

**System-Level Sustainability Assessment for Economic Viability of
Cellulosic Biofuel Manufacturing**

BY

YUNTIAN GE

B.E., Beijing Institute of Technology, Beijing, China, 2013

M.S.E., Purdue University Northwest, Hamond, IN, USA, 2015

THESIS

Submitted as partial fulfillment of the requirements
for the degree of Doctor of Philosophy
in Industrial Engineering and Operations Research
in the Graduate College of the
University of Illinois at Chicago, 2020

Chicago, Illinois

Defense Committee:

Lin Li, Chair and Advisor

David He

Houshang Darabi

Jeremiah Abiade

Jie Lin, Civil and Material Engineering

DEDICATION

To my family and friends for the unwavering support over the years.

ACKNOWLEDGEMENTS

I would like to first express my sincere appreciation to my advisor Professor Lin Li, for his guidance and patience throughout this research, without which I could not have successfully completed this dissertation. I am truly grateful for his generous help in rigorously training and preparing me for an academic career. In addition, I am thankful to the other committee members, Professors Houshang Darabi, David He, Jeremiah Abiade, and Jie Lin, for their comments and suggestions.

It was a great pleasure working with the colleagues in the SMSRL: Yiran Yang, Yong Wang, Zeyi Sun, Xufeng Yao, Fadwa Dababneh, Azadeh Haghighi, Jing Zhao, Rahul Shah, Lingxiang Yun, Minkun Xiao, Muyue Han and Xue Zhou. I surely benefited a lot from these beautiful minds through the discussions in team meetings and seminars. Thanks also go to my friends and PhD classmates in the Mechanical and Industrial Engineering Department: Miao He, Haiyang He, Jia Luo, Jie Jiang, Lu Lu, and Yizhou Jiang. Their respective research broadened my view in the field of industrial engineering.

Scholars from several universities in China have also inspired me in my research. I would like to thank Professor Wenbin Gu, Professor Yukan Hou, and Professor Weiwei Cui for providing suggestions and sharing their ideas with me.

Besides, I would like to extend my appreciation to my old friends, Zekun Lyu, Xinyuan Ji, Dengke Guo, and Yuqi Luan for their caring and encouragement all the time. Finally, thanks to my parents for their love and always being so supportive in my decision to pursue higher education.

Yuntian Ge

CONTRIBUTION OF AUTHORS

Chapter 1 is an introduction that includes the background information and literature review to highlight the significance and challenge of my research.

Chapter 2 represents a published paper (“Li L., Ge Y., 2017, System-level cost evaluation for economic viability of cellulosic biofuel manufacturing. *Applied Energy*, 203, 711-722”) for which I was the major driver of the research. My advisor, Dr. Lin Li contributed to research idea generation and paper revision.

Chapter 3 represents a published paper (“Ge Y., Li L., 2018, System-level energy consumption modeling and optimization for cellulosic biofuel production. *Appl Energy* 226: 935–46”), for which I was the primary author and the major driver of the research. My advisor, Dr. Lin Li, contributed to the idea discussion of the research and proofreading of the manuscript.

Chapter 4 represents one of my unpublished (under review) research focusing on using industrial symbiosis concept to improve the waste utilization efficiency of cellulosic biofuel. I anticipate that this work will be published soon.

Chapter 5 represents the conclusions of the research presented in this thesis. The intellectual contribution and broad impact are summarized. The future directions in this area are discussed.

TABLE OF CONTENTS

<u>CHAPTER</u>	<u>PAGE</u>
DEDICATION	ii
ACKNOWLEDGEMENTS	iii
CONTRIBUTION OF AUTHORS	iv
TABLE OF CONTENTS	v
LIST OF TABLES	vi
LIST OF FIGURES	vii
LIST OF ABBRIVIATIONS	viii
SUMMARY	ix
CHAPTER 1. INTRODUCTION.....	1
1.1. Introduction	1
1.2. Literature Review	4
1.3. Motivation and Proposed Research Framework.....	8
1.4 Organization of Dissertation.....	12
CHAPTER 2. SYSTEM-LEVEL ECONOMIC VIABILITY EVALUATION FOR CELLULOSIC BIOFUEL MANUFACTURING	13
2.1. Introduction	13
2.2. Notations.....	14
2.3. Mathematical Modeling.....	15
2.4. Solution Strategies.....	27
2.5. Case Study	29
2.6. Conclusions	39
CHAPTER 3. ENERGY EFFICIENCY MODELING AND OPTIMIZATION FOR CELLULOSIC BIOFUEL MANUFACTURING SYSTEM.....	40
3.1. Introduction	40
3.2. Notations.....	41
3.3. Process Description	42
3.4. Energy Consumption Modeling.....	44
3.5. Energy Analysis of Baseline Case.....	53
3.6. Energy Consumption Optimization Using PSO	59
3.7. Conclusions	64
CHAPTER 4. A NOVEL WASTE MANAGEMENT DESIGN VIA INDUSTRIAL SYMBIOSIS TO CO-PRODUCING ALGAL AND CELLULOSIC BIOFUELS	66
4.1. Introduction	66
4.2. Notations.....	68
4.3. Novel Industrial Symbiosis Design	70
4.4. Mass Flow and Cost Modeling.....	77
4.5. Environmental Impact Assessment	81
4.6. Results and Discussion	85
4.7. Conclusions	98
CHAPTER 5. CONCLUSIONS.....	100
5.1. Conclusions	100
5.2. Intellectual Contributions and Broader Impacts	100
5.3. Future Work.....	101
CITED LITERATURE.....	102
VITA	116
APPENDIX	118

LIST OF TABLES

<u>TABLES</u>	<u>PAGE</u>
TABLE I. INPUT DECISION VARIABLES	17
TABLE II. SOLID COMPOSITION OF CORN STOVER.....	30
TABLE III. VALUES OF INPUT DECISION VARIABLES.....	30
TABLE IV. REACTION RATE CONSTANTS	31
TABLE V. OTHER PARAMETERS.....	31
TABLE VI. COST OF CONVERTING 1 KG FEEDSTOCK TO ETHANOL (\$US)	36
TABLE VII. VALUES OF DECISION VARIABLES IN COST-EFFECTIVE CASE	38
TABLE VIII. COMPARISON OF COST BREAKDOWN	39
TABLE IX. SOLID COMPOSITION OF CORN STOVER (Humbird et al., 2011b).....	42
TABLE X REACTIONS IN CELLULOSIC BIOFUEL PRODUCTION	49
TABLE XI. BASELINE CASE DECISION VARIABLES	53
TABLE XII. ENERGY RELATED PARAMETERS.....	54
TABLE XIII. REACTION RELATED PARAMETERS.....	54
TABLE XIV. DATA OF BIOFUEL PRODUCTION ENERGY SENSITIVITY ANALYSIS ...	57
TABLE XV. THE AVERAGE TIME AND STATISTICAL RESULTS OF THE ENERGY CONSUMPTION OPTIMIZATION PROBLEM IN 6 DIFFERENT POPULATION SIZES (20 TRIAL RUNS FOR EACH SIZE)	63
TABLE XVI. COMPARISON OF NEAR-OPTIMAL SOLUTION AND BASELINE CASE...	64
TABLE XVII. MAIN REACTIONS RELATED TO BIOETHANOL PRODUCTION	71
TABLE XVIII. OXYGEN GENERATION IN THE CEP FERMENTATION PROCESS	72
TABLE XIX. COMPOSITION OF SOLUTES IN CEP WASTEWATER (CALCULATED BASED ON RELEVANT DATA FROM (Humbird et al., 2011a)).....	74
TABLE XX. COMPOSITION OF MDP SOLID WASTE	75
TABLE XXI. COMPOSITION OF CEP SOLID WASTE	75
TABLE XXII. ELEMENTAL CONSTITUTIONS OF SOLID WASTE COMPONENTS.....	76
TABLE XXIV. COMPOSITION OF THE 3 MICROALGAE SPECIES OVER A 4-DAY CULTIVATION PERIOD (Davis et al., 2014).....	85
TABLE XXIV. ELEMENTAL COMPOSITION OF SCENEDESMUS, CHLORELLA, AND ANNOCHLOROPSIS FOR DIFFERENT HARVEST STAGES	86
TABLE XXV. BIOFUEL PRODUCTION OF SCENARIOS 1, 2, 3, AND 4	87
TABLE XXVI. SUPPLEMENTARY PARAMETERS.....	87
TABLE XXVII. COMPOSITION OF SCENEDESMUS, CHLORELLA, AND NANNOCHLOROPSIS FOR DIFFERENT HARVEST STAGES.....	95

LIST OF FIGURES

<u>FIGURE</u>	<u>PAGE</u>
Figure 1. Composition of cellulosic biomass (corn stover).....	4
Figure 2. The proposed research framework.....	11
Figure 3. Biochemical pathway in cellulosic ethanol production system	15
Figure 4. Process-dependent cost breakdown.....	26
Figure 5. Mass evolutions of state variables with 1 kg feedstock converted to ethanol.....	33
Figure 6. Mass evolutions of state variables component in pretreatment.....	33
Figure 7. Accumulated energy consumption with 1 kg feedstock converted to ethanol.....	34
Figure 8. Energy consumption contribution from each process with.....	35
Figure 9. Cost breakdown from each manufacturing process	36
Figure 10. Cost and ethanol yield comparison	38
Figure 11. Block diagram of biofuel production from cellulosic biomass	42
Figure 12. Reaction temperature profile during pretreatment, enzymatic hydrolysis and fermentation process.....	46
Figure 13. Total energy consumption breakdown	55
Figure 14. Energy usage in each process from different sources	56
Figure 15. Heating energy breakdown	57
Figure 16. Effects of (a) feedstock particle size, (b) water loading, (c) acid loading, (d) pretreatment temperature, (e) pretreatment time, (f) enzymatic hydrolysis temperature, (g) enzymatic hydrolysis time, (h) fermentation temperature and (i) fermentation time on total energy consumption and ethanol yield.	59
Figure 17. Solution procedures of the energy optimization problem using PSO	62
Figure 18. Averaged optimal result of energy consumption with 95% confidence interval	63
Figure 19. Schematic overview of the proposed industrial symbiosis energy system	68
Figure 20. Proposed industrial symbiosis bioenergy production system	71
Figure 21. Capital cost analysis for Scenarios 1 and 2	89
Figure 22. Manufacturing cost comparison for the 4 scenarios.....	90
Figure 23. Comparison of the unit cost of biofuel products for the 4 scenarios.....	91
Figure 24. CO ₂ emissions breakdown for the 4 scenarios.....	92
Figure 25. Comparison of EP for the 4 scenarios.....	93
Figure 26. Comparison of AP for the 4 scenarios	93
Figure 27. Production and cost performance change of (a) microalgae production, (b) CO ₂ cost, (c) cost of cellulosic feedstock (corn stover), and (d) total manufacturing cost for <i>Scenedesmus</i> , <i>Chlorella</i> , and <i>Nannochloropsis</i> at early-, mid-, and late-harvest stages	97
Figure 28. Sensitivity analysis of selected parameters on the unit cost of	98

LIST OF ABBRIVIATIONS

AP	acidification potential
CEP	cellulosic ethanol production
CHP	combined heat and power
COD	chemical oxygen demand
EP	eutrophication potential
GGE	gallon gasoline equivalent
GHG	greenhouse gas
IS	industrial symbiosis
kWh	kilowatt hour(s)
LCA	lifecycle assessment
MDP	microalgae biofuel production
MW	million-watt(s)
NREL	National Renewable Energy Laboratory
PSO	particle swarm optimization
SHF	separate hydrolysis and fermentation

SUMMARY

In this dissertation, a framework to address economic and sustainability issues for cellulosic biofuel manufacturing is proposed. This novel framework can facilitate the technological readiness of cellulosic biofuel industrialization. Detailed research tasks of the proposed framework include the systematic modeling of material flow, energy consumption, cost, environmental impact, and waste utilization for cellulosic biofuel manufacturing. Specifically, system-level production and energy models are established considering the interrelationships among multiple manufacturing processes. In addition, a novel industrial symbiosis design is carried out to promote the material-utilization efficiency of cellulosic and algal biofuel manufacturing. New insights are acquired based on the applications of established models in economic viability analysis, energy-consumption evaluation, and waste-management approaches for cellulosic biofuel manufacturing. The findings based on case studies show that the established interrelations have great potential to reduce cost, enhance energy efficiency, and promote waste utilization without sacrificing biofuel yield. Appropriate implementation of the research outcomes can help promote economic biofuel manufacturing, improve the economic viability of the U.S. cellulosic biofuel manufacturing industry, reduce dependence on imported oil, and significantly benefit the environment and society in terms of greenhouse gas emissions and waste reduction. The systematic methodology developed in this research can be applied to various industries, such as biochemistry, medicine, and the petroleum industry.

CHAPTER 1. INTRODUCTION

1.1. Introduction

As one of the most severe challenges faced by human society, the sustainability issues associated with the increasing global energy consumption and limited fossil fuel reserves have attracted extensive attention. In 2018, global greenhouse gas (GHG) emissions reached an all-time high with 62% of these emissions from burning fossil fuels (Chen et al., 2019). The extensive use of fossil fuels has led to serious issues, e.g., climate change, environmental pollution, threats to human health, and energy supply challenges associated with the irreversible depletion of fossil fuels (Kesharwani et al., 2019). To solve these issues, a significant amount of research has been conducted to investigate renewable energy resources as sustainable energy alternatives.

As a promising substitute for traditional fossil fuels, biofuel has become popular as a renewable energy source that can be sustainably produced (Jafri et al., 2019). Generally, biofuels appear to be environmentally friendly, considering their low lifecycle carbon and sulfur emissions. In addition, using biofuels can relieve a nation's energy dependence on imported crude oil resources and have a positive impact on both the national economy and environment (House, 2014). Hence, biofuels have attracted increasing attention worldwide. As a result, the global biofuel production in 2018 was eight times greater than in 2000 (IEA, 2018). It has been estimated that biofuels will replace 30 % of the U.S.'s liquid transportation fuels by 2022 (UNCTAD, 2016).

Biofuel refers to a type of fuel produced through contemporary biological processes rather than geological processes as in conventional fuel types (e.g., fossil fuel). Based on

different types of raw materials, biofuel can be generally categorized into three generations (Alam et al., 2015). ‘First-generation’ or traditional biofuels are produced from food crops (Manochio et al., 2017), and usually refer to sugars and vegetable oils found in arable crops. To avoid competing for food resources with humans, ‘second-generation’ biofuels are produced from various types of cellulosic biomass (Ge and Li, 2018), e.g., agricultural residues and wooden crops. With the development and breakthroughs regarding the technologies to process biomass, ‘third-generation’ biofuels, which use algae as a biofuel source, have been proposed (Baudry et al., 2018).

Among different types or generations of biofuels, cellulosic biofuel is considered promising due to its capability to mitigate global climate change (Lynd, 2017). This superior capability is mainly due to the wide availability of feedstock resources and low lifecycle GHG emissions. It was reported that using cellulosic biofuel (i.e., cellulosic ethanol) could lead to up to a 90% of reduction in GHG emissions compared to petroleum fuels (Farrell et al., 2006). Owing to the outstanding performance of cellulosic biofuel in terms of relieving environmental burdens, cellulosic biofuel has become an accessible alternative energy resource that is renewable and sustainable. To further facilitate the development and implementation of cellulosic biofuel manufacturing, the U.S. government has issued a mandate requiring that national annual cellulosic biofuel production reach at least 16 billion gallons by the year 2022 (U.S. Congress, 2007).

A typical cellulosic biofuel manufacturing system consists of four main processes: pretreatment, enzymatic hydrolysis, fermentation, and product recovery (Rodionova et al., 2017). Bioethanol production begins with the feedstock handling process, in which the cellulosic feedstock is milled and cleaned before being delivered for pretreatment. In the

pretreatment process, the cell wall structures of the cellulosic feedstock are disrupted, and most hemicellulose carbohydrates are converted to soluble sugars. After pretreatment, the slurry is cooled and further hydrolyzed via cellulase in the enzymatic hydrolysis process, in which most of the remaining cellulose is converted into glucose. After enzymatic hydrolysis, the saccharified slurry is cooled for fermentation. After the product recovery process via distillation and molecular sieve adsorption, pure ethanol is produced (Humbird et al., 2011a).

However, widespread adoption of cellulosic biofuel is taking place at a much slower pace than expected. Quite simply, producing ethanol from cellulosic materials is not yet economically viable. In addition, intensive energy usage significantly undermines the large-scale implementation and long-term sustainability of cellulosic biofuel manufacturing (Li and Ge, 2017). In addition, cellulosic biofuel manufacturing yields a considerable amount of by-products and wastes. As shown in Figure 1, the convertible part (i.e., xylan and glucan) of cellulosic materials only accounts for approximately half of the total weight. Lignin and other solid residues mixed with process additives such as sulfate and cell mass will adversely impact the environment if not properly treated. Furthermore, the current economic and sustainability models for cellulosic biofuel production are mostly panel data models that neglect the interrelationships between each process, which may jeopardize the accuracy of the results.

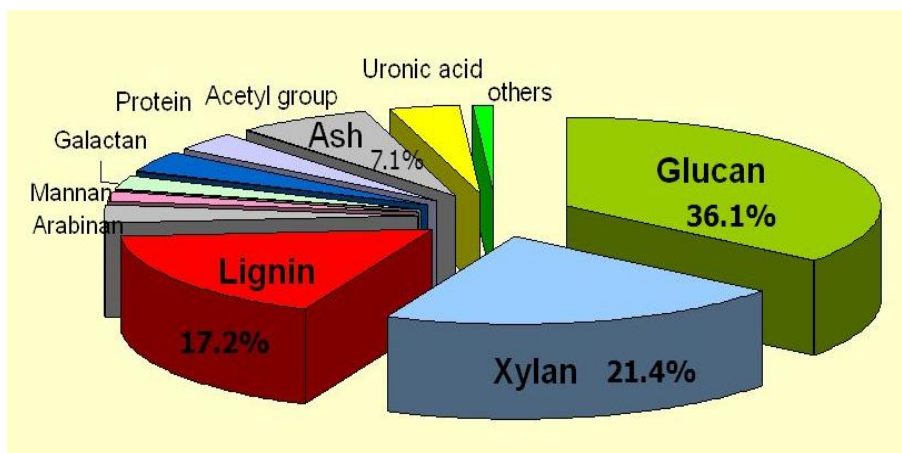


Figure 1. Composition of cellulosic biomass (corn stover)

1.2. Literature Review

In this section, an overview of current literature on cellulosic biofuel manufacturing is presented regarding economic viability, energy consumption, and waste management.

1.2.1. Literature Review on Economic Viability of Cellulosic Biofuel Manufacturing

Based on a survey of current literature, numerous studies have been performed regarding different aspects of cellulosic biofuel manufacturing. It has been reported that the feedstock accounts for the highest proportion of manufacturing costs. Considerable research is being conducted on the effects of various factors related to the biomass on biofuel production, such as feedstock types (Jung et al., 2015; Mesa et al., 2017; Somerville et al., 2010; Yu et al., 2016), feedstock size (Cadoche and López, 1989; Li et al., 2016; Miao et al., 2011; Vidal et al., 2011), and biomass particle properties (Cai et al., 2017; Mani et al., 2004; Phanphanich and Mani, 2011). In addition, research efforts have been devoted to reducing the costs of the biofuel conversion process. These efforts include optimizing the pretreatment process improvement (Fockink et al., 2015; Ko et al., 2020; Maurya et al., 2015; Mesa et al., 2017; You et al., 2017), developing cellulase enzyme

(Liu et al., 2016; Yarbrough et al., 2017), and genetically modifying fermentation microbes (Yu et al., 2011; Zheng et al., 2015), etc.

However, the majority of cost studies are performed based on the individual process in biofuel manufacturing systems. In other words, most of the cost studies do not consider the interactions between multiple processes, which oversimplifies the production problem. In a biofuel manufacturing system, most of the individual processes are highly correlated. For example, Aden and Foust (2009) studied the impact of feedstock cost in the pretreatment process. However, the feedstock cost change can be significantly affected by parameters from other processes such as enzyme loading, fermentation temperature, and biofuel yield. Generally, cost savings in one individual process might be offset by cost increases in other processes and vice versa. Therefore, reducing the cost from one process does not necessarily lead to a global cost savings considering system-level biofuel manufacturing. Hence, to conduct comprehensive cost evaluation for biofuel manufacturing, it is critical to consider the interrelations between multiple processes and study the cost-effectiveness of these processes simultaneously and systematically

1.2.2. Literature Review on Energy Consumption of Cellulosic Biofuel Manufacturing

Currently, the high energy demand in cellulosic biofuel production is still challenging. It was reported that to produce 1 MJ of ethanol, 1.27 MJ of energy is required, 63% of which is consumed in the production process (Patzek, 2004). Hence, it is necessary to comprehensively investigate and improve the energy efficiency of cellulosic biofuel production. In the literature, the majority of energy analyses adopt the life cycle assessment (LCA) approach to estimate the energy usage and analyze the associated environmental impacts (Farrell et al., 2006; Kemppainen and Shonnard, 2008; Ou et al., 2009; Schmer et

al., 2008; You et al., 2012). As these studies provide useful insights into estimating the amount of energy consumption, they cannot be used to reduce the energy use the production by adjusting the process parameters (e.g., pretreatment temperature, feedstock particle size, and fermentation time). In such cases, more comprehensive system-level energy models are generally preferred, so that the production energy consumption can be reduced by utilizing the relationships between energy consumption and production parameters.

Two popular methods are often adopted to establish energy models for biofuel manufacturing: simulation-based modeling and analytical modeling. The majority of simulation-based studies use Aspen software to simulate biofuel conversion in single or multiple processes (Cardona Alzate and Sánchez Toro, 2006; Frankó et al., 2016; Gonzalez-Salazar et al., 2014; Silva Ortiz and de Oliveira, 2014; Tian et al., 2011; Velásquez-Arredondo et al., 2010; Wang et al., 2007). The advantage of simulation-based methods is that they can capture system performance in quite complex biofuel production systems. However, like LCA models, they cannot reveal the fundamental mathematical relationships between system parameters and performance measures. Furthermore, the development and execution of simulation models to obtain statistically useful results may be prohibitively expensive and slow, making it very difficult to find optimal solutions.

Compared to simulation-based studies, much less research uses analytical modeling methods due to the difficulties in establishing mathematical relationships between biofuel production parameters and energy consumption. In only a few papers have analytical modeling methods been used to study energy consumption in cellulosic biofuel production. They focus on a single process rather the production system (Li et al., 2016; Mafe et al.,

2015). For example, in one study the authors developed a feedstock pre-processing scheme considering particle separation to reduce energy waste for the biomass size-reduction process (Li et al., 2016). Nevertheless, optimizing the energy consumption in one process will not necessarily lead to the system's energy reduction because the processes within cellulosic biofuel production systems are highly interrelated. For instance, producing coarser particles in the size reduction process usually requires less energy, which might eventually result in higher total energy consumption since coarser particles require more energy to be converted to biofuel. Furthermore, exclusively optimizing the energy consumption of different processes may cause biofuel production yield loss. Therefore, it is necessary to consider the interrelations between each process and analyze the energy consumption of multiple processes systematically.

1.2.3. Literature Review on Waste Treatment of Cellulosic Biofuel Manufacturing

Currently, most studies on the waste treatment of cellulosic biofuel manufacturing focus on replacing one or more raw materials used in biofuel production with collectible wastes, and exploring the viability of byproduct recovery technology in a biofuel production system (Doherty et al., 2011; Ghosh, 2016; Kopania et al., 2012; Rodionova et al., 2017; Sudiyani et al., 2013). For example, a method that replaces the water and nitrogen sources required for cellulosic ethanol production (CEP) with biogas slurry was carried out in (You et al., 2017), and the results indicated that at least 10% of the total cost could be saved. In addition, a cost analysis for the use of solid lignin residuals from CEP to produce hydrocarbon fuels is presented in (Ge et al., 2017), which suggested that an extra 19.9 gallons of diesel-range biofuel can be produced in addition to 83.2 gallons of cellulosic ethanol by consuming 1 ton of corn stover.

These studies provide valuable knowledge for waste management, but the analyses do not consider the interactions between the biofuel production system and the industry that renders them. For example, the utilization of CO₂ from power plant flue gas to cultivate microalgae was evaluated in (Gutiérrez-Arriaga et al., 2014). Although this study indicated that it is economically and environmentally beneficial to reuse flue gas CO₂, only the merit of ‘free’ CO₂ is considered. While the linked reactions are neglected, such as the cost of CO₂ collection, separation, and distribution, quantitative results could therefore be inaccurate without a systematic perspective.

Moreover, a few studies utilize the industrial symbiosis (IS) concept to establish a bioenergy system to enhance waste utilization efficiency. Gonela and Zhang (Gonela and Zhang, 2014) designed the optimal bioenergy-based industrial symbiosis for reducing cellulosic biofuel production costs. They found that a biorefinery plant's profit can be improved when operating in IS mode compared to standalone mode. Furthermore, Martin and Eklund designed an IS bioenergy system to co-produce first- and second-generation biofuels (Martin and Eklund, 2011), without conducting a quantitative analysis.

1.3. Motivation and Proposed Research Framework

Despite the progress made as evidenced in the literature, conducting a system-level evaluation that promotes the economic viability and sustainability is still difficult due to the following challenges:

- 1) The interrelationships among biofuel manufacturing processes are still unclear.

Most of the reported studies assumed that the individual processes were independent of each other and did not include the interrelations between different cellulosic biofuel manufacturing processes. For this reason, the experimental

studies of process parameters were isolated and inconsistent. In fact, many processes in cellulosic biofuel manufacturing are interrelated or interdependent. Input variation in one process usually causes the cost difference in one or several other processes. Cost reduction in one process may be offset by cost increases in other processes, and vice versa. There is no guarantee that separately optimized parameters of each process will lead to reduced costs for the entire biofuel manufacturing system while achieving the same amount of ethanol yield.

- 2) The studies on system-level energy consumption evaluations and energy optimization strategies for cellulosic biofuel production are far behind. Currently, most studies on the energy analysis of biofuel production adopt the LCA approach to estimate energy usage and analyze environmental impacts. However, LCA models are typically linear steady-state models and thus cannot be used to reduce the production energy usage by identifying the optimum system production parameters (e.g., pretreatment temperature, feedstock particle size, and fermentation time). These models do not reflect the interconnections between each process; thus, they suffer from the endogeneity and reversed causality resulting from these interconnections. In addition, some researchers use Aspen software to simulate biofuel conversion in single or multiple processes. The advantage of simulation-based methods is that they can capture system performance in quite complex biofuel production systems. Furthermore, the development and execution of simulation models to obtain statistically useful results may be prohibitively expensive and slow, which makes it quite challenging to find optimal solutions.

- 3) There is a lack of effective waste management plans to improve the material utilization efficiency of cellulosic biofuel manufacturing. Based on the literature review, most studies have conducted explorations of the potential of replacing one or more of the raw materials used in biofuel production with collectible wastes, as well as investigated the viability of byproduct recovery technology in a biofuel production system. Few research efforts are devoted to developing systematic planning for waste management. Research lacking systematic perspective suffers the same fate as economic panel models.

Therefore, the main goal of this thesis is to address these challenges and generate new knowledge about improving sustainability and cost performance for cellulosic biofuel production from a systematic perspective. In order to achieve this goal, a new framework will be established to evaluate and improve the cost and sustainability based on the interrelationships between process characteristics and systematic performance of cellulosic biofuel manufacturing. Moreover, detailed research tasks on modeling cellulosic biofuel production, cost, energy consumption, and waste management will be implemented. Accordingly, the proposed research framework is shown in Figure 2.

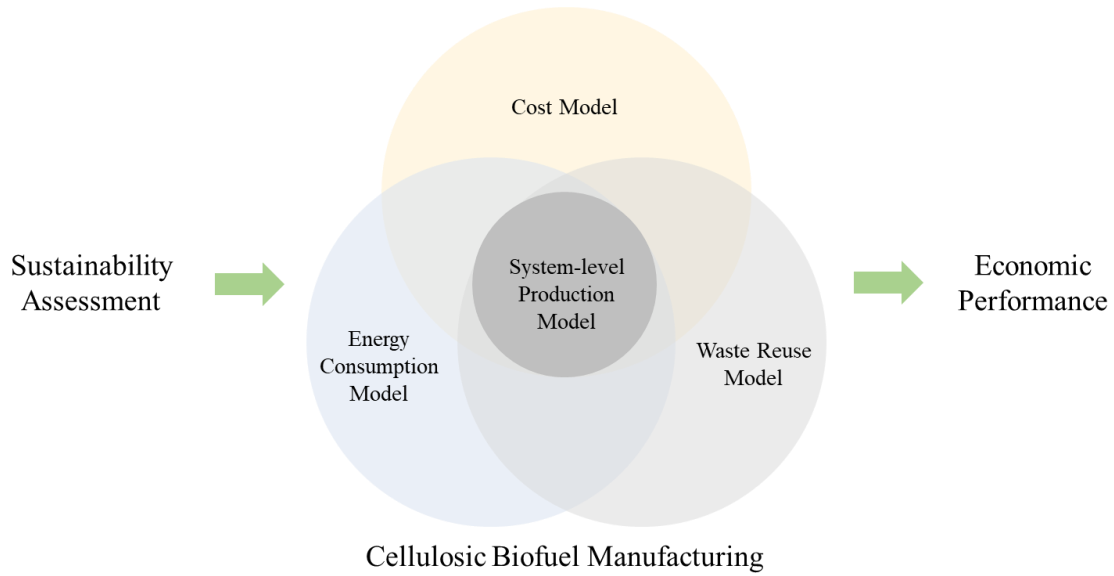


Figure 2. Proposed research framework

At the core of the framework is the new system-level production model, which maps the interrelationships between process characteristics and systematic performance of cellulosic biofuel manufacturing. It involves five main processes in cellulosic biofuel manufacturing, i.e., size reduction, pretreatment, enzymatic hydrolysis, fermentation, and biofuel recovery. The interrelationships among these processes are illustrated by introducing inter-process and intra-process decision variables. In the production model, material flow is established based on reaction kinetics by monitoring the main composition's mass evolution over time. The changes in decision variables will influence the generation and consumption of each material in all processes and finally lead to variations in biofuel yield.

Based on the production model, the cost model, energy consumption model, and waste management model are further developed. It is obvious that with different input of decision variables, the three models' output would be distinct, which renders the potential for optimization. However, unlike cost and energy consumption, to only minimize the produced waste is not the best solution for waste management. It is more favorable to reuse

these wastes and produce model value-added products. In this research, the industrial symbiosis concept is implemented to design a novel waste management strategy. The stakeholders in the industrial symbiosis system can utilize other's output waste as input, which improves environmental and economic benefits and creates a 'win-win situation' for all participants. The material flow, energy flow, cost performance, and environmental impact models are established considering the interactions of stakeholders in the IS system. The appropriate implementation of the research outcomes can provide insight into realizing cost-effective and environmentally sustainable biofuel production to rally the adoption of advanced biofuels.

1.4 Organization of Dissertation

The dissertation is organized as follows. In Chapter 1, a brief introduction is provided, followed by the literature review, motivation, and objective of this research. The system-level economic viability assessment for cellulosic biofuel production is presented in Chapter 2. In Chapter 3, the energy efficiency of cellulosic biofuel manufacturing is modeled. Energy consumption optimization using PSO is also presented in Chapter 3. In addition, a novel waste management strategy facilitated via industrial symbiosis is developed in Chapter 4. Finally, in Chapter 5 the conclusions of this research are drawn and original contributions as well as potential future work are listed.

CHAPTER 2. SYSTEM-LEVEL ECONOMIC VIABILITY EVALUATION FOR CELLULOSIC BIOFUEL MANUFACTURING

(Parts of this chapter were previously published as: *Li L., Ge Y., 2017, System-level cost evaluation for economic viability of cellulosic biofuel manufacturing. Applied Energy, 203, 711-722. <https://doi.org/10.1016/j.apenergy.2017.06.074>.*)

2.1. Introduction

In this chapter, a system-level production model of the cellulosic biofuel is created to map the relationships between process-level input variables and system-level measures such as ethanol yield. This production model can serve as basis for further modeling, analysis, and optimization on cost, energy consumption, and waste management. Based on the established interrelationships across different processes in the production model, a comprehensive cost model is further proposed, in which the input variables can be adjusted towards a cost-effective or a yield-maximized production by using the relationships between individual processes. The establishment of the model provides valuable information and more opportunities to conduct cost-effective decision-making for the entire cellulosic biofuel manufacturing system.

