VALORIZATION OF SUGARCANE BAGASSE IN THAILAND: AN ECONOMIC ANALYSIS OF BIO-ETHANOL RECOVERY VIA THE ORGANOSOLV METHOD

SUPHALERK KHAOWDANG

A Dissertation Submitted to University of Phayao
in Partial Fulfillment of the Requirements
for the Doctor of Philosophy Degree in Environmental Technology and Management
October 2025

การเพิ่มมูลค่ากากอ้อยในประเทศไทย: การวิเคราะห์เชิงเศรษฐศาสตร์ของการผลิตไบโอเอทานอลด้วยวิธีออร์กาโนซอลฟ์

ศุภฤกษ์ ขาวแดง

วิทยานิพนธ์เสนอมหาวิทยาลัยพะเยา เพื่อเป็นส่วนหนึ่งของการศึกษา
หลักสูตรปริญญาปรัชญาดุษฎีบัณฑิต
สาขาวิชาเทคโนโลยีและการจัดการสิ่งแวดล้อม
ตุลาคม 2568

VALORIZATION OF SUGARCANE BAGASSE IN THAILAND: AN ECONOMIC ANALYSIS OF BIO-ETHANOL RECOVERY VIA THE ORGANOSOLV METHOD

SUPHALERK KHAOWDANG

A Dissertation Submitted to University of Phayao
in Partial Fulfillment of the Requirements
for the Doctor of Philosophy Degree in Environmental Technology and Management
October 2025

Dissertation

Title

Valorization of Sugarcane Bagasse in Thailand: An Economic Analysis of Bio-ethanol Recovery via the Organosolv Method

Submitted by SUPHALERK KHAOWDANG

Approved in partial fulfillment of the requriements for the
Doctor of Philosophy Degree in Environmental Technology and Management
University of Phayao

Approved by

.... Chairman
(Assistant Professor Dr. Surachai Wongcharee , Ph.D.)
.... Advisor
(Associate Professor Dr. Torpong Kreetachat , D.Eng.)
.... Co Advisor
(Associate Professor Dr. Saksit Imman , Ph.D.)
.... Co Advisor
(Assistant Professor Dr. Nopparat Suriyachai , Ph.D.)
.... Examiner
(Assistant Professor Dr. Nathiya Kreetachat , D.Eng.)
.... Dean of School of Energy and Environment
(Associate Professor Dr. Torpong Kreetachat , D.Eng.)

Title: VALORIZATION OF SUGARCANE BAGASSE IN THAILAND: AN ECONOMIC ANALYSIS OF BIO-ETHANOL RECOVERY VIA THE ORGANOSOLV METHOD

Author: Suphalerk Khaowdang, Dissertation: Ph.D (Environmental Technology and Management), University of Phayao, 2025

Advisor: Associate Professor Dr. Torpong Kreetachat , D.Eng. Co-advisor Associate Professor Dr.Saksit Imman , Ph.D. Assistant Professor Dr.Nopparat Suriyachai , Ph.D.

Keywords: Lignocellulosic biomass, Organosolv pretreatment, Process simulation, Co-product utilization, Economic feasibility

ABSTRACT

A comprehensive techno-economic assessment was undertaken to determine the viability of bioethanol production from sugarcane bagasse in Thailand through organosolv fractionation, incorporating three distinct catalytic systems: sulfuric acid, formic acid, and sodium methoxide. Rigorous process simulations were executed using Aspen Plus, facilitating the derivation of detailed mass and energy balances, which served as the foundational input for downstream cost modeling. Economic performance metrics, including the total annualized cost and minimum ethanol selling price, were systematically quantified for each scenario. Among the evaluated configurations, the formic acid-catalyzed organosolv system exhibited superior techno-economic attributes, achieving the lowest unit production costs of 1.14 USD/L for ethanol and 1.84 USD/kg for lignin, corresponding to an estimated ethanol selling price of approximately 1.14 USD/L. This favorable outcome was attained with only moderate capital intensity, indicating a well-balanced trade-off between operational efficiency and investment burden. Conversely, the sodium methoxide-based process configuration imposed the highest economic burden, with a TAC of 15.27 million USD/year, culminating in a markedly elevated MESP of 5.49 USD/kg (approximately 4.33 USD/L). The sulfuric acid-driven system demonstrated effective delignification performance. Sensitivity analysis revealed that reagent procurement costs exert the greatest impact on TAC variation, highlighting chemical expenditure as the key economic driver. These findings emphasize the critical role of solvent choice, catalytic performance, and process integration in improving the cost-efficiency of lignocellulosic ethanol production. Among the examined options, the formic acid-based organosolv process stands out as the most economically viable for large-scale implementation within Thailand’s bioeconomy.

ACKNOWLEDGEMENT

This doctoral dissertation represents a significant step in enhancing the research capabilities and academic development of the author. It marks a crucial milestone in the journey toward becoming a professional researcher. The completion of this study would not have been possible without the generous support, guidance, and encouragement received from various individuals and institutions.

First and foremost, I would like to express my sincere gratitude to the University of Phayao and the Faculty of Energy and Environment, University of Phayao, for providing essential research facilities, resources, and a supportive academic environment that enabled the successful execution of this research project.

I am deeply grateful to Assoc. Prof. Dr. Torpong Kreetachat, Dean of the Faculty of Energy and Environment, University of Phayao, for his continuous academic and administrative support, as well as his inspirational leadership. His guidance has greatly contributed to the refinement of my research direction and has opened up valuable opportunities for academic growth, critical thinking, and practical problem-solving throughout the course of this study.

I would like to extend my heartfelt appreciation to my advisor, Assoc. Prof. Dr. Saksit Imman, and co-advisor, Asst. Prof. Dr. Nopparat Suriyachai, for their insightful guidance, invaluable suggestions, and constructive feedback throughout every stage of this dissertation. Their academic rigor, encouragement, and dedication have been instrumental in shaping the quality and depth of this research.

Special thanks are also due to Assoc. Prof. Dr. Santi Chuetor, from the Department of Chemical Engineering, Faculty of Engineering, King Mongkut's University of Technology North Bangkok, for his technical advice and for sharing his expertise in biomass process simulation using Aspen Plus. His contribution played a vital role in enhancing the technical foundation and practical implementation of this research model.

Finally, I would like to express my deepest appreciation to my beloved family. Their unwavering support, understanding, and encouragement have been the emotional cornerstone that sustained me through the challenges of this academic journey. Their belief in me has been a constant source of strength and inspiration.

I humbly acknowledge the kindness and support of all those mentioned above, and I offer my heartfelt thanks.

Suphalerk Khaowdang

LIST OF CONTENTS

LIST OF TABLES

Page

LIST OF FIGURES

Page

CHAPTER 1

INTRODUCTION

Rationale and Significance of the Study

At present, the world is facing a critical energy crisis due to the depletion of natural fuel resources, particularly non-renewable energy sources such as crude oil and natural gas. These fuels serve as the primary energy sources for global economic and transportation sectors. This situation highlights the imbalance between the limited availability of energy reserves and the continuously rising demand for energy driven by population and economic growth. Consequently, this leads to significant risks in energy security at both national and global levels, especially for countries that heavily rely on energy imports, such as Thailand.

According to the Energy Policy and Planning Office (EPPO), Ministry of Energy, Thailand's final commercial energy consumption in 2023 averaged approximately 2,007 thousand barrels of oil equivalent per day, representing an increase of 0.8% compared to the previous year. This growth reflects the recovery of economic and service sector activities following the gradual easing of the COVID-19 pandemic, particularly in the tourism industry, which directly impacts energy demand in the transportation sector. For instance, the consumption of aviation fuel increased significantly by 50.0% compared to 2022, driven by a substantial rise in both domestic and international tourist arrivals [1].

In terms of energy consumption structure, refined petroleum products remain the most consumed energy source. In 2023, daily consumption of refined oil was approximately 153 million liters, an increase of 0.7% from 2022. The main contributors to this increase included gasoline, aviation fuel, and liquefied petroleum gas (LPG), while the consumption of diesel and fuel oil declined. Nevertheless, Thailand still relies heavily on the importation of refined petroleum. In 2023, the average daily import volume was 11 million liters, a decrease of 8.5% from the previous year. This may indicate improvements in domestic refining capacity or be influenced by global economic conditions and market prices.

This situation underscores the challenges Thailand faces in managing sustainable energy security, particularly in reducing reliance on imported energy and developing domestic renewable energy sources to meet the increasing future energy demand.

The use of fossil fuels such as petroleum, natural gas, and coal, although long regarded as the world's primary energy sources, has significantly impacted the environment. These impacts include greenhouse gas emissions, particulate matter, and various other pollutants. Furthermore, fossil fuel prices tend to rise continuously due to uncertainties in production sources and geopolitical tensions in different regions. As a result, many countries have increasingly turned their attention to the development and promotion of clean and sustainable alternative energy sources.

In Thailand, the energy development direction has been outlined in the Alternative Energy Development Plan 2015–2036 (AEDP2015), which emphasizes three key aspects: Energy Security, focusing on diversifying energy sources to reduce dependence on imported energy; Economy, promoting efficient energy use, cost reduction, and appropriate energy pricing structures; and Ecology, which supports the domestic production of renewable energy and the adoption of clean technologies to mitigate environmental impacts [2].

Thailand is an agricultural country with an abundance of agricultural residues, such as rice straw, sugarcane bagasse, corn cobs, and oil palm residues. These materials are classified as lignocellulosic biomass and can be efficiently converted into biofuels such as bioethanol. Due to their high cellulose and sugar content, they can be processed at a lower cost compared to food-based sugar sources such as corn or cassava [3], [4]. Among these residues, sugarcane bagasse a byproduct of the sugar industry contains a high proportion of cellulose, along with hemicellulose and lignin. These components can be pretreated and biologically hydrolyzed into fermentable sugars, which are then converted into ethanol using microorganisms such as *Saccharomyces cerevisiae*, a common yeast used in fermentation processes [5]. The conventional bioethanol production process from lignocellulosic biomass comprises four principal stages: (1) pretreatment, (2) enzymatic hydrolysis (saccharification), (3) fermentation, and (4) product recovery and purification. This process is inherently complex and involves a series of interdependent operations conducted in a continuous or semi-continuous manner. It commences with the sourcing and transportation of lignocellulosic feedstock, followed by pretreatment to increase the accessibility of cellulose and hemicellulose to enzymatic action. Subsequently, polysaccharides are enzymatically hydrolyzed into fermentable sugars, which are then converted into ethanol through microbial fermentation. The resulting ethanol is recovered and purified to meet fuel-grade specifications. In addition to the core processing steps, the system requires effective management of products, by products, and waste streams. Moreover, the process depends on a wide range of inputs, including labor, equipment, utilities, and chemical reagents, all of which must be carefully integrated to ensure technical and economic feasibility [6], [7].

Although the production of bioethanol from biomass has been extensively studied at the laboratory scale, there are still limitations in scaling up the process to the industrial level, particularly in terms of appropriate process design and economic feasibility assessment. This study aims to develop a mathematical model to investigate the optimal conditions for bioethanol production from sugarcane bagasse. The simulation and analysis focus on the pretreatment, saccharification, and simultaneous saccharification and fermentation (SSF) stages. In addition, a techno economic evaluation is conducted to provide insights and guidelines for the development of pilot scale or industrial scale bioethanol production in the future.

Research Hypothesis

This study is based on the hypothesis that the integration of mathematical modeling with laboratory scale experimental data can be effectively used to develop, analyze, and simulate the bioethanol production process from agricultural biomass waste, specifically sugarcane bagasse. It is assumed that such integration can provide both technological and economic insights, particularly for the Simultaneous Saccharification and Fermentation (SSF) process, which involves complex enzyme and microbial kinetics. The research hypothesizes that a kinetic model developed from experimental data can accurately predict ethanol yields under varying operational conditions. Furthermore, it is believed that a techno-economic analysis using indicators such as Total Annual Cost (TAC) and Minimum Selling Price (MSP) derived from process modeling can assess the feasibility of scaling up the process to pilot or industrial levels. This approach is expected not only to provide technically sound information, but also to reflect the relevance and applicability within the context of Thailand's bioeconomy and sustainable agricultural development.

Research Objectives

1. To design and simulate the pretreatment process of sugarcane bagasse using mathematical modeling, aiming to enhance the breakdown efficiency of the lignocellulosic structure for ethanol production at the laboratory scale and to promote the efficient utilization of biological resources.
2. To develop a kinetic model of the Simultaneous Saccharification and Fermentation (SSF) process for converting cellulose into ethanol, based on experimental data, in order to accurately predict ethanol yields and analyze process performance.
3. To evaluate the potential and economic feasibility of ethanol production from sugarcane bagasse using Total Annual Cost (TAC) and Minimum Selling Price (MSP) as key performance indicators derived from mathematical simulation, with the aim of industrial-scale application.
4. To support the sustainable development of bioenergy technologies from agricultural waste materials in alignment with Thailand's national development strategies and the United Nations Sustainable Development Goals (SDGs).

Scope of the Study

1. This study focuses on the design and development of an ethanol production process from lignocellulosic biomass, specifically sugarcane bagasse, a byproduct of the sugar industry. The research considers the potential of bagasse as a low-cost feedstock for renewable energy production.

2. The study investigates lignin fractionation processes to enhance cellulose accessibility. It evaluates the effects of key pretreatment parameters—such as solvent type, temperature, and residence time based on previous experimental data to identify optimal conditions for maximizing ethanol yield and purity.

3. Mathematical modeling is integrated with Aspen Plus simulation software to model the ethanol production process. Experimental data are linked with process modeling analysis to examine process behavior at a level that enables scale-up to industrial applications.

4. The economic feasibility of ethanol production from sugarcane bagasse is assessed using model outputs to calculate Total Annual Cost (TAC) and Minimum Selling Price (MSP) of ethanol. These indicators support the commercial viability assessment of the process within the context of sustainable alternative energy development.

Expected Benefits of the Research

1. To obtain in-depth information on the optimal conditions for the pretreatment of sugarcane bagasse to effectively separate lignocellulose, based on mathematical model analysis. This will support the engineering design of ethanol production processes.

2. To understand the optimal conditions for ethanol production from sugarcane bagasse using the Simultaneous Saccharification and Fermentation (SSF) process, aiming to enhance ethanol yield through the application of kinetic modeling as an analytical and predictive tool.

3. To determine the recycling rates and solvent recovery efficiency within the production process, which are critical parameters for improving process performance and conducting economic feasibility analysis at the industrial scale.

4. To generate techno-economic evaluation results that demonstrate the feasibility of the ethanol production process from sugarcane bagasse, using indicators such as Total Annual Cost (TAC) and Minimum Selling Price (MSP). These findings can serve as a foundation for decision-making in future pilot or commercial-scale project development.

CHAPTER 2

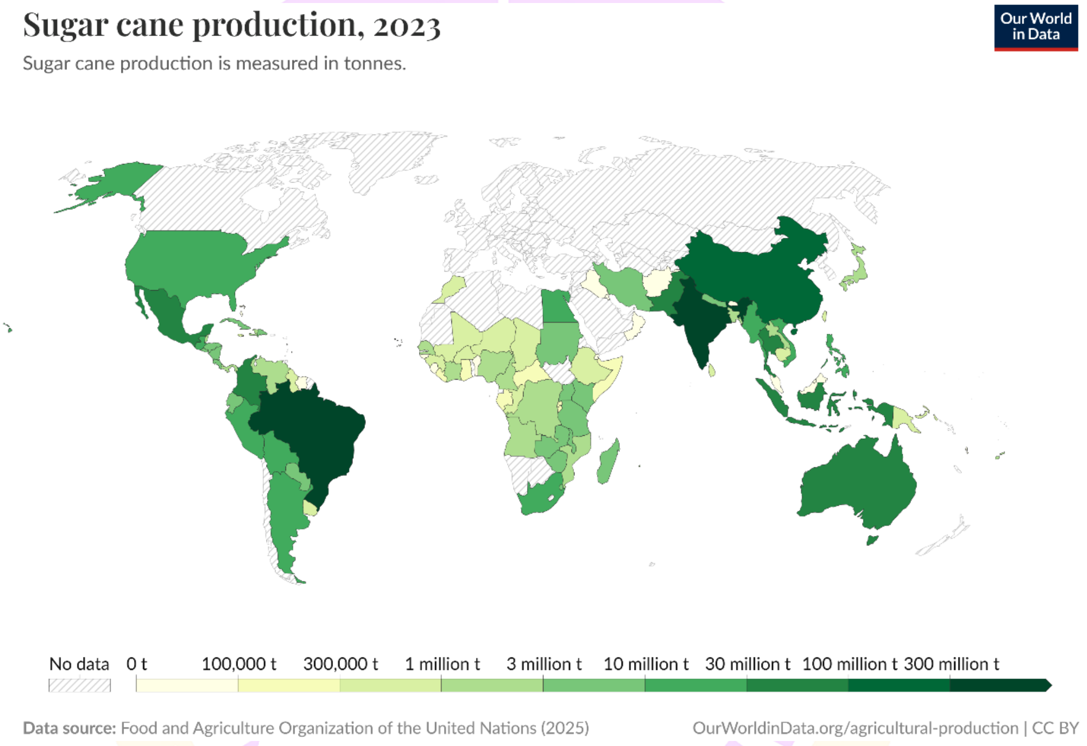
REVIEW OF RELATED LITERATURE AND RESEARCH

Sugarcane

Sugarcane (*Saccharum officinarum L.*) is a monocotyledonous plant belonging to the genus Saccharum within the family Poaceae, which is the same family as maize and sorghum. It is a tropical crop that thrives in hot and humid climates, particularly in areas with abundant sunlight, adequate rainfall, and well-drained soils. In Thailand, sugarcane can be cultivated in almost all regions, except for certain areas in the southern part of the country where excessive rainfall makes the environment unsuitable for its growth. Propagation of sugarcane is commonly done using stem cuttings. Generally, sugarcane cultivated in Thailand is classified into two main types: thick skinned varieties, which are predominantly used in the sugar manufacturing industry, and thin skinned varieties, which are mainly grown for fresh consumption in the form of sugarcane juice.

Sugarcane cultivation remains a significant agricultural activity in many countries, particularly in tropical and subtropical regions that provide favorable climatic conditions for its growth. According to the Food and Agriculture Organization of the United Nations (FAO), as presented on the Our World in Data platform (2023), the top sugarcane producing countries in 2022 were Brazil, India, China, and Thailand, respectively. As shown in Figure 1, Brazil reported the highest production volume, reaching approximately 724.4 million tonnes, accounting for about 37.7% of the world’s total sugarcane output. This was followed by India with 439.4 million tonnes, China with 103.4 million tonnes, and Thailand with 92.1 million tonnes. These figures highlight the crucial role of Latin American and Asian countries in the global sugarcane industry.

In the 2023/24 production year, Brazil is expected to maintain its position as the world's leading sugarcane producer, with an estimated output of 661.4 million tonnes an increase of approximately 6–7% compared to the previous year. This growth is attributed to favorable weather conditions and the implementation of efficient agricultural technologies. Notably, over half of Brazil's sugarcane output is utilized for ethanol production to meet the country's renewable energy demand. Additionally, Brazil maximizes the value of by products such as molasses and bagasse for biomass energy and electricity generation, aligning with the principles of circular economy and sustainable resource management.



Data source: Food and Agriculture Organization of the United Nations (2025) OurWorldinData.org/agricultural-production | CC BY

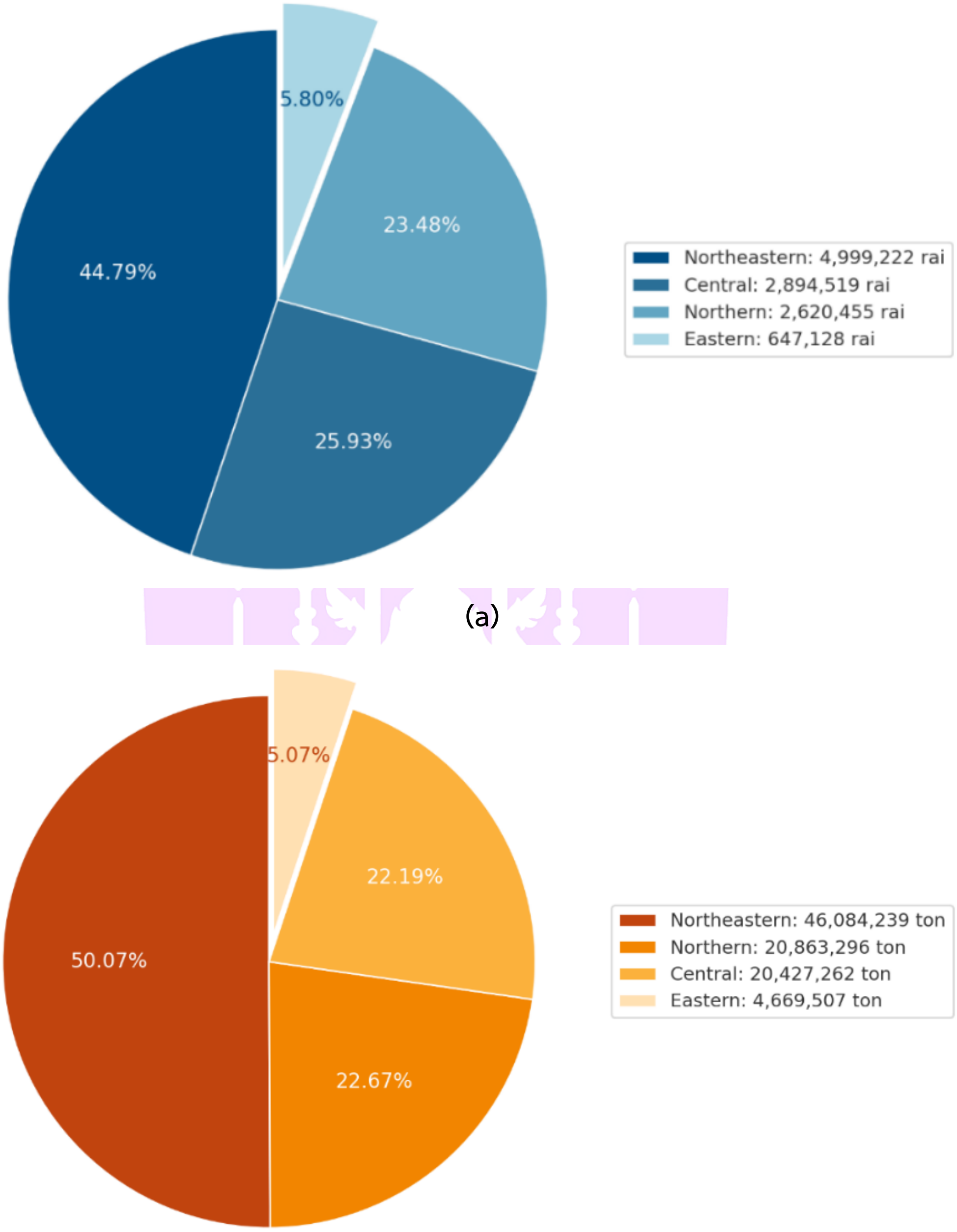
Figure 1 Global sugarcane production by country in 2023 (measured in tonnes)

Source: H. Ritchie et al., 2023

In Thailand, although the production volume is relatively lower than that of Brazil and India, the country remains a key producer in Southeast Asia, with a total output of approximately 92.1 million tonnes in 2022. The growth in Thailand’s sugarcane production is primarily driven by improvements in yield per unit area rather than an expansion of cultivated land, due to increasing land-use competition with other economic crops and limited land availability. Sugarcane typically matures for harvesting within 12–18 months after planting and can be ratooned (regrown from stubble) multiple times over a span of 4 to 6 years. This practice allows farmers to reduce production costs over the long term, thereby enhancing economic viability.

