brief introduction on the PCA as well as an explanation how this paper differentiates from previous works are provided.

Principal Component Analysis

PCA is a dimension-reducing technique used to linearly transform a large set of data into a smaller number of uncorrelated components, called "principal components", which represent most of the information in the original variables and allows for an enhanced understanding of the data. This statistical test may be more simply described as a summary of the sample variation from many variables with a smaller number of principal components [98]. These principal components are uncorrelated linear combinations of the original variables, which successively account for the variation within the original dataset; the first component will have the largest variance of all components and account for as much of the variability from the analyzed data as possible. Analyzing a dataset using this technique is useful to uncover patterns through visualizing variable interactions and can reduce a large amount of data into a subset of significant relationships; it can be used for a variety of purposes including revealing relations between variables and relations between samples through clustering, detecting outliers, finding and quantifying patterns, generating new hypotheses, among others [99].

While there are currently numerous software programs that will perform a PCA seamlessly, it is important to understand the process occurring behind the scenes to ensure full comprehension and correct interpretation of the results. PCA essentially works in steps toward solving an eigenvalue/eigenvector problem to reduce the dimensions of a dataset. Beginning with

a calculation of the first principal component, a linear combination of $x_1, x_2, ..., x_p$ (i.e., $y_1 = a_{11}x_1 + a_{12}x_2 + ... + a_{1p}x_p$) such that the variance of y_1 is maximized [100]. In a similar fashion, moving to the next set of variables, y_2 will be calculated and account for the second largest percentage of variance between all components. Further, the PCA will find the optimal weight vector for the first component ($a_{11}, a_{12}, ..., a_{1p}$) and its' associated variance; this calculation will be performed for each principal component found and will be maximized, subject to the constraint that it must be uncorrelated with the previous components. From these variable weight vectors and associated variances for each principal component, an indication of how each variable contributes to the variance is seen. Reducing the dataset in this way can considerably simplify data analysis and further exploration of the implications found can provide valuable insight.

The main uses of PCA are descriptive, rather than inferential [101]. Graphical representations of the results found through the multivariate analysis are used to visualize the PCs and draw conclusions about the original dataset. One example of this is a biplot. A biplot defines graphical markers for each original data point and uses vectors to represent variables. With principal components represented along the x and y axes, clusters of graphical markers are able to be analyzed based on what quadrant they are plotted. In addition, magnitude and direction of the vectors represented on a biplot will also aid in drawing conclusions about the dataset. A real world example as to how these values may be used to develop realistic conclusions and direct further research will be illustrated with a case study in Chapter four.

Expanding on Previous Works

Similar multivariate analyses have been performed in previous studies with the intent to simplify large amounts of data and summarize complex relationships. In research efforts

specifically aimed toward expanding knowledge of biomass preprocessing variables, this tool has proven to be advantageous. For example, a recent article was published in which chemical composition of biomass was investigated and significant results were found; Aboytes et al. [102] used PCA to gain an understanding on how biomass chemical composition contributes to the efficiency of biofuel generation and was able to illuminate the direct impact of storage days on biomass chemical composition. Studies such as these, which are able to draw significant conclusions about biomass physical and chemical properties and how they relate to controllable factors, expand research toward optimizing preprocessing of biomass. Further, Shukla et al. [103] used similar techniques to asses the relationship between soil attributes and biomass yield. Knowing biomass and grain yields depend on complex interactions among spatially variable physical and chemical properties of soil, PCA was used to determine the ideal soil treatment for maximized yield. Conclusions were drawn based on yield from four different field treatments and the field in which conventional tillage corn was used was found to return the lowest yield as well as the largest variation; these conclusions may be further used to necessitate site-specific management for optimizing the efficient use of inputs [103].

In a similar fashion, this paper uses multivariate analysis to summarize the relationship between biomass properties and controllable factors along the biomass-to-biofuel supply chain. However, this paper differentiates from previous works through exploration of biomass type and moisture content effects on preprocessing logistics. These factors have not been studied in published works using the PCA technique and will provide valuable insight towards optimizing the preprocessing of biomass and lowering logistics costs and energy consumption.