The remainder of this chapter is organized as follow. Section 2.2 introduces the notations used in this chapter. The modeling procedure is presented in Section 2.3, and the solution strategy is illustrated in Section 2.4. In addition, case studies are performed to evaluate the model performance and obtain the optimization results, shown in Section 2.5. Finally, the conclusions of this chapter are discussed in Section 2.6.

2.2. Notations

The following notations are used in this chapter.

Bold Face			
R	Reaction diagonal matrix	N_o	Amount of substance of accessible cellobiose lattices/g cellulose
F	Formation diagonal matrix	N_A	Avogadro constant
S	State variable set	$P_{i,g}$	Threshold ethanol concentration of glucose (g/mol)
		$P_{i,x}$	Threshold ethanol concentration of xylose (g/mol)
Upper Case		$P_{m,g}$	Maximum ethanol concentration of glucose (g/mol)
A	Pre-exponential factor (1/s)	$P_{m,x}$	Maximum ethanol concentration of xylose (g/mol)
A_{G2}	Area of the cellobiose lattice (m ²)	R	Gas Constant
A_{max}	Maximum enzyme adsorption per g cellulose	T	Temperature (K)
AS	Total surface area accessible to enzyme (m ²)	Lower case	
A_s	Reactor surface area (m ²)	A	Ratio of the liquid volume and solid spheres volume
C_{acid}	Active acid concentration (w/w%)	c_e	Concentration of ethanol (kg/L)
C_0	Initial acid concentration (w/w%)	c_g	Concentration of glucose (kg/L)
C^D	Process-dependent cost (\$)	c_{gb}	Concentration of cellobiose(kg/L)
C^{ID}	Process-independent cost (\$)	C_{xl}	Concentration of xylose (kg/L)
E_a	Activation energy	C_{xo}	Concentration of xylose oligomer (kg/L)
E_b	Bound enzyme concentration (g/kg)	C_z	Concentration of recombinant (kg/L)
E_{b1}	Bound concentration of endo- β -1,4-glucanase and exo- β -1,4-glucanase (g/kg)	d	Feedstock particle diameter (m)
E_{b2}	Bound concentration of β - glucosidase (g/kg)	d_r	Thickness of reactor (m)
E_f	Free enzyme concentration (g/kg)	$h_{cellubiose}$	Entropy of cellubiose (kJ/kg)
E_{f2}	Concentration of free β -glucosidase (g/kg)	h_{cond}	Conductivity of pretreatment reactor (W/m)
E_h	Energy consumption by heat transfer (kJ)	h_{conv}	Convection coefficient (W/m ²)
E_r	Energy consumption by reaction (kJ)	$h_{ethanol}$	Entropy of ethanol (kJ/kg)
E_s	Energy consumption by heating up steam (kJ)	h_{glucan}	Entropy of glucan (kJ/kg)
E_{tot}	Total energy consumption (kJ)	$h_{glucose}$	Entropy of glucose (kJ/kg)
$K_{1,gl}$	Inhibition constant of glucose when glucan transforms to glucose (g/L)	h_{xylan}	Entropy of xylan (kJ/kg)
$K_{1,gb}$	Inhibition constant of cellobiose when glucan transforms to glucose (g/L)	h_{xylose}	Entropy of xylose (kJ/kg)
$K_{1,xl}$	Inhibition constant of xylose when glucan transforms to glucose (g/L)	$h_{xylose-oligomer}$	Entropy of xylose oligomer (kJ/kg)
$K_{2,gl}$	Inhibition constants of glucose when glucan transforms to cellobiose(g/L)	k	Reaction rate (1/s)
$K_{2,gb}$	Inhibition constants of cellobiose when glucan transforms to cellobiose(g/L)	$\dot{q}$	Heat flux (W/m ²)
$K_{2,xl}$	Inhibition constants of xylose when glucan transforms to cellobiose(g/L)	$q_{emax,g}$	Overall maximum specific ethanol production rate by glucose (g)
$K_{3,gl}$	Inhibition constants of glucose when cellobiose transforms to glucose(g/L)	$q_{emax,x}$	Overall maximum specific ethanol production rate by xylose (g)
K_{3m}	Cellobiose saturation constants when cellobiose transforms to glucose(g/L)	$q_{smax,g}$	Overall maximum specific glucose utilization rate (g)
$K_{3,xl}$	Inhibition constants of xylose when cellobiose transforms to glucose(g/L)	$q_{smax,x}$	Overall maximum specific xylose utilization rate (g)
$K_{i,g}$	Inhibition constant of glucose when glucose transforms to ethanol(g/L)	p_g	Mass of glucan in feedstock (kg)

$K_{i,x}$	Inhibition constant of xylose when glucose transforms to ethanol(g/L)	p_x	Mass of xylan in feedstock (kg)
K_p	Dissociation constant in terms of L/g cellulose	Greek	
$K_{s,g}$	Limitation constant of glucose(g/L)	α	Weight factor of glucose consumption
$K_{s,x}$	Limitation constant of xylose(g/L)	β	Initial water volume (L)
M_g	Molecular weight of glucan(g/mol)	λ	Ratio of cellobiose lattices occupied to bound enzyme molecule
M_{gl}	Molecular weight of glucose(g/mol)	ρ_{solid}	Density of the solid (kg/m3)
M_x	Molecular weight of xylan(g/mol)	$\mu_{max,g}$	Maximum overall specific growth rate of glucose (1/s)
M_{xl}	Molecular weight of xylose(g/mol)	$\mu_{max,x}$	Maximum overall specific growth rate of xylose (1/s)
M_{xo}	Molecular weight of xylose oligomer(g/mol)		

2.3. Mathematical Modeling

2.3.1. Cellulosic Biofuel Manufacturing System Description

The proposed mathematical model is established based on the biochemical pathway of the cellulosic biofuel manufacturing, as shown in Figure 3. The cellulosic biofuel manufacturing system studied in this chapter consists of three main processes: pretreatment, enzymatic hydrolysis, and fermentation.

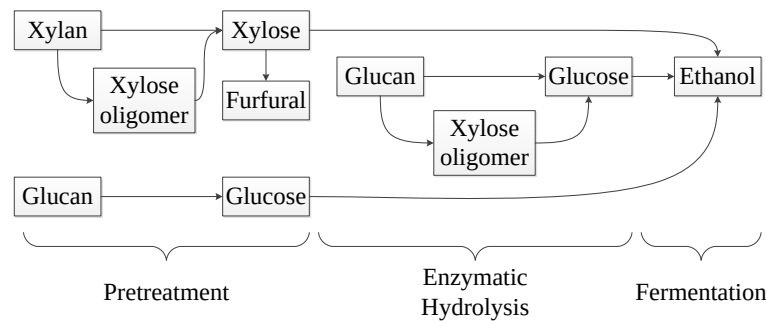


Figure 3. Biochemical pathway in cellulosic ethanol production system

In the pretreatment process, the steam-assisted diluted acid pretreatment method is adopted, where steam is used to heat the feedstock to the required reaction temperature, as well as to disrupt the outer lignin structure. Processing water is added at the beginning of the pretreatment process and its volume is assumed to be constant. Diluted acid is also added at the start of pretreatment and permeates the feedstock particles following the principle of diffusion. These particles are assumed to have a spherical shape with a

diameter of d (Crank, 1975; Kim, 2002), so that the overall bulk transportation of acid is considered to have no certain diffusional direction. During the pretreatment process, diluted acid catalyzes the conversion of hemicellulose and cellulose into simpler sugars at a high temperature ($\sim 160^{\circ}\text{C}$). In most cellulosic feedstocks, xylan accounts for more than 90% of all hemicellulose (Kumar et al., 2009). Therefore, in this proposed model, the conversion of xylan into xylose oligomers and ultimately into monomeric xylose is used to represent all the hemicellulose conversions. A part of xylose is also converted into furfural, which is an undesired degraded product that lowers the concentration of xylose and further influences the ethanol yield. At the end of pretreatment process, ammonia is used to adjust the pH value of the hydrolysate slurry.

After being exposed to the severe reaction conditions in the pretreatment process, cellulose is more easily hydrolyzed to sugar via enzymatic hydrolysis. In this model, the Separate (or sequential) Hydrolysis and Fermentation (SHF) is applied. The conversions in enzymatic hydrolysis include the transformation of cellulose simultaneous hydrolysis to cellobiose and glucose, and the conversion of cellobiose to glucose. Total enzyme loading is set as 20 mg/g feedstock to achieve a high conversion rate (Aden et al., 2002). The reaction temperature is kept around 48°C to maintain the activity of the enzyme. A modified Langmuir equation is used to model the enzyme absorption process associated with the particle size (Zhang and Lynd, 2004). It has been found that part of the saccharified slurry can be used to produce enzymes for the purpose of reducing cost (Humbird et al., 2011a). Therefore, in this model, we assume 10% of the saccharified slurry is used for the enzyme production while ensuring the final ethanol yield.

After 84 hours of hydrolysis, the saccharified slurry proceeds to the fermentation process. Two types of sugar (i.e., xylose and glucose) are simultaneously fermented into ethanol by recombinant *Zymomonas mobilis* strain ZM4 (pZB5) (*Z. mobilis* ZM4 (pZB5)) (Jeon et al., 2002). The fermentation temperature is kept around 32 °C and the substrates stay at the reactor for 36 hours until the fermentation process finishes.

2.3.2. Input Decision Variables

The interrelationships between different individual processes are characterized by introducing inter-process and intra-process decision variables into the reaction kinetics equations. Inter-process variables exist across multiple processes and have direct influence on cost and energy consumption in multiple processes. On the contrary, intra-process variables only exist in one process and are carried into the following processes as functions, hence they influence other processes indirectly. Both inter-process and intra-process decision variables are summarized in TABLE I.

TABLE I. INPUT DECISION VARIABLES

Inter-process variables	Processes
Feedstock particle diameter: d	Pretreatment, Hydrolysis
Initial input water volume: β	Pretreatment, Hydrolysis, Fermentation
Intra-process variables	Process
Initial concentration of acid: C_0	Pretreatment
Pretreatment temperature: T_p	Pretreatment
Pretreatment time: t_p	Pretreatment
Total enzyme loading: E_t	Hydrolysis
Enzymatic hydrolysis time: t_h	Hydrolysis
Enzymatic hydrolysis temperature: T_h	Hydrolysis
Fermentation temperature: T_f	Fermentation
Fermentation time: t_f	Fermentation

2.3.3. System Performance Modeling

In this section, the analytical models for the ethanol yield, energy consumption, and total cost are presented. Reaction kinetic equations are used to describe the biofuel manufacturing processes by tracking the mass evolutions of major reactants and products. Ethanol yield, energy consumption, and cost are modeled as follows: ethanol yield is the mass of ethanol at the end of fermentation process; energy consumption is calculated by combining the internal heat of steam, heat loss from heat transfer, and energy consumed by all reactions; finally, total cost is computed by summarizing all the cost-components of the biofuel manufacturing system.

2.3.3.1. Ethanol Yield Modeling

To describe the mass evolution of the reactants and products in the production system, seven major matters in the biofuel manufacturing biochemical pathway are defined as state variables: xylan mass in the feedstock p_x ; glucan mass in the feedstock p_g ; xylose-oligomers concentration c_{xo} ; xylose concentration c_{xl} ; glucose concentration c_g ; cellobiose concentration c_{gb} ; and ethanol concentration c_e . The expressions of these state variables' variation rate are different in each manufacturing process. Therefore, we divide the total manufacturing time t_{tot} into three durations: pretreatment time t_p , hydrolysis time t_h , and fermentation time t_f . The three processes occur during time slots $[0, t_p)$, $[t_p, t_p + t_h)$, $[t_p + t_h, t_p + t_h + t_f]$, respectively.

Xylan is consumed in the pretreatment process ($t \in [0, t_p)$), where it is converted to xylose-oligomers and xylose. The governing equation for the variation of p_x is given by:

$$\frac{dp_x}{dt} = \begin{cases} -(k_{xo} + k_{xl})p_x \cdot C_{acid} & t \in [0, t_p) \\ 0 & t \in [t_p, t_p + t_h) \\ 0 & t \in [t_p + t_h, t_p + t_h + t_f] \end{cases} \quad (1)$$

where k_{xo} and k_{xl} are the reaction rates of the conversion from xylan to xylose-oligomers and xylan to xylose, respectively. In this model, the reaction rates are assumed to have an Arrhenius dependence (Rodríguez-Aragón and López-Fidalgo, 2005) on temperature, shown in Eq. (2), which indicates that the reaction rate is higher if the temperature increases:

$$k = A \cdot e^{-E_a/RT} \quad (2)$$

For the acid concentration, the feedstock particles are assumed to have a spherical shape, and they are penetrated by acid from an un-infiltrated condition to a fully soaked condition. The active acid concentration C_{acid} is represented by the concentration of acid, which has infiltrated particles. The diffusion into a spherical particle is described by the following partial differential equation:

$$\frac{\partial C}{\partial t} = D_e \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right) \quad (3)$$

The analytical solution of this classical problem is given by Crank (Crank, 1975):

$$C_{acid}(t) = C_0 \cdot [1 - f(t)],$$

$$f(t) = 1 - \sum_{n=1}^{\infty} \left(\frac{6a(1+a)}{9+9a+q_n^2 a} \right) \exp\left(-\frac{q_n^2 D_e t}{(d/2)^2}\right) \quad (4)$$

where $C_{acid}(t)$ denotes the active acid concentration at time t ; and $a = 3\beta/[4\pi(d/2)^3]$ is the ratio of the liquid volume and solid spheres volume. As an inter-process input variable, particle size influences the pretreatment process by affecting acid infiltration into the particles.

Xylose-oligomers is a mid-product formed by xylan in the pretreatment process, and it will be further converted into xylose. Therefore, the governing equation for the variation of c_{xo} is given by:

$$\frac{dc_{xo}}{dt} = \begin{cases} k_{xo} \cdot \left(\frac{p_x}{M_x}\right) \left(\frac{M_x}{M_{xo}}\right) \cdot C_{acid} \cdot \frac{1}{\beta} & t \in [0, t_p) \\ -k_{x2} \cdot c_{xo} \cdot C_{acid} & t \in [t_p, t_p + t_h) \\ 0 & t \in [t_p + t_h, t_p + t_h + t_f] \end{cases} \quad (5)$$

Term β represents the initial input water volume, which determines the concentration of each matter in this system. Generally, less initial water leads to higher reactant concentration, which will then enhance the conversion rate. However, if the inhibition effect is considered in the enzymatic hydrolysis process, less initial water also results in stronger inhibitions, which will jeopardize the fermentable sugar yield. In addition, less initial water makes the slurry thicker and applies a heavier load on the agitators and pumps in the system.

Xylose is formed from xylan and xylose-oligomer in the pretreatment process. Part of the formed xylose is converted into furfural during the pretreatment process, which is an undesired secondary product that hazards the xylose yield. In the fermentation process, ($t \in [t_p + t_h, t_p + t_h + t_f]$), xylose is fermented into ethanol. The governing equation for the variation of xylose concentration is given by:

$$\begin{aligned}
& k_{xl} \cdot \left(\frac{p_x}{M_x}\right) \left(\frac{M_x}{M_{xl}}\right) \cdot C_{acid} \cdot \frac{1}{\beta} & t \in [0, t_p) \\
& + k_{x2} \cdot c_{xo} \cdot \left(\frac{M_{xo}}{M_{xl}}\right) \cdot C_{acid} - k_f \cdot c_{xl} \cdot C_{acid} \\
\frac{dc_{xl}}{dt} = & \begin{cases} 0 & t \in [t_p, t_p + t_h) \\ -(1 - \alpha) \cdot \frac{q_{smax,x}}{\beta} \cdot \left(\frac{c_{xl}}{K_{ss,x} + c_{xl}}\right) \cdot & t \in [t_p + t_h, t_p + t_h + t_f] \\ (1 - \frac{p - P_{is,x}}{P_{ms,x} - P_{is,x}}) \left(\frac{K_{is,x}}{K_{is,x} + c_{xl}}\right) \cdot c_Z & \end{cases} \quad (6)
\end{aligned}$$

where c_Z is the concentration of recombinant *Z. mobilis* ZM4 (pZB5), which uses glucose and xylose as carbon sources, converts both sugars into ethanol simultaneously (Jeon et al., 2002). The expression for the microbial growth rate is given by:

$$\begin{aligned}
\frac{dc_Z}{dt} = & \alpha \cdot \frac{\mu_{max,g}}{\beta} \cdot \left(\frac{c_g}{K_{sz,g} + c_g}\right) \left(1 - \frac{c_e - P_{iz,g}}{P_{mz,g} - P_{iz,g}}\right) \left(\frac{K_{iz,g}}{K_{iz,g} + c_g}\right) \cdot c_Z + \\
& (1 - \alpha) \cdot \frac{\mu_{max,x}}{\beta} \cdot \left(\frac{c_{xl}}{K_{sz,x} + c_{xl}}\right) \left(1 - \frac{c_e - P_{iz,x}}{P_{mz,x} - P_{iz,x}}\right) \left(\frac{K_{iz,x}}{K_{iz,x} + c_{xl}}\right) \cdot c_Z \quad (7)
\end{aligned}$$

A portion of glucan is converted into glucose in pretreatment, while the rest of the glucan is saccharificated in the enzymatic hydrolysis process ($t \in [t_p, t_p + t_h)$). The governing equation for the variation of p_g is given by:

$$\begin{aligned}
& -k_g \cdot p_g \cdot C_{acid} & t \in [0, t_p) \\
\frac{dp_g}{dt} = & \begin{cases} -\frac{k_{h1} \cdot E_{b1} \cdot p_g}{1 + \frac{c_{gl}}{K_{1,gl}} + \frac{c_{gb}}{K_{1,gb}} + \frac{c_{xl}}{K_{1,xl}}} & t \in [t_p, t_p + t_h) \\ -\frac{k_{h2} \cdot (E_{b1} + E_{b2}) \cdot p_g}{1 + \frac{c_{gl}}{K_{2,gl}} + \frac{c_{gb}}{K_{2,gb}} + \frac{c_{xl}}{K_{2,xl}}} & \\ 0 & t \in [t_p + t_h, t_p + t_h + t_f] \end{cases} \quad (8)
\end{aligned}$$

The enzymes are absorbed by feedstock particles to catalyze the reaction. A modified Langmuir equation involving particle size of feedstock developed by Zhang and Lynd, 2004, is used to describe the enzyme absorption:

$$E_b = \frac{N_0 K_p' E_f}{1 + \lambda K_p' E_f} \quad (9)$$

where $K_p' = K_p/\lambda$, $\lambda = \frac{N_0}{A_{max}}$, and $A = \frac{AS}{N_A \lambda A_{G2}}$. The total surface area of all particles AS can be calculated by the surface area of each particle S multiplied with number of particles, N :

$$AS = S \times N = (4\pi \cdot (d/2)^2) \times (mass\ of\ feedstock) / \rho_{solid} \cdot [\frac{4}{3} \cdot \pi \cdot (d/2)^3] \quad (10)$$

where particle size affects the enzymatic hydrolysis process by influencing the enzyme absorption of the particles.

Glucose is formed by glucan in both pretreatment and hydrolysis processes, and is converted into ethanol in the fermentation process. The governing equation for the variation in the glucose concentration c_g is given by:

$$\begin{aligned}
& k_g \cdot \left(\frac{p_g}{M_g}\right) \left(\frac{M_g}{M_{gl}}\right) \cdot C_{acid} \cdot \frac{1}{\beta} & t \in [0, t_p) \\
& 1.111 \times \frac{k_{h2} \cdot (E_{b1} + E_{b2}) \cdot p_g \cdot \left(\frac{1}{\beta}\right)}{1 + \frac{c_g}{K_{2,gl}} + \frac{c_{gb}}{K_{2,gb}} + \frac{c_{xl}}{K_{2,xl}}} \\
\frac{dc_g}{dt} = & \begin{cases} + 1.053 & t \in [t_p, t_p + t_h) \\ \times \frac{k_{h3} \cdot E_{f2} \cdot c_{gb}}{K_{3m}(1 + \frac{c_{gl}}{K_{3,gl}} + \frac{c_{xl}}{K_{3,xl}}) + c_{gb}} \\ - \alpha \cdot \frac{q_{smax,g}}{\beta} \cdot \left(\frac{c_g}{K_{ss,g} + c_g}\right) (1 \\ - \frac{c_e - P_{is,g}}{P_{ms,g} - P_{is,g}}) \left(\frac{K_{is,g}}{K_{is,g} + c_g}\right) \cdot c_Z & t \in [t_p + t_h, t_p + t_h + t_f] \end{cases} \quad (11)
\end{aligned}$$

As a reaction intermediate, cellobiose is formed from glucan and further converted into glucose in the enzymatic hydrolysis process. The governing equation for the variation of cellobiose concentration c_{gb} is given by:

$$\begin{aligned}
& 0 & t \in [0, t_p) \\
& - \frac{k_{h3} \cdot E_{f2} \cdot c_{gb}}{K_{3m}(1 + \frac{c_{gl}}{K_{3,gl}} + \frac{c_{xl}}{K_{3,xl}}) + c_{gb}} \\
\frac{dc_{gb}}{dt} = & \begin{cases} + 1.056 & t \in [t_p, t_p + t_h) \\ \times \frac{k_{h1} \cdot E_{b1} \cdot p_g \cdot \left(\frac{1}{\beta}\right)}{1 + \frac{c_{gl}}{K_{1,gl}} + \frac{c_{gb}}{K_{1,gb}} + \frac{c_{xl}}{K_{1,xl}}} \\ 0 & t \in [t_p + t_h, t_p + t_h + t_f] \end{cases} \quad (12)
\end{aligned}$$

Eventually, ethanol is fermented from xylose and glucose under the catalysis of recombinant *Z. mobilis* ZM4 (pZB5). The ethanol yield is determined by the value of

ethanol concentration at end of fermentation process. The governing equation for the ethanol production is given by:

$$\begin{aligned}
 & 0 & t \in [0, t_p) \\
 & 0 & t \in [t_p, t_p + t_h) \\
 \frac{dc_e}{dt} = & \begin{cases} \alpha \cdot \frac{q_{emax,g}}{\beta} \cdot \left(\frac{c_g}{K_{se,g} + c_g} \right) \\ \left(1 - \frac{c_e - P_{ie,g}}{K_{me,g} - P_{i,g}} \right) \left(\frac{K_{ie,g}}{K_{ie,g} + c_g} \right) \cdot c_Z \\ + (1 - \alpha) \frac{q_{emax,x}}{\beta} \left(\frac{c_{xl}}{K_{se,g} + c_{xl}} \right) \\ \left(1 - \frac{c_e - P_{ie,x}}{K_{me,x} - P_{i,x}} \right) \left(\frac{K_{ie,x}}{K_{ie,x} + c_{xl}} \right) \cdot c_Z \end{cases} & t \in [t_p + t_h, t_p + t_h + t_f]
 \end{aligned} \tag{13}$$

2.3.3.2. Energy Consumption Modeling

As an important component of the manufacturing cost, energy consumption is calculated in this section. The energy consumption of the cellulosic biofuel manufacturing system has three main sources: the energy used to heat up steam, the heat loss due to heat transfer, and the energy consumed by chemical thermodynamics.

1) Energy of heating steam

Before the dilute-acid pretreatment process, feedstock is exposed to overheated steam to disrupt the outer lignin structure of cellulosic feedstock. The energy consumed by heating up steam is calculated by multiplying the weight of steam m_{steam} with the entropy of steam h_{steam}^T , where superscription T indicates the entropy of steam at temperature T .

$$E_s = m_{steam} \cdot h_{steam}^T \tag{14}$$

2) Heat loss due to heat transfer

The reaction temperature for all three individual processes are higher than room temperature (25°C). Therefore, heat transfers from the internal of the reactor to the surrounding via conduction and natural convection, while radiation in this situation is neglected. According to heat transfer balance, heat flux can be expressed as:

$$\dot{q} = \frac{k_{cond} \cdot A_s}{d_r} (T_i - T_o) = h_{conv} \cdot A_s \cdot (T_o - T_\infty) \quad (15)$$

Then the governing equation of heat loss by heat transfer over time t is given by:

$$E_h^t = \dot{q} \cdot t \quad (16)$$

3) Energy consumption from chemical thermodynamics

The temperature of each reaction should be maintained at an optimal value or range to ensure the targeted ethanol yield. Therefore, additional energy is needed to balance the energy consumed/released by reaction thermodynamics. The energy consumed by reaction thermodynamics is calculated through measuring the internal energy variation between the raw materials and the materials at time t .

The set of state variables is: $\mathbf{S} = [p_x \quad p_g \quad c_{xo} \quad c_{cl} \quad c_g \quad c_{gb} \quad c_e]$. Let $\mathbf{S}_{[i]}^t$ be the concentration of i th term at time t , then the energy supplement for the reaction at time t can be calculated by:

$$E_r^t = \sum_{i=1}^2 \mathbf{S}_{[i]}^t \cdot h_i + \sum_{i=3}^7 \mathbf{S}_{[i]}^t \cdot h_i \cdot \beta - \sum_{i=1}^2 \mathbf{S}_{[i]}^0 \cdot h_i - \sum_{i=3}^7 \mathbf{S}_{[i]}^0 \cdot h_i \cdot \beta \quad (17)$$

where h_i denotes the entropy of the i th term; superscription t represents the state variables at time t ; and superscription 0 represents the state variables at time 0. For $i=1$ and 2, xylan and glucan use the unit kg, and therefore the internal energy is calculated by multiplying their mass with entropy. For $i=3, 4, \dots, 7$, these components use kg/L as the unit, and thus must be multiplied with initial water volume β to convert their units to kg.

In summary, the governing equation for total energy consumption at time t is:

$$E_{tot}^t = E_s + E_h^t + E_r^t. \quad (18)$$

2.3.3.3. Cost Modeling

The total costs of the cellulosic biofuel manufacturing system are divided into two types: process-independent cost C^{ID} and process-dependent cost C^D (as illustrated in Figure 4). The process-independent costs can be expressed by a linear summation of all the cost items such as capital recovery and labor cost. The process-dependent costs include acid, ammonia, steam, and electricity costs from the pretreatment process; enzyme and electricity costs from the enzyme hydrolysis process; and recombinant *Z. mobilis* and electricity costs from the fermentation process.

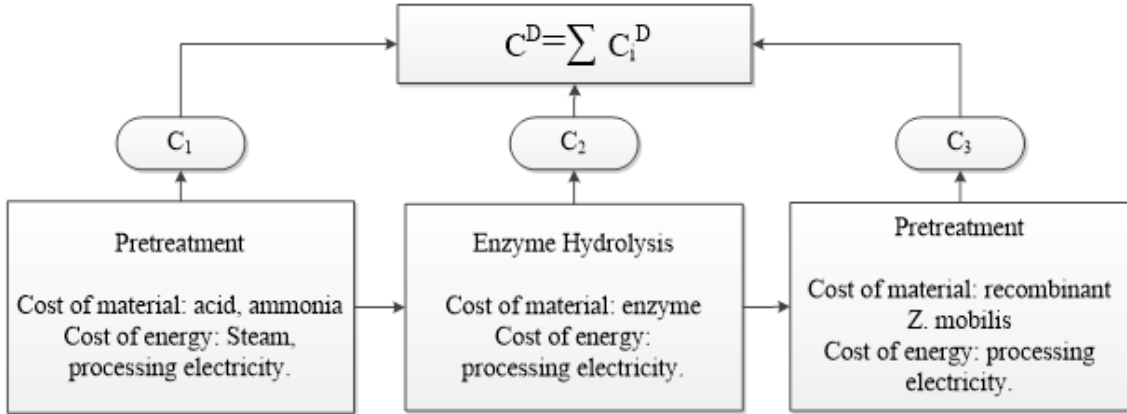


Figure 4. Process-dependent cost breakdown

Let $X_i = [x_{i1}, x_{i2}, \dots, x_{in}]$ be the set of cost items in process i , then the process-dependent cost of process i can be represented as:

$$C_i^D = \sum_n x_i \cdot C_{in} \quad (19)$$

where C_{in} denotes the unit price of n th cost item in process i . Some of the cost items are input decision variables (e.g., enzyme and dilute acid), and others are functions of input variables such as electricity usage. The process-dependent costs are expressed by an

explicit non-linear function, through which the relationships between decision variables and process-dependent costs are established. Therefore, the total cost is rendered by adding up all the process-independent costs and process-dependent costs:

$$C = \sum_i C^D + \sum C^{ID}. \quad (20)$$

2.4. Solution Strategies

In Eq. (1)-(13), time-dependent differential equations are used to describe the evolution of state variables. By introducing the input decision variables, the reaction kinetics of the biofuel manufacturing systems are characterized by the tightly coupled equations. Let $\mathbf{R}$ and $\mathbf{F}$ be the diagonal matrices which represent consumption and formation terms respectively, then the differential equations are generalized as:

$$[\mathbf{R}_p]\mathbf{S} + \mathbf{F}_p \quad t \in [0, t_p) \quad (21)$$

$$\frac{d\mathbf{S}}{dt} = \begin{cases} [\mathbf{R}_h]\mathbf{S} + \mathbf{F}_h & t \in [t_p, t_p + t_h) \end{cases} \quad (22)$$

$$[\mathbf{R}_f]\mathbf{S} + \mathbf{F}_f \quad t \in [t_p + t_h, t_p + t_h + t_f] \quad (23)$$

$$\mathbf{S} = [p_x \quad p_g \quad c_{xo} \quad c_{cl} \quad c_g \quad c_{gb} \quad c_e]^T \quad (24)$$

where $\mathbf{S}$ is the solution vector containing the state variables, and the superscript T denotes a transpose. The subscripts p , h and f represent the pretreatment, hydrolysis and fermentation, respectively. Let $\mathbf{S}^0$ be the initial state variable set for the systematic model and introduce $\mathbf{S}_0$ in pretreatment kinetic model (Eq. (21)). We are able to obtain the state variable set $\mathbf{S}_p$ after pretreatment; next, using $\mathbf{S}_p$ as the initial state variable set for enzymatic hydrolysis model (Eq. (22)), we can calculate the state variable set $\mathbf{S}_h$ after enzymatic hydrolysis; then $\mathbf{S}_h$ is considered as the initial values of fermentation model (Eq. (23)), and the final yield can be obtained. The reaction matrices and formation matrices are given by the following equations.

$$\mathbf{R}_p = \text{diag} \begin{bmatrix} -(k_{xo} + k_{x1}) \cdot C_{acid} \\ -k_g \cdot C_{acid} \\ k_{x2} \cdot C_{acid} \\ -k_f C_{acid} \\ 0 \\ 0 \\ 0 \end{bmatrix}, \mathbf{R}_h = \text{diag} \begin{bmatrix} 0 \\ -\frac{k_{h1} \cdot E_{b1}}{1 + \frac{c_{gl}}{K_{1,gl}} + \frac{c_{gb}}{K_{1,gb}} + \frac{c_{xl}}{K_{1,xl}}} \\ -\frac{k_{h2} \cdot (E_{b1} + E_{b2})}{1 + \frac{c_{gl}}{K_{2,gl}} + \frac{c_{gb}}{K_{2,gb}} + \frac{c_{xl}}{K_{2,xl}}} \\ 0 \\ 0 \\ 0 \\ \frac{k_{h3} \cdot E_{b3} \cdot c_{gb}}{K_{3m} \left(1 + \frac{c_{gl}}{K_{3,gl}} + \frac{c_{xl}}{K_{3,xl}}\right) + c_{gb}} \\ 0 \end{bmatrix}, \quad (25)$$

$$\mathbf{R}_f = \text{diag} \begin{bmatrix} 0 \\ 0 \\ 0 \\ -(1 - \alpha) \cdot \frac{q_{smax,x}}{\beta} \cdot \left(\frac{1}{K_{ss,x} + c_{xl}}\right) \cdot \\ \left(1 - \frac{p - P_{is,x}}{P_{ms,x} - P_{is,x}}\right) \left(\frac{K_{is,x}}{K_{is,x} + c_{xl}}\right) \cdot c_z \\ -\alpha \cdot \frac{q_{smax,g}}{\beta} \cdot \left(\frac{1}{K_{ss,g} + c_g}\right) \cdot \\ \left(1 - \frac{c_e - P_{is,g}}{P_{ms,g} - P_{is,g}}\right) \left(\frac{K_{is,g}}{K_{is,g} + c_g}\right) \cdot c_z \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{F}_p = \text{diag} \begin{bmatrix} 0 \\ 0 \\ k_{xo} \cdot \left(\frac{p_x}{M_x}\right) \left(\frac{M_x}{M_{xo}}\right) \cdot C_{acid} \cdot \frac{1}{\beta} \\ k_{xl} \cdot \left(\frac{p_x}{M_x}\right) \left(\frac{M_x}{M_{xl}}\right) \cdot C_{acid} \cdot \frac{1}{\beta_i} \\ + k_{x2} \cdot c_{xo} \cdot \left(\frac{M_{xo}}{M_{xl}}\right) \cdot C_{acid} \\ k_g \cdot \left(\frac{p_g}{M_g}\right) \left(\frac{M_g}{M_{gl}}\right) \cdot C_{acid} \cdot \frac{1}{\beta} \\ 0 \\ 0 \end{bmatrix}, \mathbf{F}_h = \text{diag} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1.111 \times \frac{k_{h2} \cdot (E_{b1} + E_{b2}) \cdot p_g \cdot \left(\frac{1}{\beta}\right)}{1 + \frac{c_g}{K_{2,gl}} + \frac{c_{gb}}{K_{2,gb}} + \frac{c_{xl}}{K_{2,xl}}} \\ + 1.053 \times \frac{k_{h3} \cdot E_{f2} \cdot c_{gb}}{K_{3m} \left(1 + \frac{c_{gl}}{K_{3,gl}} + \frac{c_{xl}}{K_{3,xl}}\right) + c_{gb}} \\ 1.056 \times \frac{k_{h1} \cdot E_{b1} \cdot p_g \cdot \left(\frac{1}{\beta}\right)}{1 + \frac{c_{gl}}{K_{1,gl}} + \frac{c_{gb}}{K_{1,gb}} + \frac{c_{xl}}{K_{1,xl}}} \\ 0 \end{bmatrix}, \quad (26)$$

$$\mathbf{F}_f = \text{diag} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \alpha \cdot \frac{q_{e max,g}}{\beta} \cdot \left(\frac{c_g}{K_{se,g} + c_g}\right) \cdot \\ \left(1 - \frac{c_e - P_{ie,g}}{P_{me,g} - P_{ie,g}}\right) \left(\frac{K_{ie,g}}{K_{ie,g} + c_g}\right) \cdot c_z + \\ \left(1 - \alpha\right) \cdot \frac{q_{e max,x}}{\beta} \cdot \left(\frac{c_{xl}}{K_{se,x} + c_{xl}}\right) \cdot \\ \left(1 - \frac{c_e - P_{ie,x}}{P_{me,x} - P_{ie,x}}\right) \left(\frac{K_{ie,x}}{K_{ie,x} + c_{xl}}\right) \cdot c_z \end{bmatrix}$$

To simulate the manufacturing system in a programming software, the coupled differential equations Eq. (26) are discretized using the Finite-difference Method (FDM), which is well suited for solving first order differential equations. After discretizing the total production time ($t_p + t_h + t_f$), Eq. (21)-(23) can be transformed to Eq. (27).

$$\frac{s_i^{n+1} - s_i^n}{\Delta t} = [R_i]^n S_i^{n+1} + F_i^n, \text{ where } i=p, h \text{ and } f. \quad (27)$$

where superscript n denotes the number of time steps, and $n+1$ represents the next time step from n . Time interval Δt is one second to ensure the calculation accuracy. For each state variable set at time step n (i.e., S^n), Eq. (28) is solved as a linear system to obtain the values for next time step. This discretion approach is coded and solved in MATLAB programming environment. The MATLAB function ‘linsolve’ is used to simultaneously calculate the state variable values in every time step. Subsequently, the reaction energy consumption is calculated by Eq. (17), and the total energy consumption is obtained by Eq. (18). The total cost is then determined by the product of unit price and each cost-related state variables.