The sugarcane cultivation situation in Thailand for the 2024/2025 crop year reflects the structural development of the agricultural sector, particularly in major economic crops such as sugarcane. Sugarcane serves as a key raw material for various industries, including the production of refined sugar, bioethanol, and downstream industries such as biomass-based electricity generation, organic fertilizers, and biochemicals. The expansion in cultivation area demonstrates farmers' responsiveness to price structures, government policies, and the overall growth trend of the bio-industry market. According to the Office of the Cane and Sugar Board [9] and as illustrated in Figure 2 (a), the total sugarcane cultivation area nationwide in the 2024/2025 crop year reached 11,161,324 rai, representing an increase of approximately 30,023 rai or 0.27% from the previous year. The Northeastern region recorded the largest cultivated area, totaling 4,999,222 rai equivalents to about 45% of the national sugarcane area and exhibited the highest growth rate among all regions. The Central and Northern regions followed, with approximately 2.9 and 2.6 million rai, respectively. In contrast, the Eastern region had the smallest cultivation area, accounting for only 6% or approximately 647,128 rai. Regarding regional sugarcane yield, as illustrated in Figure 2 (b), the pattern closely corresponds with the cultivated area. The Northeastern region remained the highest producer, accounting for approximately 50% of the total national sugarcane yield, or more than 46 million tons. The Central and Northern regions followed, with yields of approximately 20.4 million tons and 20.8 million tons, respectively. In contrast, the Eastern region recorded the lowest yield, producing around 4.6 million tons or about 5% of the national total.

These findings highlight the crucial role of the Northeastern region as Thailand's primary sugarcane production zone. Its significance contributes not only to the agricultural sector but also to the long-term development of the country's bio-based industries.



(a)

(b)

Figure 2 Sugarcane production data by region in Thailand for the 2024/2025 crop year: (a) Sugarcane plantation area by region (unit: rai); (b) Sugarcane yield by region (unit: ton).

Source: Office of the Cane and Sugar Board, 2024a

In quantitative terms, Thailand reported a total sugarcane supply to factories of 92.04 million tons in the 2024/2025 production year, an increase from 82.17 million tons in the previous year, representing a growth rate of 10.73%. The national average yield was 9.56 tons per rai, which is consistent with the long-term decadal average. Provinces with the highest average yield per rai included Khon Kaen and Udon Thani, both at 9.92 tons per rai, reflecting the effectiveness of field management systems, the selection of appropriate sugarcane varieties, and favorable environmental conditions such as water availability and climate. In addition, policies promoting the reduction of sugarcane field burning have been implemented to address PM2.5 air pollution. These include government support for 100% fresh cane harvesting, with a subsidy of 69 baht per ton of fresh cane, and incentives for purchasing sugarcane tops and leaves at 1,200 baht per ton for biomass energy production [9]. These measures not only help reduce environmental costs but also increase farmers' income by an average of 85 baht per ton, thereby contributing to the establishment of a tangible circular economy at the farm level.

Bagasse

Thailand's sugar industry has long been a crucial pillar of the country's agricultural economy, contributing significantly to income generation, employment, and the development of an integrated agricultural supply chain. According to the 2024/2025 production performance report [10], a total of 58 sugar mills were in operation nationwide, collectively producing approximately 13.09 million tons of sugar, comprising raw sugar, white sugar, and refined sugar. The average sugar yield was 137.18 kilograms per ton of cane, with an average Commercial Cane Sugar (C.C.S.) value of 12.60, reflecting stable production efficiency and effective feedstock management across the sector.

At the regional level, the Northeastern region continues to play a dominant role, accounting for 5.34 million tons or 53.11% of the total sugar output. This was followed by the Northern (2.16 million tons, or 21.50%), Central (2.05 million tons, or 20.38%), and Eastern regions (0.50 million tons, or 5.01%). The total amount of fresh sugarcane processed nationwide reached 92.04 million tons, with regional distribution aligning with the sugar production trends.

Bagasse, a byproduct generated from the cane-crushing process, constitutes approximately 29.13% of the fresh cane weight. This resulted in a total estimated bagasse volume of 26.80 million tons for the 2024/2025 season. However, as illustrated in Figure 3, around 3.31 million tons of bagasse remain unutilized or are inefficiently managed. The majority of this loss occurs in the Northeastern region (1.54 million tons), followed by the Northern and Central regions (approximately 0.80 million tons each), and the Eastern region (0.17 million tons). The open burning or improper disposal of such a substantial volume of residual bagasse not only represents a significant loss of potentially valuable resources but also contributes to environmental degradation through air pollution and greenhouse gas emissions.

In the context of sustainable development, it is increasingly essential to restructure the agricultural and industrial sectors toward high-efficiency resource utilization. Thailand has embraced the Bio-Circular-Green Economy (BCG Model) as a key strategy to drive a bio-based economy built upon the principles of bioeconomy, circular economy, and green economy. Utilizing bagasse in biorefinery processes such as the production of bioenergy, biochemicals, and biomaterials serves as a prominent example of transforming agricultural waste into high-value products under the BCG framework.

Moreover, this approach directly aligns with several United Nations Sustainable Development Goals (SDGs), including SDG 7: Affordable and Clean Energy; SDG 9: Industry, Innovation and Infrastructure; SDG 12: Responsible Consumption and Production; and SDG 13: Climate Action. These goals emphasize the importance of sustainable industrial development, efficient resource use, and climate change mitigation. Designing an integrated bagasse management system not only reduces waste and enhances the value chain but also stimulates local economies, reduces dependency on external raw materials, and promotes the adoption of clean technologies at the industrial scale.

Therefore, integrating bagasse utilization into the bio-based and circular economy represents a strategic pathway to achieving Thailand’s long-term economic, environmental, and social sustainability objectives. It also contributes to strengthening the agro-industrial sector and enhancing the nation's competitiveness on the global stage.

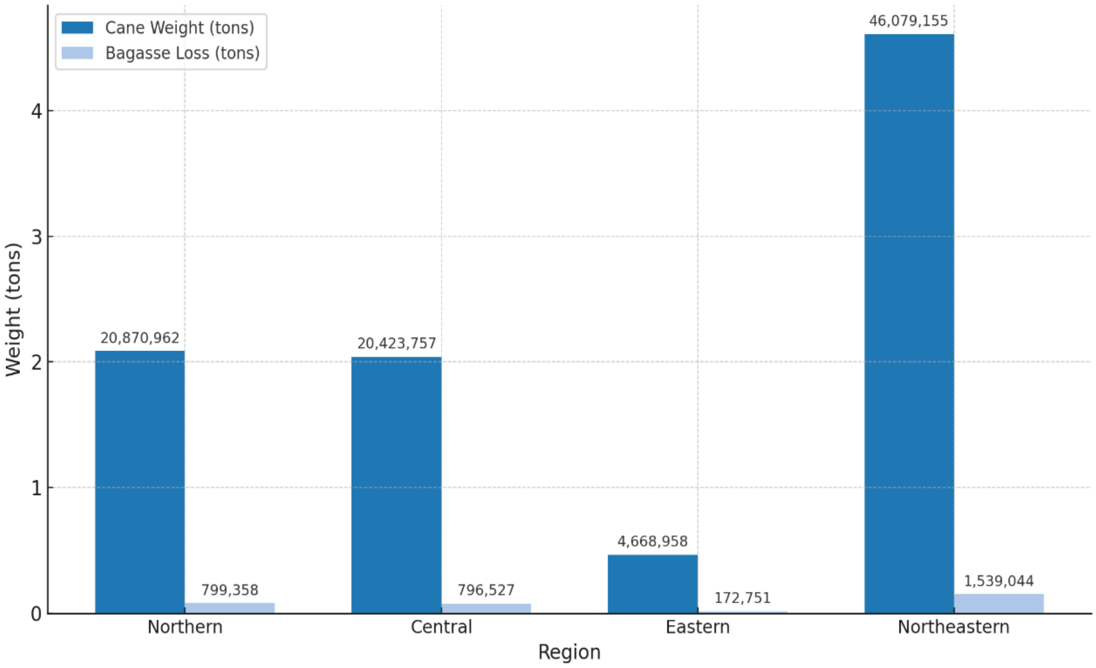


Figure 3 Sugarcane Crushing Input and Bagasse Loss by Region in Thailand for the 2024/2025 Production Season

Source: Office of the Cane and Sugar Board, 2024b

In summary, Thailand's sugarcane and sugar production system continues to play a vital role in the country's agricultural economy, reflecting positive trends in production efficiency and biomass resource management. In particular, bagasse an abundant byproduct of sugarcane processing holds substantial potential for conversion into value-added products such as bio-based chemicals, renewable energy, and sustainable materials within the framework of a bioeconomy. However, the management of residual bagasse at the regional level remains a significant challenge. In many high-production areas, inefficient practices such as open burning persist, leading to the loss of valuable resources and negative environmental impacts. Therefore, the development of systematic approaches to bagasse utilization, aligned with clean technology adoption and strategic policy planning, is essential. The BCG Model centered on Bioeconomy, Circular Economy, and Green Economy has emerged as a strategic framework for transitioning from conventional monoculture-based agriculture to an integrated biorefinery system. This model aligns closely with several United Nations Sustainable Development Goals (SDGs), particularly those related to clean energy, sustainable industrial development, responsible resource consumption, and climate action. Consequently, promoting the economic and environmental utilization of bagasse, in tandem with research and innovation that addresses local and community-specific needs, is a critical strategy for advancing Thailand’s agricultural industry toward long-term sustainability and enhancing the nation’s global competitiveness.

Bioethanol Production Process

Thailand is an agricultural country endowed with abundant natural resources and high potential for crop production, especially in the cultivation of major economic crops such as sugarcane, rice, and cassava. These crops not only yield products for consumption and processing industries but also generate substantial agricultural residues such as bagasse, rice straw, and rice husk. In the past, such by-products were often regarded as waste with little to no value. However, a study by Awoyale and Lokhat [11] revealed that agricultural biomass residues can be efficiently utilized to produce economically valuable products through the application of advanced scientific knowledge and processing technologies.

One of the key approaches to utilizing agricultural biomass residues is the production of biofuels, particularly bioethanol, which is a type of alternative energy derived from the conversion of biomass or sugar- and starch-rich crops such as molasses, cassava, and sugarcane. Bioethanol is a liquid biofuel with physical and energetic properties similar to gasoline, making it suitable for direct substitution or blending with petroleum fuels at various ratios for use in internal combustion engines. Moreover, bioethanol is considered a form of clean energy, as its combustion emits significantly fewer greenhouse gases than fossil fuels and does not produce harmful air pollutants, thereby gaining widespread interest as a sustainable and environmentally friendly energy alternative.

Therefore, research and development of technologies aimed at enhancing the efficiency of converting agricultural biomass residues into biofuels represent a highly promising direction. This approach offers economic benefits, waste reduction, and support for achieving the Sustainable Development Goals (SDGs), particularly those related to clean energy and the efficient use of resources.

Ethanol, also known as ethyl alcohol, is a hydrocarbon compound belonging to the hydroxyl group (-OH), which is bonded to a hydrocarbon chain, classifying it as an organic compound. Ethanol can be utilized as a solvent, a beverage ingredient, and as a renewable fuel alternative in internal combustion engines. Its molecular formula is CH_3CH_2OH, with a molecular weight of 46.07 g/mol. Ethanol is a colorless liquid with a boiling point of 78.32°C, characterized by high flammability, high volatility, and a high-octane number. Generally, ethanol can be produced via petrochemical synthesis or fermentation processes, as outlined below.

1. Chemical synthesis

Ethanol can be synthesized from ethylene (C_2H_4), a petrochemical-derived feedstock, through a process known as hydration, in which water is added to ethylene under specific catalytic conditions. The ethanol produced from this method is referred to as synthetic ethanol.

$$C_2H_4 + H_2O \longrightarrow CH_3CH_2OH \qquad \text{... (1)}$$

2. Microorganism fermentation process

Microbial fermentation is the most widely adopted method for ethanol production due to its low cost, operational simplicity, and the availability of abundant feedstocks such as cassava, molasses, and sugarcane. In this process, ethanol (or ethyl alcohol) is produced through the metabolic activity of microorganisms under anaerobic conditions, typically at a temperature range of 32–35°C and a pH between 4.2 and 4.5 (Jacques et al., 2003). The key biochemical reactions involve the conversion of hexose and pentose sugars such as glucose and xylose into ethanol, as illustrated below:

$$C_6H_{12}O_6\,(aq) \longrightarrow 2C_2H_5OH(1) + 2\ CO_2\,(g) \qquad \text{... (2)}$$

$$3C_5H_{10}O_5\,(aq) \longrightarrow 5C_2H_5OH(1) + 5\ CO_2\,(g) \qquad \text{... (3)}$$

According to the theoretical principles of fermentation stoichiometry, the conversion of one gram of hexose sugar under ideal anaerobic conditions, such as by the yeast *Saccharomyces cerevisiae*, can theoretically yield approximately 0.51 grams of ethanol and 0.49 grams of carbon dioxide. However, in practical fermentation processes, the actual ethanol yield often falls short of the theoretical maximum due to various limitations, including incomplete substrate utilization, cellular maintenance energy demands, the formation of metabolic by-products, and environmental stress factors encountered during fermentation [12].

3. Biomass pretreatment process

The production of ethanol from lignocellulosic biomass requires a pretreatment step to disrupt the complex and rigid structure of the lignocellulosic matrix. This process enhances the accessibility of enzymes or microorganisms to the biomass, facilitating its subsequent degradation. In the hydrolysis step, cellulose is converted into fermentable sugars, particularly reducing sugars such as glucose and xylose. Following hydrolysis, the fermentation step converts these sugars into ethanol [13]. The main types of pretreatment methods are outlined as follows:

1) Physical Pretreatment

Physical pretreatment aims to reduce the particle size of lignocellulosic biomass in the bioethanol production process. This size reduction helps to decrease the crystallinity of cellulose and increase the specific surface area, thereby enhancing enzyme accessibility. One common physical pretreatment approach is mechanical comminution, which involves the application of mechanical forces to reduce the size of biomass particles. Techniques include crushing, grinding, and milling, all of which contribute to the disruption of cellulose crystallinity and an increase in reactive surface area. After size reduction, the resulting particle sizes typically range from 0.2 to 2 millimeters [14].

2) Chemical Pretreatment

Chemical pretreatment aims to reduce the crystallinity of cellulose by removing solid components such as lignin and hemicellulose. Enzymes alone are incapable of converting lignocellulosic biomass into fermentable sugars without prior chemical treatment. Various chemical agents can be used for pretreatment, including alkaline solutions (e.g., sodium hydroxide (NaOH), hydrazine (N_2H_4)), acids (e.g., sulfuric acid and hydrochloric acid), as well as oxidizing agents and other chemicals. These treatments effectively disrupt the lignin–carbohydrate complex, enhancing the accessibility of cellulose to enzymatic hydrolysis.

2.1) Alkaline Pretreatment

Alkaline pretreatment involves the use of alkaline solutions such as sodium hydroxide (NaOH) or potassium hydroxide (KOH) to remove lignin and part of the hemicellulose from lignocellulosic biomass, thereby increasing enzyme accessibility to cellulose. This pretreatment method can be carried out at low temperatures, but typically requires extended reaction times and high alkali concentrations. The effectiveness of alkaline pretreatment depends on the nature of the lignocellulosic material, particularly the lignin content, which influences the degree of biomass deconstruction during the process. Alkaline treatment has been shown to significantly alter the structural integrity of biomass, enhancing its susceptibility to enzymatic hydrolysis [15].

2.2) Acid Pretreatment

Acid pretreatment of lignocellulosic biomass has been widely applied to enhance the efficiency of hydrolysis by effectively removing hemicellulose and lignin with minimal degradation of cellulose. Various types of acids, such as hydrochloric acid (HCl), sulfuric acid (H_2SO_4), nitric acid (HNO_3), and phosphoric acid (H_3PO_4), have been employed for this purpose. Both concentrated and dilute acid solutions can be used to facilitate the breakdown of complex biomass structures and increase the yield of fermentable sugars. Among these approaches, dilute acid pretreatment is particularly popular and has been extensively studied due to its operational feasibility and scalability (Mussatto et al., 2005). Typically, dilute sulfuric or phosphoric acid is applied at controlled temperatures to hydrolyze the hemicellulosic components of lignocellulose into soluble sugars, while cellulose remains available for subsequent enzymatic hydrolysis into glucose. This method can be implemented in two operational modes: (1) low solids loading (5–10% w/w) at high temperatures (above 433 K), or (2) high solids loading (10–40% w/w) at lower temperatures (below 433 K). The choice of method depends on the type of feedstock, process conditions, and desired sugar yield for downstream fermentation [16].

2.3) Pretreatment with the Oxidizing Agent

Pretreatment of lignocellulosic biomass using oxidizing agents, such as hydrogen peroxide (H_2O_2) or peracetic acid ($C_2H_4O_3$), has been investigated as an effective method for the removal of hemicellulose and lignin. These oxidizing compounds are typically applied in aqueous suspension to facilitate the oxidative breakdown and solubilization of lignin. Hydrogen peroxide, in particular, promotes oxidative delignification by generating reactive oxygen species that attack lignin structures, thereby disrupting the lignocellulosic matrix. This disruption enhances enzyme accessibility and improves the efficiency of enzymatic hydrolysis in subsequent steps. The oxidative pretreatment process can significantly improve the digestibility of biomass, contributing to higher sugar yields in bioethanol production [17].

3) Biological Pretreatment

Biological pretreatment is considered an environmentally friendly method, characterized by low chemical input and low energy requirements. However, it is often difficult to control due to its reliance on microbial degradation processes. In this method, specific microorganisms are employed to modify the structure of lignocellulosic biomass and enhance its susceptibility to enzymatic hydrolysis. Biological pretreatment facilitates the partial degradation of solid components such as lignin and hemicellulose, thereby improving the overall digestibility of the biomass. Several microbial strains have been identified for their high efficiency in biological pretreatment, including *Phanerochaete chrysosporium*, *Ceriporia lacerata*, *Cyathus stercoreus*, *Ceriporiopsis subvermispora*, *Pycnoporus cinnabarinus*, and *Pleurotus ostreatus*. These organisms are known for their ligninolytic enzyme systems, which play a key role in the breakdown of complex lignin structures, contributing to improved enzymatic conversion in downstream processes [18].

4) Physicochemical Pretreatment

Physicochemical pretreatment integrates both physical and chemical mechanisms to enhance the digestibility of lignocellulosic biomass. The primary objectives are to reduce the particle size of the raw material and to disrupt structural components such as hemicellulose and lignin. By combining mechanical and chemical actions, this approach improves enzyme accessibility and facilitates subsequent hydrolysis and fermentation processes. Common physicochemical pretreatment methods include steam explosion (SE), which involves rapid depressurization after high-pressure steam treatment; hot compressed water (HCW), which uses subcritical water to hydrolyze hemicellulose; ammonia fiber explosion (AFEX), which employs liquid ammonia under high pressure; and carbon dioxide explosion (CO_2 explosion), which utilizes supercritical or pressurized CO_2 to disrupt biomass structure. These methods have shown promise in enhancing the efficiency of biomass conversion while minimizing the formation of fermentation inhibitors [19].

4.1) Steam Explosion

Steam explosion is a widely used pretreatment technique for the disruption of lignocellulosic biomass. This method involves heating the biomass at high temperature and pressure, followed by a sudden decompression, which causes the material to undergo structural rupture. The rapid pressure release facilitates the breakdown of the biomass matrix, significantly increasing the surface area and improving enzyme accessibility for subsequent enzymatic hydrolysis. Steam explosion is typically conducted at temperatures ranging from 160°C to 260°C, under pressures of 0.69 to 4.82 MPa. It is particularly effective for pretreating lignocellulosic materials, as it partially removes hemicellulose and alters the lignin structure, thereby enhancing the digestibility of cellulose without extensive use of chemicals [20], [21].

4.2) Hot Compressed Water (HCW)

Hot compressed water (HCW) pretreatment is a suitable method for enhancing the hydrolysis of lignocellulosic biomass. The process is typically conducted at temperatures ranging from 150°C to 260°C for short residence times, usually between 5 to 20 minutes. The primary objective of HCW pretreatment is to solubilize hemicellulose into oligosaccharides, which remain in the liquid phase, and to disrupt the structural integrity of cellulose, hemicellulose, and lignin. This structural breakdown significantly increases the enzyme accessibility to cellulose in subsequent enzymatic hydrolysis steps. HCW operates without the use of added chemicals, relying on the unique properties of water under subcritical conditions to act as a reactive medium, making it an environmentally friendly alternative within physicochemical pretreatment strategies [22], [23].

4.3) Ammonia Fiber Explosion (AFEX)

Ammonia Fiber Explosion (AFEX) is a physicochemical pretreatment method that involves exposing lignocellulosic biomass to liquid ammonia at temperatures ranging from 60°C to 100°C under high pressure for a defined period. The process is followed by a rapid depressurization step, which disrupts the biomass structure. AFEX significantly increases sugar yields, particularly by enhancing the digestibility of cellulose, but has limited effect on hemicellulose removal and is less effective for biomass with high lignin content. One of the advantages of this method is that ammonia can be recovered and reused, making the process more sustainable and economically viable. Furthermore, unlike some other pretreatment methods, such as steam explosion, AFEX does not produce significant levels of inhibitory compounds that interfere with enzymatic hydrolysis. While steam explosion typically results in a slurry consisting of separable solid and liquid fractions, AFEX-treated biomass is recovered primarily as a solid fraction [24], [25].

4.4) Carbon Dioxide Explosion

Carbon dioxide explosion is a physicochemical pretreatment method that employs carbonic acid, generated from pressurized CO_2 and water, to disrupt the lignocellulosic structure of biomass. The process is often carried out in conjunction with organic solvents such as ethanol, which facilitate the selective solubilization and removal of lignin from the biomass matrix. Although the overall sugar yields obtained from CO_2 explosion are typically lower compared to those achieved via steam explosion or ammonia fiber explosion (AFEX), this technique offers a significant advantage in minimizing the formation of inhibitory compounds that may hinder enzymatic hydrolysis. In contrast to steam explosion, which often generates degradation products such as furfural and hydroxymethylfurfural (HMF), the CO_2 explosion process is considered milder and more environmentally benign. Consequently, it is regarded as a promising alternative for biomass pretreatment, particularly in applications where the preservation of enzyme activity and downstream fermentation efficiency is critical [26].

4. Enzymatic Hydrolysis

Enzymatic hydrolysis of lignocellulosic biomass is a critical step involving the degradation of cellulose and hemicellulose structures by specific enzymes such as cellulases and hemicelluloses. This process converts the complex polysaccharides present in pretreated biomass into simple monosaccharides and disaccharides (as illustrated in Figure 3), which serve as fermentable carbon sources for subsequent fermentation processes. Compared to acid or alkaline hydrolysis, enzymatic hydrolysis is generally more cost-effective due to its substrate specificity and lower chemical requirements. The optimal conditions for enzymatic hydrolysis typically lie within a temperature range of 45–55°C and a pH range of 4.8–5.3, which correspond to the ideal activity ranges for cellulase and hemicellulase enzymes. After hydrolysis, cellulase enzymes primarily yield glucose, whereas hemicellulases produce a mixture of sugars including glucose, galactose, mannose, xylose, and arabinose. These sugars can be further utilized as substrates for microbial fermentation, particularly by yeast species capable of metabolizing both hexose and pentose sugars [27], [28], [29].

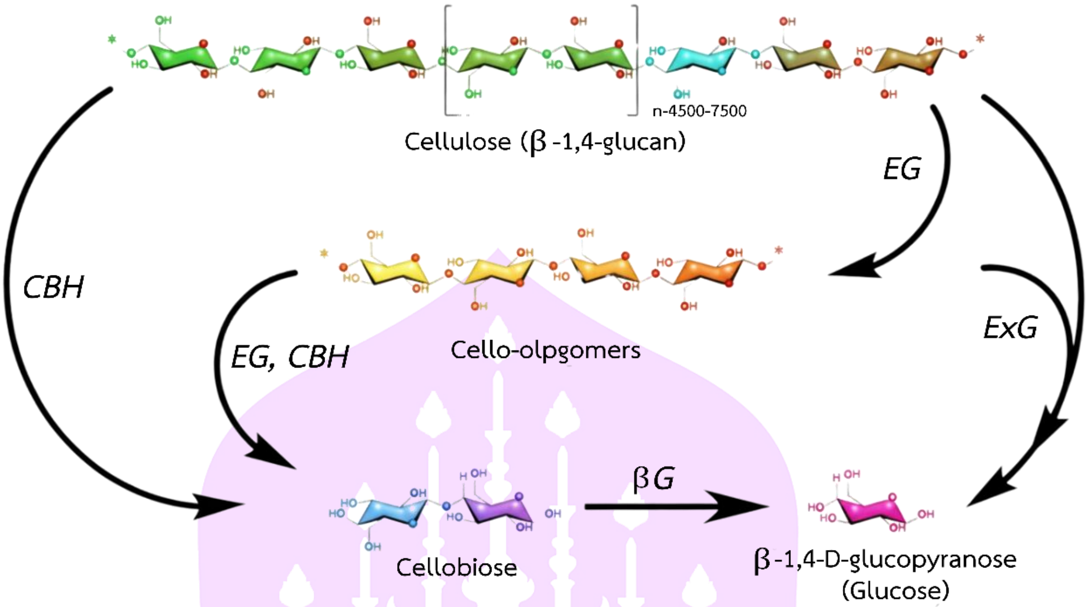


Figure 4 Reaction network of the enzymatic hydrolysis process

Source: Jon Albert Obnamia, 2014

5. Ethanol Fermentation Process

Fermentation refers to the metabolic process by which microorganisms such as bacteria, yeasts, and fungi convert sugars into other chemical products. In the case of ethanol production, specific microorganisms, most notably *Saccharomyces cerevisiae* are employed to convert fermentable sugars into ethanol and carbon dioxide under anaerobic conditions. Ethanol fermentation can be carried out using various process configurations, depending on the nature of the feedstock, desired yield, and economic or operational constraints. Examples of commonly employed fermentation processes include batch fermentation, fed-batch fermentation, continuous fermentation, and simultaneous saccharification and fermentation (SSF). Each method offers distinct advantages in terms of productivity, process control, and suitability for large-scale bioconversion systems.