CHAPTER FOUR: CASE STUDY

Data Collection

A major participant in enhancing research of biomass-to-biofuel supply chain logistics is Idaho National Laboratory (INL). INL has taken major strides in investigating the economics and sustainability of moving biomass from harvest to the throat of the biomass conversion process; these advances have been made possible, in part, through development of a full-scale, integrated feedstock preprocessing system called the Process Demonstration Unit (PDU) [104]. Through utilization of the PDU, extensive experimentation and data collection has been made possible which may provide insight on how to adapt control parameters to account for variability. Figure 1 shows a block flow diagram of the biochemical conversion process, which is the process the biomass used in PDU experiments undergoes [18]. The data used to further understand how preprocessing variables affect throughput was taken from the preprocessing operations of Stage I and II grinding blocks.

In this preprocessing arrangement, the stage I grinder takes the as-received biomass and begins the reduction process through a 3 inch screen, then continues through the dryer to the stage II grinder through a 1 inch screen to meet the target particle size [105]. Test data at INL's PDU analyzes the capability of the system in terms of the systems' throughput and the modeled logistics costs are calculated for each operation shown in the dark grey blocks. This data varies between the type of biomass and moisture content, among several other factors. Understanding how these factors are correlated to the system's performance and determining the ideal input and output values, is a vital piece of the puzzle in advancing the state of technology in biomass collection, conversion, and sustainability.

Data from a report by Idaho National Laboratory, "Enabling Sustainable Landscape Design for Continual Improvement of Operating Bioenergy Supply Systems," was used in order to analyze how the throughput, energy consumption, and system costs are affected by moisture content and type of feedstock [105]. Roni et al. [105] emphasize the importance of capturing the intricacies of multiple land management practices, feedstock production and collection practices, extended harvest windows, and potential complications of handling multiple feedstock within a logistics operation when collecting data for further analysis. With these considerations in mind, switchgrass was harvested from eight different fields and the corn stover was collected from nine fields, various harvesting methods were applied depending on fields, 3-month storage tests at INL storage simulators were used with a range of moisture content, and input moisture from different fields was taken into account while energy consumption and throughput were measured. ANTARES Group Incorporated and the FDC Enterprises provided the harvesting field data from projects that involved biomass harvesting; switchgrass harvesting data were collected from a DOE-sponsored "Growing Bioeconomy Markets: Farm-to-Fuel in Southside Virginia" [106] project and corn-stover data were collected from the DOE co-sponsored BALES project [107]. Results from the process testing, gathered from BALES Project [107] at INL PDU were used for the preprocessing throughput and energy consumption. \Box

Feedstock preprocessing is affected primarily by feedstock characteristics such as format, moisture, and particle size. This experiment focused on how moisture and type of biomass affect selected factors during preprocessing. Preprocessing includes reduction of stage size to reduce the size of particle, which occurs during stage 1 and stage 2 grinding. As particles underwent the reduction process, throughput and energy consumption were measured. Logistics cost and preprocessing cost were also considered during this study, and harvesting, storage, and

transportation costs were calculated for each source of biomass tested. Table 1 shows the test data used for analysis. Logistics cost were modeled using The Biomass Logistics Model (BLM), which incorporates information from a collection of databases that provide (1) engineering performance data for hundreds of equipment systems, (2) spatially explicit labor-cost data sets, and (3) local tax and regulation data [108]. The BLM simulates the flow of biomass through the entire supply chain while tracking changes in feedstock project information in accordance with DOE Contract No. DE-AC07-05ID1451 10 of 33 characteristics (i.e., moisture content, dry matter, ash content, and dry bulk density) and calculating cost and energy consumption [108]

Measured	Measured	Logistics	Preprocessing	Biomass	Incoming
Throughput	Energy	Cost(\$/dry ton)	Cost(\$/dry ton)		Moisture
	Consumption				
4.54	19.91	93	14.66	Switchgrass	15
5.24	6.44	45.73	11.24	Switchgrass	10
4.97	6.58	49.09	11.88	Switchgrass	13.5
4.54	19.91	48.65	13.47	Switchgrass	14.5
4.97	6.58	49.36	11.91	Switchgrass	13.7
4.97	6.58	43.45	11.66	Switchgrass	12.5
4.54	19.91	70.89	14.37	Switchgrass	16.5
4.97	6.58	57.02	11.74	Switchgrass	12
3.89	7.09	93	14.66	Switchgrass	13
5.03	6.14	45.73	11.24	Switchgrass	8
4.67	6.73	49.09	11.88	Switchgrass	11.5
4.67	6.73	48.65	13.47	Switchgrass	12.5
4.67	6.73	49.36	11.91	Switchgrass	11.7
4.86	6.38	43.45	11.66	Switchgrass	10.5
3.89	7.09	70.89	14.37	Switchgrass	14.5
4.86	6.38	57.02	11.74	Switchgrass	10
3.82	13.29	49.03	15.42	Corn Stover	14.17
4.28	15.83	39.55	13.74	Corn Stover	10.5
3.82	13.29	41.23	15.25	Corn Stover	13.64
4.04	14.33	40.25	14.37	Corn Stover	11.5
3.95	15.05	51.75	15.36	Corn Stover	12.5
3.95	15.05	49.48	15.28	Corn Stover	12.5