2.5. Case Study

In this section, two numerical cases, i.e., baseline case and cost-effective case, are conducted. The baseline case uses the parameters in the technical report from National Renewable Energy Laboratory (NREL), ‘Process design and economics for conversion of lignocellulosic biomass to ethanol’ (Humbird et al., 2011a), as input decision variables, and is compared with the cost and ethanol yield results from (Humbird et al., 2011a) to validate the proposed model. In the cost-effective case, the values of input decision variables are changed to reduce total manufacturing cost under the constraint of ethanol yield. By comparing the results of cost-effective case with the baseline case, the

effectiveness of the establishment of the interrelationships between different processes is demonstrated. The cost in the cost-effective case is reduced by 12.8% compared with the baseline case without sacrificing ethanol yield.

2.5.1. Parameter Setup

The composition of corn stover used in the baseline case is shown in TABLE II. For validation purposes, the values of input decision variables in the baseline case are shown in TABLE III. The value of parameters in the following tables are as same as in (Humbird et al., 2011a).

TABLE II. SOLID COMPOSITION OF CORN STOVER

Component	Dry weight percentage
Glucan	35.0%
Xylan	19.5%
Lignin	15.8%
Galactan	1.4%
Arabinan	2.4%
Acetate	1.8%
Ash	4.9%

TABLE III. VALUES OF INPUT DECISION VARIABLES

Inter-process variables	Values
Feedstock particle diameter: d	6.67mm in diameter (4 mesh)
Initial input water volume: β	2.2 Liter
Intra-process variables	
Initial concentration of acid: C_0	1.0% w/w
Pretreatment temperature: T_p	158°C
Pretreatment time: t_p	5min
Total enzyme loading: E_t	20mg/g feedstock
Enzymatic hydrolysis time: t_h	84hrs
Enzymatic hydrolysis temperature: T_h	48°C
Fermentation temperature: T_f	32°C
Fermentation time: t_f	36hrs

The reaction rate constants used in this model are summarized in TABLE IV. TABLE V illustrates the invariant model parameters excluding the constants associated with reaction rate.

TABLE IV. REACTION RATE CONSTANTS

Arrhenius reaction rate parameters (Esteghlalian et al., 1997; Kadam et al., 2004; Wolfrum and Sluiter, 2009),		
Reaction rate	A (1/s)	E _a (kJ/mol)
k_{xo}	1.0×10^{15}	110.0
k_{xl}	8.0×10^{17}	130.0
k_{x2}	2.5×10^{14}	110.0
k_f	7.0×10^{11}	98.0
k_g	2.0×10^{22}	180.0
k_{h1}	2.3×10^7	5540
k_{h2}	2.0×10^7	5570
k_{h3}	3.0×10^6	5810

TABLE V. OTHER PARAMETERS

Molecular weights (g/mol)		Inhibition constant (g/L) (Kadam et al., 2004)	
M_x	132 ^a	$K_{1,gl}$	0.1
M_{xo}	450 ^a	$K_{2,gl}$	0.04
M_{xl}	150 ^a	$K_{3,gl}$	3.9
M_g	162 ^a	$K_{1,gb}$	0.015
M_{gl}	180 ^a	$K_{2,gb}$	132
Overall substrate utilization rate (g/L) (Leksawasdi et al., 2001)		K_{3m}	24.3
$\mu_{max,g}$	0.31	$K_{1,xl}$	0.1
$\mu_{max,x}$	0.1	$K_{2,xl}$	0.2
$q_{max,g}$	10.9	$K_{3,xl}$	0.2
$q_{max,x}$	3.27	Heat transfer coefficients (Humbird et al., 2011a; Sinnott, 2007; Voragen, 1998; Yalkowsky and He, 2003),	
$q_{smax,g}$	5.12	k_{cond} (W/m/K)	50.2 ^a
$q_{smax,x}$	1.59	h_{conv} (W/K)	20 ^a
Substrates inhibitory concentration (g/L) (Leksawasdi et al., 2001)		A_s (m ²)	0.005
$K_{iz,x}$	200	d (m)	0.05
$K_{iz,g}$	600	T_∞ (°C)	25 ^a
$K_{is,x}$	186	m_{steam} (kg)	0.35
$K_{is,g}$	600	h_{steam} at 268°C (kJ/kg)	2853.8 ^a
$K_{ie,x}$	186	h_{glucan} (kJ/kg)	3100.0
$K_{ie,x}$	600	h_{xylan} (kJ/kg)	2812.0
Enzyme concentrations (g/g) (Bothwell et al., 1997)		$h_{glucose}$ (kJ/kg)	7061.1
E_b	0.02	h_{xylose} (kJ/kg)	6826.0
E_{b1}	0.017	$h_{xylose-oligomer}$ (kJ/kg)	4214.0
E_{b2}	0.003	$h_{cellulbiose}$ (kJ/kg)	3895.0
A_{max} (mg/g)	280	$h_{ethanol}$ (kJ/kg)	5825.0
K_p (L/mg)	0.04	R (J/mol/K)	8.314 ^a

$A_{G2} \text{ (m}^2\text{)}$	5.512×10^{-19}	Other parameters	
Threshold ethanol concentration (g/L) (Leksawasdi et al., 2001)		$d \text{ (m)}$	0.0066
$P_{i,g}$	57.4	$N_A \text{ (molecules/mol)}$	$6.023 \times 10^{23} \text{ }^a$
$P_{i,x}$	81.2	α	0.65 (Leksawasdi et al., 2001)
$P_{m,g}$	57.4	$\rho_{solid} \text{ (kg/m}^3\text{)}$	650 ^a
$P_{m,x}$	81.2		

^a Obtained from common knowledge

2.5.2. Model Performance

The mass evolutions of state variables are illustrated in Figure 5. The final ethanol yield from 1 kg feedstock is 0.236 kg by adopting the values of input decision variables as shown in TABLE III. It can be observed that most of the hemicellulose (i.e., xylan) is hydrolyzed into soluble sugar during the pretreatment process (as shown in Figure 5), while most of the cellulose is converted into glucose in the enzymatic hydrolysis process. Further observations from numerically simulated data suggest that:

- (i) In Figure 6, the slight decrease in xylose concentration at the end of the pretreatment process is due to the conversion of xylose to its secondary degradation furfural. Thus, pretreatment should not last too long to avoid loss in sugar yield.
- (ii) Although the total reaction time for enzymatic hydrolysis t_h is 84 hours, it is noticed that the concentration of glucose hardly changes at $t=60$ hours, which implies that we may be able to adopt less enzymes to save cost and maintain the same glucan conversion rate at $t=84$ hours.
- (iii) After the enzymatic hydrolysis, the mass of each state variable except ethanol drops down. This is because 10% of the saccharified slurry is removed from the stream for enzyme production. This production scheme results in about 10% of ethanol yield loss, however, it saves cost related to enzyme production.

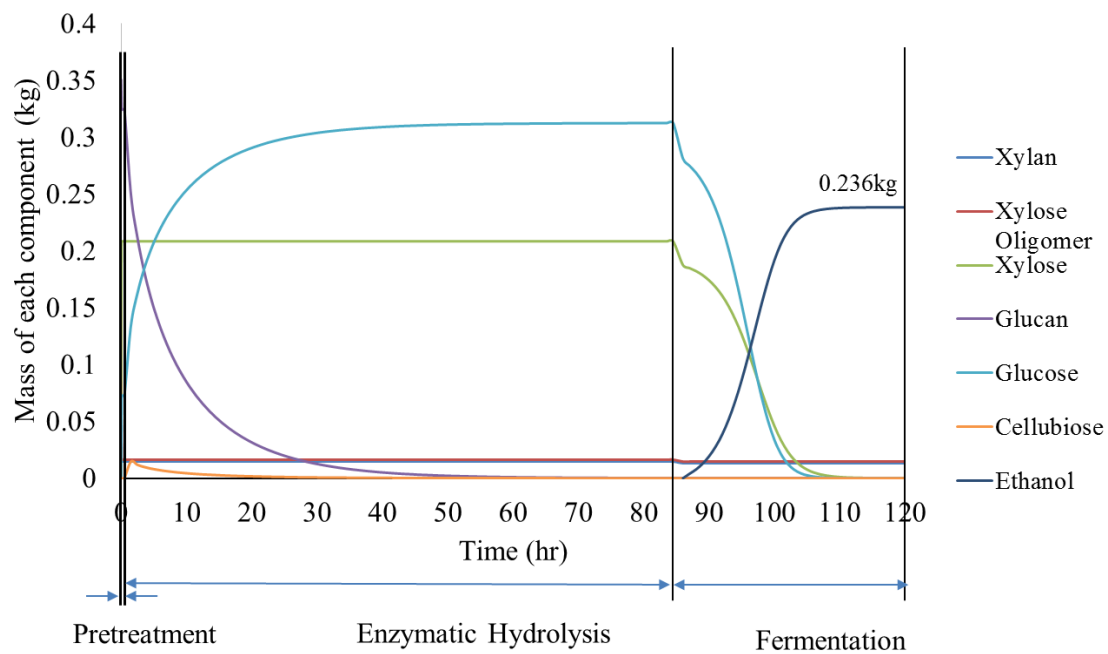


Figure 5. Mass evolutions of state variables with 1 kg feedstock converted to ethanol

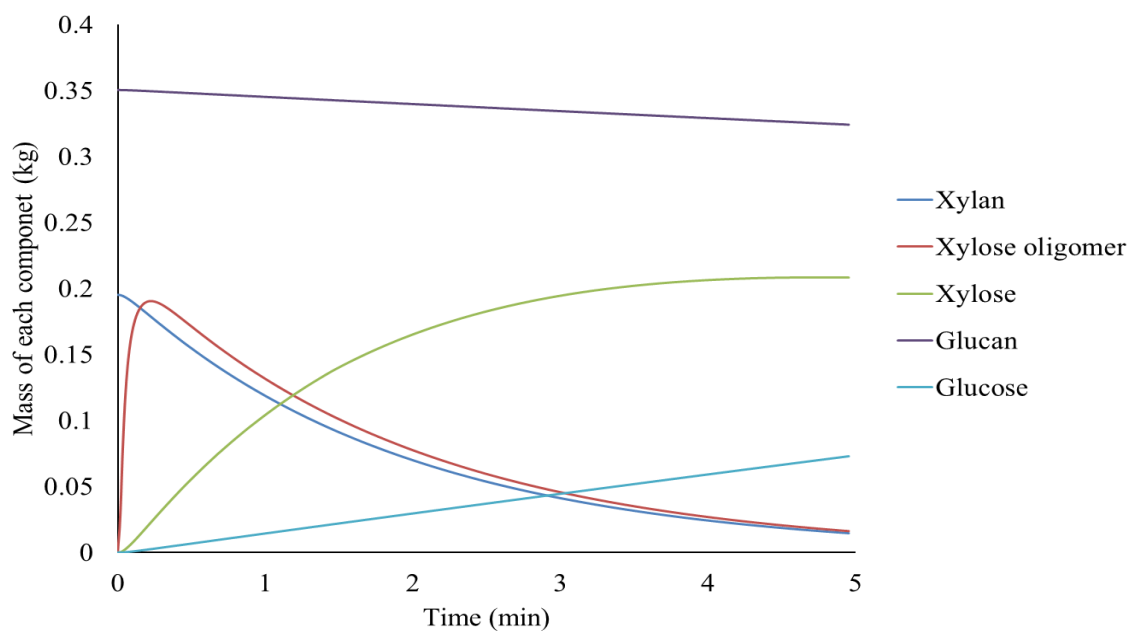


Figure 6. Mass evolutions of state variables component in pretreatment

The illustrations of the evolution of each reactant and product provide information such as the amount of reactant left, the real-time reaction rate for each reaction, the side-

product accumulation level, and the final product concentration, etc., under a set of decision variables values. By changing these values, the desired objectives can be achieved.

Figure 7 shows the cumulative energy consumption as a function of time. The results indicate that 4400 kJ of energy are consumed to convert 1 kg feedstock to ethanol with a production rate of 0.236 kg ethanol/ kg feedstock. The energy consumed by the manufacturing process is illustrated in Figure 8. Although the pretreatment process only lasts 5 minutes, it accounts for 48% of the total energy consumption due to its need for steam exposure and severe reaction conditions. Thus, the development of energy-efficient pretreatment techniques will greatly benefit the sustainability of cellulosic biofuel production. In addition, hydrolysis accounts for most proportion of the energy consumed by heat transfer. This is because the hydrolysis lasts for a comparatively long duration (84 hours) with a temperature (48°C) higher than room temperature.

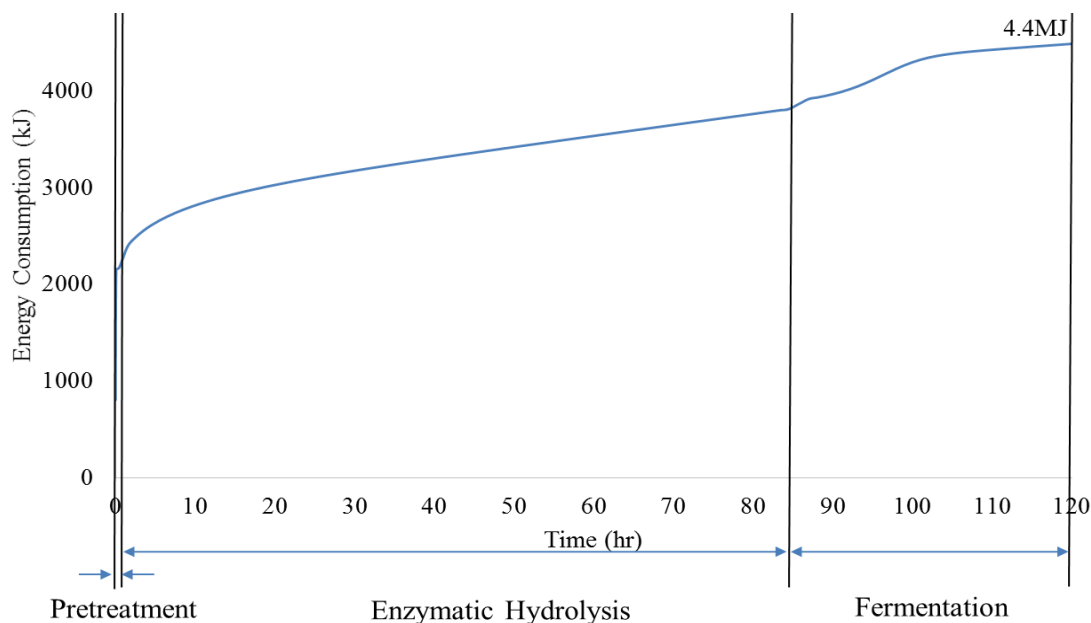


Figure 7. Accumulated energy consumption with 1 kg feedstock converted to ethanol

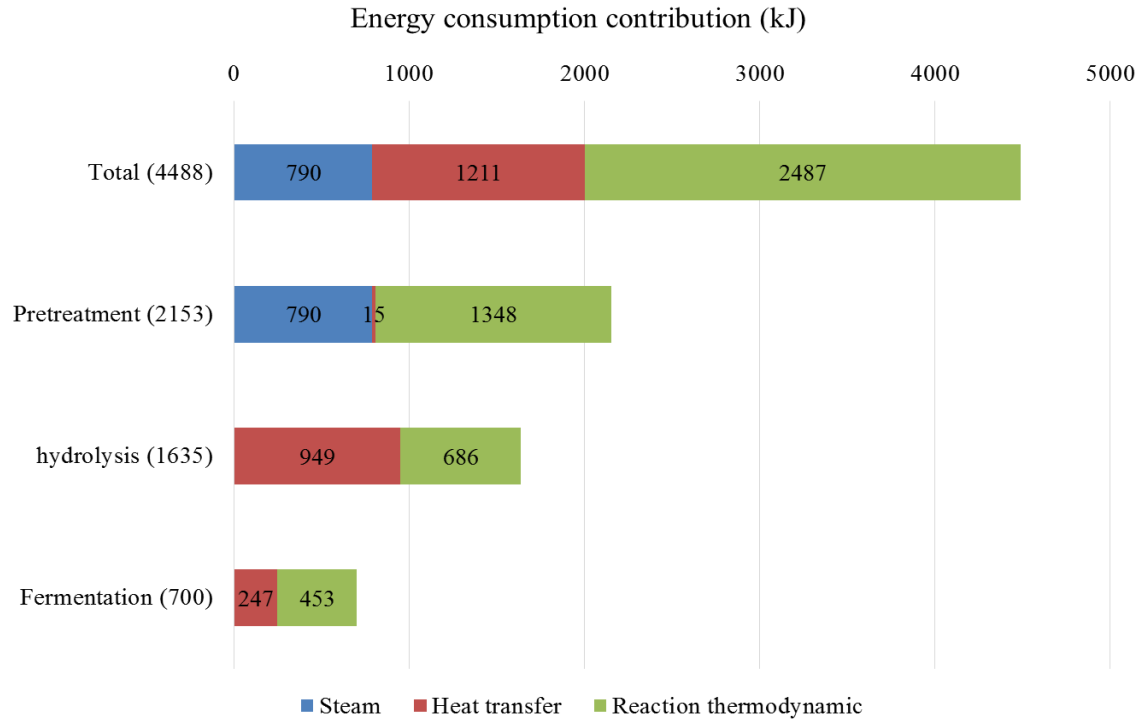


Figure 8. Energy consumption contribution from each process with 1 kg feedstock converted to ethanol

Figure 9 shows the detailed cost breakdown of converting 1 kg cellulosic feedstock to ethanol, where fixed cost includes labor cost, maintenance cost, and other miscellaneous costs. Meanwhile, TABLE VI summarizes the cost of converting 1 kg cellulosic feedstock to ethanol as found in literature (Aden et al. 2002b; Huang et al. 2009; Mcaloon et al. 2000; A. Aden and Foust 2009; Humbird et al. 2011). The results from the proposed model are at the same scale as the results from literature. It is observed that:

- (i) Overall, the largest portion of the total cost is feedstock, which accounts for 49% of overall cost. Enzyme is the second largest single cost component since it is assumed to have a complete enzyme production system including capital investment, raw material supply, utilities, labor, etc.
- (ii) It is worth noting that the cost of energy consumption is much less than other components, because of a very low electricity unit cost given in the proposed

model since most biofuel plants are designed to be able to self-supply electricity by burning biomass lignin residues onsite.

- (iii) Although it is assumed that enzyme is produced by an on-site enzyme plant (same as the baseline case in (Humbird et al., 2011a)) to reduce the cost of preservation and transportation, the cost of enzyme still accounts for approximately 25% of total cost to convert 1 kg feedstock to ethanol. The development of low-cost cellulose enzyme production method would greatly benefit the economic performance of cellulosic biofuel manufacturing.

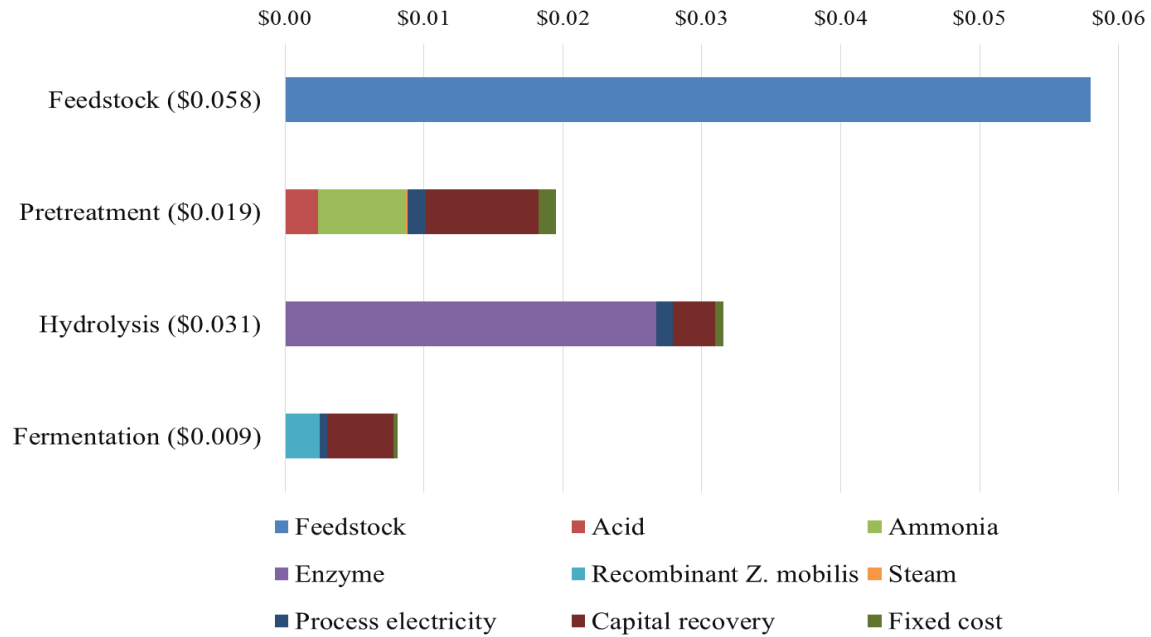


Figure 9. Cost breakdown from each manufacturing process

TABLE VI. COST OF CONVERTING 1 KG FEEDSTOCK TO ETHANOL (\$US)

Aden (Aden and Foust, 2009)	Huang (Huang et al., 2009)	Aden (Aden et al. 2002b)	McAloon (Mcaloon et al., 2000)	Humbird (Humbird et al., 2011a)	Average in literature	This study
0.130	0.109	0.132	0.105	0.122	0.120	0.117

^b These values have been adjusted to represent the cost only in manufacturing processes

2.5.3. Baseline Comparison

By adopting input decision variables in TABLE III, the baseline case obtained similar results related to the ethanol yield and total cost compared to (Humbird et al., 2011a). The ethanol yield of the baseline case is 0.4% higher and the cost is 3.9% lower than (Humbird et al., 2011a), which suggests that the proposed model is accurate and robust. Utilizing the established relationships among the characteristics of the different processes in the model, we can conduct cost-effective decision-making under the constraint of ethanol yield by adjusting the value of input decision variables. The objective function for systematic cost-effective optimization is:

$$\min(\sum C_i), \text{ subject to } Y \geq Y_b, \quad (28)$$

where Y_b is the ethanol yield in the baseline case.

TABLE VII shows the decision variables used in the cost-effective case. Instead of using fine grinded feedstock, the particles diameter in this case is raised to 25.4mm (1 mesh). Ten percent less enzyme is used to catalyze the hydrolysis of cellulose. To counterbalance the production loss that may be caused by these two changes, the initial acid concentration is elevated as well as the pretreatment temperature. The processing time of enzymatic hydrolysis is also extended to 90 hours to maintain the conversion rate of glucose.

TABLE VII. VALUES OF DECISION VARIABLES IN COST-EFFECTIVE CASE

Inter-process variables	Cost-effective case	Baseline case
Feedstock particle diameter: d	25.4mm in diameter	6.67mm in diameter
Initial input water volume: β	2.2 Liter	2.2 Liter
Intra-process variables		
Initial concentration of acid: C_0	1.2% w/w	1.0% w/w
Pretreatment temperature: T_p	162°C	158°C
Pretreatment time: t_p	5mins	5mins
Total enzyme loading: E_t	18mg/g feedstock	20mg/g feedstock
Enzymatic hydrolysis time: t_h	90hrs	84hrs
Enzymatic hydrolysis temperature: T_h	48°C	48°C
Fermentation temperature: T_f	32°C	32°C
Fermentation time: t_f	30hrs	36hrs

By adopting the current input decision variable combination, the ethanol yield is the same as baseline case. However, the cost drops down to \$0.102 for 1 kg feedstock converted to ethanol, which saves 12.8% of the total cost (as shown in Figure 10). These results demonstrate the effectiveness of the proposed model, as well as the establishment of the interrelationships between different processes. These relationships provide not only the information to conduct cost analysis, but also the opportunity to make decisions. The application of this model in industry will result in an effective decision making tool for parameter estimation, cost and yield prediction, production optimizations, etc.

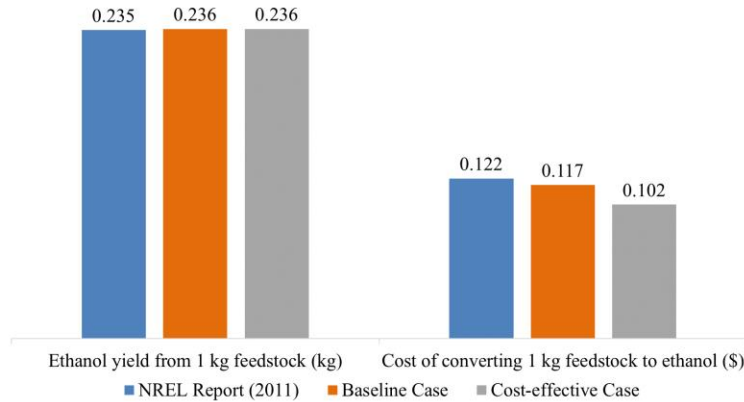


Figure 10. Cost and ethanol yield comparison

TABLE VIII summarizes the cost breakdown for both cases. The reasons for cost reduction in the cost-effective case are the expensive components are replaced with

economical alternatives, and the added costs due to the increasing usage of utility and acid are insignificant.

TABLE VIII. COMPARISON OF COST BREAKDOWN

Category	Cost-effective case		Baseline case	
	US\$/Feedstock	Share of total cost (%)	US\$/Feedstock	Share of total cost (%)
Raw Materials	0.0813	79.71	0.1014	83.11
Feedstock	0.0405	39.7	0.0560	45.90
Acid	0.0044	4.31	0.0041	3.36
Ammonia	0.0129	12.6	0.0127	10.41
Enzyme	0.0210	20.6	0.0261	21.39
Other materials	0.0025	2.45	0.0025	2.04
Utilities	0.0029	2.67	0.0026	2.13
Steam	0.00014	0.1	0.00012	0.1
Processing electricity	0.0028	2.74	0.0025	2.03
Capital recovery cost	0.0159	15.56	0.0159	13.03
Fixed cost	0.0021	2.06	0.0021	1.72
Total	0.102	100	0.122	100

2.6. Conclusions

In this chapter, a system-level cellulosic biofuel manufacturing model mapping the interrelationships between individual process characteristics and systematic performance is proposed. The interrelationships across multiple individual processes are illustrated by introducing inter-process and intra-process decision variables; subsequently the system output (i.e., ethanol yield, energy consumption and cost) are calculated from a systematic perspective. The cost-effective case shows that the total cost is significantly reduced by 12.8% compared with the baseline case without sacrificing ethanol yield. Given the systematic modeling methodology adopted in this study, the proposed model can further result in a cost-effective decision-making tool to improve the economic viability of multi-process cellulosic biofuel manufacturing.

CHAPTER 3. ENERGY EFFICIENCY MODELING AND OPTIMIZATION FOR CELLULOSIC BIOFUEL MANUFACTURING SYSTEM

(Parts of this chapter were previously published as: Ge Y., Li L., 2018, *System-level energy consumption modeling and optimization for cellulosic biofuel production. Appl Energy* 226: 935–46. <https://doi.org/10.1016/j.apenergy.2018.06.020>.)

3.1. Introduction

In this chapter, an analytical system-level energy model for the cellulosic biofuel production system is proposed by considering the interrelationships between each process. In addition, the energy consumption is optimized under the constraint of biofuel yield and solved using Particle Swarm Optimization (PSO) algorithm. The establishment of these relationships provides a powerful tool to theoretically predict, evaluate and optimize the energy consumption in cellulosic biofuel production, which will offer valuable guidance in system design and operation. Additionally, the presented optimization strategy enables manufacturers to determine the best production parameters and achieve significant energy savings without compromising biofuel yield.

The rest of this chapter is organized as follows. In Section 3.2, notations used in this chapter are introduced. In Section 3.3, a brief description of the four major processes in the biofuel production system is presented. The analytical model for the energy consumption and ethanol yield is proposed in Section 3.4. In Section 3.5, a comprehensive energy analysis is conducted, and the sensitivity analysis is performed by adjusting the baseline parameters. In Section 3.6, the optimization model is formulated and solved using

PSO approach, and the results from optimal solution is compared with the baseline case.

Finally, the conclusions and future research directions are discussed in Section 3.7.