1) Separated Hydrolysis and Fermentation (SHF) Process

The concept of the Separated Hydrolysis and Fermentation (SHF) process involves conducting hydrolysis and fermentation in separate units. In the first unit, pretreated biomass is enzymatically hydrolyzed by cellulase enzymes to convert polysaccharides into monomeric sugars. These sugars are then fermented into ethanol in a second, separate fermentation unit, as illustrated in Figure 5.

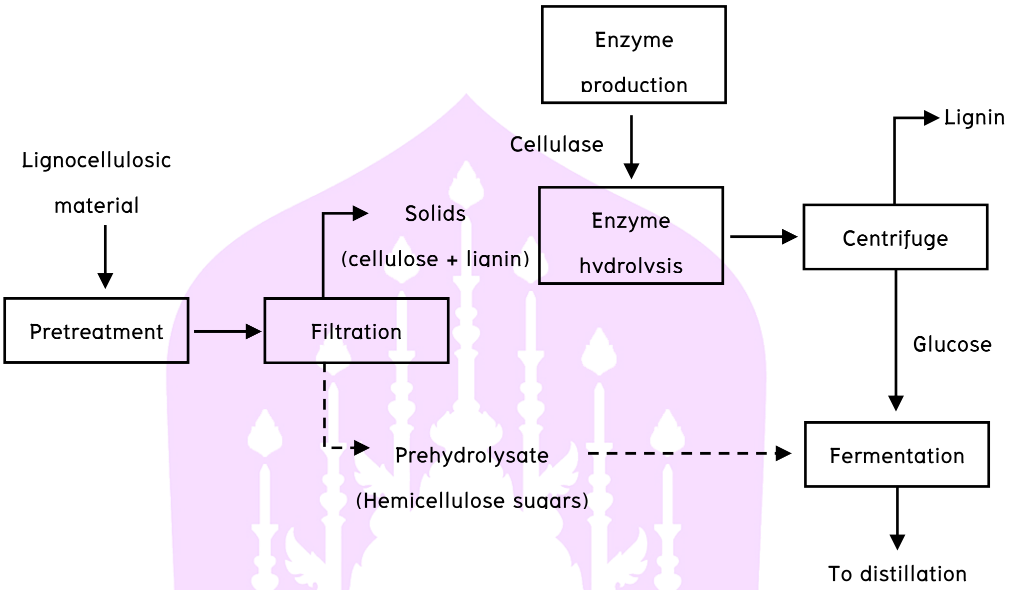


Figure 5 Process of bioethanol production via separated hydrolysis and fermentation (SHF)

The primary advantage of this approach is that both hydrolysis and fermentation can be performed under their respective optimal conditions. Cellulase enzymes have been shown to exhibit maximum efficiency at temperatures between 45–50°C during enzymatic hydrolysis, whereas the optimal temperature range for most fermentative microorganisms is typically between 30–37°C. Another benefit of SHF is the potential to recycle microbial cells for continuous fermentation processes. However, a major drawback is the need for two separate reactors, which increases system complexity and capital cost.

2) Simultaneous- Saccharification and Fermentation (SSF)

The concept of Simultaneous Saccharification and Fermentation (SSF) refers to the integration of enzymatic hydrolysis of starch or cellulose and microbial fermentation of the resulting sugars into ethanol, carried out concurrently in a single bioreactor. This approach differs from the Separated Hydrolysis and Fermentation

(SHF) process, in which hydrolysis and fermentation are performed in separate steps. SSF is particularly suitable for lignocellulosic materials such as sugarcane bagasse, rice straw, or other agricultural residues with high cellulose content. The combined use of cellulase enzymes and yeast under the same operating conditions helps prevent the accumulation of glucose in the system, which is beneficial to enzymatic activity, as cellulases are often inhibited by their own hydrolysis products in SHF processes. Therefore, SSF can enhance the efficiency of sugar conversion to ethanol while also reducing operational costs. This is because SSF requires only one reactor throughout the process, simplifying the system and lowering initial capital investment in equipment construction.

However, SSF presents several important limitations. One major challenge is the difficulty of separating yeast from the system after fermentation, which limits the feasibility of yeast recycling in subsequent fermentation cycles, particularly in industrial-scale operations where economic viability is crucial. Furthermore, SSF faces process condition constraints due to the significant difference between the optimal temperatures for enzymatic hydrolysis (approximately 45–50°C) and yeast fermentation (around 30–35°C). This necessitates a compromise in temperature selection, which may adversely affect overall process efficiency. To address these challenges, the development of SSF technologies requires the selection of enzymes and microbial strains that can tolerate suboptimal conditions, or the adjustment of process parameters to achieve a balance between hydrolysis and fermentation. Such optimization is essential to maximize ethanol yield in both technological and economic terms [31].

The process illustrated in Figure 6 represents the conversion of cellulosic biomass into ethanol using technology developed by the National Renewable Energy Laboratory (NREL). This approach has been developed to enhance the efficiency of biofuel production from agricultural residues in a sustainable manner. The process begins with cellulosic biomass, such as sugarcane bagasse, rice straw, or corn stover, which undergoes a pretreatment step to disrupt the lignin and hemicellulose structures that encase cellulose and hinder enzymatic access. This pretreatment facilitates better enzymatic hydrolysis in subsequent stages.

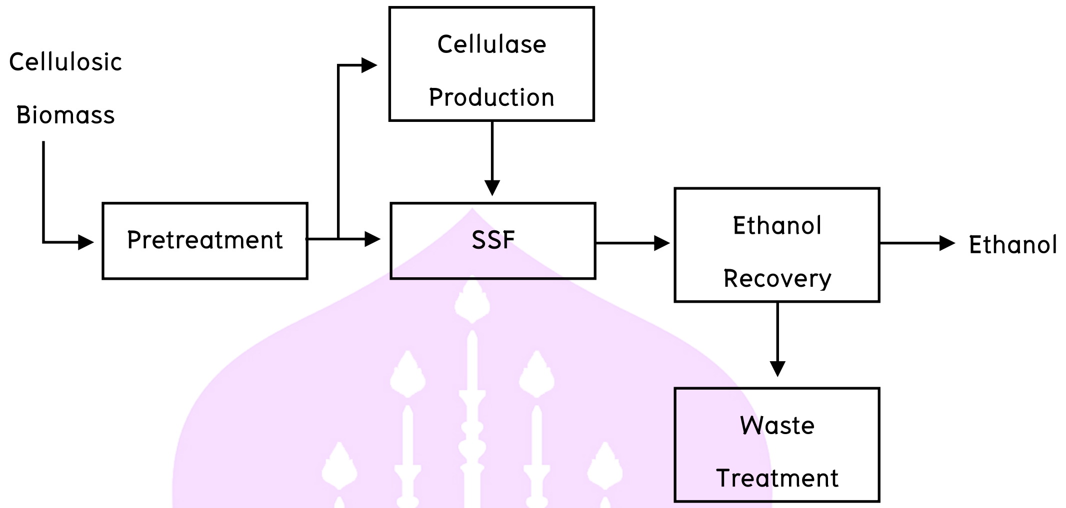


Figure 6 A simplified process of biomass-to-ethanol conversion technology developed by the National Renewable Energy Laboratory (NREL)

Following pretreatment, cellulase enzymes are produced using suitable microorganisms, such as *Trichoderma reesei*. These enzymes are then fed into a Simultaneous Saccharification and Fermentation (SSF) system. In this step, the pretreated cellulose is enzymatically hydrolyzed and fermented into ethanol in a single reactor. The main advantage of the SSF process is its ability to reduce sugar accumulation, which can inhibit enzyme activity, while simultaneously improving overall ethanol yield. Additionally, SSF reduces equipment costs and shortens the production timeline compared to separated hydrolysis and fermentation systems. Once fermentation is complete, the resulting broth is transferred to an ethanol recovery unit, typically involving distillation, to separate ethanol from the fermentation mixture. The final product is ethanol, which can be used directly as a biofuel or blended with gasoline to produce gasohol. The residual by-products from the process are sent to a waste treatment system for proper management. These wastes may be utilized for energy recovery, heat generation, or organic fertilizer production. With its integrated process design, the NREL approach serves as a viable model for sustainable ethanol production from biomass. It is particularly suitable for agricultural countries like Thailand, where abundant agricultural residues provide strong potential for renewable energy development in the future.

6. Kinetic model for Simultaneous Saccharification and Fermentation (SSF)

The study of chemical kinetics involves the investigation of the rate at which chemical reactions occur, which is influenced by the concentration of the reactants. Therefore, a chemical reaction can be represented by the following equation.

$$A \longrightarrow \text{Products} \qquad \text{... (4)}$$

$$(-r_A) = k(C_A)^n \qquad \text{... (5)}$$

Where:

Where:	r_A	is the reaction rate of compound A
	K	is the reaction rate constant or kinetic constant
	C_A	is the concentration of reactant A
	n	is the exponent of C_A

1) Kinetic Model of SSF process

The kinetics of the SSF process for lignocellulosic materials is described by an unstructured kinetic model developed by Kroumov [32]. The model corresponds to the following equations:

$$\text{Cellulose} \xrightarrow{r} \text{Glucose} \xrightarrow{r_x,\ r_g} \text{Ethanol + Cell mass + } CO_2 \text{ ... (6)}$$

The reaction mechanism in Equation (6) represents the mass balance of the reactions and the associated enzyme kinetics. The kinetic equations can be expressed sequentially as follows:

$$\text{Cellulose balance;} \quad \frac{dC}{dt} = -r \qquad \text{... (7)}$$

$$\text{Glucose balance;} \quad \frac{dG}{dt} = 1.111r - r_g \qquad \text{... (8)}$$

The coefficient “1.111” in Equation (8) is defined as the theoretical yield or stoichiometric coefficient (YGC = 1.111)

Biomass balance:

$$\frac{dX}{dt} = r_x \qquad \text{... (9)}$$

Product balance:

$$\frac{dE}{dt} = q_p X \qquad \text{... (10)}$$

Enzymatic rate of cellulose hydrolysis; r:

$$r = \frac{k \times Enz \times C}{K_m\left(1 + \frac{G}{K_G}\right) + \frac{C}{K_{sub}} + C} \qquad \text{... (11)}$$

Glucose formation and consumption rate; r_g) (g/L-h):

$$r_g = \frac{1}{Y_{XC}}\frac{dX}{dt} + \frac{1}{Y_{EC}}\frac{dE}{dt} \qquad \text{... (12)}$$

Biomass growth rate; r_x (g/L-h):

$$r_x = \mu X \qquad \text{... (13)}$$

Specific ethanol production rate; q_p (h^{-1})

$$q_p = \frac{1}{X}\frac{dP}{dt} = \frac{q_{pm} G\left[1 - \frac{E}{E_{max}}\right]}{(K_{s1} + G)\left(k_{ps1} + E + \frac{E^2}{K_{pi}}\right)} \qquad \text{... (14)}$$

2) Microbial growth kinetics

Kinetics play a crucial role in providing information related to biomass growth and product formation. The relationship between the specific growth rate (μ) of microorganisms and the glucose concentration (G) can be described by the Monod model (Equation 15), which illustrates the influence of substrate concentration on the cell growth rate.

$$\mu = \mu_{max} \frac{G}{K_s + G} \qquad \dots (15)$$

Where: μ is the specific growth rate (h^{-1})
μ_{max} is Maximum specific growth rate (h^{-1})
G is Glucose concentration (g/L)
K_s is Saturation constant (g/L)

To estimate the values of μ_{max} and K_s, the Monod equation can be linearized by taking the reciprocal of both sides, as shown in Equation (16).

$$\frac{1}{\mu} = \frac{K_s}{\mu_{max}} \frac{1}{G} + \frac{1}{\mu_{max}} \qquad \dots (16)$$

The values of μ_{max} and Ks can be determined by plotting a graph of $\frac{1}{\mu}$ versus $\frac{1}{G}$. This yields a straight line with a slope equal $\frac{K_s}{\mu_{max}}$ and a y-intercept of $\frac{1}{\mu_{max}}$

Biomass yield (g cells per g cellulose) is expressed by Equation (17).

$$Y_{XC} = \frac{\frac{dX}{dt}}{\frac{dC}{dt}} = \frac{(X_f - X_0)}{(C_0 - X_f)} \qquad \dots (17)$$

Ethanol yield (g ethanol per g cellulose) is expressed by Equation (18).

$$Y_{EC} = \frac{\frac{dE}{dt}}{\frac{dC}{dt}} = \frac{(E_f - E_0)}{(C_0 - C_f)} \qquad \dots (18)$$

Process Simulation and Applications of Aspen Plus

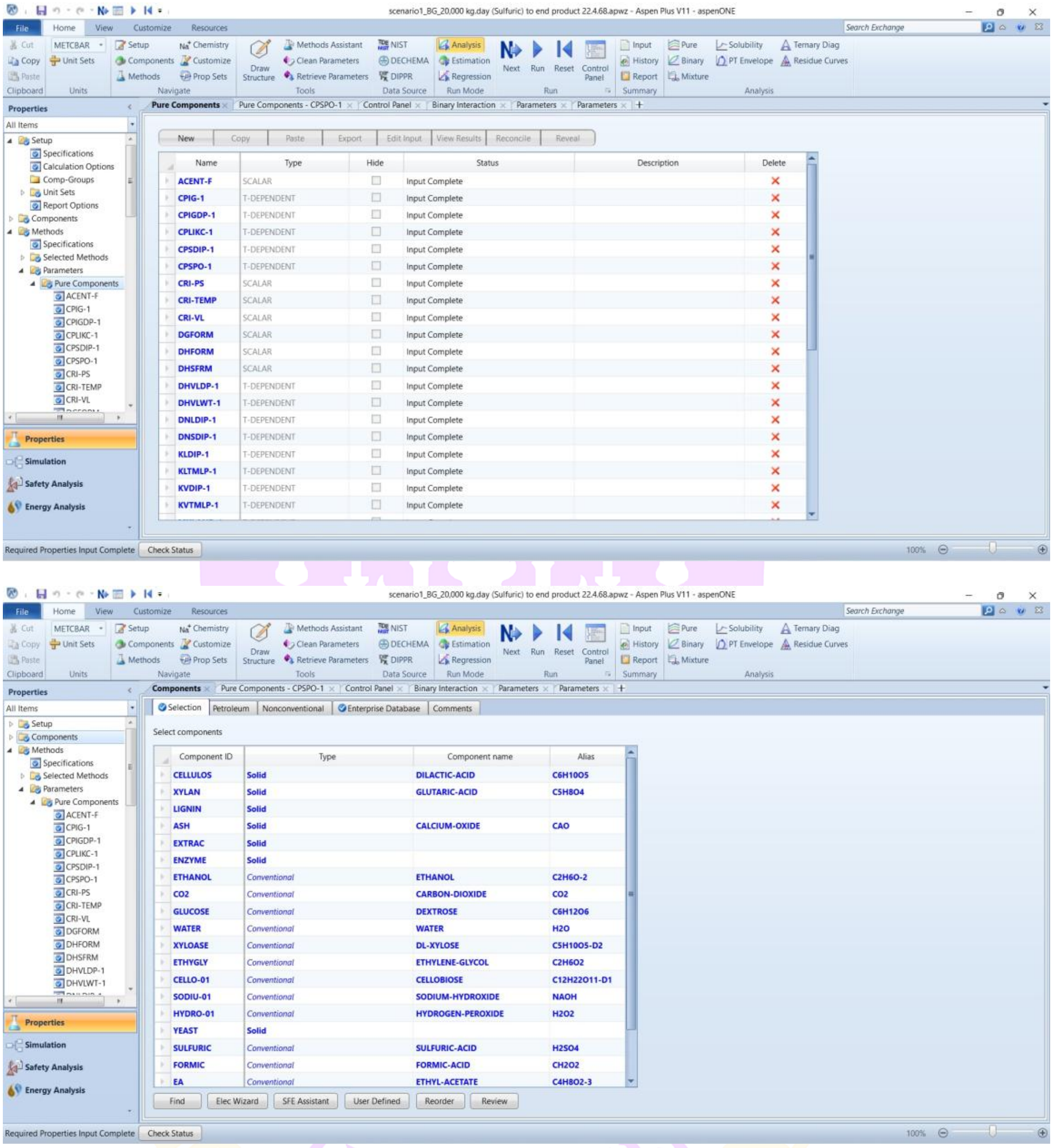
The integration of mathematical modeling with chemical process simulation software such as Aspen Plus plays a crucial role in systematically analyzing the production of bioethanol from lignocellulosic biomass. Aspen Plus serves as a virtual process modeling tool, comprising various unit operations connected through a flowsheet, representing key steps such as feedstock preparation, chemical reactions, separation, distillation, and ethanol purification. This simulation enables precise calculation of mass and energy balances, while also allowing for the evaluation of the effects of process variables on the overall efficiency and economic feasibility. For example, changes in solid loading during the hydrolysis step directly influence sugar concentration, thereby affecting ethanol yield during fermentation. Aspen Plus also supports the design and analysis of advanced distillation systems, such as multi-effect distillation or extractive distillation, to enhance the separation efficiency of ethanol from water. Additionally, it facilitates the assessment of total energy demand and the potential for energy integration, promoting sustainability from both economic and environmental perspectives. On a global scale, a key institution contributing to the development of process models and data for lignocellulosic ethanol production is the National Renewable Energy Laboratory (NREL) [33], under the U.S. Department of Energy. NREL has developed standardized baseline models and technical reports covering engineering assumptions, kinetic parameters, and operating conditions for various unit operations. These resources can be flexibly adapted to different types of biomass feedstocks.

Moreover, NREL provides tools for conducting techno-economic analysis (TEA) alongside process simulations, enabling comprehensive assessment of production costs and competitiveness of biofuels at the industrial scale. Applying NREL’s models to agricultural residues in Thailand such as rice straw, cassava peels, or sugarcane bagasse enhances the credibility of research findings and facilitates systematic comparison with international data. The combined use of Aspen Plus and NREL baseline models reduces the time required to develop new simulations, supports mass and energy balance analysis, and helps optimize ethanol yield. This approach serves as a powerful decision-making tool for shaping national bioenergy policies effectively and sustainably.

Aspen Plus is a chemical process simulation software developed by Aspen Technology, Inc. [34], widely used in both industrial sectors and academic research in chemical and bioenergy engineering. It is particularly effective for designing, analyzing, and optimizing the production systems of biofuels derived from lignocellulosic biomass, such as ethanol production from sugarcane bagasse, rice straw, or cassava peels. In version 11, Aspen Plus has been improved to offer a more user-friendly interface, allowing users to construct process flowsheets and connect unit operations such as reactors, mixers, separators, and distillation columns efficiently. This facilitates the accurate and systematic simulation of complex production processes. One of the key features of Aspen Plus v11 is its extensive chemical property database containing more than 20,000 components, along with various thermodynamic models such as NRTL, UNIQUAC, Peng–Robinson (PR), and Soave–Redlich–Kwong (SRK), which are suitable for simulating systems involving vapor, liquid, and solid phases. The software also includes essential unit operations for bioprocesses, such as RCSTR (Continuous Stirred-Tank Reactor) for fermentation, RPlug (Plug Flow Reactor) for kinetic reactions, and RadFrac for multi-stage distillation used to efficiently separate ethanol from water.

For the simulation of lignocellulosic biomass conversion, Aspen Plus version 11 fully supports the application of comprehensive bioprocess modeling. Biomass materials such as sugarcane bagasse and rice straw are typically defined as non-conventional components, which require additional configuration according to the guidelines provided by NREL, as illustrated in Figure 7. Users can input compositional data for the biomass such as the proportions of cellulose, hemicellulose, and lignin based on laboratory analyses. The RYield module is then used to simulate thermal or chemical decomposition during pretreatment or pyrolysis. The resulting products are subsequently converted into conventional components (e.g., glucose, xylose) to be used in the subsequent enzymatic hydrolysis and fermentation stages.

Users may define custom kinetic rate expressions or adopt standard models published by institutions such as the National Renewable Energy Laboratory (NREL). A typical simulation workflow for bioethanol production in Aspen Plus includes four main stages: (1) feedstock preparation and pretreatment, (2) enzymatic hydrolysis, (3) fermentation, and (4) ethanol separation and purification. The software also allows users to evaluate the influence of key process variables, such as solid loading, temperature, pH, residence time, and ethanol yield, across individual unit operations.



scenario1_BG_20,000 kg.day (Sulfuric) to end product 22.4.68.apwz - Aspen Plus V11 - aspenONE

Name	Type	Hide	Status	Description	Delete
ACENT-F	SCALAR	☐	Input Complete		✗
CPIG-1	T-DEPENDENT	☐	Input Complete		✗
CPIGDP-1	T-DEPENDENT	☐	Input Complete		✗
CPLIKC-1	T-DEPENDENT	☐	Input Complete		✗
CPSDIP-1	T-DEPENDENT	☐	Input Complete		✗
CPSPO-1	T-DEPENDENT	☐	Input Complete		✗
CRI-PS	SCALAR	☐	Input Complete		✗
CRI-TEMP	SCALAR	☐	Input Complete		✗
CRI-VL	SCALAR	☐	Input Complete		✗
DGFORM	SCALAR	☐	Input Complete		✗
DHFORM	SCALAR	☐	Input Complete		✗
DHSFRM	SCALAR	☐	Input Complete		✗
DHVLDP-1	T-DEPENDENT	☐	Input Complete		✗
DHVLWT-1	T-DEPENDENT	☐	Input Complete		✗
DNLDIP-1	T-DEPENDENT	☐	Input Complete		✗
DNSDIP-1	T-DEPENDENT	☐	Input Complete		✗
KLDIP-1	T-DEPENDENT	☐	Input Complete		✗
KLTMLP-1	T-DEPENDENT	☐	Input Complete		✗
KVDIP-1	T-DEPENDENT	☐	Input Complete		✗
KVTMLP-1	T-DEPENDENT	☐	Input Complete		✗

Required Properties Input Complete

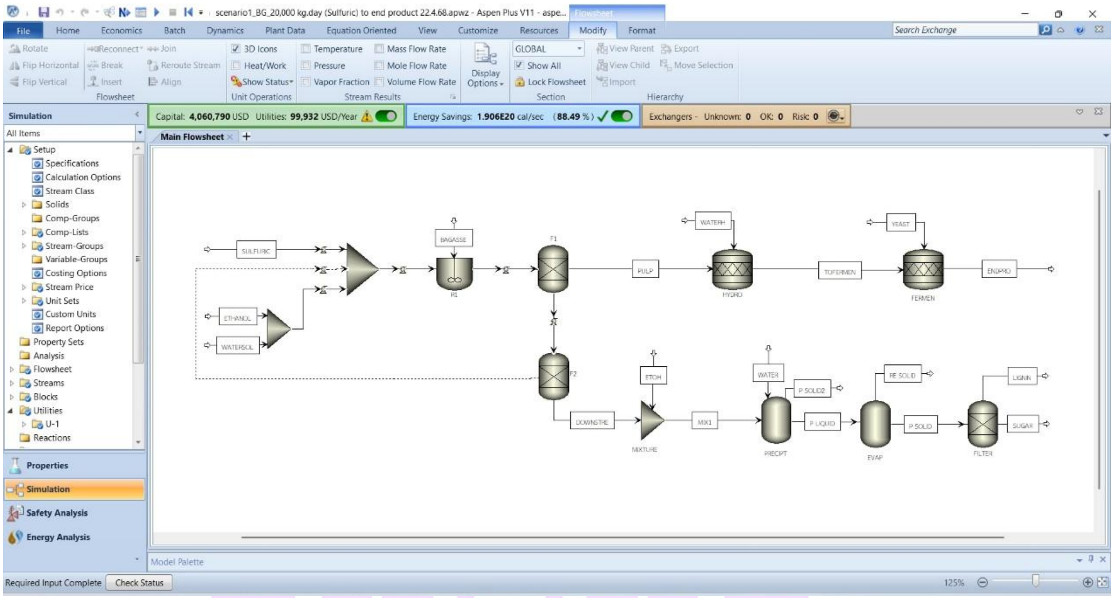
scenario1_BG_20,000 kg.day (Sulfuric) to end product 22.4.68.apwz - Aspen Plus V11 - aspenONE

Select components

Component ID	Type	Component name	Alias
CELLULOS	Solid	DILACTIC-ACID	C6H10O5
XYLAN	Solid	GLUTARIC-ACID	C5H8O4
LIGNIN	Solid		
ASH	Solid	CALCIUM-OXIDE	CAO
EXTRAC	Solid		
ENZYME	Solid		
ETHANOL	Conventional	ETHANOL	C2H6O-2
CO2	Conventional	CARBON-DIOXIDE	CO2
GLUCOSE	Conventional	DEXTROSE	C6H12O6
WATER	Conventional	WATER	H2O
XYLOASE	Conventional	DL-XYLOSE	C5H10O5-D2
ETHYGLY	Conventional	ETHYLENE-GLYCOL	C2H6O2
CELLO-01	Conventional	CELLOBIOSE	C12H22O11-D1
SODIU-01	Conventional	SODIUM-HYDROXIDE	NAOH
HYDRO-01	Conventional	HYDROGEN-PEROXIDE	H2O2
YEAST	Solid		
SULFURIC	Conventional	SULFURIC-ACID	H2SO4
FORMIC	Conventional	FORMIC-ACID	CH2O2
EA	Conventional	ETHYL-ACETATE	C4H8O2-3

Required Properties Input Complete

Figure 7 Configuration of solid molar inputs according to NREL guidelines and biomass component specification for modeling ethanol production in Aspen Plus.



scenario1_BG_20,000 kg.day (Sulfuric) to end product 22.4.68.apwz - Aspen Plus V11 - aspe...