Table 1. Preprocessing Test Data

3.69	13.15	59.71	16.26	Corn Stover	17.17
3.45	15.49	55.4	16.82	Corn Stover	20.5
3.69	13.15	58.82	16.12	Corn Stover	17.17
4.06	18.09	49.03	15.42	Corn Stover	12.17
4.91	13.39	39.55	13.74	Corn Stover	8.5
4.06	18.09	41.23	15.25	Corn Stover	11.64
4.4	13.85	40.25	14.37	Corn Stover	9.5
4.16	18.4	51.75	15.36	Corn Stover	10.5
4.16	18.4	49.48	15.28	Corn Stover	10.5
3.64	17.4	59.71	16.26	Corn Stover	15.17
3.57	15.43	55.4	16.82	Corn Stover	18.5
3.64	17.4	58.82	16.12	Corn Stover	15.17

Principal component analysis (PCA) is applied in order to find which "principal components" account for most of the variance. Minitab software is used to run the Principal Component Analysis and R software is used for further graphical representation of results.

Factors analyzed for this experiment are: type of biomass (switchgrass or corn stover) and percentage of moisture. Moisture percentage was measured prior to entering the first stage of grinding, and again prior to entering the second stage of grinding. Variables included in this PCA were measured throughput, energy consumption, logistics cost, and preprocessing cost. Table 2 shows the factors and variables needed for PCA.

Table 2. Factors and V	Variables for PCA
------------------------	-------------------

Factors	No. Groups	Variables
Biomass	2	Throughput, energy consumption, logistics cost, preprocessing cost
Moisture Percentage	Varies	Throughput, energy consumption, logistics cost, preprocessing cost

Implementation of the PCA

The first step of PCA involves calculating the correlation matrix to begin the breakdown of variables. The correlation matrix displays the correlation coefficient for each pair of variables and starts the process of developing which relationships contribute to the system's variation. Stronger correlations will return a larger value, with positive and negative correlations shown as positive or negative numbers. To help visualize relationships, shades of orange are used for negative relationships, and blue is shown for positive ones. For example, the correlation matrix which was calculated from our test data and is shown in Table 3, shows that measured throughput has a strong negative correlation coefficient with preprocessing costs, this means as preprocessing cost increases, there is a strong decrease in throughput.

Pearson's Correlation Value	Measured Throughput	Measured Energy Consumption	Logistics Cost	Preprocessing Cost
Measured Throughput	-	-0.557	-0.232	-0.934
Measured Energy Consumption	-0.557	-	0.093	0.739
Logistics Cost	-0.232	0.093	-	0.24
Preprocessing Cost	-0.934	0.739	0.24	-

Table 3. Correlation Coefficient Matrix

While reducing the factors down to individual correlations is helpful, further reduction of these relationships is desired. The second step is to find the eigenvectors; these are essentially the principal components. These principal components are meant to retain most of the variation in the original variables but summarize relationships in a manner that makes interpretation simpler. Because there are four variables, four principal components were calculated. The principal

components from this study can be found in Table 4. The first few principal components account for most of the variation and are the main principal components. As such, the first principal component is a linear combination of the original variables and explains as much variation as possible from the original data. Each subsequent component explains as much of the remaining variation as possible, under the condition that it is uncorrelated with the previous components. Table 4 shows the eigenvalue, proportion, and cumulative value. The row labeled 'eigenvalue' displays the principal components. The PCs are 2.5682, 0.9471, 0.4508, and 0.0339. The proportion row displays how much variance that PC accounts for. Thus, the first PC accounts for 64.2% of the total variance, the second PC accounts for 23.7% of the total variance, and so on. From this table, we can see that the PC1 and PC2 account for 87.9% of the total variance in this study, and this distribution is desired as our first two main components are primarily relied upon for further analysis.