3.2. Notations

Bold Face		$Q_{size\ reduction}$	Energy required in size reduction process (KJ)
S	Solution vector to the optimization problem	R	Gas constant
X	Particle position vector	R_1	Inner radius of the reactor (m)
V	Particle velocity vector	R_2	Outer radius of the reactor(m)
Upper Case		T_p	Pretreatment temperature (°C)
A	Pre-exponential factor (1/s)	T_h	Enzymatic hydrolysis temperature (°C)
A^p	Pretreatment reactor surface area (m ²)	T_f	Fermentation temperature (°C)
A^h	Hydrolysis reactor surface area (m ²)	Lower Case	
A^f	Fermentation reactor surface area (m ²)	a	Ratio of the liquid volume and solid spheres volume
C_{acid}	Active acid concentration (w/w%)	c_1	Learning factor
C_k	Kick's constant	c_2	Learning factor
C_{pw}	Specific heat capacity of water (KJ/mol/K)	C_e	Concentration of ethanol (kg/L)
C_{pb}	Specific heat capacity of biomass (KJ/mol/K)	C_g	Concentration of glucose (kg/L)
C_{pa}	Specific heat capacity of acid (KJ/mol/K)	C_{xl}	Concentration of xylose (kg/L)
D_e	Diffusion coefficient (m ² /s)	C_{xo}	Concentration of xylose oligomer (kg/L)
E_a	Activation energy (kJ/mol)	C_z	Concentration of recombinant (kg/L)
H_L	Latent heat of water vaporization (KJ/kg)	h_{out}	Convection coefficient (W/m ² /°C)
K_g	Inhibition constant of xylose (g/L)	m_a	Mass of diluted acid (kg)
K_{xl}	Inhibition constants of xylose (g/L)	m_b	Mass of biomass (kg)
L_1	Particle size before reduction (mm)	m_w	Mass of water (kg)
L_2	Particle size after reduction (mm)	k_{pipe}	Thermal conductivity of the reactor (W/m/°C)
M_g	Molecular weight of glucan (g/mol)	t_p	Pretreatment time (min)
M_{gl}	Molecular weight of glucose (g/mol)	t_f	Fermentation time (hour)
M_x	Molecular weight of xylan (g/mol)	t_h	Enzymatic hydrolysis time (hour)
M_{xl}	Molecular weight of xylose (g/mol)	k	Reaction rate (1/s)
M_{xo}	Molecular weight of xylose oligomer (g/mol)	$q_{emax,g}$	Maximum specific ethanol production rate by glucose (g/L)
N_p	Number of particles in the swarm	$q_{emax,x}$	Maximum specific ethanol production rate by xylose (g/L)
$P_{i,g}$	Threshold ethanol concentration of glucose (g/mol)	q_n	Reaction constant
$P_{i,x}$	Threshold ethanol concentration of xylose (g/mol)	$q_{smax,g}$	Maximum specific glucose utilization rate (g/L)
$P_{m,g}$	Maximum ethanol concentration of glucose (g/mol)	$q_{smax,x}$	Maximum specific xylose utilization rate (g/L)
$P_{m,x}$	Maximum ethanol concentration of xylose (g/mol)	p_g	Mass of glucan in feedstock (kg)
$Q_{heatloss}$	Energy to balance heat loss (KJ)	p_x	Mass of xylan in feedstock (kg)
$Q_{heating}$	Energy for heating (KJ)	Greek	
$Q_{reaction}$	Reaction energy (KJ)	ρ_w	Density of water (kg/m ³)
$Q_{recovery}$	Recovered energy (KJ)		

3.3. Process Description

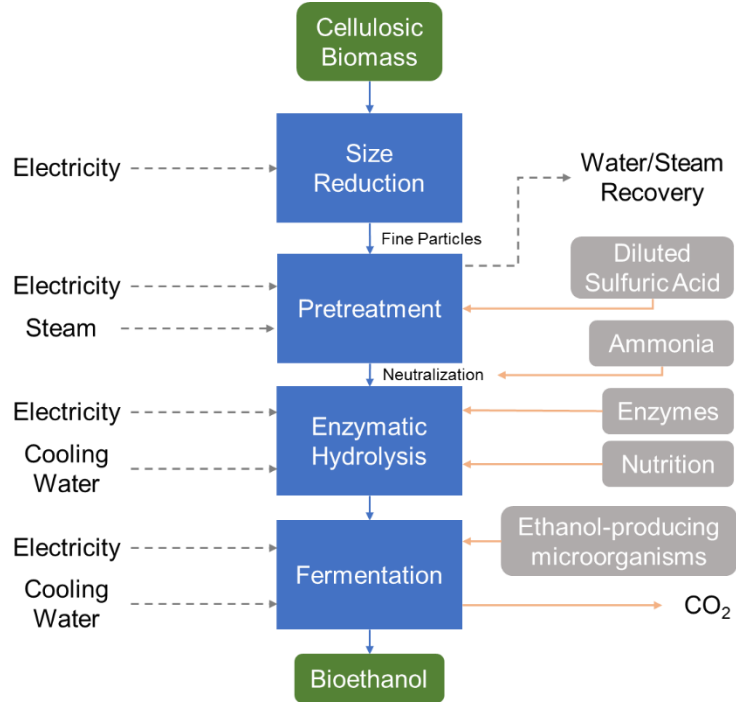


Figure 11. Block diagram of biofuel production from cellulosic biomass

The proposed energy model is based on the cellulosic biofuel production system shown in Figure 11. It consists of four major processes: size reduction, pretreatment, enzymatic hydrolysis, and fermentation. Note that in this study corn stover is used as the biomass feedstock. The solid composition of corn stover is shown in TABLE IX.

TABLE IX. SOLID COMPOSITION OF CORN STOVER (Humbird et al., 2011b)

Component	Dry weight percentage
Glucan	39.1%
Xylan	23.1%
Lignin	16.3%
Galactan	1.8%
Arabinan	3.4%
Mannan	0.3%
Acetyl	2.7%
Structural inorganics	4.8%
Protein	4.5%
Ash	4%

The biomass size reduction process usually involves grinding or cutting cellulosic feedstock into small pieces. The minced feedstock is screened by sieves with certain sizes. In this process, the biomass' contacting surface area increases greatly so that it can be hydrolyzed into soluble sugar at a fast rate. The main energy intensive activity at this stage comes from the size reduction machines' electricity consumption.

In the pretreatment process, it is assumed that the steam-assisted dilute-acid pretreatment method is adopted (Sitaraman et al., 2015). The cellulosic material is mixed with water and broken down under high-temperature ($\sim 158^{\circ}\text{C}$) and high-pressure (5 atm) reaction conditions. In the reaction, the crystallinity degree of cellulose is reduced, and the cellulose becomes more amorphous, which is the most suitable form for enzymatic attack. Most of the hemicellulose contained in the feedstock is converted into soluble pentoses (i.e., xylose) that can be utilized as substrates for fermentation. A small fraction of glucan degrades to glucose, while the majority of the glucan remains as solid residues. In this process, energy is mainly consumed by heating the feedstock-water mixture and maintaining the reaction temperature. The heat in the water/steam can be partially recovered while cooling.

In the hydrolysis process, the cellulose chains are broken down to produce glucose for fermentation. Enzymatic hydrolysis is current the most recognized technique for bioethanol hydrolysis because no degradation products of glucose are formed, although the process is rather slow (Kadam et al., 2004). After the hydrolysis process, most of the cellulosic content (hemicellulose and cellulose) is converted into fermentable sugars. Energy is consumed to cool down the hydrolysis reactor since this reaction is exothermic.

In the fermentation process, all soluble sugars (mainly xylose and glucose) are assumed to be simultaneously fermented into ethanol using recombinant *Zymomonas mobilis* strain ZM4 (pZB5) (*Z. mobilis* ZM4 (pZB5)) (Jeon et al., 2002). Meanwhile, energy is supplied to maintain the reaction temperature.

3.4. Energy Consumption Modeling

In this section, the mathematical model for the energy consumption is developed considering the biomass size reduction process (in Section 3.4.1) and biofuel chemical conversion processes (in Section 3.4.2).

3.4.1. Energy Modeling of Biomass Size Reduction Process

Generally, energy required in the grinding process can be described by three empirical equations, namely, Rittinger's law, Kick's law, and Bond's law. According to (Tanaka, 1966), Rittinger's law and Bond's law are often used for smaller particles (< 1 cm), while Kick's law can be used to model the energy consumption of grinding particles larger than 1 cm, which is within the size range of raw biomass feedstock particles. Therefore, in this research, the Kick's law is adopted to calculate the energy consumption in the size reduction process.

Based on Kick's law, it is assumed that the energy required to reduce a material in size is directly proportional to the size reduction ratio dL/L :

$$\frac{dQ_{\text{size reduction}}}{dL} = C_k \cdot L^{-1}. \quad (29)$$

Performing integration for both side of the equal sign, we have:

$$Q_{\text{size reduction}} = C_k \cdot \ln \left(\frac{L_1}{L_2} \right) \quad (30)$$

where $Q_{\text{size reduction}}$ is the energy required in this process; C_k is the Kick's constant; L_1 is the particle size before reduction; and L_2 is the particle size after reduction. Particle size is

defined as the screen size that the particles can pass through regardless of the particles' shape.

Kick's constant is an experimental constant which depends on the biomass type and grinding machines' properties. In (Bitra et al., 2009), the researchers measured the energy consumption of grinding switchgrass, wheat straw, and corn stover, where the data of corn stover is used to calculate C_k . In (Bitra et al., 2009), the corn stover used is 150 mm, and it consumes 0.02 kWh when grinded into 25.4 mm at 500 rpm rotor speed and 5 kg/min feeding rate, thus the Kick's constant can be calculated as:

$$C_k = Q_{\text{size reduction}} / \ln \left(\frac{L_1}{L_2} \right) = 72(\text{KJ/kg}) / \ln(150/25.4) = 40.55.$$

In this work, the corn stover and grinding machine properties are assumed to be the same as (Bitra et al., 2009). Hence the Kick's constant C_k of 40.55 is used for the following energy calculations.

3.4.2. Energy Modeling of Biofuel Chemical Conversion Processes

In this section, the energy modeling of the three biochemical processes, i.e., pretreatment, enzymatic hydrolysis, and fermentation is presented. Energy in these processes is mainly supplied to heat the reactants and maintain desired reaction temperature. Moreover, in the cooling stages, energy is also partially recovered.

In Figure 12, the reaction temperature profile during the pretreatment, enzymatic hydrolysis, and fermentation processes is illustrated. The timeline is slotted into 8 stages according to the temperature changes. In the heating stage (i.e., stage H), biomass is mixed with water at room temperature (25°C), and the mixture is heated up to attain the desired reaction temperature of T_p (>155°C). Energy is supplied to maintain this temperature in stage M₁, during which the oligomers are formed. Then, the heat is released in stage C₁ to

cool the contents down to 130 °C. The reactor is kept at 130 °C for about 25 minutes in stage M₂ to allow the conversion of oligomers to monomers. In stage C₂, the energy continues to be released and the products are cooled down to T_h . Stage M₃ represents the enzymatic hydrolysis process with a residence time of t_h ($t_h \approx 84$ hours), during which energy is supplied to maintain the temperature of T_h to ensure the efficiency of the cellulase enzyme. After enzymatic hydrolysis, the saccharified slurry is cooled to T_f for fermentation. Energy is supplied for t_f ($t_f \approx 36$ hours) fermentation to ensure the ethanol yield from the strain of *Z. mobilis*.

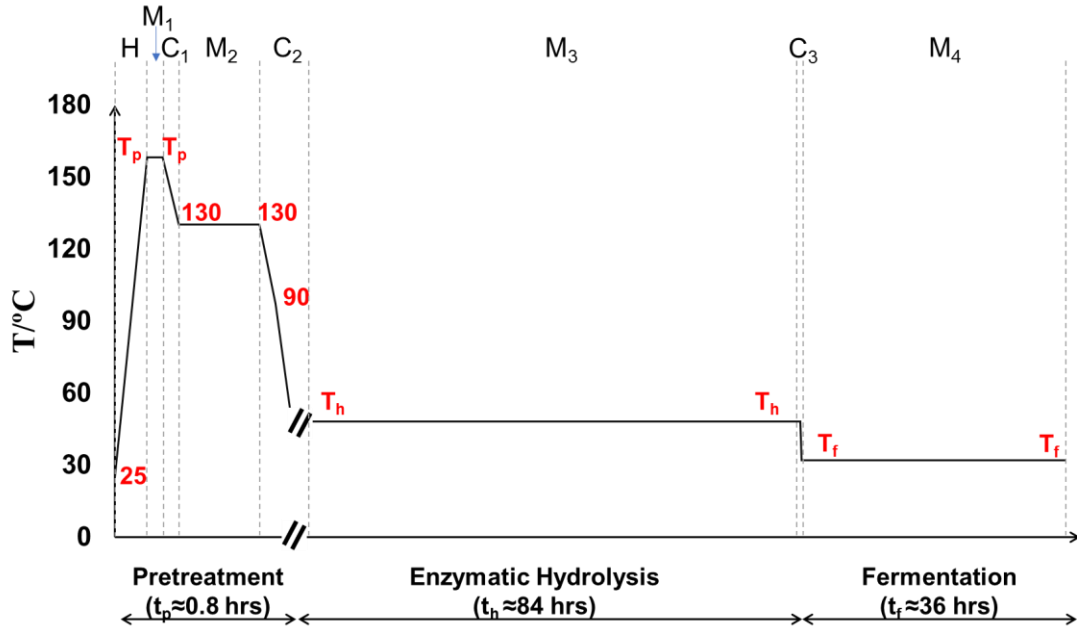


Figure 12. Reaction temperature profile during pretreatment, enzymatic hydrolysis and fermentation process

3.4.2.1. Heating Energy

In stage H, energy is supplied to heat up the biomass, water (steam), and sulfuric acid mixture. The generic equation of the heating energy is:

$$Q_{heating} = m_w \int_{25}^{T_p} C_{p_w} dT + m_b \int_{25}^{T_p} C_{p_b} dT + m_a C_{p_a} (T_p - 25) \quad (31)$$

where m_w , m_b and m_a are the mass of water, biomass, and diluted acid, respectively; C_{pw} and C_{pb} are the specific heat capacity of water and biomass, respectively; C_{pa} is the average specific heat capacity of diluted sulfuric acid; and T_p represents the pretreatment temperature.

To calculate the energy required for heating the water from 25°C to T_p , it is determined that at a pressure of 557 kPa (5.5 atm), water boils at 155°C. The latent heat of water vaporization (H_L) at 155°C is adopted. It is assumed 5% of the water evaporates at this temperature, which further results in 95% of water being heated from 155°C to T_p . According to (Poling et al., 2007), we can formulate the water and steam heat capacity expressions as:

$$C_{pw} = 0.00001T^2 - 0.0013T + 4.2085 \quad (32)$$

$$C_{ps} = 0.0000008T^2 + 0.0002T + 1.8572. \quad (33)$$

In addition, we obtain the specific heat capacity of biomass from (Mafe et al., 2015) as:

$$C_{pb} = 0.00004T^2 - 0.0015T + 0.9325. \quad (34)$$

Consequently, the expression of heating energy is:

$$\begin{aligned} Q_{\text{heating}} = & m_w \int_{25}^{155} (0.00001T^2 - 0.0013T + 4.2085)dT + 0.05m_w H_L \\ & + 0.95m_w \int_{155}^{T_p} (0.00001T^2 - 0.0013T + 4.2085)dT \\ & + 0.05m_w \int_{155}^{T_p} (0.0000008T^2 + 0.0002T + 1.8572)dT \\ & + m_b \int_{25}^{T_p} (0.00004T^2 - 0.0015T + 0.9325)dT + m_a \overline{C_{pa}} (T_p - 25). \end{aligned} \quad (35)$$

3.4.2.2. Energy Loss

Since the reaction temperatures during all the stages (as shown in Figure 12) are higher than the room temperature (i.e., 25°C), heat escapes from reactors to the ambient

via conduction and convection. In this study, the reactors are assumed to be of a cylindrical nature (Humbird et al., 2011b) and as a result, the amount of heat lost during the all processes is formulated as the heat loss of a pipe:

$$Q_{lost} = UA\Delta T \cdot t \quad (36)$$

where A is the surface area of reactor; ΔT represents the temperature difference between the inner side of the reactor and the room temperature; and t is the duration time. In addition, the overall heat transfer coefficient, U , is defined as:

$$U = 1/[(R_2 \ln(R_2/R_1)/k_{pipe}) + 1/h_{out}] \quad (37)$$

where R_1 and R_2 represent the inner and outer radius of the reactor, respectively; k_{pipe} is the thermal conductivity of the reactor; and h_{out} is the convection coefficient at the outside surface.

Since the heating stage residence time is quite short, the temperature rising of the reactor is assumed to be linear. Therefore, the total energy required to offset energy loss and maintain the reaction temperature is:

$$Q_{heatloss} = U^p A^p \int_0^{t_H} t \cdot \left(\frac{T_p - 25}{t_H}\right) dt + \left(\sum_1^2 U^p A^p \Delta T^{M_i}\right) \cdot t_{M_i} + U^h A^h \Delta T^{M_3} \cdot t_h + U^f A^f \Delta T^{M_4} \cdot t_f \quad (38)$$

where the superscript/subscript p , h , and f represent the pretreatment, hydrolysis, and fermentation processes, respectively; t_H is the residence time of the heating stage; and M_i ($i=1, 2, 3, 4$) represents the stages M_1 to M_4 .

3.4.2.3. Reaction Energy

The reaction energy model established in this work is based on the net energy balance for a closed system: the change in the internal energy is equal to the amount of

heat supplied to the system, minus the amount of work done by the system on its surroundings. Since all the reactions are taken place in isochoric reactors, the work done by the system is zero. Therefore, the energy absorbed/released due to the reactions is equal to the change of internal energy, which is measured by the internal energy variations between the input materials and output materials in each process. Consequently, the mass of the products in each process needs to be calculated.

Chemical reactions of cellulosic biofuel production

TABLE X lists nine major chemical reactions of cellulosic biofuel production. Arabinan, mannan, and galactan are assumed to have the same reactions and conversion pathways as xylan. Heat of formation represents the energy required/released for 1 kg reactant converting to product. The positive values mean that the reaction is endothermic while negative values indicate exothermic reactions.

TABLE X REACTIONS IN CELLULOSIC BIOFUEL PRODUCTION

Process	Reaction	Reactant	Heats of Formation (KJ/kg) ^a
Pretreatment	#1: (Xylan) _n + n H ₂ O → n Xylose	Xylan	248.8
	#2: (Xylan) _n + m H ₂ O → m Xylose Oligomer	Xylan	1903.2
	#3: (Glucan) _n + n H ₂ O → n Glucose	Glucan	279.1
	#4: (Arabinan) _n + n H ₂ O → n Arabinose	Arabinan	2102.2
	#5: (Mannan) _n + nH ₂ O → Mannose	Mannan	2941.5
	#6: (Galactan) _n + nH ₂ O → nGalactose	Galactan	2941.5
Enzymatic Hydrolysis	#7: (Glucan) _n + n H ₂ O → n Glucose	Glucan	-1463.1
Fermentation	#8: Glucose → 2 Ethanol + 2 CO ₂	Glucose	-1836.9
	#9: 3 Xylose → 5 Ethanol + 5 CO ₂	Xylose	-1610.3

^a Calculated based on the data in (Humbird et al., 2011b). Original data is in the unit of cal/mol.

Catalyzed by diluted acid, the xylan is converted to xylose and xylose oligomer, which finally is converted to xylose:

$$\begin{aligned}
\frac{dp_x}{dt} &= -(k_{xo} + k_{xl})p_x \cdot C_{acid} \\
\frac{dc_{xo}}{dt} &= k_{xo} \cdot \left(\frac{p_x}{M_x}\right)\left(\frac{M_x}{M_{xo}}\right) \cdot C_{acid} \cdot \frac{1}{(m_w/\rho_w)} - k_{x2} \cdot c_{xo} \cdot C_{acid} \\
\frac{dc_{xl}}{dt} &= k_{xl} \cdot \left(\frac{p_x}{M_x}\right)\left(\frac{M_x}{M_{xl}}\right) \cdot C_{acid} \cdot \frac{1}{(m_w/\rho_w)} + k_{x2} \cdot c_{xo} \cdot \left(\frac{M_{xo}}{M_{xl}}\right) \\
&\quad \cdot C_{acid}
\end{aligned} \quad t \in [0, t_{M_1}] \quad (39)$$

where p_x , c_{xo} , and c_{xl} represent xylan mass fraction in biomass, xylose-oligomers concentration and xylose concentration, respectively; k_{xo} and k_{xl} are the reaction rates of the conversion from xylan to xylose-oligomers and xylan to xylose, respectively. The reaction rates are assumed to have an Arrhenius dependence on temperature:

$$k = A \cdot e^{-E_a/RT}. \quad (40)$$

The acid concentration C_{acid} is represented by the concentration of acid which has infiltrated feedstock particle. The diffusion into a spherical particle is described by the following partial differential equation:

$$\frac{\partial C}{\partial t} = D_e \left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r} \frac{\partial C}{\partial r} \right). \quad (41)$$

The analytical solution of this problem is given by Crank (Crank, 1975):

$$\begin{aligned}
C_{acid}(t) &= c_0 \cdot [1 - f(t)], \\
f(t) &= 1 - \sum_{n=1}^{\infty} \left(\frac{6a(1+a)}{9+9a+q_n^2 a} \right) \exp\left(-\frac{q_n^2 D_e t}{(d/2)^2}\right)
\end{aligned} \quad (42)$$

where $C_{acid}(t)$ denotes the active acid concentration at time t ; and $a = 3 \times (m_w/\rho_w)/[4\pi(L_2/2)^3]$ is the ratio of the liquid volume and solid spheres volume; q_n is a reaction constant; and D_e is the diffusion coefficient.

In pretreatment, a fraction of glucan is converted into glucose:

$$\begin{aligned}
\frac{dp_g}{dt} &= -k_g \cdot p_g \cdot C_{acid}, \\
\frac{dc_g}{dt} &= k_g \cdot \left(\frac{p_g}{M_g}\right) \left(\frac{M_g}{M_{gl}}\right) \cdot C_{acid} \cdot \frac{1}{(m_w/\rho_w)}
\end{aligned}
\quad t \in [0, t_{M_1}] \quad (43)$$

where p_g and c_g represent glucan mass fraction in biomass and glucose concentration, respectively.

In the enzymatic hydrolysis process, a substrate inhibition model is adopted to simulate the glucose formation:

$$\begin{aligned}
\frac{dp_g}{dt} &= -\frac{k_h \cdot E_b \cdot p_g}{1 + \left(\frac{c_g}{K_g}\right) + \left(\frac{c_{xl}}{K_{xl}}\right)} \\
\frac{dc_g}{dt} &= 1.111 \times \frac{k_h \cdot E_b \cdot p_g \cdot \left(\frac{1}{(m_w/\rho_w)}\right)}{1 + \left(\frac{c_g}{K_g}\right) + \left(\frac{c_{xl}}{K_{xl}}\right)}
\end{aligned}
\quad t \in [0, t_h] \quad (44)$$

where E_b is the enzyme loading; K_g and K_{xl} represent the substrate inhibition coefficient of glucose and xylose, respectively.

In the fermentation process, the xylose and glucose generated from pretreatment and enzymatic hydrolysis are finally converted into ethanol. We simplified the model developed in (Leksawasdi et al., 2001), which based on substrate inhibition and product inhibition, and implement it to calculate the ethanol yield.

$$\begin{aligned}
\frac{dc_{xl}}{dt} &= -(1 - \alpha) \frac{q_{s \max, x}}{m_w} \left(1 - \frac{c_e - P_{i, x}}{P_{m, x} - P_{i, x}}\right) \left(\frac{K_{i, x}}{K_{i, x} + c_{xl}}\right) \cdot c_z \\
\frac{dc_g}{dt} &= -\alpha \cdot \frac{q_{s \max, g}}{m_w} \cdot \left(1 - \frac{c_e - P_{i, g}}{P_{m, g} - P_{i, g}}\right) \left(\frac{K_{i, g}}{K_{i, g} + c_g}\right) \cdot c_z \quad t \in [0, t_f] \quad (45) \\
\frac{dc_e}{dt} &= -\left(\frac{q_{e \max, x}}{q_{s \max, x}} \cdot \frac{dc_{xl}}{dt} + \frac{q_{e \max, g}}{q_{s \max, g}} \cdot \frac{dc_g}{dt}\right)
\end{aligned}$$

where c_e is the concentration of ethanol; c_z is the concentration of ethanol production microbial; $q_{s \max}$ is the maximum substrate uptake rate; $q_{e \max}$ is the maximum ethanol production rate; P_i is the production inhibition coefficient; P_m is the maximum production inhibition coefficient; and K_i is the substrate inhibition coefficient.

Reaction heat modeling

The total reaction energy is calculated by the sum of internal energy changes in all processes. The internal energy change is determined by the conversion rate of the reactant multiply with the heat of formation of corresponding reactions:

$$Q_{\text{reaction}} = \Delta Q_{i,p} + \Delta Q_{i,h} + \Delta Q_{i,f} = \sum_1^9 CR_i \cdot HoF_i = \sum_1^9 \left(\frac{R_i^0 - R_i^E}{R_i^0}\right) \cdot HoF_i \quad (46)$$

where R_i^0 and R_i^E are the mass of the reactant at the beginning and end of the 9 reactions from TABLE X, respectively; and HoF_i represents the heat of formation of the corresponding reaction.

3.4.2.4. Energy Recovery

In this model. We consider the energy that potentially could be recovered in Stages C₁ and C₂ (Figure 12) by calculating the enthalpy changes of the water and biomass at each stage:

$$Q_{\text{Recovery}} = \sum_{c_1, c_2} m_{b, \text{remain}} \int_{T_1}^{T_2} (0.00004T^2 - 0.0015T + 0.9325) dT \quad (47)$$

$$+ m_w \int_{T_1}^{T_2} (0.00001T^2 - 0.0013T + 4.2085) dT.$$

In summary, the total energy required to produce ethanol from size reduction process to the end of fermentation can be expressed as a linear combination of all energy components:

$$Q_{\text{total}} = Q_{\text{size reduction}} + Q_{\text{heating}} + Q_{\text{heatloss}} + Q_{\text{reaction}} - Q_{\text{recovery}}. \quad (48)$$

3.5. Energy Analysis of Baseline Case

3.5.1. Parameter Preparation

The values of input decision variables (as listed in TABLE XI) are selected from a cellulosic biofuel production design reported by NREL (Humbird et al., 2011b) as the baseline case setup. Input feedstock is assumed as 1 kg for all following analysis. For the purpose of model calculation, the energy related parameters and chemical reaction parameters are listed in

TABLE XII and TABLE XIII, respectively.

TABLE XI. BASELINE CASE DECISION VARIABLES

Decision variables	Values
Feedstock particle diameter: L_2	6.67mm (4 mesh)
Water loading (per kg feedstock): m_w	2.2 kg
Diluted acid loading: C_{acid}	1.0% w/w
Pretreatment temperature: T_p	158°C
Pretreatment time: t_p	5min
Enzymatic hydrolysis temperature: T_h	48°C
Enzymatic hydrolysis time: t_h	84hrs
Fermentation temperature: T_f	32°C
Fermentation time: t_f	36hrs

TABLE XII. ENERGY RELATED PARAMETERS

Parameter	Values (Humbird et al., 2011b; Poling et al., 2007)
C_k	40.55
C_{pa}	101.2 KJ/mol/K
H_L	2257 KJ/kg
R_1	1.3 m
R_2	1.315
k_{pipe}	13.8 W/m/°C
h_{out}	45 W/m ² /°C
A^p	47.78 m ²
A^h	250 m ²
A^f	200 m ²
R	8.314 ^a

^a Obtained from common knowledge

TABLE XIII. REACTION RELATED PARAMETERS

Arrhenius reaction rate parameters (Esteghlalian et al., 1997; Kadam et al., 2004; Wolfrum and Sluiter, 2009)			Overall substrate utilization rate (g/L) (Leksawasdi et al., 2001)	
Reaction rate	A (1/s)	E _a (kJ/mol)		
k_{xo}	1.0×10^{15}	110.0	$q_{emax,g}$	10.9
k_{x1}	8.0×10^{17}	130.0	$q_{emax,x}$	3.27
k_g	2.0×10^{22}	180.0	$q_{smax,g}$	5.12
k_{h2}	2.0×10^7	5570	$q_{smax,x}$	1.59
Molecular weights (g/mol) (Humbird et al., 2011b)			Substrates inhibitory concentration (g/L) (Leksawasdi et al., 2001)	
M_x	132		$K_{i,x}$	186
M_{xo}	450		$K_{i,g}$	600
M_{xl}	150		$K_{i,x}$	186
M_g	162		$K_{i,x}$	600
M_{gl}	180		Threshold ethanol concentration (g/L) (Leksawasdi et al., 2001)	
Inhibition constant (g/L) (Zhang and Lynd, 2004)			$P_{i,g}$	57.4
K_g	0.1		$P_{i,x}$	81.2
K_{xl}	0.1		$P_{m,g}$	57.4
			$P_{m,x}$	81.2
Other parameters				
ρ_w	1 kg/m ³		q_n	0.213 [28]
D_e	0.68×10^{-10} m ² /s (Poling et al., 2007)			

3.5.2. Energy Consumption Breakdown

In the baseline case, the total energy consumption is 2470.57 KJ, and the ethanol yield from 1 kg feedstock is 0.241 kg. The energy breakdown for each process is shown in Figure 13. It can be observed that the pretreatment process contributes nearly half of the total energy consumption, although its residence time is much shorter compared to hydrolysis and fermentation. The main reason for such high energy consumption in the pretreatment process is the high-temperature reaction condition. Hence, it is expected that the development of energy-efficient pretreatment techniques will greatly benefit the sustainability of cellulosic biofuel production.

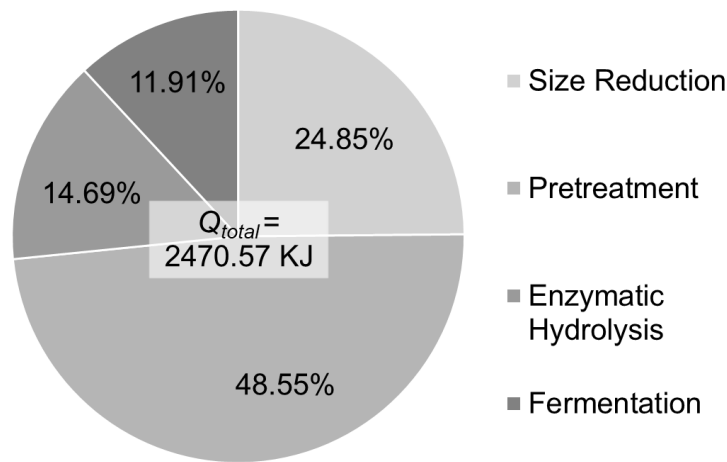


Figure 13. Total energy consumption breakdown

Figure 14 illustrates the energy input to and output from the production system in each process. The values on right side of the y-axis are the energy supplied to the system, while the left side represents the energy released from the system. It is observed that the electric energy is provided to the grinding machines in the size reduction process. In pretreatment process, energy is supplied for heating and maintaining reaction temperatures; and the energy contained in heated steam and water is released for heat recovery. It is worth noting that, in enzymatic hydrolysis and fermentation processes, more energy is released

by reactions than the energy input to balance the heat loss. Therefore, cooling energy should be provided to these two processes to keep desired temperatures. In practice, hydrolysis and fermentation reactions are cooled by circling cooling water.