Capital: **4,060,790** USD Utilities: **99,932** USD/Year

Energy Savings: **1.906E20** cal/sec (**88.49** %)

Exchangers - Unknown: **0** OK: **0** Risk: **0**

Figure 8 Simulation of lignocellulosic bioethanol production process using Aspen Plus version 11

Furthermore, Aspen Plus allows for total system energy demand analysis and energy integration through the Heat Exchanger Network (HEN) module to improve energy efficiency. It can also interface with cost evaluation tools such as Aspen Process Economic Analyzer (APEA) for preliminary economic assessment. In addition, process models and kinetic data from standard NREL reports can be integrated with localized feedstock simulations, helping reduce model development time and enhancing the reliability of technical and economic analyses for biofuel production. Overall, Aspen Plus v11 is a powerful tool for analyzing and designing bioethanol production processes from lignocellulosic biomass. It is valuable not only for technical and bioenergy engineering applications but also for informing strategic planning and policymaking in clean energy development. An example of a process flowsheet developed in Aspen Plus is shown in Figure 8, illustrating the implementation of this software in the present study.

CHAPTER 3

MATERIALS AND METHODS

Process synthesis and design

The present study applied mathematical modeling and process simulation using Aspen Plus v11 (Aspen Technology, Inc., Bedford, MA, USA) to examine the fractionation of sugarcane bagasse, a key agricultural residue in Thailand. Aspen Plus is an industry-standard tool widely used by institutions like the National Renewable Energy Laboratory (NREL) for biorefinery design. Its strong thermodynamic features, especially the Non-Random Two-Liquid (NRTL) model, support accurate simulation of non-ideal liquid systems in biomass pretreatment. The software's extensive property database, unit operations, and flexible modeling environment allow for scalable process development and detailed techno-economic analysis, enhancing the reliability of the results. The chemical composition (Table 1) with comparison of sugarcane bagasse in different countries was analyzed based on prior studies conducted by Suriyachai et al. [35] and Weerasai et al. [36]. This case study was divided into three categories according to the type of catalyst used in the organosolv fractionation process: (1) H_2SO_4-based organosolv (Industrial-grade, Qingdao Hisea Chem Co., Ltd., China), (2) CH_2O_2-based organosolv (Industrial-grade, Feicheng Acid Chemicals, China), and (3) CH_3ONa-based organosolv (CH_3Ona-based organosolv (Zhengzhou Clover Chemical Co., Ltd., China). All simulations were performed using the Non-Random Two-Liquid (NRTL) thermodynamic model for phase equilibrium calculations. Component property data were sourced from the Aspen Plus database and supplemented with information from the National Renewable Energy Laboratory (NREL) to ensure greater simulation accuracy [33].

Table 1 Comparison of chemical compositions of sugarcane bagasse from different countries.

Composition	Brazil [37]	China [38]	Thailand [36] *
Cellulose	42.19	39.52	38.30
Xylan	27.60	25.63	20.70
Lignin	21.56	30.36	23.70
Ash	2.84	1.45	4.20
Other	5.63	1.72	13.00

Note: * This research is based on the following data

The Non-Random Two-Liquid (NRTL) model is commonly applied to estimate activity coefficients, especially in liquid–liquid (LLE) and vapor–liquid equilibrium (VLE) systems [39]. Its strength lies in capturing non-ideal behaviour by accounting for molecular interactions and the uneven distribution of molecules within the liquid phase. This makes it particularly effective for systems with strong polar interactions or non-random mixing. The activity coefficient of each component in a multicomponent mixture is calculated using the NRTL equations, as illustrated in Eq. 19.

$$\ln \gamma_i = \sum_{j=1}^{N} \frac{\tau_{ji} G_{ji} x_j}{\sum_{k=1}^{N} G_{ki} x_k} + \sum_{j=1}^{N} \frac{x_j G_{ij}}{\sum_{l=1}^{N} G_{li} x_l} \left[\tau_{ij} - \frac{\sum_{m=1}^{N} \tau_{mj} G_{mj} x_m}{\sum_{k=1}^{N} G_{kj} x_k} \right] \quad \ldots (19)$$

Where:

- $\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT}$ is the interaction parameter between components *i* and *j*.
- $G_{ij} = e^{-\alpha_{ij} \tau_{ij}}$ is a weighting factor.
- x_j is the mole fraction of component *j*.
- α_{ij} is a non-randomness parameter (typically between 0.2 and 0.47).

In the NRTL equation provided, k and m are dummy indices used for summation over components in the system:

- k typically indexes all components in the denominators to normalize the interactions with respect to component i or j.
- m is used similarly to k, but specifically for summing interactions between component j and all other components m (inside the inner bracket) in the second term of the equation.

Roles:

k appears in:

- $\sum_{k=1}^{N} G_{ki} x_k$: Denominator of the first term (normalizing interaction contributions to component i).
- $\sum_{k=1}^{N} G_{kj} x_k$: Denominator inside the brackets in the second term (normalizing interactions related to component j).

m appears in:

- $\sum_{m=1}^{N} \tau_{mj} G_{mj} x_m$: Numerator inside the bracket (weighted average interaction toward j from all m).

In essence, k and m are used to iterate over all components in the mixture, similar to j, but serve distinct roles depending on where they appear in the formula.

Process setup for organosolv fractionation

In this study, the biomass feed rate was set at 20,000.00 kg/day, and the solvent recycling efficiency was assumed to be 95%. Figure 1a and 1b present the process flowsheet for biomass fractionation using the organosolv technique, employing sugarcane bagasse an agricultural residue from Thailand’s sugar industry as the primary feedstock.

The diagram outlines the ethanol production process from sugarcane bagasse, involving a series of integrated unit operations. The process starts with the introduction of sugarcane bagasse (BAG) and catalysts into reactor R1, a Recirculating Continuous Stirred-Tank Reactor (RCSTR), which ensures uniform mixing and enhances reaction efficiency. The output from R1 proceeds to unit F1, a membrane filter press, for solid-liquid separation. The resulting cellulose pulp (PULP) is transferred to the HYDRO unit, an agitated hydrolysis reactor with temperature and pH control, where water (WT-RH) is added to depolymerize cellulose into glucose. The glucose solution is then sent to the FERMEN unit for anaerobic fermentation with yeast (YEAST), converting glucose into ethanol and CO_2. Ethanol is collected in the END unit, while the liquid stream from F1 goes to the distillation column (F2) for solvent recovery. Recovered ethanol is partially recycled (S-RCY), and the residue is processed in the PRECIP unit to extract primary solids (P-SOLID). The remaining liquid is concentrated in the EVAP unit to recover additional solids (RE-SOLID), followed by filtration (FILTER) to isolate lignin (LIGNIN) as a by-product. The leftover sugar solution is directed to the SUGAR unit for further use. In the HYDRO unit, cellulose $(C_6H_{10}O_5)_n$ is hydrolyzed with water to produce glucose ($C_6H_{12}O_6$), as represented in Eq. 20.

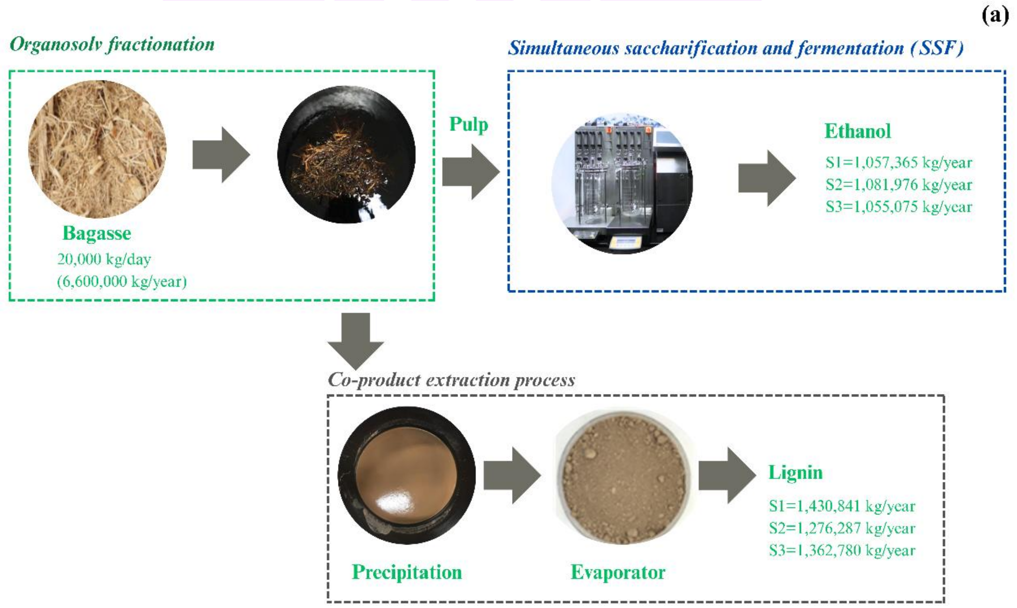
$$(C_6H_{10}O_5)_n + nH_2O \longrightarrow n\,C_6H_{12}O_6 \qquad \text{... (20)}$$

From the hydrolysis process, 1 gram of cellulose can theoretically produce around 1.11 grams of glucose due to water incorporation during the reaction. However, actual yields typically range between 80% and 95%, influenced by the catalyst type and operating conditions. The glucose-rich hydrolysate is then fed into the FERMEN unit, an anaerobic fermentation reactor operating at 30–35°C. Yeast is added to convert glucose into ethanol and carbon dioxide, as shown in Eq. 21.

$$C_6H_{12}O_6 \longrightarrow 2C_2H_5OH + 2CO_2 + ATP \qquad \text{... (21)}$$

The final product obtained from the ENDPRO unit is ethanol, which is ready for subsequent separation and purification processes.

Scenario 1 involves organosolv fractionation using a 70:30 %v/v ethanol–water solvent mixture, with 2% w/v H_2SO_4 as the catalyst. The process was carried out at 170°C, 20 bar, and a 60-minute residence time (This study). Scenario 2 depicts organosolv fractionation using CH_2O_2 as the catalyst. The reactor conditions were 159°C, 20 bar, and a 40-minute residence time. The solvent mixture comprised water, ethanol, ethyl acetate, and CH_2O_2 in a 43:20:16:21 %v/v ratio. [35]. Scenario 3 describes organosolv fractionation using 5.1% w/v CH_3ONa as the catalyst. The process runs at 150°C, 20 bar, with a residence time of 63.9 minutes. [36]. This study assumes 7,920 hours of annual plant operation and a 95% solvent recycling rate, a common value in Organosolv processes. Reported recycling efficiencies vary, with studies noting values as high as 99% [40] and as low as 68.9% [41]. Efficient solvent recycling is vital for lowering costs and environmental impact, though repeated use may degrade performance. Thus, advancing solvent regeneration methods and improving biomass preparation are key to enhancing process efficiency and economic viability.



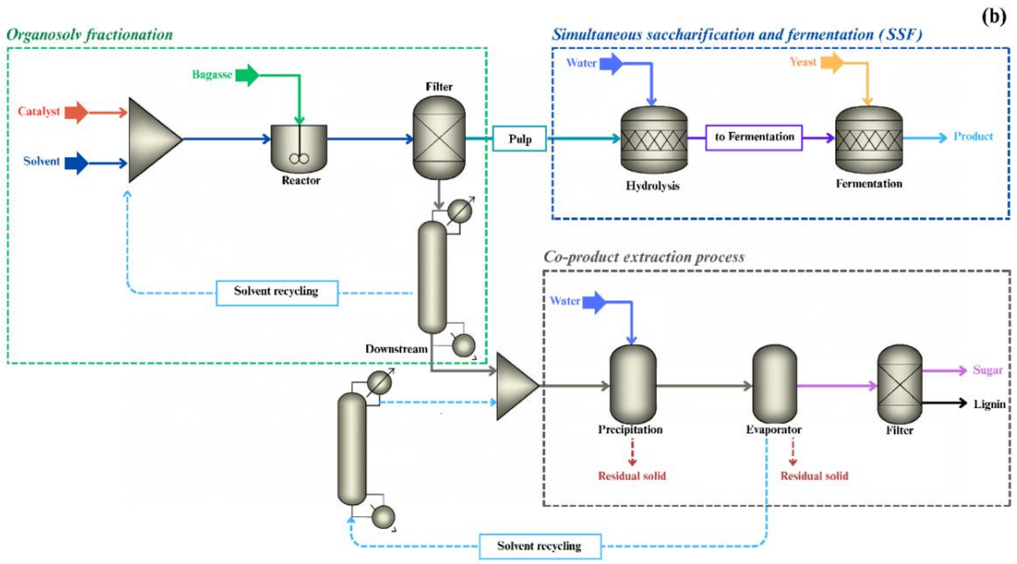


Figure 1. Flowsheet setup for ethanol production from sugarcane bagasse via the organosolv process; a) feed rate per day and b) scenario for organosolv fractionation

In the Organosolv process, lignin is efficiently extracted from lignocellulosic biomass through the use of organic solvents such as ethanol, methanol, or formic acid in combination with water and either acidic or alkaline catalysts. This process facilitates the cleavage of lignin–carbohydrate linkages within the plant cell wall matrix, particularly targeting the *β*-O-4 ether bonds, which are the most abundant interunit linkages in native lignin. Under acidic conditions, the chemical mechanism of lignin depolymerization begins with the protonation of the hydroxyl group at the α-position (α-OH), leading to the formation of a stable benzylic carbocation intermediate. This intermediate plays a crucial role in promoting the cleavage of the *β*-O-4 ether bond. The representative reaction mechanism is shown as follows (Equation (22)):

$$\text{Ar-CH(OH)-CH}_2\text{-O-Ar'} + \text{H}^+ \longrightarrow \text{Ar-CH}^+\text{-CH}_2\text{-O-Ar'} \longrightarrow \text{Ar-CHO} + \text{HO-CH}_2\text{-Ar'} \qquad \text{... (22)}$$

In this equation, Ar and Ar′ represent aromatic rings in the lignin polymer; CH(OH) denotes the hydroxyl group at the *α*-position; and CH_2–O corresponds to the *β*-O-4 ether linkage. The products Ar–CHO and HO–CH_2–Ar′ are aromatic aldehydes and alcohols, respectively, indicating the effective depolymerization of lignin. Once dissolved into the solvent phase, lignin can be recovered by precipitation through water addition or solvent evaporation. The resulting lignin is characterized by its sulfur-free composition, low ash content, and low molecular weight, making it highly suitable for the production of high-value bioproducts such as resins, carbon fibers, and bio-based composite materials. Nevertheless, the Organosolv process presents economic limitations, primarily due to the high cost of organic solvents and the need for efficient solvent recovery systems to ensure the process’s overall economic and environmental sustainability

Economic analysis

The factorial estimation method, utilizing parameters specified by Gavin and Ray [42], was employed to calculate the costs associated with both liquid and solid processing systems in this analysis. All cost calculations in this study were conducted using United States dollars as the base currency as shown in Table 2.

The Total Annual Cost (TAC), calculated using the Capital Recovery Factor (CRF), is a common method in techno-economic analysis (TEA) to estimate the annualized cost of industrial-scale processes, as outlined in Eq. 23.

$$TAC = (TCI \times CRF) + OC \qquad \text{... (23)}$$

Where, TCI is Total Capital Investment, which includes the cost of plant construction, equipment, and installation. OC refers to the Operating Cost, which encompasses annual expenses such as raw materials, chemicals, energy, and labor. The Capital Recovery Factor (CRF) serves to convert a one-time initial investment into an equivalent annual cost that accounts for the time value of money or the expected rate of return (e.g., 10% per year), as shown in Eq. 24.

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1} \qquad \text{... (24)}$$

Where:

- i = interest rate or desired rate of return (per year)
- n = project lifetime or payback period (years)

Table 2 Feedstock, chemicals, and utilities prices

Input	Unit	Price	Reference
Bagasse	USD/ton	14.00	[43]
C_2H_6O	USD/L	0.80	[44]
H_2O	USD/L	0.00028	[45]
H_2SO_4	USD/L	0.16	[44]
CH_2O_2	USD/L	0.49	[44]
$C_4H_8O_2$	USD/L	1.30	[44]
CH_3ONa	USD/kg	0.60	[44]
CH_3OH	USD/L	0.28	[44]
Electricity	USD/KV	2.1	[46]

Sensitivity analysis

Sensitivity analysis helps assess a project's robustness by examining how cost and performance respond to changes in key variables. In this study, it evaluates the economic impact of varying biomass conditions and catalyst reaction rates, highlighting the effects of process parameter shifts. The analysis also considers future technological developments, focusing on factors like raw material properties, chemical prices, and utility costs. Key variables tested include solvent type, catalyst amount, temperature, and pressure each adjusted independently to determine its specific influence on system performance [47], [48], [49].

CHAPTER 4

RESULTS AND DISCUSSION

Scenario

The organosolv fractionation of sugarcane bagasse represents a promising strategy for valorizing one of the most abundant lignocellulosic residues generated by the sugar industry in Thailand. In this study, a feedstock input of 20,000 kg/day, equivalent to 6.6 million kg/year, was considered as the basis for process simulation across three scenarios. The compositional analysis of raw sugarcane bagasse indicated the presence of 38.30% cellulose (2,527,800 kg/year), 20.70% hemicellulose (1,359,600 kg/year), 23.70% lignin (1,564,200 kg/year), 4.20% ash (277,200 kg/year), and 13.00% other minor components (871,200 kg/year).

The distribution of these chemical constituents highlights their potential applications in biorefinery pathways. Cellulose, the primary structural polysaccharide, can be hydrolyzed into fermentable sugars, serving as a key feedstock for the production of bioethanol and other bio-based chemicals. Hemicellulose, with its amorphous and highly branched structure, can be depolymerized into pentose and hexose sugars, which are precursors for high-value products such as xylitol and furfural. Lignin, traditionally treated as a low value by-product, has gained significant attention in recent years as a renewable aromatic polymer that can be utilized in the production of biopolymers, resins, adhesives, and renewable energy. Although ash represents a relatively small fraction, it contributes to the mineral content of the biomass and can influence combustion behavior if residues are used for energy recovery. The remaining fraction, classified as other components, typically consists of extractives, waxes, and water-soluble organics, which may pose challenges during downstream processing but can also be valorized in specialty chemical markets.

Overall, this quantitative analysis underscores the importance of optimizing the organosolv fractionation process to achieve maximum cellulose recovery, enhanced enzymatic digestibility, and efficient utilization of all co-products. Such optimization not only improves the economic feasibility of bagasse-based biorefineries but also strengthens their alignment with circular bioeconomy principles and national sustainability goals.

For Scenario 1, Table 3 presents the detailed mass balance of the organosolv fractionation process using H_2SO_4 as the catalytic agent. During the conditioning step of sugarcane bagasse, the solid fraction (pulp) that was subsequently directed to hydrolysis and fermentation for ethanol production contained 2,584,341.72 kg/year of cellulose, 55,377.74 kg/year of hemicellulose (xylan), 158,931.96 kg/year of lignin, 53,139.49 kg/year of ash, and trace amounts of other minor components. These values represent the partitioning of major biomass constituents after catalytic fractionation and demonstrate the effectiveness of sulfuric acid in selectively solubilizing lignin and hemicellulose while retaining cellulose in the solid stream. The calculated performance indicators further reinforce the efficiency of this process. Specifically, the organosolv system catalyzed by H_2SO_4 achieved a cellulose recovery efficiency of 92.37% and a lignin removal rate of 90.82%. These figures confirm that the majority of cellulose was preserved within the pulp fraction, making it highly suitable for subsequent enzymatic hydrolysis and fermentation. At the same time, the removal of over 90% of lignin suggests a significant improvement in substrate accessibility, since lignin is well recognized as a major barrier to enzymatic digestibility in lignocellulosic biomass. When compared with laboratory-scale experimental results reported by [50], which documented cellulose recovery efficiencies as high as 99%, the simulation results in this study exhibited slightly lower cellulose retention. This discrepancy can be attributed to the inherent limitations of process simulation in replicating ideal laboratory conditions, where reaction severity and solvent penetration can be more precisely controlled. However, it is noteworthy that the lignin removal efficiency obtained in the present simulation (90.82%) exceeded the value of 86.4% reported in the same study. This finding indicates that under industrial-scale assumptions, sulfuric acid catalysis may enhance delignification beyond laboratory expectations, possibly due to the higher solvent-to-solid ratios and extended mass transfer conditions modeled in the simulation environment. These differences highlight the intrinsic variability between laboratory-scale experimentation and large-scale process simulation. While laboratory data often represent optimized and controlled scenarios with limited system complexity, industrial-scale simulations integrate broader process dynamics, including fluid-solid interactions, heat and mass transfer constraints, and operational heterogeneity. As a result, simulation outcomes may better reflect the realistic challenges and opportunities of full-scale deployment. Importantly, such results provide valuable insights into the techno-economic feasibility of sugarcane bagasse valorization. From a broader perspective, the relatively high cellulose recovery combined with substantial lignin removal demonstrates that sulfuric acid remains an effective catalyst for biomass fractionation in organosolv systems. The cellulose-enriched pulp stream represents a promising substrate for downstream conversion to bioethanol, while the solubilized lignin fraction could be isolated and valorized in biopolymer or energy applications. Moreover, the favorable balance between cellulose preservation and lignin extraction under Scenario 1 underscores the role of acid-catalyzed organosolv pretreatment as a scalable approach for integrating sugarcane bagasse into the circular bioeconomy. In summary, Scenario 1 results indicate that the use of H_2SO_4 as a catalyst delivers efficient cellulose recovery and strong delignification performance, with outcomes comparable to or surpassing laboratory benchmarks in some respects. These findings emphasize the necessity of integrating both experimental and simulation approaches to capture the full spectrum of biomass fractionation behavior, bridging the gap between controlled laboratory trials and the complexities of industrial application.