Table 4. Eigenvalues of Correlation Matrix

Eigenanalysis of the Correlation Matrix

Eigenvalue	2.5682	0.9471	0.4508	0.0339
Proportion	0.642	0.237	0.113	0.008
Cumulative	0.642	0.879	0.992	1.000

Figure 8 exhibits the scree plot, which depicts the relation between the eigenvalues and the PCAs; PCAs with an eigenvalue larger than 1 should be used in the analysis. From Figure 8 we can see that PC1 and PC2 have an eigenvalue greater than 1.



Figure 7. Scree Plot of PCA Variables

Once the main PCs are found, the eigenvectors are calculated in order to find the associated variance of each variable for the calculated PCs. The calculated eigenvectors are seen in Table 5. The larger the magnitude of the eigenvector, the greater the correlation between it and the variable listed. The sign tells if that variable is directly or indirectly proportional to the component.

Table 5. Eigenvectors

Eigenvectors

Variable	PC1	PC2	PC3	PC4
Measured Throughput	-0.574	-0.031	0.561	0.596
Measured Energy Consumption	0.504	0.267	0.785	-0.241
Logistics Cost(\$/dry ton)	0.208	-0.960	0.185	-0.024
Preprocessing Cost(\$/dry ton)	0.611	0.078	-0.184	0.766

From this table, it is concluded that PC1 consists mainly of all variables excluding logistics cost. The eigenvectors matrix also shows that the measured throughput has a negative correlation with the first principal component. Additionally, the correlation for each Principal Component is deducted from the following variables:

- PC1: Measured Throughput, Measured Energy Consumption, and Preprocessing Cost.
- PC2: Logistics Cost and Measured Energy Consumption
- PC3: Measured Throughput and Measured Energy Consumption
- PC4: Measured Throughput and Preprocessing Cost

Thus, for PC2, if measured energy consumption and preprocessing cost increased, then measured throughput would decrease. The same conclusions may also be applied to the remaining components based on these rules.

Once the eigenvalues and eigenvectors are calculated, the scores of the original data based on the two main components are found. The scores result from PCA and they are the transformed variables from the original set of data. As seen in figure 9, the biomass types return significantly different scores with respect to either PC. This confirms that there is a statistically significant difference in observations between varying biomass.



Figure 8. Score Plot of Variables

From this transformation of data, a monoplot and bi-plot chart are constructed in order to view the segregation of the factors versus the main PCs. If no segregation occurs, then there is no difference between the factors. If segregation occurs, then that factor did have effect on the main PCs.

Using PCA to Understand Biomass Preprocessing Variables

A two-dimensional monoplot is a valuable tool to assess the relationship between the variables. It allows for a visualization of the first two principal components and illustrates the original variables as vectors pointing away from the origin. The angles between the vectors approximates the correlation between the variables, with a small angle indicative of a positive correlation, no correlation would show a perpendicular vector, and an angle closer to 180 degrees is interpreted as a negative correlation. The length of each vector shows how well each variable is represented in the plot, with the poorly represented vectors being shorter. With the monoplot

shown in Figure 10, we can now analyze each variable is represented within our main principal components and conclude their representation as well as their correlation to one another. The small angle between energy consumption and preprocessing cost indicates that these variables are positively correlated, and the opposite may be said about preprocessing cost and throughput.



Figure 9. Monoplot of Variables

A biplot chart analysis is used to understand the similarities between observations. It's easier to first reduce the dimensionality of the data using principal components and then develop a biplot that simultaneously plots information on the observations and the variables by distinguishing the factors used. The biplots represent variables using calibrated axes and observations are represented using points. To analyze the factors, biplots are constructed using R software and are seen below in Figure 11 and Figure 12. Each point shown on the biplot represents the data taken from each observation with varying moisture content and biomass source. To aid in visualizing how biomass type and moisture content falls amongst observations, a legend is displayed. Thus, the points on these bi plots are the scores, which can be differentiated, based on color. Further, the distance between points represents the similarity between them, with closer points signifying a similar profile. For example, our ideal observations would return a higher throughput and would therefore fall closely to our throughput vector as many switchgrass observations have. We can quickly deduct that corn stover observations are contributing higher logistics and preprocessing costs. In addition, patterns are visible in which clustered points fall closer to the axes. For example, Figure 11 shows that observations in which switchgrass is used returns higher throughput values, but a cluster of switchgrass observations also had higher logistics costs.