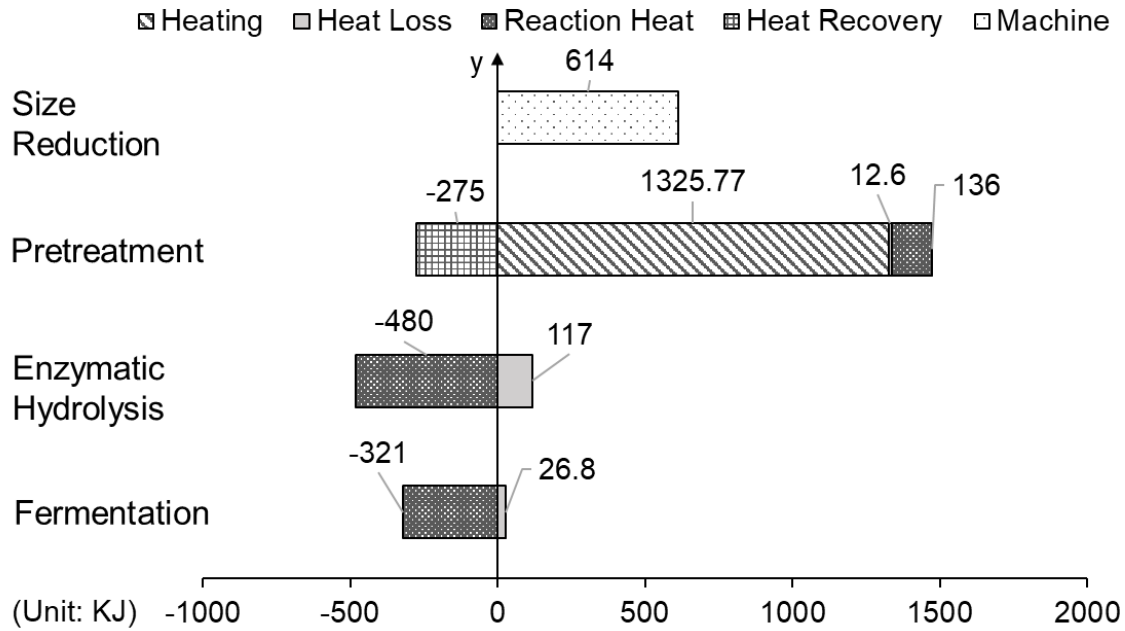


Figure 14. Energy usage in each process from different sources

It is also observed in Figure 14 that 275 KJ of energy is recovered in the pretreatment process, which can lead to more than 10% of total energy saving. In a commercial-scale biofuel production plant, energy efficiency could be significantly improved by adopting advanced heat recovery system. In addition, the energy consumed in the pretreatment process is 1474.4 KJ, 88% of which is contributed by heating.

The heating energy breakdown is shown in Figure 15, where the energy for heating water and steam is accounted for more than 90%. Note that in this study, it is assumed that the biomass loading is a constant (1 kg), which makes the heating energy for biomass is unchanged. In addition, the specific heat capacity of water is much larger than biomass, therefore, the water/biomass mass ratio becomes a main energy driver in this process.

Further discussions on the impact of water/biomass ratio to the production system will be presented in Section 3.5.3.

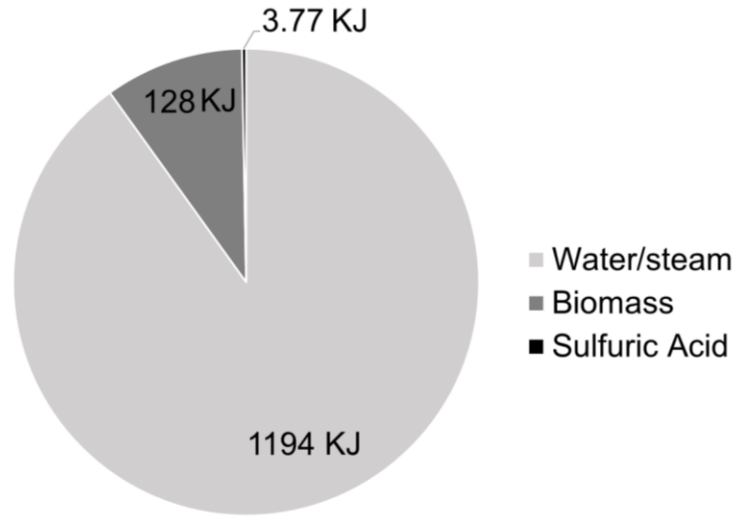


Figure 15. Heating energy breakdown

3.5.3. Sensitivity Analysis

The nine decision variables considered for sensitivity analysis are shown in TABLE XIV. Their reasonable ranges are selected based on estimations of the most probable ranges obtained from literature. Both total energy consumption and final ethanol yield are analyzed.

TABLE XIV. DATA OF BIOFUEL PRODUCTION ENERGY SENSITIVITY ANALYSIS

Decision variables	Baseline setup	Range	Increment
Feedstock particle diameter: L_2	6.67 mm	2.54 – 25.4 mm	2.54 mm
Water loading (per kg feedstock): m_w	2.2 kg	1.5 - 3 kg	0.15 kg
Diluted acid loading: C_{acid}	2.0% w/w	1% - 3% w/w	0.1% w/w
Pretreatment temperature: T_p	158 °C	150 – 170 °C	2 °C
Pretreatment time: t_p	5 min	4 – 6 minutes	0.2 minute
Enzymatic hydrolysis temperature: T_h	48 °C	44°C - 52°C	1 °C
Enzymatic hydrolysis time: t_h	84 hours	72 – 96 hours	2 hours
Fermentation temperature: T_f	32 °C	28 – 36 °C	1 °C
Fermentation time: t_f	36 hours	30 – 42 hours	1 hours

In Figure 16, it can be observed that the total energy consumption and biofuel yield has a positive correlation for most decision variables, while their relation tends to be more

complex as feedstock particle size, water/biomass ratio, and pretreatment temperature are the arguments. The water/biomass ratio is most sensitive variable to total energy consumption followed by the pretreatment temperature; while acid loading and fermentation time have the least impact on total energy consumption.

The water/biomass ratio has the most significant impact on total energy consumption. When water loading increases from 2 to 3 kg per kg feedstock, the production system consumes additional 25% energy, while the ethanol yield is decreasing. This indicates that a pretreatment reactor that can accommodate high solids loading will lead to the reduction of water usage and thus the energy consumed. However, in practice, high solid loading rate requires larger power of agitator and pumping machines, and sometimes is not necessarily pumpable. In addition, the ethanol yield reaches the maximum when the water/biomass ratio equals to 2, yet the yield is low when the ratio is at extreme values of its range.

In the case of feedstock size and pretreatment temperature, the total energy consumption shows non-monotonicity. The energy consumption reaches the maximum at feedstock size equals to 4 mesh. This may be because that it consumes more energy to produce smaller feedstock particle size, which however, requires less energy in later biochemical conversions. Similarly, low pretreatment temperature will cause more energy consumption in the following processes and less energy recovery; however, high pretreatment temperature will cause substantial energy demand to increase in the heating stage. Therefore, in Figure 16 (d), the lowest total energy consumption is achieved when the pretreatment temperature is at 166°C.

Moreover, it is also observed that the effects of pretreatment time, enzymatic hydrolysis time, fermentation temperature and fermentation time on total energy consumed are near-linear, and the change of fermentation time has almost no impact on total energy consumption.

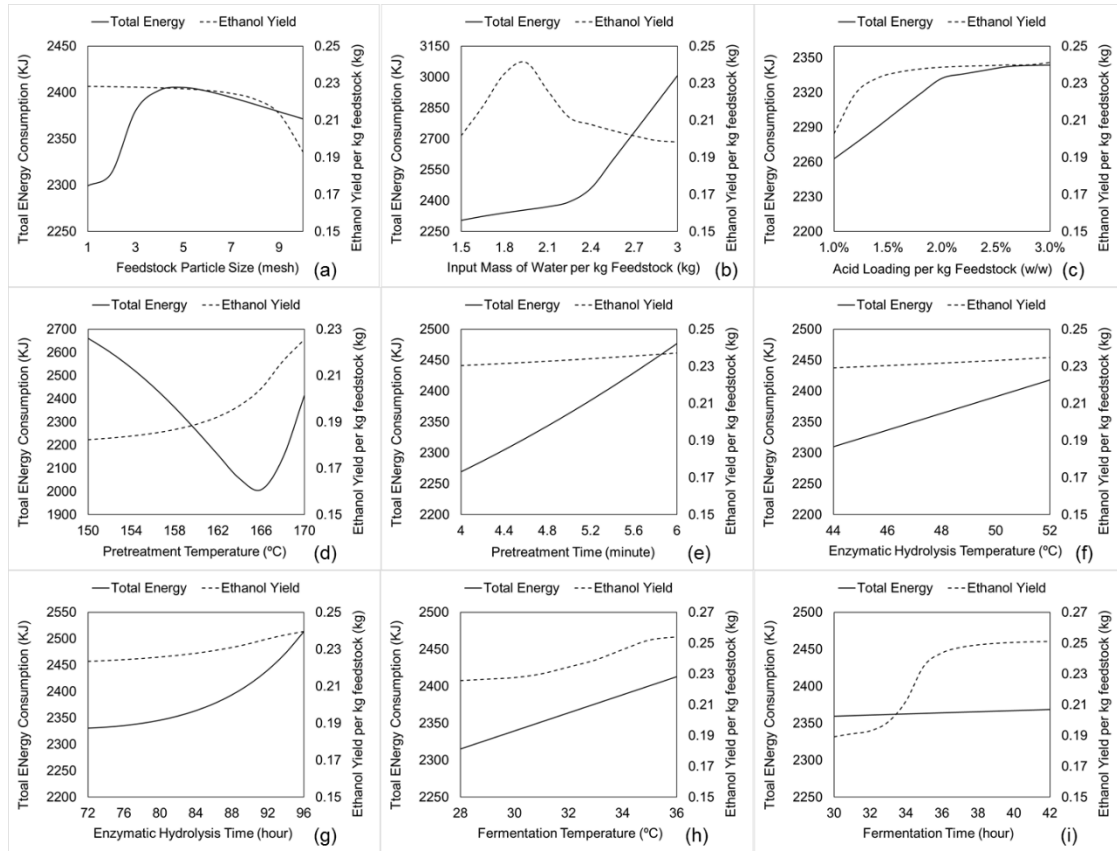


Figure 16. Effects of (a) feedstock particle size, (b) water loading, (c) acid loading, (d) pretreatment temperature, (e) pretreatment time, (f) enzymatic hydrolysis temperature, (g) enzymatic hydrolysis time, (h) fermentation temperature and (i) fermentation time on total energy consumption and ethanol yield.

3.6. Energy Consumption Optimization Using PSO

PSO is a metaheuristic technique for solving optimization problems, and it is originally proposed based on social-psychological principles to simulate the movement behavior of swarms such as bird flocks. Such swarms exhibit a property called swarm intelligence so that the complex behaviors of a big system can be accomplished efficiently

by the combination of a group of subsystems (population) with simple individual behaviors (Kennedy et al., 2001).

In the research, the energy consumption optimization problem is formulated as minimizing the total energy under the constraint of ethanol yield. The decision variables are selected to be the nine variables shown in TABLE XI. The nature of the biofuel production system energy consumption problem makes PSO an ideal approach because it is developed to solve problems with high complexity and non-linearity in high dimensional space.

3.6.1. Problem Formulation

Let $\mathbf{S} = [L_2 \quad m_w \quad C_{acid} \quad T_p \quad t_p \quad T_h \quad t_h \quad T_f \quad t_f]$ be a potential solution that contains all the decision variables of the biofuel energy consumption problem. Based on the developed model, the optimization problem can be formulated as searching the variable values of $\mathbf{S}$ to minimize Q_{total} (Eq. (48)) while maintaining the desired ethanol yield. Let the final ethanol yield in baseline case (0.2411kg ethanol/kg feedstock) be the minimum value for the optimization solution, then the problem can be formulated by Eq. (49)-(59), where Eq. (49) represents the objective function; Eq. (50) shows the yield constraint; and Eq. (51)-(59) define the feasible range of each decision variable.

$$\text{Objective function:} \quad \min (Q_{total}) \quad (49)$$

$$\text{s.t.} \quad ce_f \geq ce_{f,baseline} \quad (50)$$

$$2.54mm \leq L_2 \leq 25.4mm \quad (51)$$

$$1.5 \text{ kg} \leq m_w \leq 3 \text{ kg} \quad (52)$$

$$1\% \text{ w/w} \leq C_{acid} \leq 3\% \text{ w/w} \quad (53)$$

$$150^\circ\text{C} \leq T_p \leq 170^\circ\text{C} \quad (54)$$

$$4 \text{ mins} \leq t_p \leq 6 \text{ mins} \quad (55)$$

$$44^\circ\text{C} \leq T_h \leq 52^\circ\text{C} \quad (56)$$

$$72 \text{ hrs} \leq t_h \leq 96 \text{ hrs} \quad (57)$$

$$28^\circ\text{C} \leq T_f \leq 36^\circ\text{C} \quad (58)$$

$$28 \text{ hrs} \leq t_f \leq 36 \text{ hrs} \quad (59)$$

3.6.2. Solution Procedure

In PSO, each possible solution is considered as a particle in the swarm. The population size (number of particles in the swarm) is denoted by N_p . Each particle is characterized by a position vector $\mathbf{X}$ and velocity vector $\mathbf{V}$, so it can fly around the searching space over iterations. A series of random numbers is generated for all decision variables in solution $\mathbf{S}$ from their ranges and is used as the initial solution.

After initialization, the position and velocity are updated according to the optimality of the found solution:

$$\begin{aligned} \mathbf{V}_i(n+1) = & \mathbf{V}_i(n) + c_1 w_1 (\mathbf{S}_{PB,i}(n) - \mathbf{S}_i(n)) + c_2 w_2 (\mathbf{S}_{GB}(n) \\ & - \mathbf{S}_i(n)), \quad i = (1, \dots, N_p) \end{aligned} \quad (60)$$

$$\mathbf{X}_i(n+1) = \mathbf{X}_i(n) + \mathbf{V}_i(n+1), \quad i = (1, \dots, N_p) \quad (61)$$

where n and $n+1$ represent the n^{st} and $(n+1)^{\text{st}}$ iteration; c_1 and c_2 are learning factors; w_1 and w_2 are random numbers drawn from the unit uniform distribution Uniform (0,1); $\mathbf{S}_{PB,i}$ is the personal best solution (P_{best}) of the i th particle in n iterations; and $\mathbf{S}_{GB}$ represents the global best solution (G_{best}) of all particles in n iterations.

The fitness function of individual particles can be formulated by Eq. (62) with ethanol yield constraints integrated as penalty terms, where M is a positive large real

number. If the calculated ethanol yield is smaller than the baseline value, the fitness function will return a very large value so that the result will be rejected.

$$y = Q_{total} + M \cdot [\min(ce_f - ce_{f,baseline}, 0)]^2 \quad (62)$$

The learning factor c_1 and c_2 are set as 2; the maximum iteration number $N_{I,m}$ is set to be 100. The population size of 10, 20, 30, 50, 100 and 200 are tested to approach the near optimal solution. The algorithm terminates when the number of iterations reaches 100. The overall PSO algorithm is illustrated in Figure 17.

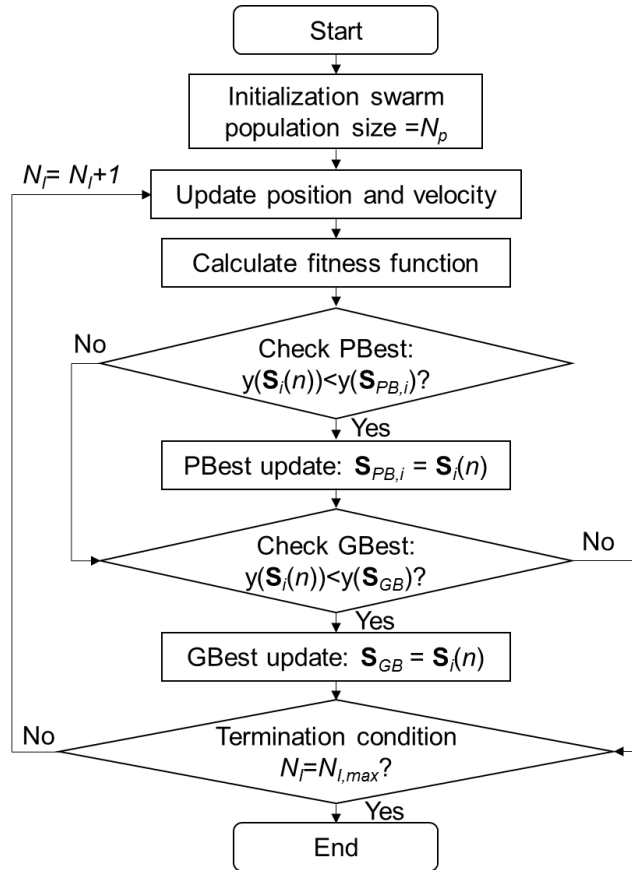


Figure 17. Solution procedures of the energy optimization problem using PSO

3.6.3. Results Analysis and Discussion

The optimization results are obtained for population sizes of 10, 20, 30, 50, 100, and 200, where 20 trial runs are conducted for each size. The algorithm is coded in MATLAB and run by a desktop with 4GB memory and 2.4 GHz Intel i5 CPU. The

averaged time and statistical results to finish 100 iterations for the 6 population sizes (20 independent trial runs each) are provided in TABLE XV.

TABLE XV. THE AVERAGE TIME AND STATISTICAL RESULTS OF THE ENERGY CONSUMPTION OPTIMIZATION PROBLEM IN 6 DIFFERENT POPULATION SIZES (20 TRIAL RUNS FOR EACH SIZE)

Population Size	Avg. time (second)	Min (KJ)	Mean (KJ)	Max (KJ)	Std. Dev.
10	0.2625	1964.3782	2101.1899	2242.9214	132.74
20	0.2944	1949.9644	1989.6188	2094.5133	54.9090
30	0.3418	1949.9644	1964.0309	1987.1477	13.3324
50	0.4268	1949.3492	1952.6224	1965.2769	4.7360
100	0.5814	1949.3472	1951.3232	1963.6914	4.4136
200	0.9316	1949.3468	1949.6940	1950.9635	0.5325

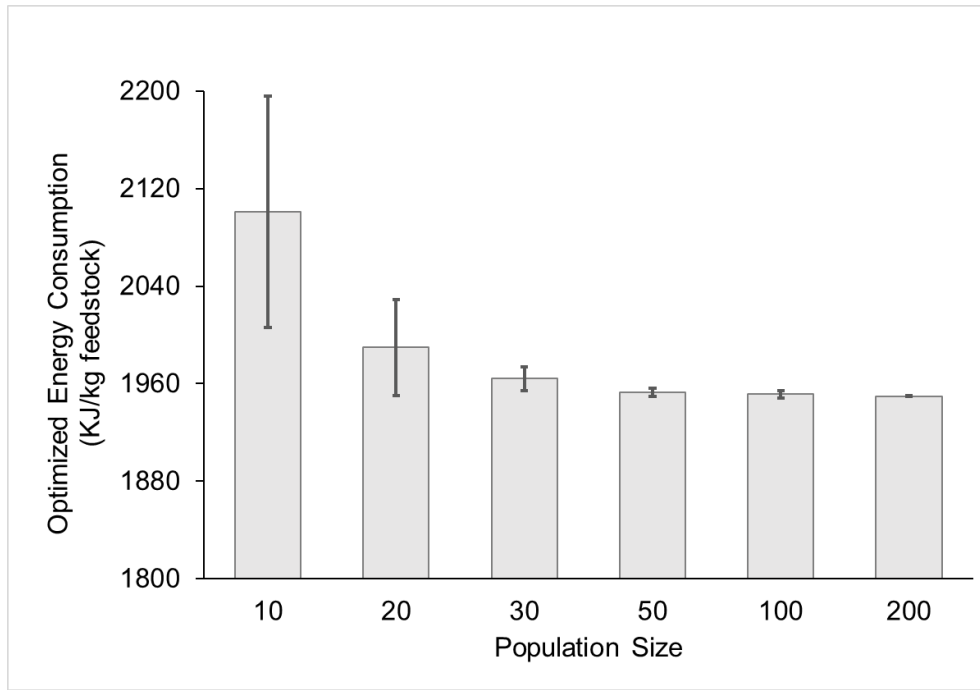


Figure 18. Averaged optimal result of energy consumption with 95% confidence interval

Figure 18 shows the average values in 20 independent trial runs and 95% confidence interval of the optimized energy consumption for the 6 population sizes. When increasing the population size, the optimal value converges to around 1950 KJ/kg feedstock input, and the 95% confidence interval is also narrowed to (-0.38, 0.39). Therefore, we use the solution which results in the least total energy consumption among the 20 runs at

population size of 200 as the near-optimal solution for the biofuel production energy consumption problem.

The results for the baseline case and solution obtained using the proposed optimization problem are shown in in TABLE XVI. Using solution obtained using the proposed optimization problem, 21.09% of the total energy consumed by the biofuel production system is saved compared to the baseline case while maintain ethanol yield. The water loading in the solution lies on the lower side of its range. It is also worth noting that pretreatment time, hydrolysis temperature, fermentation time, and fermentation temperature are taking extreme values in their range. Further widening their range may lead to better results, however, it also may not be practical in real production settings.

TABLE XVI. COMPARISON OF NEAR-OPTIMAL SOLUTION AND BASELINE CASE

Decision variables	Baseline case	Near-optimal solution
Feedstock particle diameter: L_2	6.67 mm (4 mesh)	20.32 mm (8 mesh)
Water loading (per kg feedstock): m_w	2.2 kg	1.62 kg
Diluted acid loading: C_{acid}	1.0% w/w	2.49% w/w
Pretreatment temperature: T_p	158 °C	168.21 °C
Pretreatment time: t_p	5 min	4 min
Enzymatic hydrolysis temperature: T_h	48 °C	44 °C
Enzymatic hydrolysis time: t_h	84 hours	93.68 hours
Fermentation temperature: T_f	32 °C	28 °C
Fermentation time: t_f	36 hours	42 hours
Ethanol yield:	0.2411 kg/ kg feedstock	0.2416 kg/ kg feedstock
Total energy consumption:	2470.57 KJ/ kg feedstock	1949.347 KJ/ kg feedstock (21.09% reduction)

3.7. Conclusions

In this chapter, we propose an analytical system-level energy model for the cellulosic biofuel production system. In addition, an energy optimization problem is formulated under the constraint of biofuel yield and solved using Particle Swarm Optimization (PSO) algorithm. In the proposed model, the fundamental relationships between the system energy consumption and production parameters are characterized, and

the connection between energy and ethanol yield is established by mathematically modeling the chemical reactions. In the case study results, pretreatment is shown to be most energy-intensive of all processes in the cellulosic biofuel production system. The sensitivity analysis further indicates that the input water/biomass ratio has the most impact on the total energy consumption. Moreover, the near-optimal solution obtained from solving the optimization problem leads to 21.09% reduction in total energy consumption compared to the baseline case with no ethanol yield loss. The research outcomes will help realize energy-efficient biofuel production and enhance the sustainability of the cellulosic biofuel.

CHAPTER 4. A NOVEL WASTE MANAGEMENT DESIGN VIA INDUSTRIAL SYMBIOSIS TO CO-PRODUCING ALGAL AND CELLULOSIC BIOFUELS

(Parts of this chapter are submitted to Journal of Cleaner Production for Peer Review: Ge Y., Li L., Xiao M., 2020, *Towards Biofuel Generation III+: A sustainable industrial symbiosis design of co-producing algal and cellulosic biofuels*, *Journal of Cleaner Production*, under review.)

4.1. Introduction

The widespread adoption of cellulosic biofuel is taking place at a much slower pace than expected. In November 2017, DuPont Corporation announced it would be halting operations at a cellulosic ethanol plant in Iowa, USA due to the undercutting of government financial support (Reuters, 2017). Poor material utilization efficiency is one of the main drawbacks for cellulosic biofuel industrialization. Furthermore, a huge amount of CO₂ is generated in the anaerobic fermentation of hydrolyzed sugars into ethanol at an near equimolar rate (Humbird et al., 2011a), which greatly impedes the sustainability of cellulosic ethanol production (CEP).

In the literature, the sustainability issues of CEP are largely neglected. In fact, these wastes can be reused to produce value-added products to enhance the economic viability of CEP. In this chapter, a novel industrial symbiosis (IS) design is proposed to produce the second-generation cellulosic biofuel and the third-generation algal biofuel. The proposed IS system includes three main stakeholders, i.e., the CEP plant, microalgae biodiesel production (MDP) plant, and utility facilities. They can utilize other's output waste as input, which improves environmental and economic benefits and creates a 'win-win situation' for all participants (see Figure 19). Specifically, microalgae can capture the CO₂ generated

from the CEP fermentation process as a cultivation carbon source; wastewater from CEP could supplement nitrogen nutrients for algae growth; the lipid-depleted residual biomass from MDP can be further converted into ethanol along with cellulosic feedstock in a CEP plant; and the solid waste from both types of plants can be used to generate electricity and heat to power the IS bioenergy system. It is worth noting that, unlike cellulosic biomass, microalgae contain starch, lipid, and protein without any lignin. Lignin hinders the ability of celluloses to release mono-sugars in two aspects: 1) it forms a stable lignocellulosic matrix in the cell walls that requires a severe reaction condition or catalyst to disrupt; and 2) lignin can irreversibly absorb proteins, such as cellulase enzyme, thus leading to a high enzyme loading to be applied (Tatsumoto et al., 1988). It is reported that enzyme accounts for approximately 15.8% of the total manufacturing cost for CEP (Humbird et al., 2011a). Therefore, the utilization of residual algae biomass to produce ethanol can reduce the requirements for pretreatment equipment and reduce the need for enzymes.

In this chapter, a novel IS system for co-producing second- and third-generation biofuels is proposed based on mathematically modeling the material/energy flow, manufacturing cost, and environmental impacts. The synergies among the bioenergy IS system stakeholders are proved to be viable and beneficial to enhance the economic viability, efficiency of waste utilization, and environmental sustainability, which are quantitatively evaluated by comparing 4 proposed scenarios. In addition, the impact of different microalgae species and cultivation on the performance of the IS system is analyzed. The research outcomes provide insight into realizing cost-effective and environmentally sustainable biofuel production to rally the adoption of advanced biofuels.

The rest of this chapter is organized as follows. In Section 4.2, notations used in this chapter are introduced. In Section 4.3, the IS design for integrating CEP and MDP is presented. The mass/energy flow and cost modeling are presented in Section 4.4. In Section 4.5, the mathematical modeling for environmental impact indicators are illustrated. In addition, the result and discussion of cost analysis, environmental impact evaluation and sensitivity analysis on selected indicators are illustrated in Section 4.6. Finally, the conclusions are discussed in Section 4.7.

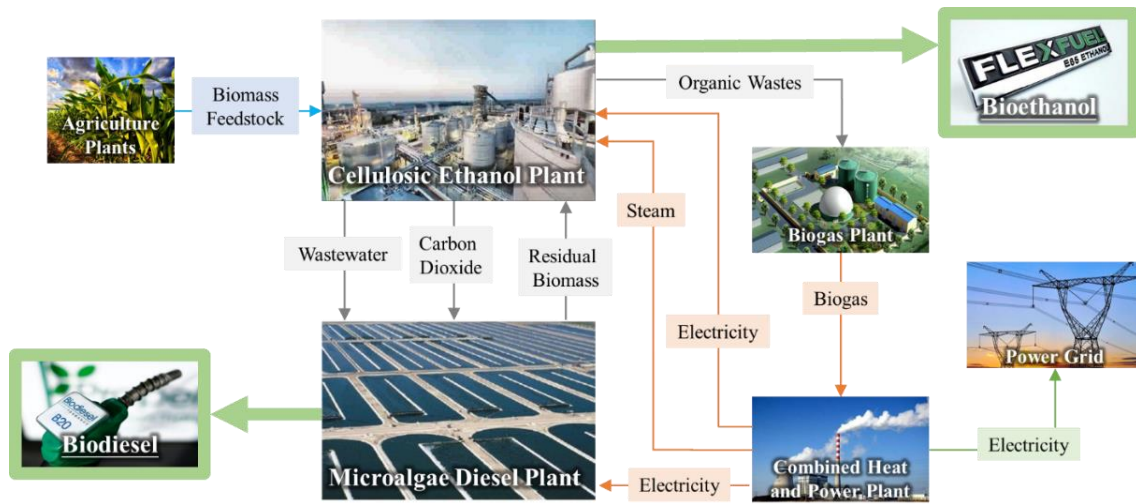


Figure 19. Schematic overview of the proposed industrial symbiosis energy system

4.2. Notations

Greek		p_{MB}	The overall annual production rate of algal biomass
α_x^p	The efficiency of xylan converting to xylose in pretreatment process	r_{CO_2}	The generation rate of CO ₂
α_G^p	The efficiency of glucan converting to glucose in pretreatment process.	r_{CH_4}	The generation rate of methane
α_G^h	The efficiency of glucan converting to glucose in enzymatic hydrolysis process	Upper case	
α_{XL}^f	The efficiency of xylose converting to ethanol in fermentation process	C_{CAP}	The total capital cost
α_{GL}^f	The efficiency of glucose converting to ethanol in fermentation process	$C_{CAP,C}$	The capital cost for CEP plant
α_{MB}^h	The efficiency of microalgae harvest	$C_{CAP,M}$	The capital cost for MDP plant
α_{MB}^o	The efficiency of oil extraction from microalgae biomass	$C_{CAP,W}$	The capital cost for waste treatment facility
α_{OD}^{bg}	The efficiency of converting COD to methane	$C_{CAP,U}$	The capital cost for utility facilities
α_{CD}^c	The efficiency of carbon dioxide utilization in microalgae culture	C_M	The total manufacturing cost

τ	The cultivation time (days) in a year	C_E	The unit cost of bioethanol
κ	Index of combustibles, $\kappa = CH_4, LG, CC, P, LP$	C_D	The unit cost of biodiesel
γ_G	The percentage of glucan consumed in the CEP	C_{GGE}	The unit cost of biofuel in GGE
γ_X	The percentage of xylan consumed in the CEP	F_{COD}	The flow rate of chemical oxygen demand (COD) in anaerobic digestion in the biogas plant
$\sigma_{CO_2/\kappa}$	The ratio of carbon content for one mole CO_2 and one mole combustible κ	M_E	The ethanol produced in the fermentation process
σ_{p/NO_2}	The ratio of nitrogen content for one mole protein and one mole NO_2	M_F	The total mass of feedstock in CEP system
σ_{AI/NO_2}	The ratio of nitrogen content for one mole ammonia ion and one mole NO_2	M_{CS}	The mass of corn stover as feedstock (in dry weight)
$\sigma_{p/PP}$	The ratio of phosphorus content for one mole protein and one mole phosphorus pentoxide	M_{RB}	The residual biomass after oil extraction process (in dry weight)
$\sigma_{PP/PH}$	The ratio of phosphorus content for one mole phosphorus pentoxide and phosphate ion.	M_{XL}^p	The xylose produced in the pretreatment process
σ_{p/SO_2}	The ratio of sulfur content for one mole protein and one mole SO_2	M_{GL}^p	The glucose produced in the pretreatment process
ω_{GGE}^E	The GGE converting factor for bioethanol	M_{GL}^h	The glucose produced in the enzymatic hydrolysis process
ω_{GGE}^D	The GGE converting factor for biodiesel	M_E	The ethanol produced in the fermentation process
Lower case		M_{CD}^f	The carbon dioxide produced in the fermentation process
af_{ND}	The SO_2 equivalent factors for NO_2	M_{MB}^c	The microalgae biomass produced in the microalgae cultivation process
af_{SD}	The SO_2 equivalent factors for SO_2	M_{MB}^h	The microalgae biomass produced in the harvest process
f_X	The mass fraction of xylan in the feedstock	M_O^o	The lipid recovered from microalgae biomass in the oil extraction process
f_G	The mass fraction of glucan in the feedstock	M_{RB}	The residual biomass after oil extraction process (in dry weight)
f_{LG}	The mass fraction of lignin in feedstock	M_D	The final biodiesel produced
$f_{P,CS}$	The mass fraction of protein in corn stover feedstock	M_{Ni}	The nitrogen requirements for microalgae cultivation
f_{LP}	The mass fraction of lipid in corn stover feedstock	M_{Ph}	The phosphorus requirements for microalgae cultivation
f_O	The mass fraction of lipid content in microalgae biomass	$M_{FC,M}$	The mass of fermentable carbohydrates from MDP sent to CEP
$f_{f,c,M}$	The mass fraction of fermentable carbohydrates in microalgae biomass	$M_{p,M}$	The mass of protein from MDP sent to CEP
$f_{p,M}$	The mass fraction of protein in microalgae biomass	M_{AI}	The mass of NH_4^+
ef_{ND}	The phosphate equivalent factors for NO_2	M_{PP}	The mass of phosphorus pentoxide
ef_{NT}	The phosphate equivalent factors for NO_3^-	M_{LG}	The lignin sent for combustion
ef_{PH}	The phosphate equivalent factors for PO_4^{3-}	M_{CC}	The carbohydrates sent for combustion
ef_{COD}	The phosphate equivalent factors for COD	M_P	The protein sent for combustion
i	Index of biofuel production, $i=CEP, MDP$	M_{LP}	The lipid sent for combustion
j	Index of resource, $j =$ raw material cost, fixed cost, tax and capital cost, and by-product credit	M_{CD}^{IS}	The total CO_2 emitted from the IS system
m_{CH_4}	The molar mass of methane	M_{CD}^{em}	The CO_2 emitted from algae cultivation pond
m_κ	The molar mass of combustible κ	$M_{CH_4}^{bg}$	The methane emitted from biogas plant
m_P	The molar mass of protein contained in the biomass residue	M_{CD}^{bg}	The CO_2 generated in the anaerobic digestion in biogas plant
m_{NO_2}	The molar mass of NO_2	M_{CD}^{cb}	The CO_2 generated from the combustion
m_{NT}	The molar mass of nitrate ion	$M_{CD}^{K,c}$	The CO_2 generated from the combustion by κ
m_{AI}	The molar mass of ammonia ion	M_{ND}^{IS}	The NO_2 generated from the IS system
m_{PH}	The molar mass of phosphate ion	M_{NT}^{IS}	The NO_3^- generated from the IS system

m_{PP}	The molar mass of phosphorus pentoxide	M_{PH}^{IS}	The PO_4^- generated from the IS system
m_{SO_2}	The molar mass of SO_2	M_{COD}^{IS}	The COD generated from the IS system
m_{CO_2}	The molar mass of carbon dioxide	M_{SD}^{IS}	The SO_2 generated from the IS system
$m_{ethanol}$	The molar mass of ethanol		

4.3. Novel Industrial Symbiosis Design

The scheme of planned industrial symbiosis is shown in Figure 20. The industrial symbiosis design involves 3 main stakeholders: the CEP plant, MDP plant, and utility system. The CEP plant utilizes outsource cellulosic biomass and recycled lipid-depleted algal biomass from MDP to produce bioethanol and provide CO_2 for algae cultivation. The economic viability of MDP could be greatly improved by saving the cost of purchasing outsourced CO_2 , and the greenhouse gas emission of CEP would also be reduced. The wastewater from CEP is then discharged to an over-liming treatment for sulfate removal and used as make-up water and a nitrogen source for microalgae. Since a considerable amount of wastewater is discharged from the CEP plant, this recycling strategy can greatly enhance the utilization efficiency of water resources. The waste solid from CEP and MDP is designed to be combusted in a combined heat and power (CHP) system in order to generate power and heat for the IS system. The net electricity (if any) will be sold to the grid.