The Aspen Plus simulation of the organosolv-based biorefinery process provided insights into the efficiency of ethanol production during the fermentation stage. According to the simulation results, the fermentation stream received 2,297,087.79 kg/year of glucose from the hydrolysis step. This glucose was subsequently converted into 1,057,365.16 kg/year of ethanol in the product unit. The calculated glucose-to-ethanol conversion efficiency was approximately 46.04% by mass, which is lower than the theoretical maximum of around 51% reported in the literature [12]. This deviation highlights the inherent complexity of simulating biological processes at a process scale, where empirical assumptions and process limitations must be integrated into mass and energy balances. The lower-than-theoretical conversion efficiency can be explained by several mechanisms reflected in the simulation. A portion of the glucose was diverted to by-product formation, including organic acids, glycerol, and other soluble metabolites, which are often modeled as loss factors in Aspen Plus. Additionally, the simulation accounted for the inhibitory effects of compounds generated during fractionation and hydrolysis, such as furfural, hydroxymethylfurfural (HMF), acetic acid, and phenolic derivatives. These inhibitors are known to reduce yeast viability and metabolic efficiency, leading to lower ethanol yields. Furthermore, ethanol losses during separation and distillation were incorporated into the simulation, reflecting volatilization, azeotrope formation, and incomplete recovery. Overall, the Aspen Plus simulation demonstrates that ethanol production efficiency in lignocellulosic biorefineries is constrained not only by theoretical biochemical pathways but also by operational and downstream limitations. The results emphasize the importance of integrated optimization, including pretreatment strategies to minimize inhibitor formation, fermentation condition adjustments to enhance microbial tolerance, and improved separation technologies to reduce ethanol losses. Addressing these challenges is essential to bridge the gap between theoretical yields and practical performance, thereby advancing the economic and environmental sustainability of sugarcane bagasse–based ethanol production.

Although the organosolv fractionation process using H_2SO_4 demonstrated high efficiencies in cellulose recovery and lignin removal, the ethanol production results revealed certain limitations that require further improvement. The fermentation stage, in particular, plays a decisive role in determining the overall glucose-to-ethanol conversion efficiency, and the simulation indicated that its performance fell below the theoretical maximum. Several factors may account for this gap. One major issue is the presence of fermentation inhibitors such as furfural, hydroxymethylfurfural (HMF), acetic acid, and phenolic derivatives, which are commonly generated during fractionation and hydrolysis. These compounds can suppress yeast activity, reduce cell viability, and alter metabolic pathways, leading to lower ethanol yields. Additionally, glucose diversion into secondary metabolites such as organic acids and glycerol further reduces ethanol productivity. Ethanol losses also occur during recovery and distillation due to volatilization, azeotrope formation, and incomplete separation. These limitations highlight the need for process optimization across multiple stages. Possible improvements include pretreatment adjustments to minimize inhibitor formation, development of inhibitor-tolerant yeast strains, optimization of fermentation operating conditions, and the design of more efficient separation technologies.

In summary, addressing these issues is essential to enhance glucose-to-ethanol conversion efficiency at the commercial scale, thereby strengthening both the economic feasibility and environmental sustainability of sugarcane bagasse-based biorefinery systems.

For Scenario 2, Table 3 and Figure 2(B) illustrate the mass balance of the organosolv fractionation process using CH_2O_2 as the catalyst. During the sugarcane bagasse conditioning step, the solid stream (Pulp) designated for subsequent hydrolysis and fermentation consisted of 2,644,494.74 kg/year of cellulose, 153,342.18 kg/year of hemicellulose (xylan), 328,771.02 kg/year of lignin, 131,498.77 kg/year of ash, and 94,979.61 kg/year of extractives. In summary, organosolv fractionation using CH_2O_2 achieved a cellulose recovery efficiency of 94.52% and a lignin removal rate of 81.01%. The simulation results indicate that the cellulose recovery rate is nearly identical to that reported in the study by [35], which observed a recovery of 94.6%. However, the lignin removal in this simulation was slightly higher 81.01% compared to 80.4% in the same study. These differences are likely due to process efficiency variations under simulated industrial-scale conditions. The Aspen Plus simulation of Scenario 2, which employed CH_2O_2 as the catalyst, produced results that align closely with reported experimental studies while also providing additional insights into industrial-scale applications. The pulp stream generated after sugarcane bagasse conditioning contained 2,644,494.74 kg/year of cellulose, 153,342.18 kg/year of hemicellulose (xylan), 328,771.02 kg/year of lignin, 131,498.77 kg/year of ash, and 94,979.61 kg/year of extractives. These values correspond to a cellulose recovery efficiency of 94.52% and a lignin removal rate of 81.01%. The high cellulose recovery achieved in this scenario demonstrates the ability of CH_2O_2 to preserve the carbohydrate fraction in a form that is highly suitable for enzymatic hydrolysis and subsequent ethanol production. At the same time, lignin removal of 81.01% reflects a substantial reduction in biomass recalcitrance, even though it is somewhat lower than the 90.82% removal observed in Scenario 1 with H_2SO_4. This difference highlights the trade-off between maximizing cellulose recovery and achieving extensive delignification, suggesting that catalyst selection strongly influences the balance between these outcomes. When compared to the study by [35], which reported a cellulose recovery of 94.6% and lignin removal of 80.4%, the simulation results are remarkably consistent. The cellulose recovery efficiency of 94.52% is nearly identical to the experimental benchmark, while the lignin removal rate of 81.01% is slightly higher, suggesting that process assumptions at an industrial scale may offer marginal advantages in delignification. Such differences likely arise from improved solvent penetration and mass transfer modeled under large-scale conditions. Overall, the results of Scenario 2 reinforce the potential of CH_2O_2 as an alternative catalyst for organosolv fractionation. The combination of high cellulose recovery and effective lignin removal suggests that formic acid–based processes can support efficient biorefinery operations, particularly when integrated with downstream hydrolysis and fermentation. Moreover, the consistency between simulation and experimental data enhances the reliability of these findings and underscores the importance of simulation tools in bridging laboratory-scale knowledge with industrial-scale feasibility.

The Aspen Plus v11 simulation of Scenario 2, which employed CH_2O_2 as the organosolv catalyst, provided detailed insights into the performance of hydrolysis and fermentation processes as well as the downstream product distribution. The hydrolysis stage successfully converted a significant portion of the cellulose fraction into fermentable sugars, yielding 2,350,554.71 kg/year of glucose directed to the fermentation unit. Subsequent fermentation resulted in an ethanol output of 1,081,976.34 kg/year in the product stream. This corresponds to a glucose-to-ethanol conversion efficiency of 46.03% by mass. Although this value closely matches the performance of Scenario 1, it remains below the theoretical maximum of 51.14%, suggesting that process inefficiencies persist. The gap between experimental and theoretical efficiency highlights important areas for optimization, particularly in relation to fermentation bottlenecks and downstream recovery losses. The lower conversion efficiency can be attributed to several potential factors. First, a fraction of glucose may have been diverted toward the synthesis of metabolic by-products rather than ethanol, reflecting the inherent limitations of microbial fermentation under industrially simulated conditions. Second, inhibitors such as furfural, hydroxymethylfurfural (HMF), and weak organic acids are typically generated during pretreatment and may have impaired microbial activity, leading to incomplete sugar utilization. Third, losses during ethanol separation and purification particularly evaporation, entrainment, and solvent recovery inefficiencies are likely to have contributed to the suboptimal yield. These findings reinforce the importance of integrating robust detoxification methods and improving separation efficiency to enhance overall process performance.

A notable observation in Scenario 2 was the significantly higher cellulose content in the solid pulp stream, recorded at 2,644,494.74 kg/year, which exceeded that of Scenario 1. This indicates that CH_2O_2 is more effective in preserving cellulose integrity under the simulated conditions, minimizing degradation during pretreatment. Such preservation is advantageous for ensuring sustained glucose supply to the hydrolysis stage and improving long-term process stability. However, this improvement in cellulose retention came at the expense of lignin removal efficiency. The pulp stream contained 328,771.02 kg/year of residual lignin, considerably higher than in the H_2SO_4 based process. The reduced lignin solubilization efficiency suggests that CH_2O_2 is less effective at disrupting lignin–carbohydrate complexes, thereby leaving behind structural barriers that limit enzyme accessibility during hydrolysis. This limitation is critical because incomplete delignification directly hinders enzymatic saccharification and reduces the fraction of cellulose that can be converted into fermentable sugars.

From a biorefinery perspective, the trade off observed in Scenario 2 improved cellulose preservation but weaker lignin removal has important implications for process development. While maintaining cellulose integrity ensures a more reliable carbohydrate feedstock, the presence of residual lignin reduces overall process efficiency and may increase enzyme demand, raising operational costs. Moreover, the ethanol yield achieved in this scenario is insufficient to justify immediate commercial scale-up without further refinement. Strategies such as optimizing catalyst concentration, extending residence time, or integrating hybrid pretreatment methods could help achieve a more balanced outcome between cellulose preservation and lignin removal. Additionally, metabolic engineering of fermentation strains and advanced separation technologies could mitigate the conversion losses observed.

In summary, Aspen Plus simulation results demonstrate that the CH_2O_2 based organosolv process offers certain advantages in cellulose recovery but faces significant challenges in lignin removal and ethanol conversion efficiency. These findings underscore the dual importance of catalyst selection and process integration in organosolv fractionation and downstream fermentation. For industrial scale biorefinery applications, further optimization is required to reduce inhibitory compound formation, enhance delignification, and maximize ethanol yields. The insights gained from this scenario highlight the value of process simulation in identifying critical performance bottlenecks and guiding targeted improvements for sustainable bioethanol production.

For Scenario 3, Table 3 presents the detailed mass balance of the organosolv fractionation process using CH_3ONa as the catalyst, with methanol as the solvent system. During the conditioning step of sugarcane bagasse, the solid pulp stream, which was directed to subsequent hydrolysis and fermentation, yielded 2,578,746.09 kg/year of cellulose, 1,081,069.87 kg/year of hemicellulose, 233,723.48 kg/year of lignin, 219,154.38 kg/year of ash, and 416,367.47 kg/year of other extractive components. These values highlight the catalytic role of CH_3ONa in preserving the carbohydrate fractions, particularly hemicellulose, while ensuring effective delignification. The cellulose recovery achieved was 92.17%, while lignin removal reached 86.50%. Compared with the experimental findings reported in Weerasai et al. [36], which observed cellulose recovery of 93.1% and lignin removal efficiency of 86.5%, the simulation results showed only a slight deviation in cellulose recovery but an identical lignin removal performance. This close agreement confirms the reliability and stability of the CH_3ONa-based organosolv pretreatment under industrial-scale simulated conditions.

One of the most notable features of Scenario 3 is the high hemicellulose retention, with xylan recovery reaching 1,081,069.87 kg/year. This is significantly higher than the values reported in Scenario 1 (H_2SO_4-based) and Scenario 2 (CH_2O_2-based). Since hemicellulose is more susceptible to degradation during pretreatment due to its amorphous structure and lower thermal stability, the ability of the CH_3ONa–methanol solvent system to maintain such a high fraction of hemicellulose is a remarkable advantage. This preservation enhances the potential of the feedstock to yield a broader spectrum of fermentable sugars, including both glucose from cellulose and xylose from hemicellulose, which could be exploited through co-fermentation strategies using engineered microorganisms. Such an outcome not only increases the theoretical ethanol yield but also contributes to improving process economics and sustainability in a biorefinery context.

In the fermentation stage, the hydrolysate stream provided 2,292,114.13 kg/year of glucose, resulting in an ethanol production of 1,055,075.74 kg/year. This corresponds to a glucose-to-ethanol conversion efficiency of 46.04%, a value consistent with those observed in Scenario 1 and Scenario 2. Although comparable, this value remains below the theoretical maximum conversion efficiency of 51.14%. This discrepancy suggests partial glucose losses, which may arise from the formation of side-products such as organic acids, glycerol, or other metabolites during fermentation, or from the inhibitory effects of residual solvents and salts, including methanol and sodium compounds, on yeast metabolism. Therefore, while the pretreatment performance of Scenario 3 is favorable for carbohydrate preservation, careful consideration must be given to the downstream impacts of residual chemicals on microbial activity and ethanol recovery efficiency.

When compared across all three scenarios, clear trade-offs emerge. Scenario 1 (H_2SO_4-based) exhibited the highest lignin removal efficiency (90.82%) but retained lower amounts of hemicellulose. Scenario 2 (CH_2O_2-based) achieved the highest cellulose recovery (2.64 million kg/year), though lignin removal was relatively modest (81.01%). Scenario 3 (CH_3ONa with methanol) demonstrated the most balanced performance, combining high cellulose recovery (2.58 million kg/year), the highest hemicellulose retention (1.08 million kg/year), and a moderate lignin removal efficiency (86.50%). Despite these differences in pretreatment outcomes, all three scenarios converged on similar fermentation efficiencies (~46%). This finding suggests that the bottleneck for ethanol yield lies less in pretreatment differences and more in fermentation constraints, particularly the presence of inhibitors and operational limitations in microbial conversion.

In summary, Scenario 3 highlights the potential of sodium methoxide–based organosolv pretreatment with methanol as a solvent system to provide a balanced recovery of biomass components, particularly excelling in hemicellulose preservation while maintaining high cellulose yields and consistent lignin removal. The advantages of this approach could be maximized through integrated strategies that couple effective detoxification, inhibitor management, and advanced fermentation technologies. Such integration is essential for translating the promising outcomes observed in simulation into viable industrial scale biorefinery applications, ensuring both technical efficiency and economic competitiveness.

Economic evaluation

Table 4 presents a comprehensive breakdown of the capital investment, operating expenses, and raw material costs associated with ethanol production via the organosolv process under three simulated scenarios. The results clearly indicate that Scenario 1 incurred the highest overall costs compared to Scenarios 2 and 3. Specifically, the total capital cost in Scenario 1 was estimated at USD 4,358,930.00, while the annual operating cost reached USD 3,368,230.00. In addition, the total raw materials cost was USD 1,957,890.00, which was slightly higher than that of Scenario 2 but markedly lower than Scenario 3. These findings suggest that the process configuration and operating conditions applied in Scenario 1 may be more resource- and energy-intensive, thereby necessitating higher investments in equipment and utilities.

From a technical standpoint, the elevated capital cost in Scenario 1 could be attributed to the requirements of H_2SO_4-based pretreatment, which often involves more robust materials of construction to resist corrosion, larger solvent recovery units, and higher safety specifications. These design factors typically lead to greater equipment complexity and higher procurement costs. Likewise, the relatively high operating costs may stem from the intensive energy demand for heating, neutralization, and solvent recovery steps inherent to the acid-catalyzed process. Although the raw material cost in Scenario 1 was lower than that in Scenario 3, it was still substantial, reflecting the additional chemicals and neutralizing agents required during pretreatment.

When comparing the three scenarios, Scenario 1 illustrates a trade-off: while achieving superior delignification performance, it does so at the expense of increased capital and operating expenditures. This highlights the importance of conducting techno-economic assessments that balance process efficiency with cost feasibility. For industrial-scale implementation, the higher expenses observed in Scenario 1 could limit economic competitiveness unless offset by improved ethanol yields, co-product valorization, or energy integration strategies. Therefore, while Scenario 1 demonstrates strong technical performance, its economic limitations underline the necessity of exploring cost reduction strategies and optimizing process integration to enhance overall feasibility.

Table 3 Mass balance for organosolv fractionation experiments into 3 Scenarios.

Scenario 1; Organosolv fractionation by H_2SO_4

	Units	Bagasse	Downstream	Lignin	Sugar	Pulp	to Fermentation	Product
Cellulose	kg/year	2,797,815.00	213,473.28	196,395.42	17,077.86	2,584,341.72	516,868.34	516,868.34
Xylan	kg/year	1,504,830.00	1,449,452.26	246,406.88	1,203,045.37	55,377.74	55,377.74	55,377.74
Lignin	kg/year	1,731,285.00	1,572,353.04	1,430,841.26	141,511.77	158,931.96	158,931.96	158,931.96
Ash	kg/year	306,810.00	253,670.51	-	253,670.51	53,139.49	53,139.49	53,139.49
Extractives	kg/year	964,260.00	904,668.73	-	904,668.73	59,591.27	59,591.27	59,591.27
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	2,041,590.44	-	3,583.91	-	-	1,057,365.16
Co_2	kg/year	-	-	-	-	-	-	1,010,101.99
Glucose	kg/year	-	-	-	-	-	2,297,087.79	229,708.78
Water	kg/year	-	1,089,128.38	-	155,788.26	-	8,536,287.65	10,603,698.80
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,823,742.37
H_2SO_4	kg/year	-	73,050.00	-	73,048.73	-	-	-
CH_2O_2	kg/year	-	-	-	-	-	-	-
CH_3OH	kg/year	-	-	-	-	-	-	-

Table 3 (continued)

Scenario 2; Organosolv fractionation by CH_2O_2								
Cellulose	kg/year	2,797,815.00	153,320.26	141,054.64	12,265.62	2,644,494.74	528,898.95	528,898.95
Xylan	kg/year	1,504,830.00	1,351,487.82	229,752.93	1,121,734.89	153,342.18	153,342.18	153,342.18
Lignin	kg/year	1,731,285.00	1,402,513.98	1,276,287.72	126,226.26	328,771.02	328,771.02	328,771.02
Ash	kg/year	306,810.00	175,311.23	-	175,311.23	131,498.77	131,498.77	131,498.77
Extractives	kg/year	964,260.00	869,280.39	-	869,280.39	94,979.61	94,979.61	94,979.61
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	583,311.56	-	-	-	-	1,081,976.34
Co_2	kg/year	-	-	-	-	-	-	1,033,613.08
Glucose	kg/year	-	-	-	-	-	2,350,554.71	235,055.47
Water	kg/year	-	1,561,084.02	-	-	-	8,530,940.88	10,646,472.99
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,775,662.21
H_2SO	kg/year	-	-	-	-	-	-	-
CH_2O_2	kg/year	-	709,162.09	-	-	-	-	-
CH_3OH	kg/year	-	687,926.46	-	-	-	-	-

Table 3 (continued)

Scenario 3; Organosolv fractionation by CH_3ONa								
Cellulose	kg/year	2,797,815.00	219,068.91	201,543.40	17,525.51	2,578,746.09	515,749.22	515,749.22
Xylan	kg/year	1,504,830.00	423,760.13	72,039.22	351,720.91	1,081,069.87	1,081,069.87	1,081,069.87
Lignin	kg/year	1,731,285.00	1,497,561.53	1,362,780.99	134,780.54	233,723.48	233,723.48	233,723.48
Ash	kg/year	306,810.00	87,655.62	-	87,655.62	219,154.38	219,154.38	219,154.38
Extractives	kg/year	964,260.00	547,892.53	-	547,892.53	-	416,367.47	416,367.47
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	-	-	-	-	-	1,055,075.74
Co_2	kg/year	-	-	-	-	-	-	1,007,914.91
Glucose	kg/year	-	-	-	-	-	2,292,114.12	229,211.41
Water	kg/year	-	-	-	-	-	8,536,785.02	10,599,719.80
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,828,214.94
CH_2O_2	kg/year	-	-	-	-	-	-	-
CH_3OH	kg/year	-	2,896,143.95	-	-	-	-	-
CH_3ONa	kg/year	-	365,250.00	-	-	365,250.00	-	-

Table 4 TAC breakdown for the organosolv fractionation processes.

Cost analysis	Unit	Scenario 1	Scenario 2	Scenario 3
Total Capital Cost	USD	4,358,930	3,671,550	3,640,210
Total Operating Cost	USD/Year	3,368,230	3,183,650	14,526,300
Total Raw Materials Cost	USD/Year	1,957,890	1,791,750	12,292,500
Total Product Sales	USD/Year	43,710,900	43,291,000	43,950,800
Total Utilities Cost	USD/Year	94,615	92,066	92,288
Desired Rate of Return	Year	20	20	20
Equipment Cost	USD	295,500	242,900	262,300
Total Installed Cost	USD	1,391,500	1,066,700	1,079,100
Electricity rate	kW	79.64	77.49	77.68
Electricity cost	USD/H	11.94	11.62	11.65
TAC	USD	4,263,365	3,927,396	15,273,841
TAC	million USD	4.26	3.92	15.27

Scenario 2 demonstrates a reduction in overall costs compared with Scenario 1, particularly in terms of raw materials and operating expenses. The raw material cost in Scenario 2 was USD 1,791,750.00, while the annual operating cost amounted to USD 3,183,650.00. The corresponding total capital investment was USD 3,671,550.00. Despite these relatively lower values, Scenario 2 incurred the highest utilities cost among all three scenarios, at USD 92,066.00. This elevated utilities cost may reflect the presence of energy-intensive process steps, such as heating and solvent recovery, or the requirement for additional environmental control systems to ensure safe operation. The results suggest that while Scenario 2 offers an advantage in terms of reduced raw material consumption and operating expenditure, its higher utility demand may offset some of these economic benefits. In contrast, Scenario 3 recorded the highest overall costs across all major categories, highlighting its less favorable economic performance. Specifically, raw material expenses reached USD 12,292,500.00, significantly surpassing those of both Scenario 1 and Scenario 2. Operating costs were also substantially elevated, at USD 14,526,300.00 per year, while the total capital investment and utilities costs were USD 3,640,210.00 and USD 92,288.00, respectively. Collectively, these values contributed to a Total Annualized Cost (TAC) of USD 15,273,841.00, equivalent to 15.27 million USD, making Scenario 3 the most cost-intensive option.

Although Scenario 3 achieved the highest total product sales of USD 43,950,800.00 per year, its disproportionately high raw material and operating expenditures suggest reduced economic viability. This outcome may be linked to the reliance on expensive catalysts or solvents, along with more resource-intensive operating conditions compared to the other scenarios. These findings underscore the importance of balancing process efficiency and product revenue with the sustainability of raw material supply and the cost of utilities. From an industrial perspective, while Scenario 3 demonstrates superior product generation potential, its high costs raise concerns regarding scalability and long-term competitiveness.

Based on the data presented in Table 4, a clear distinction in the Total Annualized Cost (TAC) among the three scenarios can be observed. Scenario 2 demonstrates the lowest TAC, at USD 3.92 million, making it the most economically favorable option despite recording the highest utilities cost among all scenarios. This suggests that, although Scenario 2 requires greater energy consumption or environmental control measures, its lower raw material and operating costs compensate for this, resulting in superior overall economic performance. In contrast, Scenario 1 exhibits the highest capital investment, amounting to USD 4.36 million, which reflects the greater complexity of the process design. The reliance on H_2SO_4 for pretreatment likely necessitates the use of more robust equipment, corrosion-resistant materials, and additional waste-handling systems, thereby driving up the capital requirement. While Scenario 1 achieves strong technical performance, particularly in lignin removal, its elevated investment and operating costs highlight significant economic limitations when considered for industrial-scale applications.

Meanwhile, Scenario 3 recorded the highest TAC, reaching USD 15.27 million, which is considerably higher than the other two scenarios. This is largely due to its significantly higher raw material cost (USD 12.29 million) and operating cost (USD 14.53 million). Although Scenario 3 generated the highest annual product sales

(USD 43.95 million), its disproportionately high expenditures undermine its economic feasibility. The elevated costs may be attributed to the use of expensive chemicals, higher solvent requirements, or more resource-intensive process conditions. As a result, despite its technical advantages in carbohydrate preservation and high ethanol yield, Scenario 3 faces substantial economic challenges that could limit its scalability.

In summary, the comparative analysis of the three scenarios reveals distinct trade-offs between technical efficiency and economic viability. Scenario 2 stands out as the most economically viable configuration, offering the lowest TAC while maintaining competitive technical performance. Scenario 1 provides strong delignification results but at the expense of higher costs, whereas Scenario 3, despite delivering the greatest product sales, demonstrates the weakest economic competitiveness due to its high raw material and operational demands. These findings emphasize the importance of integrating both technical performance and economic feasibility into process design decisions to ensure long-term sustainability of organosolv-based ethanol production at an industrial scale.