Figure 10. Biplot of Variables against Biomass Type

Figure 12 illustrates how moisture content correlates with each variable. The darker points represent observations in which biomass with a lower moisture content are used and are

found to have a higher throughput value and lower costs. In agreeance with initial assumptions, higher moisture content will result in higher preprocessing costs.



Figure 11. Biplot of Variables against Moisture Contents

This analysis can be used to further explore the intricacies of biomass-to-biofuel supply chains. The focus of this analysis is on cost reduction, increasing throughput, and decreasing preprocessing energy consumption with respect to varying biomass and moisture content. The type of biomass had the largest effect, which caused the most variance. Based on the results discussed, it is advised that switchgrass with lower moisture content between 0-15 percent, will return the higher throughput and lower logistics and preprocessing costs.

CHAPTER FIVE: CONCLUSIONS

Concluding Remarks

The maturity of the bioenergy industry is dependent on highly efficient supply chains and minimal logistic costs that are competitive with fossil fuels and other conventional sources of energy. An aspect that is often overlooked in research related to biomass-to-biorefinery supply chain optimization is the inclusion of biomass quality uncertainty for decision-making. Biomass quality characteristics (e.g., ash, moisture, chemical composition, among others) have demonstrated to impact storage, processing, transportation, and many other operations along the supply chain. Although biomass quality can prove difficult to model due to its variability, ignoring the effects of such characteristics could result in suboptimal designs and cost underestimations. This thesis presents an overview of biomass quality characteristics being addressed in current literature pertaining to quantitative methods to model and analyze biomass-to-biorefinery supply chains and continues to illustrate this necessary consideration through a case study exploring the effects of biomass type and quality on preprocessing logistics.

A total of 88 published articles written in English are reviewed and classified based on modeling approach and quality characteristic(s) are considered. It is concluded that the majority of papers discussed utilized a deterministic, single objective approach, while accounting for the moisture content of biomass. Through further development of these existing models and incorporating uncertainty, quality considerations such as dry matter loss and composition, and inclusion of multiple objectives, knowledge of the biomass-to-biofuel supply chain will be significantly expanded. This literature review summarizes the current state of research in this

domain and sets the foundation for further studies on the quantification and control of biomass quality in analytical models.

Regarding the methodological aspect of this study, the biomass data is analyzed using Principal Component Analysis (PCA) implemented in Minitab and R software. PCA tests for the "main components" that cause the most variance and reduce data in a way that is simpler to understand. Once the main components are found, a monoplot and biplot are created to test the correlation of the main components and factors. The goal of this study is to find a suitable biomass type and moisture content to reduce logistics cost and energy consumption while increasing throughput rate. Results indicate that type of biomass and percentage of moisture strongly influence the throughput, energy consumption, preprocessing cost, and logistics cost. PCA results show segregation when testing corn stover as opposed to switchgrass and varying the amount of moisture. The graphical results indicate that *decreasing costs and energy, while* increasing throughput, may be achieved when switchgrass is used rather than corn stover. The PCA results for moisture content show that lower moisture content between 0-15% increase throughput and decrease logistics cost, energy consumption, and preprocessing cost; these correlations can be seen in the biplots shown in Figures 11 and 12. To further quantify the impact of these factors, a cost comparison of using these recommended settings versus the opposition may be analyzed; using a moisture content between 0-15% results in preprocessing cost reductions of \$2.54 per dry ton, which is a 15.7% preprocessing cost reduction from using a higher moisture content. Data from type of biomass used may also be quantified as an 18% preprocessing cost reduction when using switchgrass as opposed to corn stover. It is therefore recommended for improved operations, to use switchgrass with lower moisture content (between

0-15%), which returns the highest possible throughput and lower logistics and preprocessing costs.

PCA is a dimensionality-reduction technique and, in an area of study such as the biomass-tobiofuel supply chain, where there are a substantial number of correlated variables to consider within each process, this tool is capable of expanding knowledge using existing data.

Both the case study and literature review presented can be used to further investigate the intricacies of biomass-to-biofuel supply chain optimization. The implications found on cost reduction, increasing throughput, and decreasing preprocessing energy consumption with respect to varying biomass and moisture content are intended to direct academics toward future research.