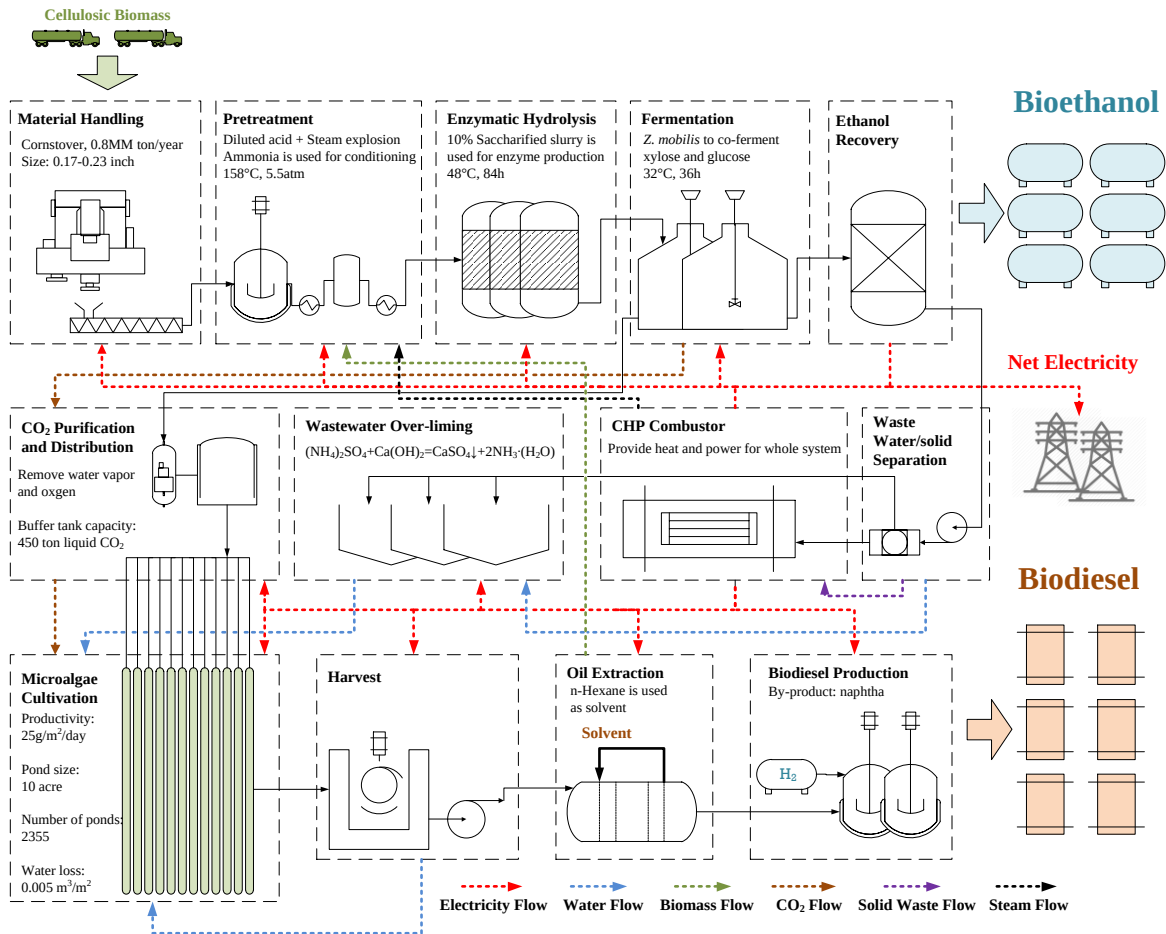


Figure 20. Proposed industrial symbiosis bioenergy production system

4.3.1. Reuse of Waste Gas from CEP Fermentation

During the CEP fermentation process, carbon dioxide is generated along with ethanol at an equimolar rate (TABLE XVII).

TABLE XVII. MAIN REACTIONS RELATED TO BIOETHANOL PRODUCTION

Process	Reaction	Reactant	% Converted to product
Pretreatment	$(\text{Glucan})_n + n \text{ H}_2\text{O} \rightarrow n \text{ Glucose}$	Glucan	9.9%
Pretreatment	$(\text{Xylan})_n + n \text{ H}_2\text{O} \rightarrow n \text{ Xylose}$	Xylan	5.0%
Enzymatic Hydrolysis	$(\text{Glucan})_n + n \text{ H}_2\text{O} \rightarrow n \text{ Glucose}$	Glucan	81.09%
Fermentation	$\text{Glucose} \rightarrow 2 \text{ Ethanol} + 2 \text{ CO}_2$	Glucose	95.0%
Fermentation	$3 \text{ Xylose} \rightarrow 5 \text{ Ethanol} + 5 \text{ CO}_2$	Xylose	85.0%

In the baseline case, 61 million gallons of ethanol is produced annually, resulting in the generation of 174,249.9 tons of CO₂. In the IS design, the microalgae fix the vented CO₂ through photosynthesis and use the carbon source for growth. The gas from the fermentation vent is a mixture of CO₂, water vapor, and a small amount of oxygen (TABLE XVIII). It is first pumped into a compression dryer to eliminate the vapor and cooled to 20°C or below. The mixed gas is then released into a separation tank with 8 MPa pressure, in which oxygen remains in its gaseous form and CO₂ is liquefied for collection. The CO₂ storage tanks are capable of containing 450 m³ liquid CO₂, which is the amount of CO₂ generated from CEP in 1 day. Moreover, in the baseline case, the total number of algae cultivation ponds is 2,355, as determined using the following equation:

$$N = \frac{M_{CD}^f \cdot \gamma_{uptake}}{p_{MB} \cdot \tau \cdot a \cdot \beta_{CO_2} \cdot 10^{-6} \cdot (\frac{ton}{g})} \quad (63)$$

where M_{CD}^f is the mass of CO₂ generated from the CEP fermentation process, γ_{uptake} is the overall CO₂ uptake efficiency of 90% (Song et al., 2019), p_{MB} is the overall annual algal biomass production rate of 25 g/m²/day (Davis et al., 2014), τ is the annual cultivation time of 360 days/year, a is the area of 1 cultivation pond (4046.8 m²), and β_{CO_2} is the CO₂ supply ratio of 1.83 tons/ton of algal biomass (Chisti, 2007).

TABLE XVIII. OXYGEN GENERATION IN THE CEP FERMENTATION PROCESS

Process	Reaction	Reactant	% Converted to product
Fermentation	Glucose + 2 H ₂ O → 2 Glycerol + O ₂	Glucose	0.6%
Fermentation	3 Xylose + 5 H ₂ O → 5 Glycerol + 2.5 O ₂	Xylose	0.3%
Fermentation	Xylose + H ₂ O → Xylitol + 0.5 O ₂	Xylose	4.6%

4.3.2. Reuse of Wastewater from CEP

After ethanol recovery, the wastewater and solid waste are separated using a pressure filter. The wastewater contains abundant monosaccharides and ammonium, which can provide carbon and nitrogen sources for algae cultivation (Min et al., 2011). The arabinose, galactose, xylose, xylitol, glucose, and mannose are simple sugars or polyalcohol that can be consumed by microalgae. The acetic acid, acetate, succinic acid, and glycerol are intermediate products or microalgae photosynthesis products which do not impede the algae growth (Chen et al., 2017). The high concentration of sulfate ions is lowered by feeding moderate amounts of calcium hydroxide, such that most of the calcium sulfate would precipitate, while maintaining a trace of sulfate ion as the sulfur source for algae cultivation. The ammonium would then exist in the water in aqueous form, thus providing the nitrogen source for the algae. Lignin has high chemical stability and does not impede algae growth (Ge et al., 2017).

Some studies, however, have mentioned that large amounts of furfural could be toxic (Brune et al., 1983; Koopman et al., 2010). Although the relationship between microalgae growth and furfural concentration has not been explored in previous research, some investigations have shown that certain bacteria can evolve a particular adaptability to furfural (Heer and Sauer, 2008). The furfural concentration level in CEP wastewater is much lower than the level considered to be toxic; moreover, the make-up freshwater would further dilute the furfural concentration. Therefore, the wastewater is suitable for supplementing the waste and nutrients following the over-liming process (using excess calcium hydroxide to precipitate sulfate ions).

TABLE XIX. COMPOSITION OF SOLUTES IN CEP WASTEWATER (CALCULATED BASED ON RELEVANT DATA FROM (Humbird et al., 2011a))

Component	Concentration (g/L)	Production (ton/year)
(NH ₄) ₂ SO ₄	6.6	20,837
Arabinose	4.6	16,160
Acetic acid	3.8	12,670
Acetate	3.6	12,670
Lactic acid	3.3	11,595
Galactose	2.8	9,710
Xylose	2.6	9,011
Xylitol	1.8	6,406
Soluble lignin	1.6	5,516
Glucose	1.4	4,971
Furfural	1.4	4,430
Mannose	1.2	4,074
Succinic acid	1.1	3,563
Glycerol	0.4	1,430

The nitrogen and phosphate requirements for microalgae cultivation are 5,445 tons and 1,167 tons, respectively. From TABLE XIX, the nitrogen contained in (NH₄)₂SO₄ is 5,953 tons, which could meet the nitrogen demand, whereas a minimum of 5,141 diammonium phosphate should be supplied.

Based on the number and size of the algae cultivation ponds, the amount of water needed to fill every pond is 2.38 million tons. The water loss due to evaporation is assumed to be 0.005 m³/m² (Gutiérrez-Arriaga et al., 2014), i.e., 17.1 million tons of water loss per year. Based on the baseline study, the annual amount of reusable wastewater from CEP is 3.41 million tons (Humbird et al., 2011a). Considering the cultivation water recycling, the required replenishment freshwater is 13.69 million tons. As mentioned previously, there is evidence that furfural could be toxic; it is assumed, however, that 13.69 tons of make-up freshwater can maintain the furfural concentration at a safe level.

4.3.3. Reuse of Solid Waste from MDP and CEP

It is assumed that all fuel-related lipids of the algal biomass are recovered from the oil extraction process in MDP, and the residual biomass is considered to be solid waste and transported to the CEP plant as feedstock. In TABLE XX, the microalgae *Scenedesmus* sp. after a 4-day cultivation is presented as an example to illustrate the composition of MDP solid waste. With the exception of fermentable carbohydrates, the remainder of the components are not involved in the ethanol conversion reactions and are delivered to be combusted along with the solid waste from CEP.

TABLE XX. COMPOSITION OF MDP SOLID WASTE
(Davis et al., 2014; Laurens et al., 2014)

Component (<i>Scenedesmus</i>)	Wt.% (dry basis)
Ash	2.4
Fermentable carbohydrates	47.8
Other carbohydrates	5
Proteins	13.2
Non-fuel related lipids	2.7
Cell mass	1.5
Total	72.6 ^a

^a The fuel-related lipids account for 27.4% dry weight of *Scenedesmus*, which is extracted in the oil extraction process.

TABLE XXI. COMPOSITION OF CEP SOLID WASTE

Component	Wt.% (dry basis)
Lignin	44.6
Glucan	5.1
Cell mass	8.2
Xylan	1.5
Ash	14.8
Proteins	25.3
Nucleic acids	0.6
Total	100

The fermentable carbohydrates in the MDP solid waste can be further converted into mono-sugars, such that they can act as a supplement for corn stover as cellulosic feedstock. Higher fermentable carbohydrate content leads to a lower demand for corn stover when producing the same amount of ethanol. Since no literature could be found to

further illustrate the composition of fermentable carbohydrates in MDP, for simplification purposes, all fermentable carbohydrates are assumed to be glucan. In addition, the proteins in TABLE XX and TABLE XXI are considered to have the same elemental constitution, the cell mass is assumed to have the same ingredients as the proteins, and the ash in both tables are presumed to be non-combustible. The elemental constitution of the components in the solid waste are presented in TABLE XVII. Note that the elemental constitutions are all converted on a unit carbon basis and do not reflect the organic structure of the components.

TABLE XXII. ELEMENTAL CONSTITUTIONS OF SOLID WASTE COMPONENTS

Component	Elemental constitution	Source
Glucan	CH _{1.67} O _{8.33}	(Humbird et al., 2011a)
Lignin	CH _{1.18} O _{0.36}	(Humbird et al., 2011a)
Non-fuel related lipids	CH _{1.5} O _{0.11}	(Laurens et al., 2014)
Nucleic acids	CH _{0.15} O _{0.56} N _{0.03} S _{0.004} P _{0.004}	(Ecologycenter, 2020)
Other carbohydrates	CH ₂ O	(Ecologycenter, 2020)
Proteins	CH _{0.14} O _{0.46} N _{0.32} S _{0.03} P _{0.03}	(Ecologycenter, 2020)
Xylan	CH _{1.6} O _{0.8}	(Humbird et al., 2011a)

The solid wastes are presumed to be fully combusted in an on-site combined heat and power (CHP) system to produce the steam for the pretreatment process and the electricity to power the IS system. The waste steam is recycled to heat the circulation water used to maintain the desired temperature for enzymatic hydrolysis and the fermentation process. It is assumed that all combustibles in the CHP system are fully oxidized, meaning only CO₂, NO₂, H₂O, SO₂, and P₂O₅ are generated from the combustion chamber. The power generated is calculated based on a previous study by the authors on energy consumption optimization for CEP systems (Ge and Li, 2018).

$$E_p = \mu_1(E_s^I - E_s^O) = \mu_1(\mu_0 \sum_i q_i \cdot m_i - E_s^O) \quad (64)$$

In Eq. (64), μ_1 represents a turbine efficiency of 90% used to generate power (power-eng, 2007); E_s^I and E_s^O are the steam inner energy before and after the turbine process, respectively; μ_0 is the 88% efficiency of the combustor used to generate steam (Boiler-efficiency, 2018); q_i is the calorific value of each combustible, which collected from various sources; and m_i is the annual supply (in kg) of each combustible. It is assumed that the outlet steam (after the turbine) has a temperature of 170°C and a flow rate of 19,533kg/hour (Humbird et al., 2011a). Therefore, the total power generated for the system is 77 MW for the stand-alone system, in which the combustibles from CEP contribute 41 MW, and the remaining 36 MW is contributed by MDP solid waste (using *Scenedesmus sp.* as inoculum). It is worth noting that in the IS design, the power generation from CEP will be inherently lower than that in the standalone system since no methane is produced by the wastewater treatment.

4.4. Mass Flow and Cost Modeling

Based on the analysis in Section 4.3, the detailed mathematical modeling for the mass flow and cost are shown as follows.

The total mass of fermentable feedstock is given by:

$$M_F = M_{CS} + M_{RB} \quad (65)$$

where M_{CS} is the mass of corn stover as feedstock (in dry weight), and M_{RB} is the residual biomass after the oil extraction after oil extraction process (in dry weight).

The xylose produced in the pretreatment process is given by:

$$M_{XL}^p = M_F \cdot f_X \cdot \alpha_X^p \quad (66)$$

where M_F is mass of feedstock in CEP system, f_X is the mass fraction of xylan in the feedstock, α_X^p is the efficiency of xylan converting to xylose in pretreatment process.

The glucose produced in the pretreatment process is given by:

$$M_{GL}^p = M_F \cdot f_G \cdot \alpha_G^p \quad (67)$$

where f_G is the mass fraction of glucan in the feedstock, α_G^p is the efficiency of glucan converting to glucose in pretreatment process.

The glucose produced in the enzymatic hydrolysis process is given by:

$$M_{GL}^h = M_F \cdot f_G \cdot \alpha_G^h \quad (68)$$

where α_G^p is the efficiency of glucan converting to glucose in enzymatic hydrolysis process.

The ethanol produced in the fermentation process is given by:

$$M_E = \alpha_{XL}^f \cdot M_{XL}^p + \alpha_{GL}^f \cdot (M_{GL}^p + M_{GL}^h) \quad (69)$$

where α_{XL}^f is the efficiency of xylose converting to ethanol in fermentation process, and α_{GL}^f is the efficiency of glucose converting to ethanol in fermentation process.

The CO₂ produced in the fermentation process is given by:

$$M_{CD}^f = M_E \cdot \frac{m_{CO2}}{m_{ethanol}} \quad (70)$$

where m_{CO2} is the molar mass of carbon dioxide and $m_{ethanol}$ is the molar mass of ethanol.

The microalgae biomass produced in the microalgae cultivation process is given by:

$$M_{MB}^c = p_{MB} \cdot A \cdot \tau \cdot 10^6 \cdot \left(\frac{ton}{g}\right) \quad (71)$$

where p_{MB} is the overall annual production rate of algal biomass, A is the total area of cultivation ponds, and τ is cultivation time (days) in a year.

The microalgae biomass produced in the harvest process is given by:

$$M_{MB}^h = M_{MB}^c \cdot \alpha_{MB}^h \quad (72)$$

where α_{MB}^h is the efficiency of microalgae harvest.

The lipid recovered from microalgae biomass in the oil extraction process is given by:

$$M_O^o = M_{MB}^h \cdot \alpha_{MB}^o \cdot f_O \quad (73)$$

where α_{MB}^o is the efficiency of oil extraction from microalgae biomass, and f_O is the mass fraction of lipid content in microalgae biomass.

The final biodiesel produced is given by:

$$M_D = M_O^o \quad (74)$$

The residual biomass after the oil extraction is given by:

$$M_{RB} = (1 - \alpha_{MB}^o \cdot f_O) \cdot M_{MB}^h \quad (75)$$

The nitrogen and phosphorus requirements for microalgae cultivation can be determined from the following equations:

$$M_{Ni} = (0.182) \cdot M_D \quad (76)$$

$$M_{Ph} = (0.039) \cdot M_D \quad (77)$$

The mass fermentable carbohydrates and protein from MDP sent to CEP is given by:

$$M_{FC,M} = M_{MB}^h \cdot f_{fc,M} \quad (78)$$

$$M_{P,M} = M_{MB}^h \cdot f_{p,M} \quad (79)$$

where $f_{fc,M}$ and $f_{p,M}$ are the mass fraction of fermentable carbohydrates in microalgae biomass, respectively.

The lignin, carbohydrates, protein, and lipid sent for combustion is given by:

$$M_{LG} = M_F \cdot f_{LG} \quad (80)$$

$$M_{CC} = M_F \cdot f_G \cdot (1 - \gamma_G) + M_F \cdot f_X \cdot (1 - \gamma_X) \quad (81)$$

$$M_P = M_{CS} \cdot f_{P,CS} + M_{MB}^c \cdot f_{P,MA} \quad (82)$$

$$M_{LP} = M_F \cdot f_{LP} \quad (83)$$

where f_{LG} is the mass fraction of lignin in feedstock; γ_G and γ_X are the percentage of glucan and xylan consumed in the CEP; $f_{P,CS}$ and $f_{P,MA}$ are the mass fraction of protein in corn stover feedstock and microalgae biomass, respectively; f_{LP} is the lipid mass fraction in corn stover feedstock.

The total capital cost is given by:

$$C_{CAP} = C_{CAP,C} + C_{CAP,M} + C_{CAP,W} + C_{CAP,U} \quad (84)$$

where $C_{CAP,C}$, $C_{CAP,M}$, $C_{CAP,W}$, and $C_{CAP,U}$ are the capital cost for CEP plant, MDP plant, waste treatment facility, and utility facilities, respectively.

The total manufacturing cost can be calculated as:

$$C_M = C_{M,R} + C_{M,F} + C_{M,T} - C_{M,B} \quad (85)$$

where $C_{M,R}$, $C_{M,F}$, $C_{M,T}$, and $C_{M,B}$ are the raw material cost, fixed cost, tax and capital cost, and by-product credit, respectively; which can be further expressed as:

$$C_{M,R} = \sum_{i=C,M} C_{M,R}^i \quad (86)$$

$$C_{M,F} = \sum_{i=C,M} C_{M,F}^i \quad (87)$$

$$C_{M,T} = \sum_{i=C,M} C_{M,T}^i \quad (88)$$

$$C_{M,B} = \sum_{i=C,M} C_{M,B}^i \quad (89)$$

where the C and M under the summation sign represent the cost items in CEP and MDP, respectively; therefore, the manufacturing cost for CEP and MDP are given by:

$$C_M^C = \sum_{i=R,F,T,B} C_{M,i}^C \quad (90)$$

$$C_M^M = \sum_{i=R,F,T,B} C_{M,i}^M \quad (91)$$

Accordingly, the unit cost of bioethanol and biodiesel are given by:

$$C_E = C_M^C / M_E \quad (92)$$

$$C_D = C_M^M / M_D \quad (93)$$

Finally, the unit biofuel cost in GGE can be calculated by:

$$C_{GGE} = (M_E \cdot \omega_{GGE}^E + M_D \cdot \omega_{GGE}^D) \cdot C_G \quad (94)$$

where ω_{GGE}^E and ω_{GGE}^D are the GGE converting factor for bioethanol and biodiesel, respectively; and C_G is the unit price of gasoline.

4.5. Environmental Impact Assessment

In this study, three indicators are considered to evaluate the environmental impact of the IS system: CO₂ emissions, eutrophication potential (EP), and acidification potential (AP). For the standalone system (no IS implementation), carbon dioxide is emitted from the fermentation vent, biogas production, cultivation ponds, and solid waste combustion. It is assumed that the CO₂ collection rate for algae cultivation is 100% in the IS system. Although this is an ideal number, it is achievable in actual production, since fermentation is an anaerobic process in which the fermenters must be airtight. The CO₂ is only emitted from the vent; hence, the recovery rate could reach 100%.

Eutrophication refers to the pollution state of aquatic ecosystems in which the over-fertilization of water and soil has led to the increased growth of undesired biomass, and acidification potential is a consequence of acids being emitted to the atmosphere and subsequently deposited in surface soils and water (UNEP/SETAC, 2005). Based on Section

4.3.3, the proteins and nucleic acids contained in the solid wastes are presumed to have been fully combusted in the CHP combustor, so that the nitrogen, sulfur, and phosphorus would be transformed into NO_2 , SO_2 , and P_2O_5 . Therefore, the eutrophication potential and acidification potential caused by these products are considered in this study, and are expressed in PO_4^- equivalent and SO_2 equivalent, respectively. The results of these factors with and without IS implementation are compared in Section 4.6. The detailed modeling used for the environmental impact indicators is provided as follow.

The CO_2 emitted from algae cultivation pond is given by:

$$M_{CD}^{em} = M_{CD}^f \cdot (1 - \alpha_{CD}^e) \quad (95)$$

The methane is produced from biogas plant is given by:

$$M_{CH_4}^{bg} = F_{COD} \cdot \alpha_{OD}^{bg} \cdot \tau \quad (96)$$

where F_{COD} is the flow rate of chemical oxygen demand (COD) in anaerobic digestion in the biogas plant, α_{OD}^{bg} is the efficiency of converting COD to methane, and τ represent the reaction time.

The CO_2 generated in the anaerobic digestion in biogas plant is given by:

$$M_{CD}^{bg} = M_{CH_4}^{bg} \cdot \frac{m_{CO_2}}{m_{CH_4}} \cdot \frac{r_{CO_2}}{r_{CH_4}} \quad (97)$$

where m_{CH_4} is the molar mass of methane, r_{CO_2} is the generation rate of CO_2 , and r_{CH_4} is the generation rate of methane.

The CO_2 generated from the combustion is given by:

$$M_{CD}^{cb} = \sum_{i=CH_4, LG, CC, P, LP} M_{CD}^{i,c} = \sum_{i=CH_4, LG, CC, P, LP} \frac{M_i}{m_i} \cdot \sigma_{CO_2/i} \cdot m_{CO_2} \quad (98)$$

where combustibles include methane generated in biogas plant, lignin from corn stover feedstock, residual glucan from corn stover feedstock and lipid-depleted microalgae,

residue xylan from corn stover feedstock, protein from corn stover feedstock and lipid-depleted microalgae, lipid from corn stover feedstock; $M_{CD}^{i,c}$ indicates the CO₂ generated by burning combustible i , M_i is the mass of combustible i , m_i is the molar mass of combustible i , $\sigma_{CO_2/i}$ is the ratio of carbon content for one mole CO₂ and one mole combustible i .

The total CO₂ emitted from the IS system is given by:

$$M_{CD}^{IS} = M_{CD}^{em} + M_{CD}^{bg} + M_{CD}^{cb} \quad (99)$$

The NO₂ generated from the IS system is considered to be from combusting the protein contained in the solid waste from CEP, which is given by:

$$M_{ND}^{IS} = M_P \cdot \frac{m_{NO_2}}{m_P} \cdot \sigma_{P/NO_2} \quad (100)$$

where M_P is the mass of protein contained in the biomass residues, m_P is the molar mass of protein contained in the biomass residues, m_{NO_2} is the molar mass of NO₂, σ_{P/NO_2} is the ratio of nitrogen content for one mole protein and one mole NO₂.

The NO₃⁻ generated from the IS system is considered to be from converting NH₄⁺ into NO₃⁻ in the nitrification reactions in the wastewater treatment process, which is given by:

$$M_{NT}^{IS} = M_{AI} \cdot \frac{m_{NT}}{m_{AI}} \cdot \sigma_{AI/NO_2} \quad (101)$$

where M_{AI} is the mass of NH₄⁺; m_{NT} and m_{AI} are the molar mass of nitrate ion and ammonia ion, respectively; and σ_{AI/NO_2} is the ratio of nitrogen content for one mole ammonia ion and one mole NO₂.

Combusting the protein contained in the solid waste from CEP would lead to P_2O_5 that is emitted in the flue. The PO_4^- is then computed by the converting P_2O_5 into PO_4^- , which is given by:

$$M_{PH}^{IS} = M_{PP} \cdot \frac{m_{PH}}{m_{PP}} \cdot \sigma_{PP/PH} = M_p \cdot \left(\frac{m_{PP}}{m_p}\right) \cdot \sigma_{p/PP} \cdot \left(\frac{m_{PH}}{m_{PP}}\right) \cdot \sigma_{PP/PH} \quad (102)$$

where M_{PP} is the mass of phosphorus pentoxide; m_{PH} and m_{PP} are the molar mass of phosphate ion and phosphorus pentoxide, respectively; $\sigma_{p/PP}$ is the ratio of phosphorus content for one mole protein and one mole phosphorus pentoxide, and $\sigma_{PP/PH}$ is the ratio of phosphorus content for one mole phosphorus pentoxide and phosphate ion.

Finally, the Eutrophication Potentials (EP) can be calculated by:

$$EP = M_{ND}^{IS} \cdot ef_{ND} + M_{NT}^{IS} \cdot ef_{NT} + M_{PH}^{IS} \cdot ef_{PH} + M_{COD}^{IS} \cdot ef_{COD} \quad (103)$$

where M_{COD}^{IS} is the mass of COD, and ef_{ND} , ef_{NT} , ef_{PH} , ef_{COD} are the phosphate equivalent factors for NO_2 , NO_3^- , PO_4^- , and COD, respectively.

The SO_2 generated from the IS system is considered to be from combusting the protein contained in the solid waste from CEP, which is given by:

$$M_{SD}^{IS} = M_p \cdot \frac{m_{SO_2}}{m_p} \cdot \sigma_{p/SO_2} \quad (104)$$

where m_{SO_2} is the molar mass of SO_2 , σ_{p/SO_2} is the ratio of sulfur content for one mole protein and one mole SO_2 .

Therefore, the Acidification Potential (AP) can be calculated by:

$$AP = M_{ND}^{IS} \cdot af_{ND} + M_{SD}^{IS} \cdot af_{SD} \quad (105)$$

where af_{ND} and af_{SD} are the SO_2 equivalent factors for NO_2 and SO_2 , respectively.

4.6. Results and Discussion

4.6.1. Alternative Scenarios with Different Microalgae Species

Based upon the material and energy flow of the standalone and IS designs, alternative scenarios are implemented to examine the current IS performance for different microalgae species, i.e., *Scenedesmus*, *Chlorella*, and *Nannochloropsis*. The logic behind this experimental design is that each species would have different compositions of lipid, carbohydrate, and protein content over the same cultivation period (TABLE XXIII). While lipid content determines the production of biodiesel, carbohydrate content can replace part of the CEP feedstock, and protein is related to the generation of contaminations.

TABLE XXIII. COMPOSITION OF THE 3 MICROALGAE SPECIES OVER A 4-DAY CULTIVATION PERIOD (Davis et al., 2014)

Microalgae species	<i>Scenedesmus</i>	<i>Chlorella</i>	<i>Nannochloropsis</i>
Fermentable carbohydrates	47.8	39.2	11
Fuel-relevant lipids	27.4	23.6	32
Proteins	13.2	14.3	28.9

The impacts of different species on the IS system could be complex and significant in terms of yield and economic viability, as well as environmental performance. It is assumed that the production rate of the 3 microalgae were the same, i.e., 25 g/m²/day. The 4 scenarios considered in the case studies are:

Scenario 1: No IS system with *Scenedesmus* as inoculum

Scenario 1 is the baseline scenario, in which the 2 biofuel production systems (i.e., CEP and MDP) have no material or energy exchange. The CO₂ for the microalgae cultivation is purchased from an outsource supplier.

Scenario 2: IS system with *Scenedesmus* as inoculum

Scenario 2 considers the synergies among the bioenergy IS system stakeholders, which applies in Scenarios 3 and 4 as well.

Scenario 3: IS system with *Chlorella* as inoculum

Scenario 4: IS system with *Nannochloropsis* as inoculum

In order to determine the amount of cellulosic feedstock cost that could be saved, the 4 scenarios are assumed to have the same annual ethanol production as the baseline case, i.e., 61 million gallons/year. In the baseline case, 800,000 tons of corn stover is consumed to meet the production target. In the IS cases, it is assumed that the captured CO₂ would be the only carbon source for the microalgae; thus, any differences in the algal biomass production for Scenarios 2, 3, and 4 would be due to the distinct elemental compositions of the 3 microalgae species (TABLE XXIV).