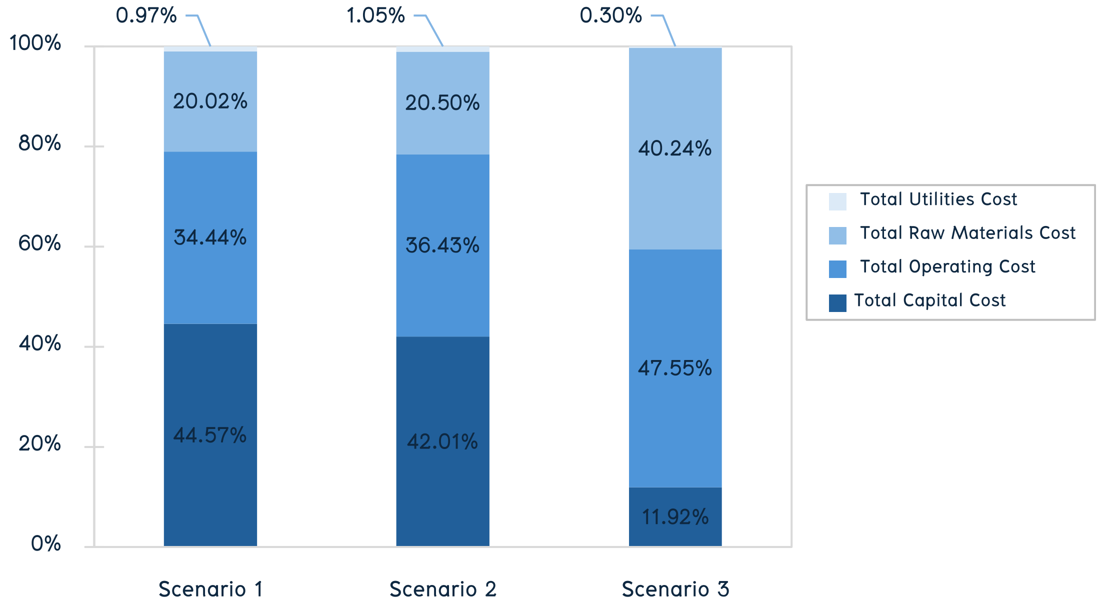


Figure 9 TAC contributions from each fractionation method

Figure 9 illustrates the percentage contributions of each cost component to the Total Annualized Cost (TAC) for the three organosolv fractionation scenarios. The analysis shows that the capital cost is the largest contributor in Scenarios 1 and 2, accounting for 44.6% and 42.0%, respectively, while it is significantly lower in Scenario 3 at only 11.9%. In contrast, the operating cost becomes the dominant component in Scenario 3 (47.5%), and also contributes substantially in Scenarios 1 and 2 at 34.4% and 36.4%, respectively. The raw materials cost is highest in Scenario 3 at 40.2%, compared to 20.0% and 20.5% in Scenarios 1 and 2, respectively. The utilities cost has the least impact in all scenarios, contributing less than 1.1% across the board.

These findings confirm that operating and raw materials costs are significant contributors to the Total Annualized Cost (TAC). Notably, the capital cost contribution observed in this study varies significantly among the scenarios, ranging from 11.9% in Scenario 3 to 44.6% in Scenario 1. In comparison, previous studies reported relatively consistent and higher capital cost shares. For example, Cheng et al. reported a capital cost share of 28.17% for liquid hot water pretreatment of sugarcane bagasse [51]. Similarly, Sganzerla et al. noted that approximately 35% of the fixed capital investment in subcritical water hydrolysis was attributed to the reactor system [52], and a 34.7% capital cost share was reported for organosolv pretreatment of olive leaves [53]. These comparisons suggest that the capital intensity in the organosolv processes evaluated in this study can vary widely depending on the specific process configuration, solvent system, and plant design, with Scenario 3 demonstrating a notably lower capital burden.

Regarding operating costs, this study reports a substantial share ranging from 34.4% to 47.5%, which is slightly lower than the 54.78% previously reported for organosolv pretreatment [53]. In contrast, the raw material costs in this study are notably higher, accounting for 20.0% to 40.2%, compared to approximately 30% reported in earlier research [54]. The increased share may be attributed to variations in solvent systems, process design, or cost assumptions applied in the simulation. In particular, the high raw material cost in Scenario 3 reflects the greater influence of input chemical prices and usage rates in that configuration.

Sensitivity analysis

A sensitivity analysis was conducted to evaluate the potential impacts of future technological changes on the economic viability of the organosolv biomass fractionation process, with a particular focus on the total annual cost (TAC), which serves as a key indicator of economic feasibility at the industrial scale. In general, sensitivity analyses in process simulation commonly adopt variation ranges of ±10–30% for operating and utility costs, ±15–40% for capital investment, and up to ±50% for raw material and product prices [54], [55]. However, to ensure a consistent and comparable assessment across all scenarios in this study, a fixed variation of ±10% was uniformly applied.

As shown in Table 5 and Figure 10, changes in chemical costs (Case 2) exerted the most substantial influence on TAC. Scenario 2, which utilized CH_2O_2, showed the highest TAC fluctuation at ±0.18%, followed by Scenario 3 (CH_3ONa) at ±0.12%, and Scenario 1 (H_2SO_4) at ±0.01%. In contrast, fluctuations in raw material costs (Case 1), utility costs (Case 3), utility consumption (Case 4), operating temperature (Case 5), and pressure (Case 6) resulted in negligible changes in TAC, typically within ±0.01% or even 0.00% in several cases. Among the scenarios, Scenario 1 exhibited the highest cost stability, as all parameters resulted in a TAC variation of no more than ±0.01%. These results confirm that chemical cost is the most sensitive and economically influential parameter in organosolv fractionation, particularly when employing CH_2O_2 and CH_3ONa as catalysts.

These findings align with previous studies such as Parascanu et al. [56], who identified chemical and energy inputs as key cost drivers in lignocellulosic biorefineries, and Gadkari et al. [57], who emphasized the significance of chemical cost control in reducing the minimum product selling price. To improve the economic viability of organosolv-based biorefineries, it is recommended to adopt strategies such as low-cost or free lignocellulosic feedstock sourcing, solvent recovery optimization, and scaling up production capacity to exploit economies of scale.

Table 5 Sensitivity analysis of price fluctuations on TAC across different scenarios.

Parameter changed		Min	Baseline	Max	Unit	TAC (million US$/year)				
						Min	Change (%)	Baseline	Max	Change (%)
Scenario 1; Organosolv fractionation by H_2SO_4 catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	4.25	-0.01	4.26	4.27	0.01
Chemicals cost	Case 2	different for water, ethanol and H_2SO_4				4.25	-0.01	4.26	4.27	0.01
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	4.25	-0.01	4.26	4.27	0.01
Utilities consumption	Case 4	75.71	84.12	92.53	KW	4.26	0.00	4.26	4.26	0.00
Temperature change	Case 5	153.00	170.00	187.00	°C	4.26	0.00	4.26	4.26	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	4.26	0.00	4.26	4.26	0.00
Scenario 2; Organosolv fractionation by CH_2O_2 catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	3.91	-0.01	3.92	4.02	0.01
Chemicals cost	Case 2	different for water, ethanol and CH_2O_2				3.74	-0.18	3.92	4.10	0.18
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	3.91	-0.01	3.92	3.93	0.01
Utilities consumption	Case 4	69.74	77.49	85.24	KW	3.92	0.00	3.92	3.92	0.00
Temperature change	Case 5	143.10	159.00	174.90	°C	3.92	0.00	3.92	3.92	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	3.91	-0.01	3.92	3.93	0.01

Table 5 (continued)

Scenario 3; Organosolv fractionation by CH_3ONa catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	15.26	-0.01	15.27	15.28	0.01
Chemicals cost	Case 2	different for water, ethanol and CH_3ONa				15.15	-0.12	15.27	15.15	0.12
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	15.26	-0.01	15.27	15.28	0.01
Utilities consumption	Case 4	69.91	77.68	85.45	KW	15.27	0.00	15.27	15.27	0.00
Temperature change	Case 5	135.00	150.00	165.00	°C	15.27	0.00	15.27	15.27	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	15.27	0.00	15.27	15.27	0.00

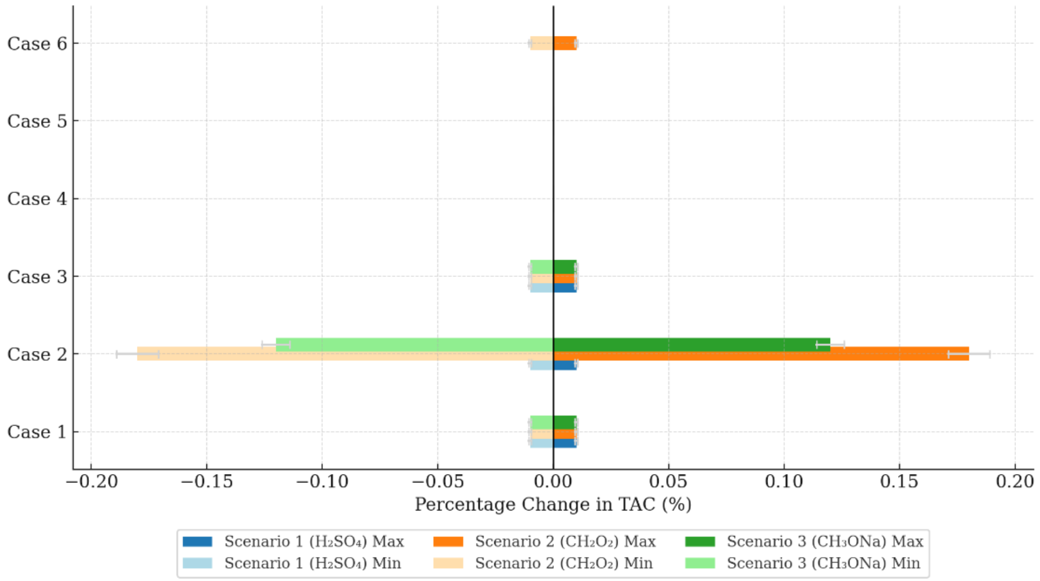


Figure 10 Sensitivity analysis of price fluctuations on TAC across different scenarios.

able 6 presents the annual ethanol production, total annual cost (TAC), total product sales, and fractionation costs of cellulose, lignin, and ethanol across three organosolv process scenarios. Among these, Scenario 2 demonstrates the most favorable economic performance. It achieves the highest ethanol yield at 977,555.63 kg/year and the greatest total product sales revenue of 88,138,800.00 USD/year. Although the TAC of Scenario 2 (23,493,394.47 USD/year) is slightly higher than that of Scenario 3, it remains lower than Scenario 1, resulting in a competitive ethanol unit cost.

Table 6 Value-based distribution of TAC for ethanol and lignin recovery.

Scenario	Ethanol Production	Lignin Production	TAC	Total Product Sales	Cost of Lignin Production	Cost of Ethanol Production	
	(kg/Year)	(kg/Year)	USD/Year)	(USD/Year)	(USD/kg)	(USD/kg)	(USD/L)*
1	1,057,365	1,430,841	4,263,365	43,710,900	1.88	1.49	1.20
2	1,081,976	1,276,287	3,927,396	43,291,000	1.84	1.45	1.14
3	1,055,075	1,362,780	15,273,841	43,950,800	6.96	5.49	4.33

Note: * Data are calculated based on an ethanol density of 0.789 kg/L [33].

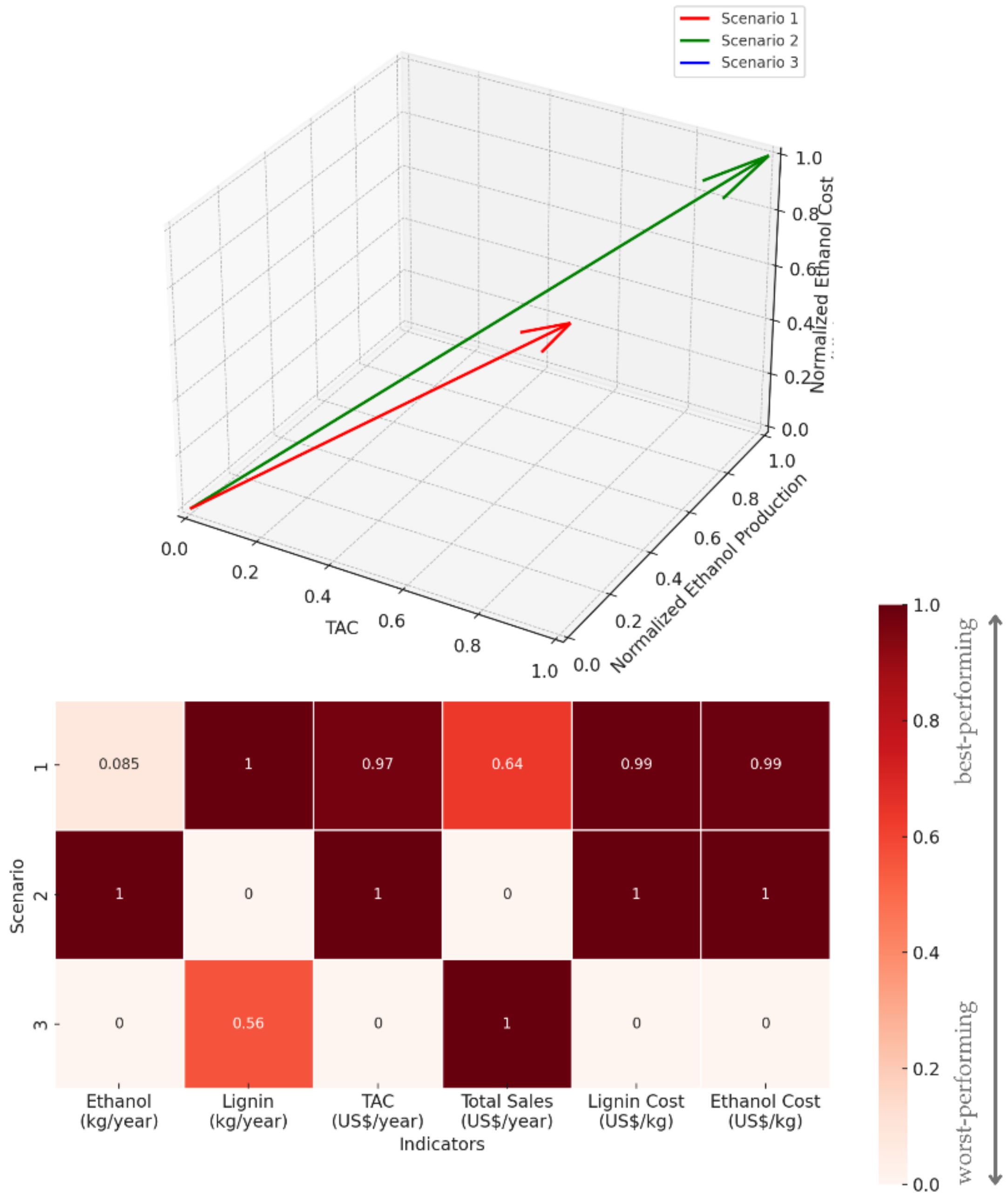
The value-based allocation approach was applied to distribute TAC between the main products, ethanol and lignin. This method allocates costs according to the economic value of each product rather than their mass proportions (as in mass-based allocation). The economic value of each product was first calculated by multiplying its annual production quantity (kg/year) by its respective market price (USD/kg). The total value was then used to determine each product’s value fraction, which was subsequently multiplied by TAC to derive the allocated cost for each product. Finally, the allocated cost was divided by the product’s annual production to obtain the unit production cost. This method improves economic accuracy, especially in cases where the co-products differ significantly in market value. It has been widely recognized in techno-economic assessments, such as the work by [58], and in life cycle analysis (LCA) studies, including that of [59], as a standard and appropriate method for cost allocation in biorefinery systems and product life cycle evaluations [60].

Table 6 presents the value-based allocation of TAC for ethanol and lignin production across three scenarios. Scenario 2 exhibits the lowest production costs for both ethanol (1.45 USD/kg) and lignin (1.84 USD/kg), while maintaining comparable total product sales to the other scenarios, indicating superior economic performance. In contrast, Scenario 3, despite achieving the highest total product sales, incurs a significantly higher TAC, resulting in markedly elevated unit production costs. Scenario 1 shows intermediate values in terms of both costs and revenues. Overall, the value-based allocation approach highlights Scenario 2 as the most cost-effective option, offering the lowest unit production costs for both primary products.

Priadi et al. [61] reported an ethanol production cost of ~1.11 USD/L using enzymatic hydrolysis, notably lower than the 1.14–4.32 USD/L range observed in Table 6. The discrepancy likely arises from differences in feedstock, process scale, and regional costs. Similarly Gubicza et al. [62] and Kautto et al. [63] achieved lower MESPs (~1.03 and 0.81 USD/L, respectively) through optimized organosolv pretreatment and lignin valorization. These findings emphasize the impact of feedstock type, pretreatment efficiency, and co-product recovery on production economics. Using a value-based cost allocation approach, Scenario 2 showed the highest economic feasibility, with the lowest ethanol 1.14 USD/L (1.45 USD/kg) and lignin costs (1.84 USD/kg). Further cost reductions could be achieved through lignin valorization (e.g., eugenol production) and the fermentation of residual sugars such as xylose, enhancing overall resource utilization and process viability in the Thai context.

A strategic evaluation of ethanol production efficiency under the three proposed scenarios was conducted using Normalized 3D Vector Analysis in combination with heatmap visualization. This integrated approach serves as a systematic method for assessing multidimensional process performance. It applies Min–Max normalization to rescale variables with differing units into a common range (0–1), enabling equitable comparisons. The normalized values are then represented as three-dimensional vectors, $\vec{v} = (x',y',z')$, typically corresponding to ethanol yield, TAC, and total product sales. The direction and magnitude of each vector reflect the overall efficiency and balance among key indicators. Simultaneously, the heatmap visualizes the normalized values using a color gradient to highlight the strengths and weaknesses of each scenario. Together, these tools facilitate a comprehensive techno-economic comparison, supporting strategic decision-making in complex biorefinery systems.

Figure 5 presents a comparative techno-economic analysis of ethanol production from sugarcane bagasse under three scenarios (Scenario 1–3). The assessment incorporates both normalized three-dimensional vector plots (ranging from 0 to 1) and heatmaps to evaluate strategic indicators, including ethanol and lignin yields, total annual cost (TAC), total sales revenue, lignin production cost, and ethanol production cost per unit. Based on the 3D vector analysis, Scenario 2 demonstrates the most outstanding performance, characterized by the longest vector length indicating an optimal balance between high ethanol yield and reasonable production cost. In contrast, Scenario 1, while achieving the highest lignin output, exhibits higher TAC and ethanol cost. Scenario 3, although offering the lowest TAC, yields minimal ethanol output, resulting in the weakest overall economic performance. The heatmap further corroborates this trend. Scenario 2 achieves superior values in key performance indicators (e.g., ethanol production, revenue, and low unit costs), whereas Scenario 3 records the lowest values in several critical dimensions. From a strategic perspective, Scenario 2 emerges as the most favorable option for ethanol production from sugarcane bagasse using the organosolv process.



Scenario	Ethanol (kg/year)	Lignin (kg/year)	TAC (US$/year)	Total Sales (US$/year)	Lignin Cost (US$/kg)	Ethanol Cost (US$/kg)
1	0.085	1	0.97	0.64	0.99	0.99
2	1	0	1	0	1	1
3	0	0.56	0	1	0	0

Figure 11 Comparative analysis of techno-economic performance for ethanol production from sugarcane bagasse via the organosolv process using normalized 3D vectors and heatmaps.

Discussion

The evaluation of organosolv fractionation for ethanol production from sugarcane bagasse underscores the pivotal influence of catalyst and solvent selection on biomass deconstruction efficiency, ethanol yield, and overall process economics at an industrial scale. Among the three catalytic scenarios examined, distinct trade-offs were observed in terms of biomass component recovery, conversion efficiency, and economic performance.

Scenario 1, employing H_2SO_4, achieved the highest lignin removal efficiency at 90.82%, alongside a glucose-to-ethanol conversion efficiency of 46.04%, which was comparable to the other scenarios. However, the corrosive nature of H_2SO_4 and the associated environmental burdens, including intensive wastewater treatment, contributed to elevated operational and maintenance costs, resulting in a higher TAC. In contrast, Scenario 2, utilizing CH_2O_2, demonstrated superior cellulose preservation with the highest recovery rate of 94.52%. When evaluated using a value-based cost allocation approach, Scenario 2 yielded the most economically favorable outcome, with unit production costs of 1.45 USD/kg for ethanol and 1.84 USD/kg for lignin, corresponding to approximately 1.14 USD/L of ethanol. These results, combined with moderate capital requirements, position Scenario 2 as the most viable candidate for large-scale deployment. Scenario 3, based on sodium methoxide (CH_3ONa) in methanol, exhibited the strongest performance in retaining total carbohydrates, particularly hemicellulose. Nevertheless, its economic viability was undermined by the highest TAC of 15.27 million USD/year, primarily driven by elevated chemical and operational expenditures, despite achieving the greatest total revenue from product sales.

Parametric sensitivity analysis revealed that chemical costs were the most influential drivers of TAC variability across all configurations, particularly in Scenarios 2 and 3. In contrast, other factors such as feedstock price, reaction temperature, and pressure exerted minimal economic impact. These insights reinforce the necessity of stringent chemical cost management to improve process economics. Strategic performance benchmarking using Normalized 3D Vector Analysis and heatmap visualization further validated Scenario 2 as the most balanced and robust configuration. It excelled across key performance indicators, including ethanol yield, revenue generation, and production cost minimization, thus affirming its suitability for industrial-scale implementation within Thailand's emerging bioeconomy.

A comparative analysis (Table 7) with the existing literature highlights the variation in minimum ethanol selling price (MESP) across different studies, shaped by feedstock type, pretreatment strategy, and co-product valorization potential. This work emphasizes the economic impact of catalyst selection in the organosolv fractionation process. The catalyst CH_2O_2 yielded the most favorable MESP at 1.14 USD/L, followed by H_2SO_4 at 1.20 USD/L and CH_3ONa at 4.33 USD/L. These findings indicate that organic acids present a more cost-effective pathway for lignocellulosic ethanol production in Thailand. Gubicza et al. [54] and Martinez-Hernandez et al. [58] reported MESPs as low as 0.50–0.63 USD/L through advanced fermentation techniques and lignin valorization. Kautto et al. [62] demonstrated further cost reduction with assumptions of high lignin market prices. Conversely, Correia et al. [66] reported higher MESPs (2.41–2.70 USD/L) due to less favorable biomass and lower conversion yields. Within this context, the MESP achieved in Scenario 2 (1.14 USD/L) is competitive, while Scenario 3 reflects cost limitations despite technical strengths. In conclusion, the findings emphasize that the integration of optimal catalyst-solvent systems, effective co-product recovery (particularly lignin valorization), mitigation of fermentation inhibitors, and comprehensive process optimization are essential for enhancing the economic sustainability of lignocellulosic biorefineries. Such strategic advancements are imperative for the successful transition of Thailand toward a high-value, bio-based economy.