CHAPTER SIX: FUTURE AREAS OF RESEARCH

Biomass promises a viable alternative to fossil fuels. Further exploration of feedstock logistics and the handling of biomass, as well as how these aspects relate to biomass quality, is essential to facilitating the transition into a new bioeconomy.

Biomass quality has had a limited focus in past research, but holds an important role in operations such as harvest and collection, storage, preprocessing and transportation. This thesis presented and discussed an array of relevant literature, which includes characteristics related to biomass quality and their effects on the biomass-to-biorefinery supply chain. With this prerequisite, many papers were excluded for overlooking biomass quality, creating a large space of opportunity for future research in this topic. Fortunately, biomass quality seems to be gathering recent attention, as papers with quality considerations discussed in this review were increasingly prevalent within the last few years. Addressing the influence of biomass quality on supply chain related decisions and quantifying this impact is a fruitful are of research, especially, the modeling and optimization of holistic biomass-to-biorefinery supply chain networks.

Regarding the inherent variability of biomass quality, there is opportunity for research on exploring multistage stochastic programming methods, as well as simulation-based optimization approaches on biofuel supply chain optimization; these approaches allow for the modeling of complexities associated with the biomass supply chain and variability in biomass quality. This survey also concludes that simulation approaches are not as heavily represented in the literature. For example, only 3% of papers discussed took an agent-based simulation approach, yet this approach is versatile in that it may assess the effect of various individual behaviors on the system in its entirety. In addition, simulation-based optimization methods made

up a mere 5% of all papers reviewed, yet this method allows for an in-depth and realistic approach. Although these approaches may require more computational power and advanced complexity, methods such as these are under-utilized and have the power to significantly expand current research. Many authors suggested their deterministic models be used as building blocks to develop stochastic models or extending existing models to use multi-objective optimization methods. For example, Xie et al. [64] suggest extensions to investigate the effects of various optimization formulations on the solution quality in the face of different types of uncertainties. Malladi et al. [63] also stress the importance of incorporating such dynamics, and including uncertainties in supply and demand quantities of biomass and suggests it may enhance the applicability of the models. An extension of existing research is the key to continuous development of the current knowledge of biomass supply chain logistics and these efforts will allow for more realistic goals of replacing fossil fuel dependency with sustainable resources such as biomass.

Future areas of study also include utilizing statistical techniques such as Principal Component Analysis to investigate a larger scale of data and incorporate more variables/factors. An incredible amount of data is generated from the PDU at INL; using techniques shown in this study, conclusions can be made which have the potential to reduce costs and increase efficiency. Further, the biplot graphs resulting from this PCA have the capability to inform future implications. The clusters within the resulting graphs can guide research iteratively through prescriptive models. For example, the finding that data points which clustered towards a higher throughput were between 0-15% moisture content, could be used to further reduce data and find a more focused threshold of ideal moisture content. Performing a PCA on additional data taken from the PDU is recommended; factors such as screen size, ash content, feed rate, etc. should be

considered to further summarize ideal setup to maximize throughput and reduce cost and energy consumption. PCA becomes more useful as the number of variables increase; including more variables such as bulk density, ash content, particle size, and many others, will return principal components which can summarize a wider range of implications.

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Amanda Hydar is from Canandaigua, NY. She studied Mechanical Engineering with a focus in Advanced Manufacturing and Enterprise Process Engineering and earned both a Bachelor's and Master's degree from The University of Texas at San Antonio. Throughout her academic studies, she worked as a Graduate Mechanical Design Engineer for the Space Science and Engineering division of Southwest Research Institute. She has extensive experience with research and development projects, as well as the accomplishment of being the lead Mechanical Engineer on two successful Rocket Sounding Missions to investigate Cusp Electrodynamics II (TRICE II). Amanda has also dedicated her time as a Graduate Research Assistant for The Texas Sustainable Energy Research Institute. Through this position, she has evaluated and expanded upon the current state of research for biomass-to- biofuel supply chain optimization. She has written a comprehensive literature review, which provides an in-depth overview of how currently published works have addressed biomass quality and aligned her thesis work with the current research agenda set forth by the U.S. Department of Energy. Her future plans include beginning her career in green manufacturing and renewable energy research in Denver, Colorado and ultimately contribute towards making our society one that relies on sustainable sources of energy and reduces waste.