TABLE XXIV. ELEMENTAL COMPOSITION OF SCENEDESMUS, CHLORELLA, AND ANNOCHLOROPSIS FOR DIFFERENT HARVEST STAGES

Wt.% (dry basis)	<i>Scenedesmus</i> (Scenario 2)			<i>Chlorella</i> (Scenario 3)			<i>Nannochloropsis</i> (Scenario 4)		
	Early	Mid	Late	Early	Mid	Late	Early	Mid	Late
C	52.2	54	57.4	51.8	51.3	56.3	51.4	53.2	63.8
H	7.5	8.2	8.7	7.3	7.7	8.5	7.7	8.1	9.9
N	8.8	1.8	1.6	9.3	2.8	2.2	7.3	5	2
O	30.4	35.5	31.8	29.8	37.7	32.4	32	32.6	23.7
S	0	0.2	0.2	0.6	0.4	0.4	0.7	0.5	0.3
P	1.03	0.22	0.2	1.15	0.15	0.11	0.88	0.6	0.24
Total	100	100	100	100	100	100	100	100	100

Consequently, the biodiesel production (TABLE XXV) could be calculated based on the fuel-related lipid content of each species and the algal biomass yield. Note that since *Scenedesmus* is used as inoculum in both Scenarios 1 and 2, they produce the same biodiesel yield. The parameters used for biofuel production calculation as well as other results in this section are given in TABLE XXVI.

TABLE XXV. BIOFUEL PRODUCTION OF SCENARIOS 1, 2, 3, AND 4

	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Bioethanol (MM gal/year)	61	61	61	61
Biodiesel (MM gal/year)	9.3	9.3	8.0	10.9

TABLE XXVI. SUPPLEMENTARY PARAMETERS

Mass fractions of each components (Davis et al., 2016, 2014; Humbird et al., 2011a)		Molecular mass ^a	
f_X	24.8%	m_{CO_2}	44
f_G	35.0%	m_{CH_4}	16
f_{LG}	15.8%	m_P	25.54
$f_{P,CS}$	3.7%	m_{NO_2}	46
f_{LP}	2.2%	m_{NT}	62
f_O	27.4%	m_{AI}	18
$f_{f_c,M}$	47.8%	m_{PH}	94
$f_{p,M}$	13.2%	m_{PP}	140
Equivalence factors for EP and AP (Liu et al., 2011)		m_{SO_2}	64
ef_{ND}	0.13 kg eq. PO_4^-	Elemental ratio ^b	
ef_{NT}	0.42 kg eq. PO_4^-	σ_{p/NO_2}	0.32
ef_{PH}	3.07 kg eq. PO_4^-	σ_{AI/NO_2}	1
ef_{COD}	0.022 kg eq. PO_4^-	$\sigma_{p/PP}$	0.01
af_{ND}	0.7 kg eq. SO_2	$\sigma_{PP/PH}$	2
af_{SD}	1 kg eq. SO_2	σ_{p/SO_2}	0.02
GGE converting factor (Tao et al., 2014)		Other factors (Davis et al., 2016, 2014; Humbird et al., 2011a)	
ω_{GGE}^E	0.68	F_{COD}	96%
ω_{GGE}^D	1.05	α_{OD}^{bg}	99.5%
Material prices (Davis et al., 2016, 2014; Humbird et al., 2011a)		Interest rate	8%
Corn stover	\$49.28/ton	Depreciation rate	10%
Ammonia	\$438.46/ton	Electricity selling price	\$0.068/kWh
Sulfuric acid	\$87.78/kg	Naphtha selling price	\$3.25/gal
H ₂	\$1.6/kg		
Glucose	\$0.57/kg		
(NH ₄) ₂ ·HPO ₄	\$0.96/kg		
n-Hexane	\$1.19/kg		

^a Basic chemistry data collected from various sources.^b Calculated data based on chemical formulae.

4.6.2. Cost Analysis

4.6.2.1. Capital Cost Comparison

The different microalgae species utilized in Scenarios 2–4 do not require significant changes in equipment. For simplification purposes, it is assumed that the installed equipment is the same for Scenarios 2–4, and the capital comparison is presented between Scenarios 1 and 2.

Compared with the standalone system, the IS system reduces the capital cost by 11.9% (Figure 21). For the CEP plant, since no equipment changes are applied in the CEP system, the expenses remained the same. The capital cost of the MDP plant increases primarily due to the fact that the MDP plant requires the CO₂ delivery system, including the compression dryer, CO₂ separation tanks, storage tanks, and distribution pipes to transport CO₂ from the CEP plant to the microalgae cultivation ponds. In addition, the delivery equipment to transport the lipid-depleted biomass to the CEP also adds to the capital cost. In the standalone system, the wastewater treatment is located in the CEP plant, which uses biochemical reactions to eliminate the nitrogen, phosphate, and other organic matter. In the IS system, wastewater is simply discharged to microalgae cultivation ponds after over-liming to remove sulfate ions, thus eliminating corresponding equipment costs. Since the anaerobic/aerobic digestion equipment now only needs to deal with solid waste, the equipment cost also decreases significantly.

	Scenario 1			Scenario 2		
	\$MM				\$MM	
Pretreatment	29.9	Capital of CEP \$104.7MM	0%	Capital of CEP \$104.7MM	29.9	
Neutralization/Conditioning	3.0				3.0	
Saccharification & Fermentation	31.2				31.2	
On-site Enzyme Production	18.3				18.3	
Distillation and Solids Recovery	22.3				22.3	
Production Ponds	78.0	Capital of MDP \$139.5MM	+8.4%	Capital of MDP \$151.2MM	78.0	
Inoculum Ponds	7.9				7.9	
CO ₂ Delivery	3.2				14.2	
Makeup Water Delivery & One-site Circulation	3.5				4.2	
Dewater	21.6				21.6	
Lipid Extraction and Solvent Recovery	15.1				15.1	
Lipid Purification and Upgrading	10.2				10.2	
Wastewater Treatment	49.4	Waste Treatment \$129.0MM	-45.1%	Waste Treatment \$70.8MM	0.2	
Anaerobic/Aerobic Digestion	13.6				4.6	
Boiler/Turbogenerator	66.0				66.0	
Utilities	17.7	Utilities \$17.7MM	0%	Utilities \$17.7MM	17.7	
Total Installed Equipment Cost	385.6	\$389.9MM	-11.9%	\$343.4MM	343.4	

Figure 21. Capital cost analysis for Scenarios 1 and 2

4.6.2.2. Manufacturing Cost Analysis

Compared with Scenario 1 (the baseline scenario), in which the CEP and MDP are independent production systems, the synergies in the IS design leads to more than 10% annual cost reduction in Scenarios 2–4. Scenario 4, in which *Nannochloropsis* is used as inoculum, featuring the best economic performance by a large margin to reduce the annual manufacturing cost by 10.82%.

All three IS scenarios exhibits different reductions of raw material costs, which are mainly due to the fact that the CO₂ for algae cultivation does not need to be purchased from an outsource supplier. Scenario 4 displays the smallest decrease since *Nannochloropsis* contains the smallest amount of fermentable carbohydrates after the 4-day cultivation, causing it to deliver less lipid-depleted biomass to replace corn stover for cellulosic bioethanol production than Scenarios 2 and 3. The taxes and capital costs for Scenarios 2–4 are all the same, and lower than those of Scenario 1 since the investment in wastewater treatment in the CEP plant is saved in the IS design. The cost of ammonia in the IS scenarios decreases by 1.4 million \$US/year, while the cost of the phosphorus source

remains the same, which is due to the fact that the wastewater from CEP is rich in nitrogen but contains almost no phosphorus for algae cultivation. The ammonia is only consumed for conditioning the pretreated biomass in the CEP plant. Since hexane solvent, natural gas, and hydrogen are used for the hydrodeoxygenation of crude algal lipids to produce biodiesel, the costs of these materials vary as well.

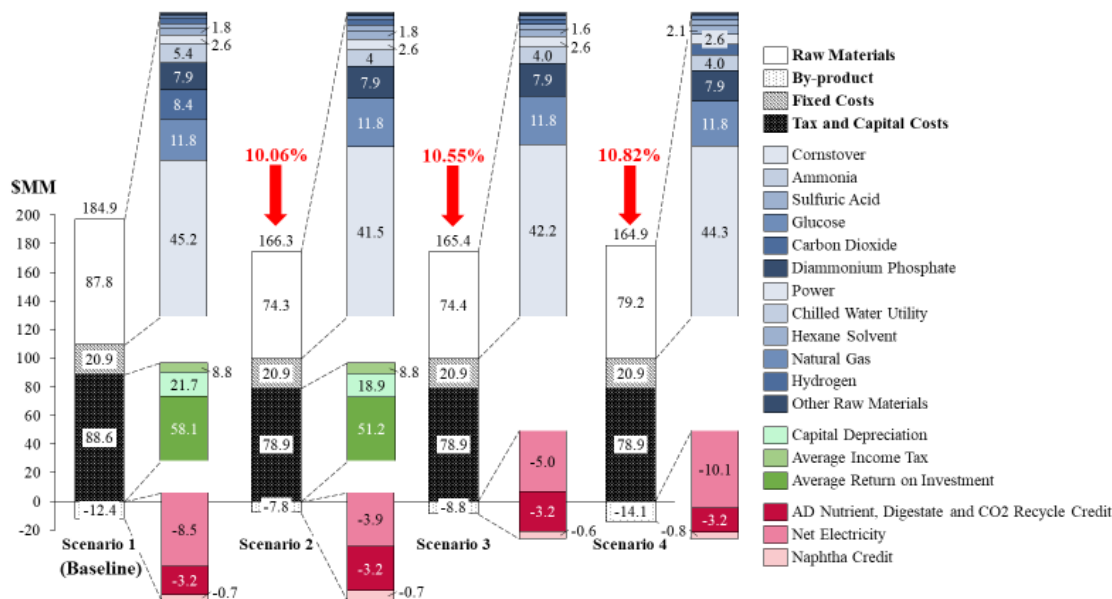


Figure 22. Manufacturing cost comparison for the 4 scenarios

The unit prices of bioethanol and biodiesel (\$US/gal) for all 4 scenarios are illustrated in Figure 23. Scenario 4 exhibits the lowest unit price for both biofuels, due to its high yield of biodiesel and overall low manufacturing cost. Compared with the baseline case, in Scenario 2, the unit prices for bioethanol and biodiesel are reduced by 8.3% and 16.2%, respectively, and the gasoline gallon equivalent (GGE) is reduced by 10.1%. The reduction in bioethanol price is mainly due to the savings in cellulosic feedstock demand and the simplification of wastewater treatment equipment, while the biodiesel cost decrease is largely due to the utilization of the CO₂ emitted during the fermentation process in CEP. Since both Scenarios 1 and 2 used *Scenedesmus* as inoculum, the results indicate that the

IS design has great potential to reduce the unit cost of biofuel production. It is worth noting that in Scenario 3, although the unit cost of biodiesel is less than the cost in the baseline scenario, it is higher than Scenarios 2 and 4. This is because *Chlorella* has a lower lipid content after cultivation, which leads to a low biodiesel yield.

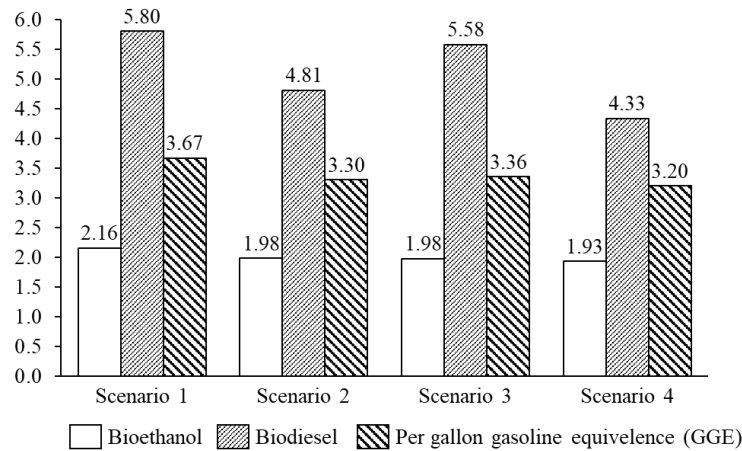


Figure 23. Comparison of the unit cost of biofuel products for the 4 scenarios

4.6.3. Environmental Impact Analysis

4.6.3.1. Carbon Dioxide Emissions

In the baseline case, the total CO₂ emission is 606,227 tons, of which combustion contributes more than half of the total. In Scenario 2, CO₂ emission is reduced by 36% compared to the baseline as a result of the CO₂ recycling for algae cultivation. It is found that the amounts of CO₂ emitted from the cultivation ponds in Scenarios 3 and 4 are slightly higher than the amounts in Scenarios 1 and 2. This is because the carbon elemental contents (TABLE XXIV) in *Chlorella* (Scenario 3) and *Nannochloropsis* (Scenario 4) are lower than that in *Scenedesmus* (Scenarios 1 and 2). For the same productivity, after a 4-day cultivation, the carbon fixed in the *Chlorella* and *Nannochloropsis* algae is less than that in *Scenedesmus*, whereas more CO₂ is emitted. Although *Chlorella* and *Nannochloropsis* have lower overall carbon content, their non-fermentable sugar and protein compositions

are higher than those of *Scenedesmus*, thus resulting in a higher CO₂ emission from combustion.

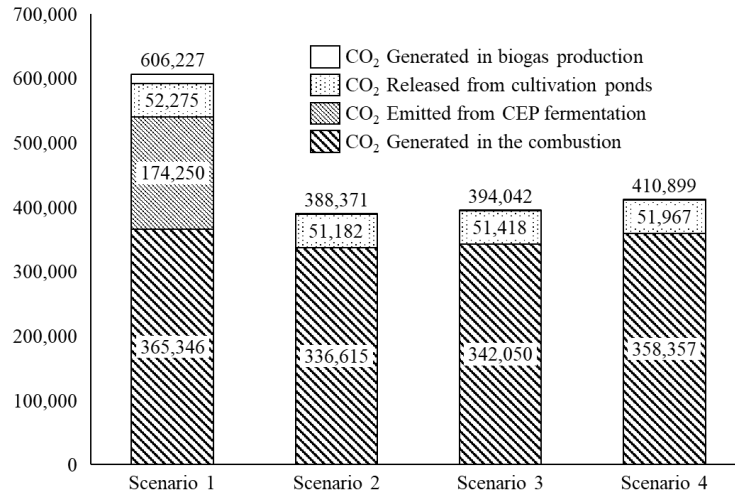


Figure 24. CO₂ emissions breakdown for the 4 scenarios

4.6.3.2. Eutrophication Potential (EP) and Acidification Potential (AP)

It is observed that the EP due to phosphorus provides the largest contribution in all four scenarios. The EP of Scenario 2 is 9.4% lower than the baseline case, indicating that the IS design can alleviate the aquatic pollution of CEP and MDP production while achieving the same biofuel yield. The eutrophication potentials from chemical oxygen demand (COD) and nitrogen (water) almost disappeared in Scenarios 2–4 because the wastewater from CEP is reused for the microalgae cultivation. It is worth noting that the EP in Scenario 4 is 29% higher than the baseline value. This is because the protein content in *Nannochloropsis* is much higher than that of either *Chlorella* or *Scenedesmus*. Thus, when the solid residues are combusted in the CHP system, more P₂O₅ and NO₂ are generated. The acidification potential variations among the four scenarios follows the same logic as the EP differences. The AP in Scenario 2 is 7.5% lower than that of the baseline. The algae species with the highest protein content, i.e., *Nannochloropsis*, exhibits the worst performance in terms of acidification.

In summary, it is interesting to discover that using *Nannochloropsis* as inoculum is most economically viable in terms of unit cost per GGE, while its negative environmental impact is the most significant. Although it is currently not practical to precisely determine the appropriate cost penalty of these impacts, this result provides some insights into the trade-off between economic viability and environmental sustainability in the CEP-MDP symbiosis system.

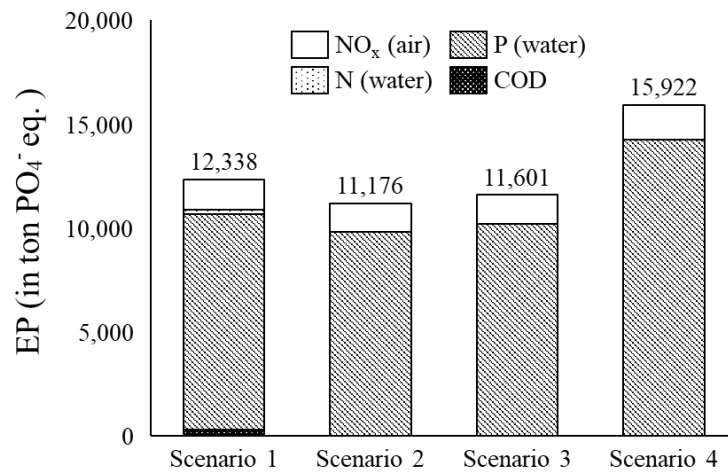


Figure 25. Comparison of EP for the 4 scenarios

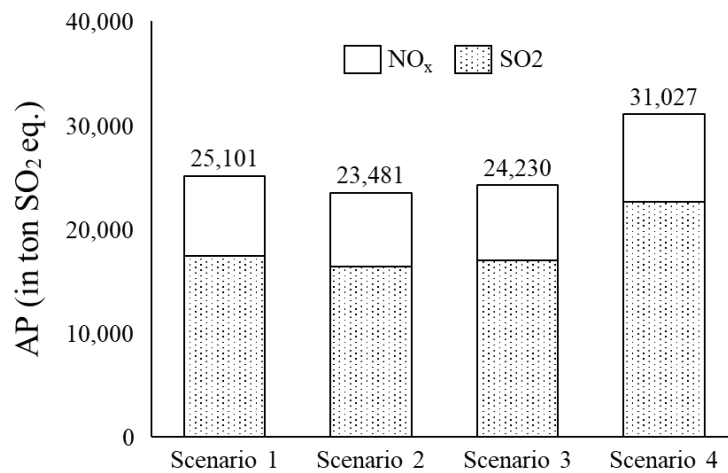


Figure 26. Comparison of AP for the 4 scenarios

4.6.4. Sensitivity Analysis

The harvest stage is one of the most important factors affecting the economic and environmental performance of the IS system. The cultivation duration alters the compositions of microalgae. In general, early-harvest, mid-harvest, and late-harvest correspond to high-protein, high carbohydrate, and high-lipid content algal biomass, respectively. While the early-harvest/high-protein scenario would most easily allow the achievement of high biomass productivity targets, the low lipid and carbon content of the biomass would be expected to lead to poor yields during downstream conversion. Alternatively, the late-harvest/high-lipid case would allow for the highest fuel yields during downstream conversion but would place additional burdens on achievable cultivation biomass productivity. In this study, the cultivation duration for the three harvest stages are assumed 2, 4, and 8 days, respectively (Davis et al., 2016).

Since the harvest stage mainly influences the composition of the algae biomass, no significant difference is expected between Scenarios 1 and 2. Therefore, the comparison is only conducted among Scenarios 2, 3, and 4. TABLE XXVII lists the compositions of *Scenedesmus*, *Chlorella*, and *Nannochloropsis* for the different harvest stages. The basis of the comparison is the target annual ethanol and biodiesel production of 61 and 9.3 million gallons, respectively, which is consistent with the baseline case. The changes in microalgae production, CO₂ cost, corn stover cost, and manufacturing are examined. The results are illustrated in Figure 27.

TABLE XXVII. COMPOSITION OF SCENEDESMUS, CHLORELLA, AND NANNOCHLOROPSIS FOR DIFFERENT HARVEST STAGES

Wt.% (dry basis)	<i>Scenedesmus</i>			<i>Chlorella</i>			<i>Nannochloropsis</i>		
Cultivation stage	Early	Mid	Late	Early	Mid	Late	Early	Mid	Late
Productivity (g/m ² /day)	35	25	15	35	25	15	35	25	15
Fermentable carbohydrates	26.2	47.8	38.2	6.8	39.2	25.2	8.2	11	9.8
Fuel-related lipids	8.3	27.4	41.2	15.2	23.6	43.3	16.8	32	63.2
Proteins	43.2	13.2	9.0	47.8	14.3	13.8	44.6	28.9	10.4
Other carbohydrates	12.8	5.0	3.9	20.7	16.0	11.2	11.9	9.0	6.6
Non-fuel related lipids	0.8	2.7	2.1	1.5	2.4	2.2	1.7	3.2	3.2
Cell mass	1.9	1.5	3.5	1.8	1.6	1.6	2.7	2.3	1.7
Ash	6.8	2.4	2.1	6.2	2.9	2.7	14.1	13.5	5.0
Total	100	100	100	100	100	100	100	100	100

For *Scenedesmus*, no change takes place after the mid-harvest strategy, which is adopted in Scenario 2. In the early harvest stage, the fuel-related lipid accumulation of *Scenedesmus* is lower than the other 2 species, and the algae production increases significantly to meet the biodiesel production target. Consequently, the CO₂ collected from fermentation is inadequate, resulting in an 18.4 million U.S. dollar increase in the outsource purchase of CO₂. In addition, it requires more cultivation ponds to produce the extra 0.122 million tons of biomass; thus, it can be expected that the capital cost for construction would also increase (not shown in Figure 27). Nonetheless, due to the high content of fermentable carbohydrates, using *Scenedesmus* as inoculum leads to a savings of nearly 3 million U.S. dollars if the early harvest is adopted. Ultimately, the early-harvest stage results in a \$50 million increase in the total manufacturing cost, which is the greatest of all compared cases.

As for *Chlorella*, its biomass production needs to be increased no matter which harvest stage is chosen. This is because during the early stage, its fuel-related lipid content is still low, while in the late stage, the lipid content increase cannot offset the productivity loss. An extra \$6.1 million is required to supplement the CO₂ shortage if the early harvest

is adopted. In total, the manufacturing costs increases by \$16.1, 5.1, and 3.9 million in order to meet the production goal for the early-, mid-, and late-harvest stages, respectively.

For *Nannochloropsis*, its fuel-related lipids are higher than those of *Scenedesmus* and *Chlorella* in all 3 harvest stages, which leads to a decrease in the biomass production requirement. Its need for extra CO₂ during the early-harvest stage is also the lowest among the 3 species. However, due to the low fermentable carbohydrate content, it requires the most corn stover to achieve the ethanol production goal. The 63.2% of fuel-related lipids ultimately results in a decrease in total manufacturing cost, which is consistent with our analysis in Section 4.6. The results in Section 4.6, however, reveals that although *Nannochloropsis* is more economically viable, its negative impact on environmental sustainability is the greatest.

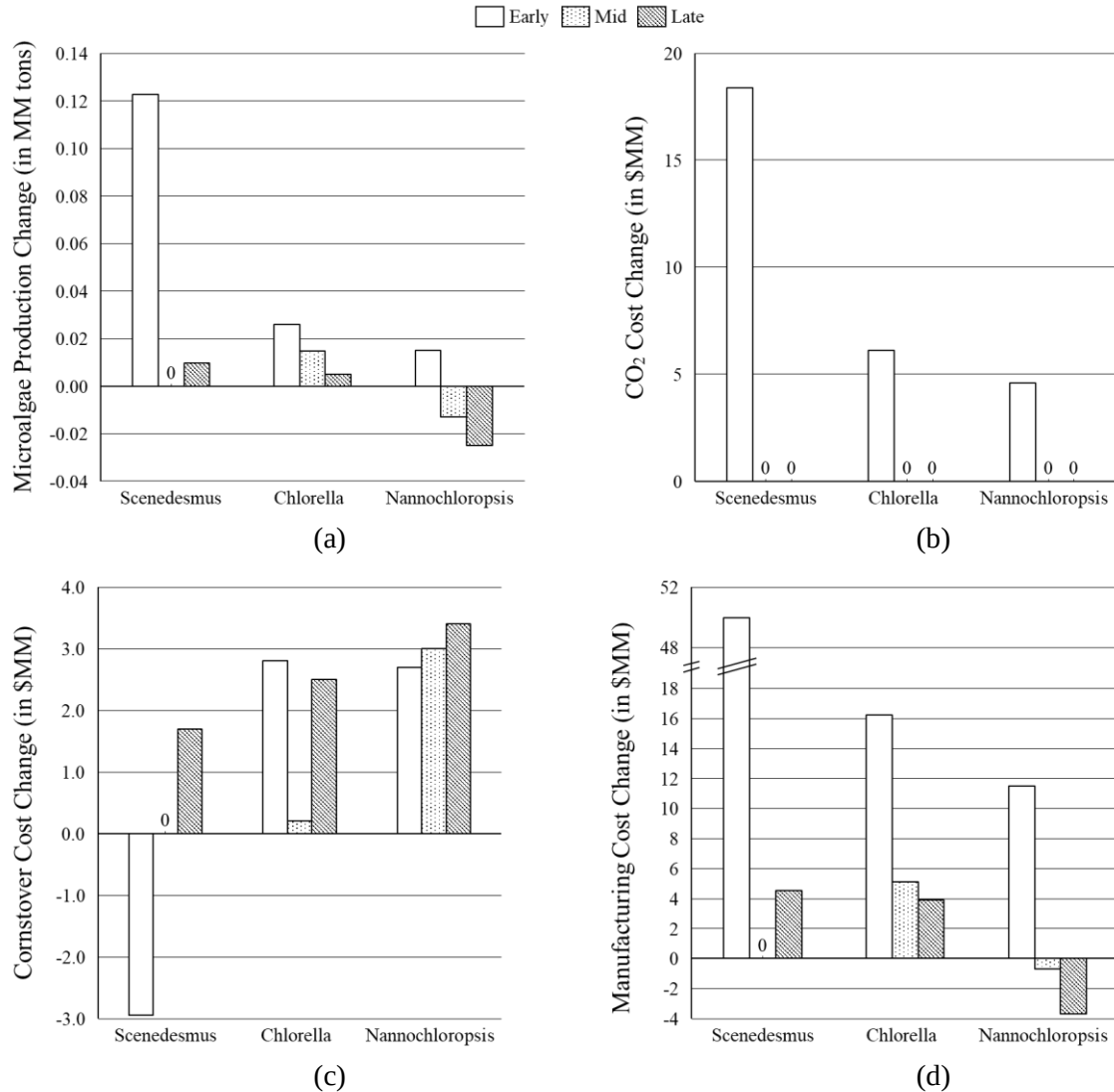


Figure 27. Production and cost performance change of (a) microalgae production, (b) CO₂ cost, (c) cost of cellulosic feedstock (corn stover), and (d) total manufacturing cost for *Scenedesmus*, *Chlorella*, and *Nannochloropsis* at early-, mid-, and late-harvest stages

A sensitivity analysis is conducted on selected parameters in order to assess their impacts on the unit cost of biofuel products, in \$/GGE (Figure 28). The CO₂ price is actually a reflection of the percentage of CO₂ purchased from outside sources. In the IS design, all the CO₂ consumed for algae cultivation is from the CEP plant, which can be viewed as ‘free’. Correspondingly, a CO₂ price equal to \$45/ton (Humbird et al., 2011a) indicates that all of the CO₂ is purchased. The results revealed that the CO₂ price exerts a significant influence, with a 4.5% of unit cost increase from the current design associated

with the maximum CO₂ price. It is also found that the cost is slightly more sensitive to glucose yield and ethanol yield from glucose than xylose yield and ethanol yield from xylose. This is probably because in the IS design we assumed that all fermentable carbohydrates are glucan, so that the proportion of glucan was higher than xylan.

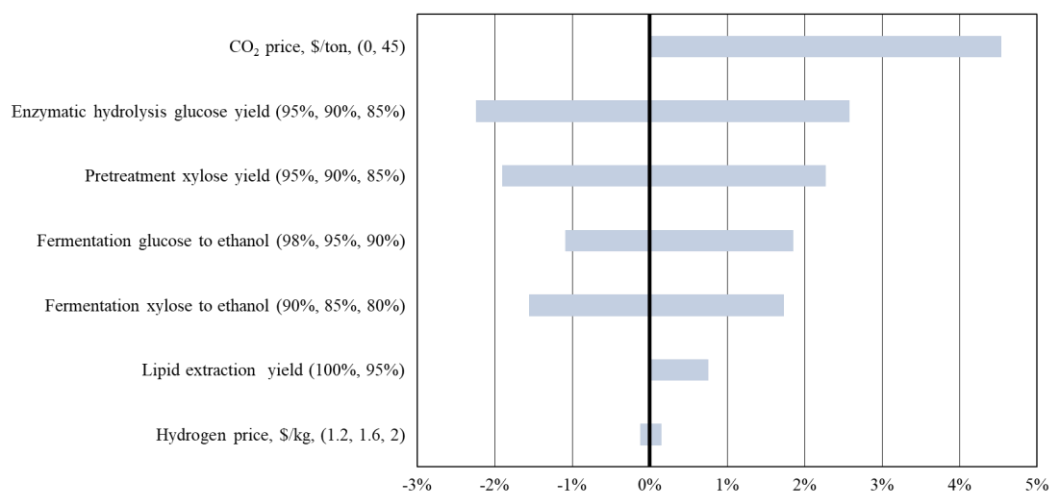


Figure 28. Sensitivity analysis of selected parameters on the unit cost of biofuels in \$/GGE

4.7. Conclusions

In this chapter, a novel IS system for co-producing the second- and third-generation biofuels is proposed to address the issues of high production cost, low biomass utilization rate, and negative environmental impact in CEP and MDP. Four scenarios, consisting of the baseline study and 3 different microalgae species, are comprehensively compared in terms of various economic and sustainability performance indicators. The total capital cost of the IS system exhibits a reduction of 11.9% compared to the standalone system due to its simpler wastewater treatment method. Manufacturing costs are more than 10% lower in all IS scenarios. The results also reveal that the IS synergies could lead to a 36% reduction in CO₂ emissions, a 9.4% decrease in EP, and a 7.5% reduction in AP when adopting the same algal inoculum. In addition, the effects of different microalgae species and cultivation

duration on the performance of the IS system are analyzed. It is discovered that using *Nannochloropsis* microalgae to produce biodiesel exhibits the best economic performance when a late-harvest strategy is adopted. It was interesting to find that although using *Nannochloropsis* is the most favorable in terms of cost, its negative impact on environmental sustainability is the most significant.

CHAPTER 5. CONCLUSIONS

5.1. Conclusions

The main objective of this dissertation is to generate new knowledge on improving sustainability and cost performance for cellulosic biofuel production from a systematic perspective. In order to achieve the objective, a novel framework that maps the interrelationships between individual process characteristics and the systematic performance of cellulosic biofuel manufacturing is established. Then, system-level models are proposed to illustrate the manufacturing cost and energy consumption. In addition, a novel waste management strategy based on the concept of industrial symbiosis is proposed. It utilizes waste materials from CEP and MDP systems to produce cellulosic biofuel and algal biofuel simultaneously.

5.2. Intellectual Contributions and Broader Impacts

The intellectual contributions of this dissertation are summarized as follows.

A system-level cellulosic biofuel manufacturing model mapping the interrelationships across multiple individual processes by introducing inter-process and intra-process decision variables is proposed. Subsequently, the system output (i.e., ethanol yield, energy consumption, and cost) can be calculated from a systematic view. This model has addressed the challenge of unclear relationships between individual process characteristics and systematic performance. In addition, the proposed systematic economic and energy models show significant potential to achieve considerable cost and energy consumption reductions. Moreover, the concept of industrial symbiosis is introduced to develop an advanced waste utilization strategy for both cellulosic and algal biofuel manufacturing. To the best of our knowledge, this research is one of the first studies to

explore the potential benefits of integrating second- and third-generation biofuels as a sustainable energy system. The synergies in the bioenergy industrial symbiosis system are proved to be viable and beneficial to enhancing economic viability, waste utilization efficiency, and environmental sustainability. The research results provide insights into achieving cost-effective and environmentally sustainable biofuel production, which can promote the adoption of advanced biofuels.