Table 7 Comparison of minimum ethanol selling price from various biomass feedstocks and conversion technologies

Biomass	Main Process	Technical Notes	MESP (USD/L)	Study / Scenario
Sugarcane bagasse	Liquefaction + SSF + Co-Ferm	*Recombinant E. coli (LY01);* pH 6.0; no detoxification required	0.50 – 0.63	[64]
Hardwood (generic)	Organosolv + enzymatic hydrolysis	Ethanol-water 50:50; no catalyst or organic solvent recovery reported	0.81 (base), 0.53 (lignin @1000 USD/t)	[65]
Wheat straw	Organosolv + lignin valorization (eugenol)	H_2SO_4 used as catalyst in organosolv; lignin valorized into eugenol	0.53	[58]
Eucalyptus residues	Steam explosion + enzymatic hydrolysis + fermentation	Steam explosion at 200°C for 10 min; enzyme: Cellic CTec2; fed-batch fermentation	2.37	[66]
Corn stover	Steam explosion + enzymatic hydrolysis + fermentation	Similar to eucalyptus; low yield from corn stover contributes to high MESP	2.65	[66]

Table 7 (continued)

Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by H_2SO_4	1.20	This study (Scenario 1)
Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by CH_2O_2	1.14	This study (Scenario 2)
Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by CH_3ONa	4.33	This study (Scenario 3)

CHAPTER 5

CONCLUSIONS

A comprehensive techno-economic evaluation was conducted to determine the industrial viability of ethanol production from sugarcane bagasse via organosolv fractionation, utilizing three catalytic systems: H_2SO_4, CH_2O_2, and CH_3ONa. Each catalytic configuration exhibited specific advantages with respect to biomass deconstruction, ethanol and lignin recovery, and cost efficiency. Among the evaluated scenarios, the CH_2O_2 catalyzed process demonstrated superior performance, achieving the highest cellulose recovery (94.52%), a competitive ethanol output of 1,081,976 kg/year, and the lowest production costs 1.14 USD/L for ethanol and 1.84 USD/kg for lignin. Capital investment remained moderate at 3.67 million USD, while TAC was the lowest among all scenarios at 3.93 million USD/year. Despite a slightly lower lignin removal efficiency (81.01%) compared to the H_2SO_4 based configuration (90.82%), the CH_2O_2 pathway maintained higher cellulose integrity and more favorable economic indices, which offset its minor limitations. In contrast, the CH_3ONa based system retained a larger proportion of hemicellulose but incurred substantial raw material and reagent expenses, resulting in the highest ethanol (4.33 USD/L) and lignin (6.96 USD/kg) production costs and TAC exceeding 15 million USD/year. Chemical input costs emerged as the dominant sensitivity parameter, particularly for CH_2O_2 and CH_3ONa configurations, while variations in feedstock prices, temperature, and pressure had negligible impacts on overall cost structure. The sulfuric acid route, though efficient in delignification, was constrained by corrosion risks and the need for extensive wastewater treatment, thereby raising operating and maintenance costs. Strategic performance evaluation using normalized 3D vector analysis and heatmap visualization revealed that the CH_2O_2 based process offered the most balanced and economically viable solution, with favorable alignment across ethanol yield, revenue, and unit cost metrics. These findings underscore the potential of formic acid-catalyzed organosolv pretreatment as a scalable and sustainable approach for lignocellulosic ethanol production in Thailand. To enhance long-term viability, future process development should prioritize solvent recovery optimization, inhibitor mitigation during fermentation, and lignin valorization into higher-value bio-based chemicals. Such advancements will further strengthen the role of sugarcane bagasse valorization in supporting Thailand's transition toward a circular, bio-based economy.

In the context of Thailand's Bio-Circular-Green (BCG) economy, the valorization of bagasse aligns with national goals for sustainable resource use and clean energy. Converting bagasse to ethanol and lignin-derived bioproducts reduces environmental impacts from open burning, supports local industry, and strengthens energy security. This research supports key UN Sustainable Development Goals (SDGs), including SDG 7 (Clean Energy), SDG 9 (Innovation and Industry), and SDG 12 (Sustainable Production). With Thailand being one of the world's top sugarcane producers, it has strong potential to advance second-generation biofuel technologies. Targeted investments in R&D, along with policy and industry support, could position Thailand as a regional biorefinery leader.

In conclusion, formic acid–based organosolv pretreatment by CH_2O_2 shows strong promise for industrial ethanol production. Future work should focus on solvent recovery optimization, inhibitor reduction, and enhanced valorization of co-products. Additionally, integrating efficient glucose fermentation via SSF or SHF could further improve ethanol yield and reduce production costs, ensuring economic and environmental sustainability in alignment with the BCG model and SDG framework.

Research Recommendations

Thailand possesses significant potential for utilizing its abundant agricultural biomass residues to advance the development of bioethanol production and other biotechnological innovations. With appropriate support from the government particularly in the form of strategic investment in research and development (R&D), formulation of conducive policies, and the promotion of collaboration among academic institutions, industries, and local communities the country can position itself as a regional hub for green energy and biorefinery technologies.

Future research should emphasize the integration of biomass fractionation processes with high-efficiency enzymatic saccharification, particularly focusing on enhancing the conversion of cellulose to glucose and its subsequent fermentation into ethanol. The application of Simultaneous Saccharification and Fermentation (SSF) or Separate Hydrolysis and Fermentation (SHF) approaches offers promising potential to reduce processing time, minimize enzyme usage, and increase ethanol yield per unit of biomass.

A key strategy to reduce the overall production cost of ethanol involves improving the efficiency of glucose fermentation. This can be achieved by developing robust strains of yeast or microorganisms capable of tolerating fermentation inhibitors generated during pretreatment and efficiently utilizing glucose. In addition, optimizing fermentation parameters such as temperature, initial sugar concentration, and pH can significantly influence the fermentation rate and final ethanol concentration. Research in this direction would contribute to higher ethanol yields from sugarcane bagasse, lower unit production costs, and enhanced competitiveness of commercial-scale bioethanol production systems.

In conclusion, the application of CH_2O_2 in the organosolv pretreatment process demonstrates strong potential for industrial-scale deployment. Nevertheless, future research should aim to enhance the performance of saccharification and fermentation processes, improve solvent recovery systems, mitigate the formation of fermentation inhibitors, and increase the market value of co-products such as lignin and hemicellulose derivatives. These efforts are critical to achieving a sustainable bioethanol production platform that is economically viable, environmentally sound, and socially beneficial fully aligned with Thailand’s Bio-Circular-Green (BCG) Economy Model and the global Sustainable Development Goals (SDGs).

BIBLIOGRAPHY

[1] Energy Policy and Planning Office (EPPO). (2024). **Energy statistics of Thailand 2024**. Bangkok, Thailand. Available online: www.eppo.go.th (accessed on July 7, 2025).

[2] Department of Alternative Energy Development and Efficiency (DEDE). (2015). **Alternative energy development plan (AEDP 2015): 2015–2036**. Bangkok, Thailand.

[3] Cazier, E. A., Pham, T.-N., Cossus, L., Abla, M., Ilc, T., and Lawrence, P. (2024). Exploring industrial lignocellulosic waste: Sources, types, and potential as high-value molecules. **Waste Management,** 188, 11–38.

[4] Barciela, P., Perez-Vazquez, A., Fraga-Corral, M., and Prieto, M. A. (2023). Utility aspects of sugarcane bagasse as a feedstock for bioethanol production: Leading role of steam explosion as a pretreatment technique. **Processes,** 11(11), 3116.

[5] Kumar, A., Techapun, C., Sommanee, S., Mahakuntha, C., Feng, J., Htike, S. L., Khemacheewakul, J., et al. (2023). Production of phenylacetylcarbinol via biotransformation using the co-culture of *Candida tropicalis* TISTR 5306 and *Saccharomyces cerevisiae* TISTR 5606 as the biocatalyst. **Journal of Fungi,** 9(9), 928.

[6] Broda, M., Yelle, D. J., and Serwanska, K. (2022). Bioethanol production from lignocellulosic biomass: Challenges and solutions. **Molecules,** 27(24), 8717.

[7] Novia, N., Melwita, E., Jannah, A. M., Selpiana, S., Yandriani, Y., Afrah, B. D., et al. (2025). Current advances in bioethanol synthesis from lignocellulosic biomass: Sustainable methods, technological developments, and challenges. **Journal of Umm Al-Qura University for Applied Sciences.**

[8] Ritchie, H., Rosado, P., and Roser, M. (2023). Sugar cane production. **Our World in Data.** https://ourworldindata.org/grapher/sugar-cane-production (accessed on July 7, 2025).

[9] Office of the Cane and Sugar Board. (2024). **Report on sugarcane plantation situation for the 2024/2025 production year**. Bangkok, Thailand.

[10] Office of the Cane and Sugar Board. (2024). **Report on the efficiency of sugar production for the 2024/2025 production year**. Bangkok, Thailand.

[11] Awoyale, A. A., and Lokhat, D. (2018). Harnessing the potential of bioethanol production from lignocellulosic biomass in Nigeria – a review. **Biofuels, Bioproducts and Biorefining,** 13(1), 192–207.

[12] Varriale, L., Geib, D., and Ulber, R. (2024). Short-term adaptation as a tool to improve bioethanol production using grass press-juice as fermentation medium. **Applied Microbiology and Biotechnology,** 108(1), 393.

[13] Kululo, W. W., Habtu, N. G., Abera, M. K., Sendekie, Z. B., Fanta, S. W., and Yemata, T. A. (2025). Advances in various pretreatment strategies of lignocellulosic substrates for the production of bioethanol: A comprehensive review. **Discover Applied Sciences,** 7(5), 748.

[14] Di Domenico, G., et al. (2025). A systematic review of mechanical pretreatment techniques of wood biomass for bioenergy. **Energies,** 18(13), 3294.

[15] Shi, R., et al. (2024). A comparative study on enhanced enzymatic hydrolysis of diverse herbaceous and woody wastes by promising dilute acid and alkaline pretreatments. **Biomass Conversion and Biorefinery,** (in press). ISSN 2197-4365.

[16] Hoang, A. T., Nizetic, S., Ong, H. C., Chong, C. T., Atabani, A. E., and Pham, V. V. (2021). Acid-based lignocellulosic biomass biorefinery for bioenergy production: Advantages, application constraints, and perspectives. **Journal of Environmental Management,** 296, 113194.

[17] Tian, D., et al. (2021). Self-generated peroxyacetic acid in phosphoric acid plus hydrogen peroxide pretreatment mediated lignocellulose deconstruction and delignification. **Biotechnology for Biofuels,** 14(1), 224.

[18] Wu, Z., et al. (2022). Lignocellulose dissociation with biological pretreatment towards the biochemical platform: A review. **Materials Today Bio,** 16, 100445.

[19] Gladysheva, E. K. (2025). Liquid hot water and steam explosion pretreatment methods for cellulosic raw materials: A review. **Polymers,** 17(13), 1783.

[20] Wojtasz-Mucha, J., Hasani, M., and Theliander, H. (2017). Hydrothermal pretreatment of wood by mild steam explosion and hot water extraction. **Bioresource Technology,** 241, 120–126.

[21] Sahay, S. (2020). Impact of pretreatment technologies for biomass to biofuel production. **Substrate analysis for effective biofuels production**, 173–216.

[22] Li, M., et al. (2017). The effect of liquid hot water pretreatment on the chemical–structural alteration and the reduced recalcitrance in poplar. **Biotechnology for Biofuels,** 10(1), 237.

[23] Jimenez-Gutierrez, J. M., Verlinden, R. A. J., van der Meer, P. C., van der Wielen, L. A. M., and Straathof, A. J. J. (2021). Liquid hot water pretreatment of lignocellulosic biomass at lab and pilot scale. **Processes,** 9(9), 1518.

[24] Mohammadi, M., Alian, M., Dale, B., Ubanwa, B., and Balan, V. (2024). Multifaced application of AFEX-pretreated biomass in producing second-generation biofuels, ruminant animal feed, and value-added bioproducts. **Biotechnology Advances,** 72, 108341.

[25] Chundawat, S. P. S., et al. (2020). Ammonia fiber expansion (AFEX) pretreatment of lignocellulosic biomass. **Journal of Visualized Experiments (JoVE),** (154), e57488.

[26] Bertran-Llorens, S., Perondi, F., Slama de Freitas, A. L., Chen, J., van Erven, G., and Deuss, P. J. (2024). Supercritical CO2 as effective wheat straw pretreatment for subsequent mild fractionation strategies. **Chemical Engineering Journal,** 497, 154491.

[27] Guo, H., Zhao, Y., Chang, J. S., and Lee, D. J. (2023). Enzymes and enzymatic mechanisms in enzymatic degradation of lignocellulosic biomass: A mini-review. **Bioresource Technology,** (in press). ISSN 1873-2976.

[28] Amândio, M. S. T., Rocha, J. M. S., and Xavier, A. M. R. B. (2023). Enzymatic hydrolysis strategies for cellulosic sugars production to obtain bioethanol from *Eucalyptus globulus* bark. **Fermentation,** 9(3), 241.

[29] Ntunka, M. G., Khumalo, S. M., Makhathini, T. P., Mtsweni, S., Tshibangu, M. M., and

Bwapwa, J. K. (2023). Valorization of lignocellulosic biomass to biofuel: A systematic review. **ChemEngineering,** 9(3), 58.

[30] Obnamia, J. A. (2014). **Modeling the reaction kinetics of the enzymatic hydrolysis of lignocellulosic biomass.** Master of Applied Science thesis. University of Toronto, Canada.

[31] Tang, C., Cavka, A., Bui, M., and Jonsson, L. J. (2024). Comparison of simultaneous saccharification and fermentation with LPMO-supported hybrid hydrolysis and fermentation. **Frontiers in Bioengineering and Biotechnology,** 12, 1419723.

[32] Kroumov, A. D., Módenes, A. N., and Tait, M. C. d. A. (2006). Development of new unstructured model for simultaneous saccharification and fermentation of starch to ethanol by recombinant strain. **Biochemical Engineering Journal,** 28(3), 243–255.

[33] Humbird, D., Davis, R., Tao, L., Kinchin, C., and Hsu, D. (2011). **Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol**. National Renewable Energy Laboratory, 275–3000.

[34] Aspen Technology, Inc. (2019). **Aspen Plus® V11 user guide**. Bedford, MA, USA.

[35] Suriyachai, N., Champreda, V., Kraikul, N., Techanan, W., and Laosiripojana, N. (2018). Fractionation of lignocellulosic biopolymers from sugarcane bagasse using formic acid-catalyzed organosolv process. **3 Biotech,** 8(5), 221.

[36] Weerasai, K., Laosiripojana, N., Imman, S., Kreetachat, T., and Suriyachai, N. (2023). Reusable alkaline catalyzed organosolv pretreatment and delignification of bagasse for sugar platform biorefinery. **Biomass Conversion and Biorefinery,** 13, 1269.

[37] Rocha, G. J. d. M., Silva, F. T., Curvelo, A. A. d. S., and Araujo, G. T. (1997). A fast and accurate method for determination of cellulose and polyoses by HPLC. **Journal of Chromatography A,** 785(1), 301–306.

[38] Tiwari, S., et al. (2022). Multistep structural and chemical evaluation of sugarcane bagasse, pretreated with alkali for enhancing the enzymatic saccharification by cellulase and xylanase of the *Pseudomonas sp.* CVB-10 (MK443365) and *Bacillus*

paramycoides T4 (MN370035) mix-culture system. **Frontiers in Energy Research,** 9, 726010.

[39] Oh, H. W., Lee, S. C., Woo, H. C., and Kim, Y. H. (2022). Energy-efficient recovery of fermented butyric acid using octyl acetate extraction. **Biotechnology for Biofuels and Bioproducts,** 15(1), 46.

[40] Viell, J., Harwardt, A., Seiler, J., and Marquardt, W. (2013). Is biomass fractionation by organosolv-like processes economically viable? A conceptual design study. **Bioresource Technology,** 150, 89–97.

[41] da Silva, A. R. G., Errico, M., and Rong, B.-G. (2017). Solvent recycle and impurity purge evaluation for organosolv pretreatment method for bioethanol production from lignocellulosic biomass. In Espuña, A., Graells, M., and Puigjaner, L. (Eds.), **Computer Aided Chemical Engineering,** 40, 1141–1146. Elsevier.

[42] Gavin, T., and Ray, S. (2021). **Chemical engineering design: Principles, practice and economics of plant and process design (3rd ed.)**. London: Elsevier.

[43] Prachuab, P. (2019). **Renewable energy strategies for sustainable development in Thailand**. Doctoral dissertation, Thammasat University.

[44] Echemi. (2025). **Weekly chemical prices**. Echemi. Available online: https://www.echemi.com/weekly-price (accessed on July 7, 2025).

[45] Provincial Waterworks Authority (PWA). (2025). **Provincial Waterworks Authority website**. PWA. Available online: https://www.pwa.co.th (accessed on July 7, 2025).

[46] Electricity Generating Authority of Thailand (EGAT). (2025). **EGAT price**. EGAT. Available online: https://www.egat.co.th/home/egat-price (accessed on July 7, 2025).

[47] Lim, K. L., Wong, W. Y., Rubinsin, N. J., Loh, S. K., and Lim, M. T. (2022). Techno-economic analysis of an integrated biorefinery for the production of biofuels and value-added chemicals from oil palm empty fruit bunches. **Processes,** 10(10), 1965.

[48] Hafyan, R. H., et al. (2024). Integrated biorefinery for bioethanol and succinic acid co-

production from bread waste: Techno-economic feasibility and life cycle assessment. **Energy Conversion and Management,** 301, 118033.

[49] Wirawan, S. S., et al. (2024). Unlocking Indonesia's sweet sorghum potential: A techno-economic analysis of small-scale integrated sorghum-based fuel grade bioethanol industry. **Bioresource Technology Reports,** 25, 101706.

[50] Nair, L. G., Agrawal, K., and Verma, P. (2023). Organosolv pretreatment: An in-depth purview of mechanics of the system. **Bioresources and Bioprocessing,** 10(1), 50.

[51] Cheng, M.-H., Wang, Z., Dien, B. S., Slininger, P. J. W., and Singh, V. (2019). Economic analysis of cellulosic ethanol production from sugarcane bagasse using a sequential deacetylation, hot water and disk-refining pretreatment. **Processes,** 7(10), 642.

[52] Sganzerla, W. G., Lachos-Perez, D., Buller, L. S., Zabot, G. L., and Forster-Carneiro, T. (2022). Cost analysis of subcritical water pretreatment of sugarcane straw and bagasse for second-generation bioethanol production: A case study in a sugarcane mill. **Biofuels, Bioproducts and Biorefining,** 16(2), 435–450.

[53] Romero-García, J. M., et al. (2024). Olive leaves upgrading applying a novel two-stage organosolv pretreatment: Techno-economic and environmental assessment. **Biochemical Engineering Journal,** 207, 109317.

[54] Peng, J., Xu, H., Wang, W., Kong, Y., Su, Z., and Li, B. (2021). Techno-economic analysis of bioethanol preparation process via deep eutectic solvent pretreatment. **Industrial Crops and Products,** 172, 114036.

[55] Turton, R., Bailie, R. C., Whiting, W. B., and Shaeiwitz, J. A. (2018). **Analysis, synthesis, and design of chemical processes (5th ed.)**. Pearson.

[56] Parascanu, M. M., Sanchez, N., Sandoval-Salas, F., Carreto, C. M., Soreanu, G., and Sanchez-Silva, L. (2021). Environmental and economic analysis of bioethanol production from sugarcane molasses and agave juice. **Environmental Science and Pollution Research,** 28(45), 64374–64393.

[57] Gadkari, S., et al. (2023). Techno-economic analysis of 2,3-butanediol production from sugarcane bagasse. **ACS Sustainable Chemistry & Engineering,** 11(22),

8337–8349.

[58] Martinez-Hernandez, E., Cui, X., Scown, C. D., Amezcua-Allieri, M. A., Aburto, J., and Simmons, B. A. (2019). Techno-economic and greenhouse gas analyses of lignin valorization to eugenol and phenolic products in integrated ethanol biorefineries. **Biofuels, Bioproducts and Biorefining,** 13(4), 978–993.

[59] Liu, F., Dong, X., Zhao, X., and Wang, L. (2021). Life cycle assessment of organosolv biorefinery designs with the complete use of biomass. **Energy Conversion and Management,** 246, 114653.

[60] Wenger, J., Pichler, S., Näyhä, A., and Stern, T. (2022). Practitioners' perceptions of co-product allocation methods in biorefinery development A case study of the Austrian pulp and paper industry. **Sustainability,** 14(5), 2619.

[61] Priadi, H., Awad, S., Villot, A., Andres, Y., and Purwanto, W. W. (2024). Techno-enviro-economic analysis of second-generation bioethanol at plant-scale by different pre-treatments of biomass from palm oil waste. **Energy Conversion and Management: X,** 21, 100522.

[62] Gubicza, K., Nieves, I. U., Sagues, W. J., Barta, Z., Shanmugam, K. T., and Ingram, L. O. (2016). Techno-economic analysis of ethanol production from sugarcane bagasse using a liquefaction plus simultaneous saccharification and co-fermentation process. **Bioresource Technology,** 208, 42–48.

[63] Kautto, J., Realff, M., Ragauskas, A., and Kässi, T. (2014). Economic analysis of an organosolv process for bioethanol production. **Bioresources,** 9(4), 6041–6072.

[64] Gubicza, K., Nieves, I. U., Sagues, W. J., Barta, Z., Shanmugam, K. T., and Ingram, L. O. (2016). Techno-economic analysis of ethanol production from sugarcane bagasse using a liquefaction plus simultaneous saccharification and co-fermentation process. **Bioresource Technology,** 208, 42–48.

[65] Kässi, T., Realff, M. J., Ragauskas, A. J., and Kautto, J. (2014). Economic analysis of an organosolv process for bioethanol production. **Bioresources,** 9(4), 6041–6072.

[66] Correia, B., Matos, H. A., Lopes, T. F., Marques, S., and Gírio, F. (2024).

Sustainability assessment of 2G bioethanol production from residual lignocellulosic biomass. **Processes,** 12(5), 987.

APPENDIX

Appendix A. Applied Science and Engineering Progress

Applied Science and Engineering Progress, Vol. 18, No. 4, 2025, 7794 1

Research Article

Comparative Study on Techno-Economic Analysis for Various Organosolv Fractionation of Bagasse in Thailand

Suphalerk Khaowdang, Nopparat Suriyachai, Saksit Imman and Torpong Kreetachat*
School of Energy and Environment, University of Phayao, Tambon Maeka, Amphur Muang, Phayao, Thailand

Santi Chuetor
Department of Chemical Engineering, Faculty of Engineering, King Mongkut's University of Technology North Bangkok, Bang Sue, Bangkok, Thailand

Surachai Wongcharee
Faculty of Engineering, Mahasarakham University, Khamriang, Mahasarakham, Thailand

Kowit Suwannahong
Department of Environmental Health, Faculty of Public Health, Burapha University, Chonburi, Thailand
Technology, Faculty of Mechanical Engineering, Technical University of Chemnitz, Chemnitz, Germany

* Corresponding author. E-mail: torpong.kr@up.ac.th

DOI: 10.14416/j.asep.2025.06.011
Received: 27 January 2025; Revised: 31 March 2025; Accepted: 6 May 2025; Published online: 30 June 2025

Abstract

Process simulation is a crucial tool for conducting techno-economic analyses of biomass fractionation processes, providing insights into technical and economic aspects to optimize efficiency, reduce costs, and enhance the viability of production. This study focuses on the development and comparison of three scenarios based on organosolv fractionation methods. The mass balance analysis revealed significant differences in product yields, with scenario 2 achieving the highest cellulose (7,240.23 kg/day) and lignin (900.13 kg/day) outputs, scenario 3 showing a balanced profile with high hemicellulose recovery (2,959.81 kg/day), and Scenario 1 offering moderate outputs for cellulose and lignin. Economic evaluation indicated that scenario 3 was the most cost-efficient, driven by reduced operating costs, while scenario 1 had the highest total capital and operating expenses. Sensitivity analysis demonstrated minimal variability across scenarios but highlighted the need to study product pricing and future returns. Toxicity evaluation identified scenarios 1 and 3 as safer options due to the lower hazard classification of chemicals used compared to scenario 2. Overall, Scenario 3 emerged as the most favorable for cost-efficient and safe production of cellulose and lignin, supporting its potential for industrial-scale applications.

Keywords: Bagasse, Fractionation, Organosolv fractionation, Process simulation, Techno-economic analysis, Toxicity evaluation

1 Introduction

The energy crisis caused by the depletion of natural fuel sources such as petroleum and crude oil, which are finite, is exacerbated by the escalating demands of humanity for unlimited energy. This has led to a significant energy shortage. According to the Energy Statistics Report of Thailand published by the Energy Policy and Planning Office (EPPO) of the Ministry of Energy in 2023, the final commercial energy consumption in Thailand for 2022 was 1,520 thousand barrels of crude oil equivalent per day, an increase of 9.3 percent [1]. This rise was primarily due to the utilization of refined oil products, which accounted for 53 percent of the final energy consumption. Additionally, the overall consumption of refined oil products was 137 million liters per day, with oil imports reaching 12 million liters per day, reflecting a substantial increase of 123.9 percent. The use of certain types of energy directly impacts the environment on a significant scale, coupled with continuously rising fuel prices. Therefore, many countries are increasingly aware of the importance of adopting various alternative energy sources. The environmental impacts of using fossil resources have further prompted the utilization of agricultural waste materials as alternative energy sources, such as cellulose-based materials from plants [2].