In terms of broader impact, the research outcomes will help realize energy-efficient biofuel production and enhance the sustainability of cellulosic biofuel. This research also provides a systems perspective and useful information for decision-makers to develop a cost-effective and sustainable biofuel manufacturing system. The methodology applied in this research can provide a new perspective for addressing the economic dilemma of current biofuel production and promote bioenergy development to the next stage: Biofuel Generation III+.

5.3. Future Work

The future work of this thesis is summarized as follows. The current system-level models can be developed to establish a dynamic decision-making strategy for biofuel manufacturing systems that monitors the real-time production conditions and maintains the system energy consumption and cost at a low level without ethanol yield loss. Moreover, this research can be extended to examine the lifecycle performance of the proposed industrial symbiosis bioenergy system. In addition, it is also interesting to introduce new factors into the current waste reuse design, thereby establishing a more energy-efficient, cost-effective, and environmentally friendly bioenergy industry cluster.

CITED LITERATURE

- Aden, A., Foust, T., 2009. Technoeconomic analysis of the dilute sulfuric acid and enzymatic hydrolysis process for the conversion of corn stover to ethanol. *Cellulose* 16, 535–545. <https://doi.org/10.1007/s10570-009-9327-8>
- Aden, A., Ruth, M., Ibsen, K., Jechura, J., Neeves, K., Sheehan, J., Wallace, B., Montague, L., Slayton, A., Lukas, J., 2002. Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover. Other Inf. PBD 1 Jun 2002 Medium: ED; Size: 154 pages. <https://doi.org/NREL/TP-510-32438>
- Alam, F., Mobin, S., Chowdhury, H., 2015. Third generation biofuel from Algae, in: *Procedia Engineering*. <https://doi.org/10.1016/j.proeng.2015.05.068>
- Baudry, G., Macharis, C., Vallée, T., 2018. Can microalgae biodiesel contribute to achieve the sustainability objectives in the transport sector in France by 2030? A comparison between first, second and third generation biofuels through a range-based Multi-Actor Multi-Criteria Analysis. *Energy*. <https://doi.org/10.1016/j.energy.2018.05.038>
- Bitra, V.S.P., Womac, A.R., Igathinathane, C., Miu, P.I., Yang, Y.T., Smith, D.R., Chevanan, N., Sokhansanj, S., 2009. Direct measures of mechanical energy for knife mill size reduction of switchgrass, wheat straw, and corn stover. *Bioresour. Technol.* 100, 6578–6585. <https://doi.org/10.1016/j.biortech.2009.07.069>
- Boiler-efficiency, 2018. Boiler Efficiency [WWW Document]. URL <https://www.sciencedirect.com/topics/engineering/boiler-efficiency> (accessed 5.27.20).
- Bothwell, M.K., Daughhetee, S.D., Chaua, G.Y., Wilson, D.B., Walker, L.P., 1997.

Binding capacities for *Thermomonospora fusca* E3, E4 and E5, the E3 binding domain, and *Trichoderma reesei* CBHI on Avicel and bacterial microcrystalline cellulose. *Bioresour. Technol.* 60, 169–178. [https://doi.org/10.1016/S0960-8524\(96\)00179-4](https://doi.org/10.1016/S0960-8524(96)00179-4)

Brune, G., Schoberth, S.M., Sahm, H., 1983. Growth of a strictly anaerobic bacterium on furfural (2-furaldehyde). *Appl. Environ. Microbiol.* <https://doi.org/10.1128/aem.46.5.1187-1192.1983>

Cadoche, L., López, G.D., 1989. Assessment of size reduction as a preliminary step in the production of ethanol from lignocellulosic wastes. *Biol. Wastes* 30, 153–157. [https://doi.org/10.1016/0269-7483\(89\)90069-4](https://doi.org/10.1016/0269-7483(89)90069-4)

Cai, J., He, Y., Yu, X., Banks, S.W., Yang, Y., Zhang, X., Yu, Y., Liu, R., Bridgwater, A. V., 2017. Review of physicochemical properties and analytical characterization of lignocellulosic biomass. *Renew. Sustain. Energy Rev.* <https://doi.org/10.1016/j.rser.2017.03.072>

Cardona Alzate, C.A., Sánchez Toro, O.J., 2006. Energy consumption analysis of integrated flowsheets for production of fuel ethanol from lignocellulosic biomass. *Energy* 31, 2111–2123. <https://doi.org/10.1016/j.energy.2005.10.020>

Chen, H., Zheng, Y., Zhan, J., He, C., Wang, Q., 2017. Comparative metabolic profiling of the lipid-producing green microalga *Chlorella* reveals that nitrogen and carbon metabolic pathways contribute to lipid metabolism. *Biotechnol. Biofuels.* <https://doi.org/10.1186/s13068-017-0839-4>

Chen, J., Shen, L., Shi, Q., Hong, J., Ochoa, J.J., 2019. The effect of production structure on the total CO₂ emissions intensity in the Chinese construction industry. *J. Clean.*

Prod. <https://doi.org/10.1016/j.jclepro.2018.12.203>

Chisti, Y., 2007. Biodiesel from microalgae. *Biotechnol. Adv.* <https://doi.org/10.1016/j.biotechadv.2007.02.001>

Crank, J., 1975. *the Mathematics of Diffusion*. 2nd Ed. Oxford Univ. Press. UK. [https://doi.org/10.1016/0306-4549\(77\)90072-X](https://doi.org/10.1016/0306-4549(77)90072-X)

Davis, R., Kinchin, C., Markham, J., Tan, E.C.D., Laurens, L.M.L., 2014. *Process Design and Economics for the Conversion of Algal Biomass to Biofuels : Algal Biomass Fractionation to Lipid- Products Process Design and Economics for the Conversion of Algal Biomass to Biofuels : Algal Biomass Fractionation to Lipid- and Carbohydr* NREL/TP-5100-62368.

Davis, R., Markham, J., Kinchin, C., Grundl, N., Tan, E., Humbird, D., 2016. *Process Design and Economics for the Production of Algal Biomass: Algal Biomass Production in Open Pond Systems and Processing Through Dewatering for Downstream Conversion*. *Natl. Renew. Energy Lab.* 128. <https://doi.org/10.2172/1239893>

Doherty, W.O.S., Mousavioun, P., Fellows, C.M., 2011. Value-adding to cellulosic ethanol: Lignin polymers. *Ind. Crops Prod.* <https://doi.org/10.1016/j.indcrop.2010.10.022>

Ecologycenter, 2020. *Elemental Composition of Biomolecules - Population Dynamics* [WWW Document]. URL <https://www.ecologycenter.us/population-dynamics-2/elemental-composition-of-biomolecules.html> (accessed 5.27.20).

Esteghlalian, A., Hashimoto, A.G., Fenske, J.J., Penner, M.H., 1997. Modeling and optimization of the dilute-sulfuric-acid pretreatment of corn stover, poplar and switchgrass. *Bioresour. Technol.* 59, 129–136. <https://doi.org/10.1016/S0960->

- Farrell, A.E., Plevin, R.J., Turner, B.T., Jones, A.D., O'Hare, M., Kammen, D.M., 2006. Ethanol can contribute to energy and environmental goals. *Science* (80-.). 311, 506–508. <https://doi.org/10.1126/science.1121416>
- Fockink, D.H., Maceno, M.A.C., Ramos, L.P., 2015. Production of cellulosic ethanol from cotton processing residues after pretreatment with dilute sodium hydroxide and enzymatic hydrolysis. *Bioresour. Technol.* 187, 91–96. <https://doi.org/10.1016/j.biortech.2015.03.096>
- Frankó, B., Galbe, M., Wallberg, O., 2016. Bioethanol production from forestry residues: A comparative techno-economic analysis. *Appl. Energy* 184, 727–736. <https://doi.org/10.1016/j.apenergy.2016.11.011>
- Ge, Y., Dababneh, F., Li, L., 2017. Economic Evaluation of Lignocellulosic Biofuel Manufacturing Considering Integrated Lignin Waste Conversion to Hydrocarbon Fuels. *Procedia Manuf.* <https://doi.org/10.1016/j.promfg.2017.07.037>
- Ge, Y., Li, L., 2018. System-level energy consumption modeling and optimization for cellulosic biofuel production. *Appl. Energy* 226, 935–946. <https://doi.org/10.1016/j.apenergy.2018.06.020>
- Ghosh, S.K., 2016. Biomass & Bio-waste Supply Chain Sustainability for Bio-energy and Bio-fuel Production. *Procedia Environ. Sci.* <https://doi.org/10.1016/j.proenv.2016.02.005>
- Gonela, V., Zhang, J., 2014. Design of the optimal industrial symbiosis system to improve bioethanol production. *J. Clean. Prod.* 64, 513–534. <https://doi.org/10.1016/j.jclepro.2013.07.059>

- Gonzalez-Salazar, M.A., Morini, M., Pinelli, M., Spina, P.R., Venturini, M., Finkenrath, M., Poganietz, W.R., 2014. Methodology for estimating biomass energy potential and its application to Colombia. *Appl. Energy* 136, 781–796. <https://doi.org/10.1016/j.apenergy.2014.07.004>
- Gutiérrez-Arriaga, C.G., Serna-González, M., Ponce-Ortega, J.M., El-Halwagi, M.M., 2014. Sustainable integration of algal biodiesel production with steam electric power plants for greenhouse gas mitigation. *ACS Sustain. Chem. Eng.* <https://doi.org/10.1021/sc400436a>
- Heer, D., Sauer, U., 2008. Identification of furfural as a key toxin in lignocellulosic hydrolysates and evolution of a tolerant yeast strain. *Microb. Biotechnol.* <https://doi.org/10.1111/j.1751-7915.2008.00050.x>
- House, W., 2014. The All-of-the-above Energy Strategy as A Path to Sustainable Economic Growth 1–43.
- Huang, H.J., Ramaswamy, S., Al-Dajani, W., Tschirner, U., Cairncross, R.A., 2009. Effect of biomass species and plant size on cellulosic ethanol: A comparative process and economic analysis. *Biomass and Bioenergy* 33, 234–246. <https://doi.org/10.1016/j.biombioe.2008.05.007>
- Humbird, D., Davis, R., Tao, L., Kinchin, C., Hsu, D., Aden, A., 2011a. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol. NREL Tech. Rep. NREL/LTP-5100-47764 147. <https://doi.org/10.2172/1013269>
- Humbird, D., Davis, R., Tao, L., Kinchin, C., Hsu, D., Aden, A., Schoen, P., Lukas, J., Olthof, B., Worley, M., Sexton, D., Dudgeon, D., 2011b. Process design and economics for conversion of lignocellulosic biomass to ethanol. NREL Tech. Rep.

NREL/TP-5100-51400 303, 275–3000.

IEA, 2018. Global Energy and CO2 Status Report. Oecd-Iea.

Jafri, Y., Wetterlund, E., Anheden, M., Kulander, I., Håkansson, Å., Furusjö, E., 2019. Multi-aspect evaluation of integrated forest-based biofuel production pathways: Part 2. economics, GHG emissions, technology maturity and production potentials. Energy. <https://doi.org/10.1016/j.energy.2019.02.036>

Jeon, Y.J., Svenson, C.J., Joachimsthal, E.L., Rogers, P.L., 2002. Kinetic analysis of ethanol production by an acetate-resistant strain of recombinant *Zymomonas mobilis*. Biotechnol. Lett. 24, 819–824. <https://doi.org/10.1023/A:1015546521000>

Jung, S.J., Kim, S.H., Chung, I.M., 2015. Comparison of lignin, cellulose, and hemicellulose contents for biofuels utilization among 4 types of lignocellulosic crops. Biomass and Bioenergy. <https://doi.org/10.1016/j.biombioe.2015.10.007>

Kadam, K.L., Rydholm, E.C., McMillan, J.D., 2004. Development and validation of a kinetic model for enzymatic saccharification of lignocellulosic biomass. Biotechnol. Prog. 20, 698–705. <https://doi.org/10.1021/bp034316x>

Kemppainen, A.J., Shonnard, D.R., 2008. Comparative Life-Cycle Assessments for Biomass-to-Ethanol Production from Different Regional Feedstocks. Biotechnol. Prog. 21, 1075–1084. <https://doi.org/10.1021/bp049548q>

Kennedy, J., Eberhart, R.C., Shi, Y., 2001. Swarm Intelligence. Scholarpedia 2, 1462. <https://doi.org/10.4249/scholarpedia.1462>

Kesharwani, R., Sun, Z., Dagli, C., Xiong, H., 2019. Moving second generation biofuel manufacturing forward: Investigating economic viability and environmental sustainability considering two strategies for supply chain restructuring. Appl. Energy.

<https://doi.org/10.1016/j.apenergy.2019.03.098>

Kim, S., 2002. Diffusion of sulfuric acid within lignocellulosic biomass particles and its impact on dilute-acid pretreatment. *Bioresour. Technol.* 83, 165–171.

[https://doi.org/10.1016/S0960-8524\(01\)00197-3](https://doi.org/10.1016/S0960-8524(01)00197-3)

Ko, C.H., Yang, B.Y., Lin, L.D., Chang, F.C., Chen, W.H., 2020. Impact of pretreatment methods on production of bioethanol and nanocrystalline cellulose. *J. Clean. Prod.*

<https://doi.org/10.1016/j.jclepro.2019.119914>

Koopman, F., Wierckx, N., De Winde, J.H., Ruijsenaars, H.J., 2010. Identification and characterization of the furfural and 5-(hydroxymethyl)furfural degradation pathways of *Cupriavidus basilensis* HMF14. *Proc. Natl. Acad. Sci. U. S. A.*

<https://doi.org/10.1073/pnas.0913039107>

Kopania, E., Wietecha, J., Ciechańska, D., 2012. Studies on isolation of cellulose fibres from waste plant biomass. *Fibres Text. East. Eur.*

Kumar, P., Barrett, D.M., Delwiche, M.J., Stroeve, P., 2009. Methods for pretreatment of lignocellulosic biomass for efficient hydrolysis and biofuel production. *Ind. Eng. Chem. Res.* <https://doi.org/10.1021/ie801542g>

Laurens, L.M.L., Van Wychen, S., McAllister, J.P., Arrowsmith, S., Dempster, T.A., McGowen, J., Pienkos, P.T., 2014. Strain, biochemistry, and cultivation-dependent measurement variability of algal biomass composition. *Anal. Biochem.*

<https://doi.org/10.1016/j.ab.2014.02.009>

Leksawasdi, N., Joachimsthal, E.L., Rogers, P.L., 2001. Mathematical modelling of ethanol production from glucose/xylose mixtures by recombinant *Zymomonas mobilis*. *Biotechnol. Lett.* 23, 1087–1093. <https://doi.org/10.1023/A:1010599530577>

- Li, L., Ge, Y., 2017. System-level cost evaluation for economic viability of cellulosic biofuel manufacturing. *Appl. Energy*. <https://doi.org/10.1016/j.apenergy.2017.06.074>
- Li, L., Sun, Z., Yao, X., Wang, D., 2016. Optimal production scheduling for energy efficiency improvement in biofuel feedstock preprocessing considering work-in-process particle separation. *Energy* 96, 474–481. <https://doi.org/10.1016/j.energy.2015.12.063>
- Liu, G., Zhang, J., Bao, J., 2016. Cost evaluation of cellulase enzyme for industrial-scale cellulosic ethanol production based on rigorous Aspen Plus modeling. *Bioprocess Biosyst. Eng.* 39, 133–140. <https://doi.org/10.1007/s00449-015-1497-1>
- Liu, Q., Jiang, P., Zhao, J., Zhang, B., Bian, H., Qian, G., 2011. Life cycle assessment of an industrial symbiosis based on energy recovery from dried sludge and used oil. *J. Clean. Prod.* 19, 1700–1708. <https://doi.org/10.1016/j.jclepro.2011.06.013>
- Lynd, L.R., 2017. The grand challenge of cellulosic biofuels. *Nat. Biotechnol.* 35, 912–915. <https://doi.org/10.1038/nbt.3976>
- Mafe, O.A.T., Davies, S.M., Hancock, J., Du, C., 2015. Development of an estimation model for the evaluation of the energy requirement of dilute acid pretreatments of biomass. *Biomass Bioenergy* 72, 28–38. <https://doi.org/10.1016/j.biombioe.2014.11.024>
- Mani, S., Tabil, L.G., Sokhansanj, S., 2004. Grinding performance and physical properties of wheat and barley straws, corn stover and switchgrass. *Biomass and Bioenergy* 27, 339–352. <https://doi.org/10.1016/j.biombioe.2004.03.007>
- Manochio, C., Andrade, B.R., Rodriguez, R.P., Moraes, B.S., 2017. Ethanol from biomass: A comparative overview. *Renew. Sustain. Energy Rev.*

<https://doi.org/10.1016/j.rser.2017.05.063>

Martin, M., Eklund, M., 2011. Improving the environmental performance of biofuels with industrial symbiosis. *Biomass and Bioenergy*.

<https://doi.org/10.1016/j.biombioe.2011.01.016>

Maurya, D.P., Singla, A., Negi, S., 2015. An overview of key pretreatment processes for biological conversion of lignocellulosic biomass to bioethanol. *3 Biotech* 5, 597–609.

<https://doi.org/10.1007/s13205-015-0279-4>

Mcaloon, A., Taylor, F., Yee, W., Ibsen, K., Wooley, R., 2000. Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic Feedstocks Determining the Cost of Producing Ethanol from Corn Starch and Lignocellulosic. *Agriculture* 44.

<https://doi.org/NREL/TP-580-28893>

Mesa, L., Martínez, Y., Barrio, E., González, E., 2017. Desirability function for optimization of Dilute Acid pretreatment of sugarcane straw for ethanol production and preliminary economic analysis based in three fermentation configurations. *Appl. Energy* 198, 299–311. <https://doi.org/10.1016/J.APENERGY.2017.03.018>

Miao, Z., Grift, T.E., Hansen, A.C., Ting, K.C., 2011. Energy requirement for comminution of biomass in relation to particle physical properties. *Ind. Crops Prod.*

33, 504–513. <https://doi.org/10.1016/j.indcrop.2010.12.016>

Min, M., Wang, L., Li, Y., Mohr, M.J., Hu, B., Zhou, W., Chen, P., Ruan, R., 2011. Cultivating chlorella sp. in a pilot-scale photobioreactor using centrate wastewater for microalgae biomass production and wastewater nutrient removal. *Appl. Biochem. Biotechnol.*

<https://doi.org/10.1007/s12010-011-9238-7>

Ou, X., Zhang, X., Chang, S., Guo, Q., 2009. Energy consumption and GHG emissions of

- six biofuel pathways by LCA in (the) People's Republic of China. *Appl. Energy* 86, S197–S208. <https://doi.org/10.1016/J.APENERGY.2009.04.045>
- Patzek, T.W., 2004. Thermodynamics of the Corn-Ethanol Biofuel Cycle, *Critical Reviews in Plant Sciences*. <https://doi.org/10.1080/07352680490886905>
- Phanphanich, M., Mani, S., 2011. Impact of torrefaction on the grindability and fuel characteristics of forest biomass. *Bioresour. Technol.* 102, 1246–1253. <https://doi.org/10.1016/j.biortech.2010.08.028>
- Poling, B.E., Thomson, G.H., Friend, D.G., Rowley, R.L., Wilding, W.V., 2007. Perry's Chemical Engineers' Handbook, Perry's Chemical Engineers' Handbook. <https://doi.org/10.1036/0071511253>
- power-eng, 2007. Steam Generator Efficiency | Power Engineering [WWW Document]. URL <https://www.power-eng.com/2007/06/01/steam-generator-efficiency/#gref> (accessed 5.27.20).
- Reuters, 2017. DuPont to sell cellulosic ethanol plant in blow to biofuel - Reuters [WWW Document]. URL <https://www.reuters.com/article/us-dowdupontethanol/dupont-to-sell-cellulosic-ethanol-plant-in-blowto-biofuel-idUSKBN1D22T5> (accessed 5.30.20).
- Rodionova, M. V., Poudyal, R.S., Tiwari, I., Voloshin, R.A., Zharmukhamedov, S.K., Nam, H.G., Zayadan, B.K., Bruce, B.D., Hou, H.J.M., Allakhverdiev, S.I., 2017. Biofuel production: Challenges and opportunities. *Int. J. Hydrogen Energy*. <https://doi.org/10.1016/j.ijhydene.2016.11.125>
- Rodríguez-Aragón, L.J., López-Fidalgo, J., 2005. Optimal designs for the Arrhenius equation. *Chemom. Intell. Lab. Syst.* <https://doi.org/10.1016/j.chemolab.2004.06.007>
- Schmer, M.R., Vogel, K.P., Mitchell, R.B., Perrin, R.K., 2008. Net energy of cellulosic

- ethanol from switchgrass. *Proc. Natl. Acad. Sci.* 105, 464–469.
<https://doi.org/10.1073/pnas.0704767105>
- Silva Ortiz, P., de Oliveira, S., 2014. Exergy analysis of pretreatment processes of bioethanol production based on sugarcane bagasse. *Energy* 76, 130–138.
<https://doi.org/10.1016/j.energy.2014.04.090>
- Sinnott, M., 2007. *Carbohydrate Chemistry and Biochemistry: Structure and Mechanism*. Royal Society of Chemistry.
- Sitaraman, H., Kuhn, E.M., Nag, A., Sprague, M.A., Tucker, M.P., Stickel, J.J., 2015. Multiphysics modeling and simulation of high-solids dilute-acid pretreatment of corn stover in a steam-explosion reactor. *Chem. Eng. J.* 268, 47–59.
<https://doi.org/10.1016/j.cej.2015.01.020>
- Somerville, C., Youngs, H., Taylor, C., Davis, S.C., Long, S.P., 2010. Feedstocks for lignocellulosic biofuels. *Science* (80-.). <https://doi.org/10.1126/science.1189268>
- Song, C., Xie, M., Qiu, Y., Liu, Q., Sun, L., Wang, K., Kansha, Y., 2019. Integration of CO₂ absorption with biological transformation via using rich ammonia solution as a nutrient source for microalgae cultivation. *Energy*.
<https://doi.org/10.1016/j.energy.2019.05.039>
- Sudiyani, Y., Styarini, D., Triwahyuni, E., Sudiyarmanto, Sembiring, K.C., Aristiawan, Y., Abimanyu, H., Han, M.H., 2013. Utilization of biomass waste empty fruit bunch fiber of palm oil for bioethanol production using pilot - Scale unit, in: *Energy Procedia*.
<https://doi.org/10.1016/j.egypro.2013.05.005>
- Tanaka, T., 1966. Comminution laws: Several Probabilities. *Ind. Eng. Chem. Process Des. Dev.* 5, 353–358. <https://doi.org/10.1021/i260020a001>

- Tao, L., Tan, E.C.D., McCormick, R., Zhang, M., Aden, A., He, X., Zigler, B.T., 2014. Techno-economic analysis and life-cycle assessment of cellulosic isobutanol and comparison with cellulosic ethanol and n-butanol. *Biofuels, Bioprod. Biorefining*. <https://doi.org/10.1002/bbb.1431>
- Tatsumoto, K., Baker, J.O., Tucker, M.P., Oh, K.K., Mohagheghi, A., Grohmann, K., Hlmmel, M.E., 1988. Digestion of pretreated aspen substrates - Hydrolysis rates and adsorptive loss of cellulase enzymes. *Appl. Biochem. Biotechnol.* <https://doi.org/10.1007/BF02930823>
- Tian, S., Zhu, W., Gleisner, R., Pan, X.J., Zhu, J.Y., 2011. Comparisons of SPORL and dilute acid pretreatments for sugar and ethanol productions from aspen. *Biotechnol. Prog.* 27, 419–427. <https://doi.org/10.1002/btpr.545>
- U.S. Congress, 2007. Energy independence and security act of 2007. Public Law 1–311. <https://doi.org/papers2://publication/uuid/364DB882-E966-450B-959F-AEAD6E702F42>
- UNCTAD, 2016. Second generation biofuel markets: satet of play, trade and developing country perspectives. United Nations Conf. Trade Dev.
- UNEP/SETAC, 2005. Life Cycle approaches: The road from analysis to practice, Assessment.
- Velásquez-Arredondo, H.I., Ruiz-Colorado, A.A., De Oliveira, S., 2010. Ethanol production process from banana fruit and its lignocellulosic residues: Energy analysis. *Energy* 35, 3081–3087. <https://doi.org/10.1016/j.energy.2010.03.052>
- Vidal, B.C., Dien, B.S., Ting, K.C., Singh, V., 2011. Influence of feedstock particle size on lignocellulose conversion - A review. *Appl. Biochem. Biotechnol.* 164, 1405–1421.

<https://doi.org/10.1007/s12010-011-9221-3>

Voragen, A.G.J., 1998. Technological aspects of functional food-related carbohydrates.

Trends Food Sci. Technol. [https://doi.org/10.1016/S0924-2244\(98\)00059-4](https://doi.org/10.1016/S0924-2244(98)00059-4)

Wang, M., Wu, M., Huo, H., 2007. Life-cycle energy and greenhouse gas emission impacts of different corn ethanol plant types. Environ. Res. Lett. 2.

<https://doi.org/10.1088/1748-9326/2/2/024001>

Wolfrum, E.J., Sluiter, A.D., 2009. Improved multivariate calibration models for corn stover feedstock and dilute-acid pretreated corn stover. Cellulose 16, 567–576.

<https://doi.org/10.1007/s10570-009-9320-2>

Wooley, R., Ruth, M., Sheehan, J., Majdeski, H., Galvez, A., 1999. Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis Current and Futuristic Scenarios Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current D. Contract 132. <https://doi.org/NREL/TP-510-32438>

Yalkowsky, S.H., He, Y., 2003. Handbook of Aqueous Solubility Data, CRC Press. <https://doi.org/10.1017/CBO9781107415324.004>

Yarbrough, J.M., Zhang, R., Mittal, A., Vander Wall, T., Bomble, Y.J., Decker, S.R., Himmel, M.E., Ciesielski, P.N., 2017. Multifunctional Cellulolytic Enzymes Outperform Processive Fungal Cellulases for Coproduction of Nanocellulose and Biofuels. ACS Nano 11, 3101–3109. <https://doi.org/10.1021/acsnano.7b00086>

You, F., Tao, L., Graziano, D.J., Snyder, S.W., 2012. Optimal design of sustainable cellulosic biofuel supply chains: Multiobjective optimization coupled with life cycle assessment and input-output analysis. AIChE J. 58, 1157–1180.

<https://doi.org/10.1002/aic.12637>

- You, Y., Wu, B., Yang, Y.W., Wang, Y.W., Liu, S., Zhu, Q.L., Qin, H., Tan, F.R., Ruan, Z.Y., Ma, K.D., Dai, L.C., Zhang, M., Hu, G.Q., He, M.X., 2017. Replacing process water and nitrogen sources with biogas slurry during cellulosic ethanol production. *Biotechnol. Biofuels*. <https://doi.org/10.1186/s13068-017-0921-y>
- Yu, M., Zhang, Y., Tang, I.-C., Yang, S.-T., 2011. Metabolic engineering of *Clostridium tyrobutyricum* for n-butanol production. *Metab. Eng.* 13, 373–382. <https://doi.org/10.1016/j.ymben.2011.04.002>
- Yu, T.E., English, B.C., He, L., Larson, J.A., Calcagno, J., Fu, J.S., Wilson, B., 2016. Analyzing Economic and Environmental Performance of Switchgrass Biofuel Supply Chains. *Bioenergy Res.* <https://doi.org/10.1007/s12155-015-9699-6>
- Zhang, Y.H.P., Lynd, L.R., 2004. Toward an aggregated understanding of enzymatic hydrolysis of cellulose: Noncomplexed cellulase systems. *Biotechnol. Bioeng.* <https://doi.org/10.1002/bit.20282>
- Zheng, J., Tashiro, Y., Wang, Q., Sonomoto, K., 2015. Recent advances to improve fermentative butanol production: Genetic engineering and fermentation technology. *J. Biosci. Bioeng.* 119, 1–9. <https://doi.org/10.1016/J.JBIOOSC.2014.05.023>

VITA

Education

MS (2015), Department of Mechanical Engineering, **Purdue University Northwestern (PUN)**, Hammond, IN, USA.

BE (2013), School of Aerospace Engineering, **Beijing Institute of Technology (BIT)**, Beijing, China.

Published Journal papers

1. **Yuntian Ge** and Lin Li, "System-level energy consumption modeling and optimization for cellulosic biofuel production". *Applied Energy*, 226 (2018): 935-948.
2. Lin Li and **Yuntian Ge**, "System-level cost evaluation for economic viability of cellulosic biofuel manufacturing." *Applied Energy*, 203 (2017): 711-722.
3. **Yuntian Ge**, Lin Li, and Yong Wang. "Modeling of Bernoulli production line with the rework loop for transient and steady-state analysis." *Journal of Manufacturing Systems*, 44 (2017):22-41.
4. Yukan Hou, **Yuntian Ge**, Lin Li, Yuan Li and Shoushan Jiang A new modeling method for both transient and steady-state analyses of inhomogeneous assembly systems. *Journal of Manufacturing Systems*, 49 (2018): 46-60.
5. Yukan Hou, **Yuntian Ge**, Yuan Li and Shoushan Jiang, "Modeling of Assembly Systems with Complex Structures for Transient and Steady-State Throughput Analysis". *Assembly Automation*, 39(2019):262-271.
6. Xiaolin Chu, **Yuntian Ge**, Xue Zhou, Lin Li, and Dong Yang, "Modeling and Analysis of Electric Vehicle-Power Grid-Manufacturing Facility (EPM) Energy Sharing System under Time-of-Use Electricity Tariff", *Sustainability*, 12(2020): 4836.

Submitted journal papers

1. **Yuntian Ge**, Lingxiang Yun, and Lin Li, “Modeling and Economic Optimization of Cellulosic Biofuel Supply Chain Considering Multiple Conversion Pathways”, *Applied Energy*, under review.
2. **Yuntian Ge**, Minkun Xiao, and Lin Li, “A novel industrial symbiosis design of cellulosic ethanol and microalgae biofuel production: analysis of environmental sustainability and integration potentials”, *Journal of Cleaner Production*, under review.
3. Shuaiyin Ma, Yingfeng Zhang, Jingxiang Lv, **Yuntian Ge**, Haidong Yang, and Lin Li, “Big data driven predictive production planning for energy-intensive manufacturing industries”, *Energy*, under review.
4. Lingxiang Yun; **Yuntian Ge**; Lin Li, and Jiawei Zhang, “Integrated Modeling and Study of Production Systems and Material Handling Systems with an Analytically Solvable Solution”, *Journal of Manufacturing Systems*, under review.

Published conference papers

1. **Yuntian Ge**, Fadwa Dababneh, and Lin Li. "Economic Evaluation of Lignocellulosic Biofuel Manufacturing Considering Integrated Lignin Waste Conversion to Hydrocarbon Fuels." *45th SME North American Manufacturing Research Conference, (NAMRC 45)*, LA, USA. *Procedia Manufacturing* 10 (2017): 112-122.
2. **Yuntian Ge**, and Xiuling Wang. "Yawed Effect on Wind Turbine Near Wake." *ASME 2014 International Mechanical Engineering Congress and Exposition (ASME-IMECE)*. American Society of Mechanical Engineers, 2014.
3. **Yuntian Ge**, Rui Zhang, and Xiuling Wang. "3D Wind Field Construction for Suburban Environment by Parallel Computational Fluid Dynamics Techniques." *ASME 2013 International Mechanical Engineering Congress and Exposition (ASME-IMECE)*. American Society of Mechanical Engineers, 2013.

APPENDIX

Elsevier Copyright Permission Policy Excerpt

(<https://www.elsevier.com/about/policies/copyright>)

Authors can use their articles, in full or in part, for a wide range of scholarly, non-commercial purposes as outlined below:

- Use by an author in the author's classroom teaching (including distribution of copies, paper or electronic)
- Distribution of copies (including through e-mail) to known research colleagues for their personal use (but not for Commercial Use)
- Inclusion in a thesis or dissertation (provided that this is not to be published commercially)
- Use in a subsequent compilation of the author's works
- Extending the Article to book-length form
- Preparation of other derivative works (but not for Commercial Use)
- Otherwise using or re-using portions or excerpts in other works
- These rights apply for all Elsevier authors who publish their article as either a subscription article or an open access article. In all cases we require that all Elsevier authors always include a full acknowledgement and, if appropriate, a link to the final published version hosted on Science Direct.