In agricultural countries such as Thailand, economically important crops are extensively cultivated, resulting in significant biomass waste. Research has focused on utilizing this biomass waste to produce bioethanol, a clean and sustainable alternative energy source suitable for replacing fossil fuels [3]. Biomass waste typically consists of carbohydrate compounds, making it an inexpensive raw material for bioethanol production. Through the process of fermentation, often relying on yeast, this biomass waste can be converted into renewable energy in the form of bioethanol. The sugar industry is a crucial part of the Thai economy, serving both domestic consumption and export markets. Currently, Thailand ranks second globally in sugar exports. Over a 5-year period (2011–2015), the average economic value of the Thai sugar industry was approximately 3,222 million US dollars. Additionally, the by-products of sugar production, such as bagasse, can be utilized as raw materials for the renewable energy industry, including electricity generation and ethanol production. Therefore, sugarcane is an important biomass resource in Thailand's agricultural sector. According to the Department of Alternative Energy Development and Efficiency, Thailand had an excess sugarcane supply of approximately 44.69 million tons in 2023, and the amount of bagasse is expected to increase to 52.70 million tons by 2027 [4].

The production of bioethanol typically consists of four key steps: 1) biomass fractionation, 2) hydrolysis, 3) fermentation, and 4) purification. Most research on bioethanol production from biomass has been concentrated on laboratory-scale processes, with relatively limited focus given to the design, synthesis, and simulation of larger-scale industrial processes [5]. Among these steps, the fractionation process is considered one of the most energy-intensive stages in bioethanol production, making it a critical target for optimization in scale-up and industrial implementation [6]. This research aims to address this gap by focusing on the techno-economic feasibility of the fractionation process at a commercial scale. A critical factor influencing the economic viability of a large-scale fractionation process is the efficiency of the bioenergy production [7], [8]. Among the various fractionation technologies, organosolv fractionation is of particular interest due to its reliance on solvent penetration into the biomass pores, which leads to the effective physical deconstruction of the lignocellulosic structure. Numerous organic solvents, such as alcohols (e.g., methanol (CH_3OH) and ethanol (C_2H_6O)), esters, and ketones, have been investigated for their ability to modify and fractionate lignocellulosic materials. The efficiency of biomass fractionation, particularly lignin and hemicellulose removal, depends on the solvent used in the fractionation process.

Biomass fractionation is a crucial step that enhances enzyme accessibility to cellulose by removing lignin and hemicellulose, reducing the recalcitrance of lignocellulosic structures, and improving hydrolysis efficiency. This process directly impacts sugar and ethanol yields. Numerous studies have investigated the use of various solvents, considering both process efficiency and industrial feasibility. According to the study by Weerasai *et al*., [9] investigated the use of sodium methoxide (CH_3ONa) in CH_3OH as an alkaline catalyst, achieving up to 86.5% lignin removal and a glucose yield of 83.9%. However, this process has high chemical costs and requires strict process control. Meanwhile, Suriyachai *et. al.,*[10] reported that the use of formic acid (CH_2O_2) in the organosolv process enhanced cellulose purity, leading to more efficient hydrolysis. Additionally, CH_2O_2 is easily recyclable and has a low environmental impact. However, precise process control is required to prevent unwanted cellulose degradation. Furthermore, Panakkal *et. al.,* [11] studied the effect of sulfuric acid (H_2SO_4) on sugarcane bagasse hydrolysis. The optimal conditions were found to be 3.50% H_2SO_4 concentration, a temperature of 136.08 °C, and a reaction time of 75.36 minutes, resulting in a maximum reducing sugar yield of 180.15 mg/g of bagasse, 3.06 times higher than untreated bagasse. Despite its low cost and availability, H_2SO_4 poses challenges such as the formation of fermentation inhibitors, high corrosiveness, and the need for removal to mitigate environmental impacts. In conventional organosolv fractionation, H_2SO_4 is often employed for its strong catalytic activity, but the corrosiveness and high cost of neutralization and wastewater treatment limit its feasibility at industrial scales [12]. Organic acids like CH_2O_2 are milder and more recoverable, making them environmentally attractive. However, their lower acid strength can compromise delignification and hemicellulose removal efficiency [13]. On the alkaline side, CH_3ONa emerges as a promising candidate due to its high catalytic efficiency, offering a potential substitute for sodium hydroxide (NaOH) in enhancing cellulose purity and reducing processing costs [9]. Thus, biomass fractionation techniques using various solvents and catalysts have both advantages and limitations. Technical and economic considerations must be carefully evaluated to ensure their effective application on an industrial scale [14], [15].

Therefore, selecting an appropriate solvent system, such as acids, alkalis, organosolv, or ionic liquids, should consider its effectiveness in biomass deconstruction and solvent recovery. [16]. In particular, organosolv fractionation is an effective pretreatment method for lignin removal while preserving the structure of cellulose and hemicellulose. A key advantage of this process is its ability to recover and recycle organic solvents, which helps reduce costs and environmental impact, thereby enhancing its feasibility and attractiveness in techno-economic terms [16].

Previous studies on the use of different solvents for biomass fractionation have highlighted various advantages and limitations in terms of process efficiency, cost, and environmental impact. Therefore, process simulation at the industrial scale is essential for the techno-economic analysis of biomass fractionation, as it provides an in-depth understanding of both technical and economic aspects [17]–[21]. Process simulation not only helps optimize the process and reduce costs but also assesses the economic feasibility of bioethanol production. By analyzing the entire system, it is possible to identify cost-intensive steps and explore alternatives that could lower overall expenses. Furthermore, selecting the most appropriate approach requires careful consideration of environmental impacts to ensure that biomass fractionation processes remain sustainable and environmentally friendly in the long term [22]–[24]..

This study focuses on developing an organosolv fractionation process for bagasse from the sugarcane industry in Thailand to assess its economic feasibility. It is based on previous experiments and examines the comparative use of different catalysts, including H_2SO_4, CH_2O_2, and CH_3ONa, while adjusting the conditions for various fractionation processes. The research utilizes data and assumptions derived from laboratory experiments and extends its findings to predict future industrial-scale production. Additionally, mathematical modeling is employed to analyze the technological and economic feasibility of the process.

2 Methods

2.1 *Process synthesis and design*

In this study, mathematical modeling has been applied using Aspen Plus (version 11) for process simulation. The selected biomass is sugarcane bagasse available in Thailand from the sugar production industry. The biomass composition is determined based on previous studies conducted by Suriyachai *et. al.,* [10] and Weerasai *et al*., [9]. The simulations are divided into 3 groups based on the use of different reaction accelerators, namely 1) Organosolv fractionation by H_2SO_4, 2) Organosolv fractionation by CH_2O_2, and 3) Organosolv fractionation by CH_3ONa. The process was modeled using the NRTL (Non-Random Two-Liquid) model, and component properties from Aspen's original data banks were used along with the application of properties from the report by the National Renewable Energy Laboratory (NREL) [25].

2.2 *Non-Random Two-Liquid model (NRTL)*

In this study, a new set of thermodynamic parameters was applied for process design using Aspen Plus [26]. The Non-Random Two-Liquid (NRTL) model, developed by Renon and Prausnitz in the 1960s, was employed to represent the non-ideal behavior of liquid-phase mixtures. The NRTL model is widely used for predicting activity coefficients in non-ideal mixtures, especially for liquid-liquid equilibrium (LLE) and vapor-liquid equilibrium (VLE) systems. It accounts for molecular interactions and non-randomness in the liquid phase, making it suitable for systems with strong molecular associations and significant differences in component polarities. The activity coefficient (γ_i) for component i in a multi-component system is calculated using the following Equation (1):

$$ln\,\gamma_i = \sum_{j=1}^{N} \frac{\tau_{ji} G_{ji} x_j}{\sum_{k=1}^{N} G_{ki} x_k} + \sum_{j=1}^{N} \frac{x_j G_{ij}}{\sum_{l=1}^{N} G_{li} x_l} \left[\tau_{ij} - \frac{\sum_{m=1}^{N} \tau_{mj} G_{mj} x_m}{\sum_{k=1}^{N} G_{kj} x_k} \right] \quad (1)$$

Where:

- $\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT}$ is the interaction parameter between components i and j.
- $G_{ij} = e^{-\alpha_{ij}\tau_{ij}}$ is a weighting factor.
- x_j is the mole fraction of component j.
- α_{ij} is a non-randomness parameter (typically between 0.2 and 0.47).

This model is particularly useful for simulating liquid-liquid extraction, azeotropic distillation, and reactive distillation, among other separation and reaction processes. In the NRTL equation provided, k and m are dummy indices used for summation over components in the system:

- k typically indexes all components in the denominators to normalize the interactions with respect to component i or j.
- m is used similarly to k, but specifically for summing interactions between component j and all other components m (inside the inner bracket) in the second term of the equation.

Roles:

k appears in:

- $\sum_{k=1}^{N} G_{ki} x_k$: Denominator of the first term (normalizing interaction contributions to component i).
- $\sum_{k=1}^{N} G_{kj} x_k$: Denominator inside the brackets in the second term (normalizing interactions related to component j).

m appears in:

- $\sum_{m=1}^{N} \tau_{mj} G_{mj} x_m$: Numerator inside the bracket (weighted average interaction toward j from all m).

In essence, k and m are used to iterate over all components in the mixture, similar to j, but serve distinct roles depending on where they appear in the formula.

2.3 *Process setup for organosolv fractionation*

Figure 1 presents the process flowsheet used for organosolv fractionation. All experiments were conducted using the same type of biomass, namely sugarcane bagasse, which consists of 38.30% cellulose, 20.70% hemicellulose, 23.70% lignin, 4.20% ash, and 13.00% other components [9]. The basis of this study involves a biomass feed rate of 20,000.00 kg/day of sugarcane bagasse. The recycling process was assumed to have a recovery rate of 95%. The required separation process of co-products (rich fraction of hemicellulose and lignin) was not considered in the total process cost. For equipment design, the fractionation reactor (R1) is modeled using a Recirculating Continuous Stirred-Tank Reactor (RCSTR) unit to enhance catalytic efficiency. This configuration maintains system equilibrium through continuous stirring, ensuring uniform distribution of reactants and products. Filtration (F1) was carried out using a membrane filter press unit, which serves to separate the solid and liquid components of the mixture. For solvent recovery (F2), a fractional distillation unit was employed, with the primary purpose of separating and recovering the solvent for reuse in the process. The experiments were classified into three scenarios as follows: Scenario 1 presents the process flow setup for organosolv fractionation in a solvent mixture of C_2H_6O/water (H_2O) using H_2SO_4 as a catalyst. The reactor operates at a temperature of 170 °C, a pressure of 20 bar, and a total residence time of 60 minutes. The solvent mixture consists of C_2H_6O and H_2O at a 70:30 %v/v ratio, with H_2SO_4 at a concentration of 2% w/v based on the solvent (This study).

Scenario 2: the flowsheet setup for organosolv fractionation with CH_2O_2 catalyst. The reactor operates at a temperature of 159 °C and a pressure of 20 bar, with a total residence time of 40 min. The process employs a solvent mixture consisting of H_2O/C_2H_6O/ethyl acetate ($C_4H_8O_2$)/CH_2O_2 in a ratio of 43:20:16:21% v/v, respectively [10].

Scenario 3: process flow configuration for organosolv fractionation using CH_3ONa as a catalyst. The process operates at a temperature of 150 °C and a pressure of 20 bar, with a total residence time of 63.9 minutes under conditions involving CH_3ONa at a concentration of 5.1% w/v [9].

After the reaction period for all scenarios, the pressure is released, and the fractionated material undergoes filtration. This process yields a solid stream rich in cellulose (PULP). The liquid stream rich in dissolved components, which flows into the downstream process for further treatment (DOWNSTREM).

In this study, the plant is designed to operate for 7,920 hours per year. The solvent recycling rate is set at 95%, which is a typical value in the organosolv process. However, previous studies have reported varying recycling rates, such as 99% [27] and 68.9% [28]. Solvent recycling helps reduce costs and environmental impact; however, repeated use may lead to a decline in efficiency. Therefore, further research on solvent regeneration methods is necessary to enhance recycling efficiency. Meanwhile, improvements in the biomass preparation process aim to reduce costs and increase economic feasibility.

2.4 *Economic analysis*

The method of factorial estimation, using parameters specified by Gavin and Ray [29], has been employed to calculate the costs of both liquid and solid processes in the analysis. Factors related to construction, equipment installation, piping, instrumentation, measurement tools and control, electrical system installation, direct costs, structural and building costs, design and engineering, and contingency costs have been assessed. The currency used in this study is specified as United States dollars. Table 1 shows the parameters for variable cost calculation, including utility and chemical costs, which were obtained from the research document and adjusted to current prices.

$$TAC = \frac{cc}{n} + UC + ChemC + RM \qquad (2)$$

Table 1: Feedstock, chemicals, and utilities prices.

Input	Unit	Price	Ref.
Bagasse	USD/ton	14.00	[30]
C_2H_6O	USD/L	~0.80	[31]
H_2O	USD/L	~0.00028	[32]
H_2SO_4	USD/L	~0.16	[31]
CH_2O_2	USD/L	~0.49	[31]
$C_4H_8O_2$	USD/L	~1.30	[31]
CH_3ONa	USD/kg	~0.60	[31]
CH_3OH	USD/L	~0.28	[31]
Electricity	USD/KV	2.1	[33]

The total annual cost (TAC) in this study is calculated by dividing the total capital cost (CC) by the payback period (n), which is set at 5 years, and adding the annual value of variable costs. These variable costs include utility cost (UC), chemical cost (ChemC), and raw material cost (RM), as shown in Equation (2).

2.5 *Sensitivity analysis*

Sensitivity Analysis is particularly beneficial for evaluating the resilience of a project in the face of potential future changes from its original scenario. It provides insights into how the costs and outcomes of the project may deviate from the original plan in different situations. In this case, it assesses the project cost when adapting biomass conditions with different catalyst reaction rates, revealing the impact of variations in project parameters. Parameters involved in multi-step processes can impact the cost and efficiency of a project. The examination includes assessing the technological landscape in the future and its effects on the plant and economy. The analysis encompasses variations in raw materials, chemical costs, and public utility expenses. It considers the solvent used, the quantity of catalysts employed, the impact of temperature adjustments, and the effects of pressure changes in the conditioning apparatus. Each process and economic variable is altered independently, while keeping other processes constant [34]–[36].

3 Results and Discussion

From the initial 20,000.00 kg/day of sugarcane bagasse feedstock, simulation results show that the product stream from organosolv fractionation experiments is divided into 3 Scenarios . The components of sugarcane bagasse were cellulose 38.30% (7,660.00 kg/day), hemicellulose 20.70% (4,120.00 kg/day), lignin 23.70% (4,740.00 kg/day), ash 4.20% (840.00 kg/day), and others 13.00% (2,640.00 kg/day).

For scenario 1, Table 2 and Figure 2(a) present mass balance for organosolv fractionation by H_2SO_4. From the sugarcane bagasse conditioning process in this procedure, it was found that the results from the PULP stream for subsequent hydrolysis and fermentation processes to produce ethanol yielded the following proportions of products: cellulose, hemicellulose, lignin, ash, and others were 7,075.54 kg/day, 151.62 kg/day, 435.13 kg/day, 145.49 kg/day, and 163.15 kg/day, respectively. In summary, the organosolv fractionation by H_2SO_4 catalyst can produce cellulose at 92.37% with the removal of lignin at 90.82%. The simulation results indicate that the cellulose recovery efficiency is lower than that reported in the study [37], which states that the use of H_2SO_4 can achieve cellulose recovery of up to 99%. However, the reported lignin removal rate in that study is 86.4%, which is lower than the results obtained from this simulation. These findings highlight the differences between industrial-scale process simulations and laboratory experiments, which may arise from variations in operating conditions, process scale, and technical limitations that influence the efficiency of biomass fractionation.

For scenario 2, Table 2 and Figure 2(b) illustrate the mass balance for the organosolv fractionation process using a CH_2O_2 catalyst. During the sugarcane bagasse conditioning in this procedure, the PULP stream results for subsequent hydrolysis and fermentation to produce ethanol showed the following product proportions: cellulose (7,240.23 kg/day), hemicellulose (419.83 kg/day), lignin (900.13 kg/day), ash (360.02 kg/day), and others (260.04 kg/day). Overall, the organosolv fractionation with a CH_2O_2 catalyst achieved a cellulose yield of 94.52% and a lignin removal efficiency of 81.01%. The simulation results indicate that the percentage of cellulose recovery is slightly lower than that reported in the study [10], which achieved a cellulose recovery of 94.6%. However, the simulation results show that lignin removal is slightly higher, at 81.01%, compared to 80.4% in the study. This difference is attributed to industrial-scale conditions that influence process efficiency.

For scenario 3, Table 2 and Figure 2(c) present the mass balance for organosolv fractionation by CH_3ONa catalyst. From the sugarcane bagasse conditioning process in this procedure, it was found that the results from the PULP stream for subsequent hydrolysis and fermentation processes to produce ethanol yielded the following proportions of products: cellulose, hemicellulose, lignin, ash, and others were 7,060.22 kg/day, 2,959.81 kg/day, 639.90 kg/day, 600.01 kg/day, and 1,139.95 kg/day, respectively. In summary, the organosolv fractionation by CH_3ONa catalyst can produce cellulose at 92.17% with the removal of lignin at 86.50%. The simulation results indicate that the efficiency of cellulose recovery after pretreatment with CH_3ONa is 92.17%, whereas the experimental results show an efficiency of 93.1% [9]. This suggests that the simulation yields a slightly lower efficiency compared to the experimental data. In terms of lignin removal percentage, both the simulation and experimental results demonstrate the same efficiency at 86.5%, indicating the stability of the pretreatment process.

Various operational conditions may influence production efficiency at the industrial scale, which should be considered for further optimization and improvement of the production process. The mass balance study of the three fractionation scenarios for bagasse demonstrates substantial variations in product distribution and efficiency, predominantly determined by the selection of catalyst and the particular organosolv fractionation method utilized. The comparison of cellulose yields showed that Scenario 2 achieved the highest cellulose products (7,240.23 kg/day), aligning with the highest co-products of lignin (900.13 kg/day). Scenario 1 had slightly lower products of cellulose and co-products. Scenario 3 yields a balanced profile with cellulose at 7,060.22 kg/day and a moderate amount of recovered lignin (639.90 kg/day), along with the highest hemicellulose recovery (2,959.81 kg/day), reflecting a more comprehensive preservation of carbohydrates.

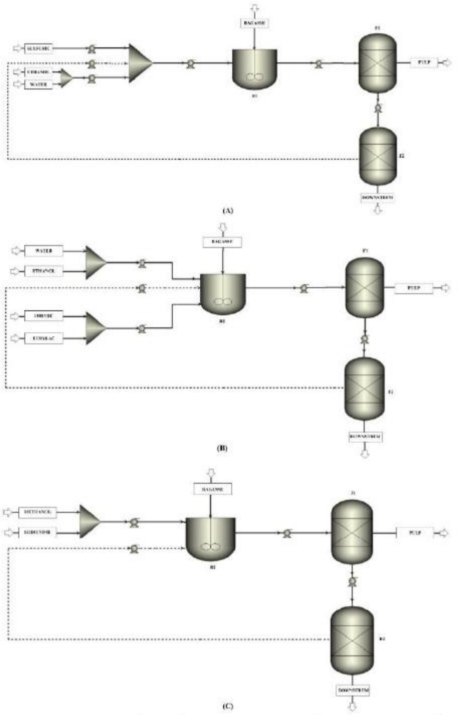
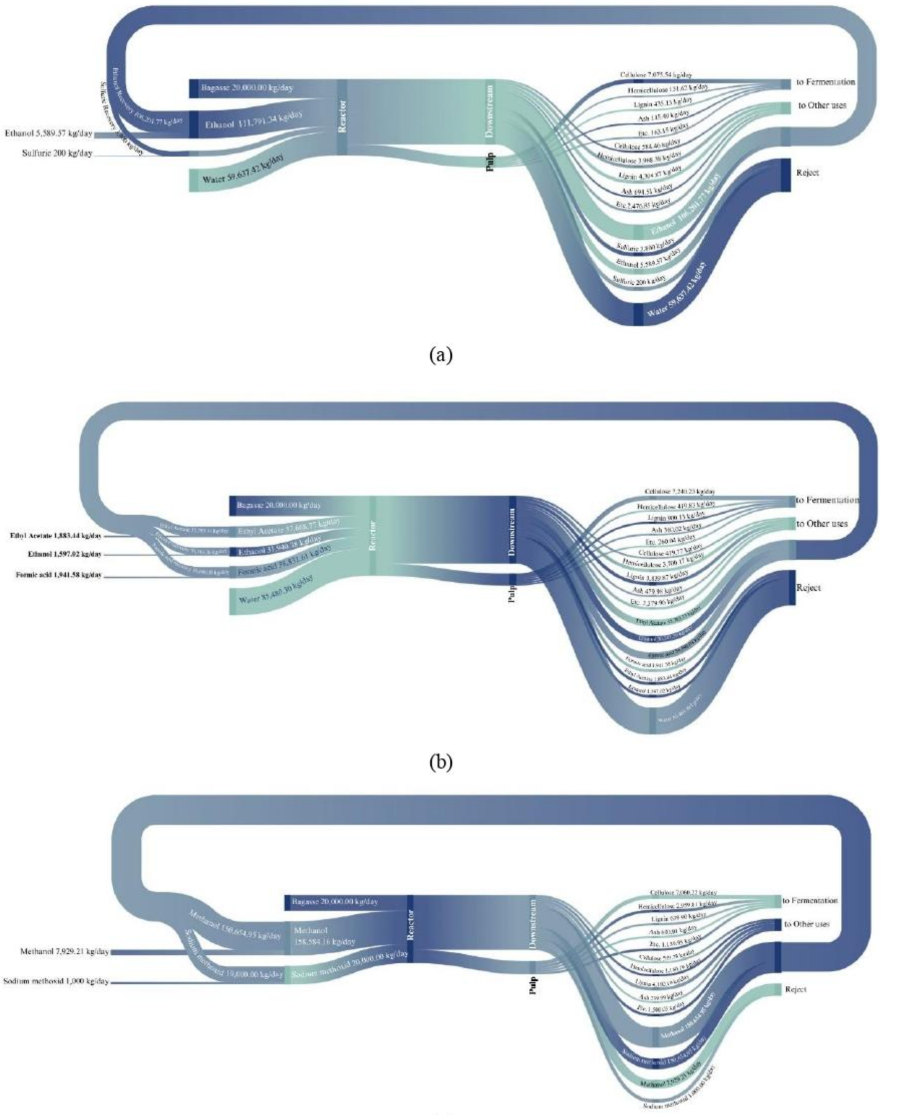


Figure 1: Flowsheet setup for organosolv fractionation experiments into 3 scenarios. (a) Scenario 1: organosolv fractionation by H_2SO_4 catalyst, (b) Scenario 2: organosolv fractionation by CH_2O_2 catalyst and (c) Scenario 3: organosolv fractionation by CH_3ONa catalyst.

Table 2: Mass balance for organosolv fractionation experiments into 3 Scenarios.

Scenario 1; Organosolv fractionation by H_2SO_4								
	Units	**Bagasse**	**H_2SO_4**		**C_2H_6O**	**H_2O**	**Pulp**	**Downstream**
Phase		Solid	Liquid		Liquid	Liquid	Solid	
Temperature	°C	25.00	25.00		25.00	25.00	170.00	170.00
Pressure	bar	1.01	1.01		1.01	1.01	20.00	20.00
Mass Flows	kg/day	20,000.00	200.00		5,589.57	59,637.42	7,970.93	77,456.06
Cellulose	kg/day	7,660.00	-		-	-	7,075.54	584.46
Hemicellulose	kg/day	4,120.00	-		-	-	151.62	3,968.38
Lignin	kg/day	4,740.00	-		-	-	435.13	4,304.87
Ash	kg/day	840.00	-		-	-	145.49	694.51
Etc.	kg/day	2,640.00	-		-	-	163.15	2,476.85
C_2H_6O	kg/day	-	-		5,589.57	-	-	5,589.57
H_2O	kg/day	-	-		-	59,637.42	-	59,637.42
H_2SO_4	kg/day	-	200.00		-	-	-	200.00
Scenario 2; Organosolv fractionation by CH_2O_2								
			H_2O	**C_2H_6O**	**CH_2O_2**	**$C_4H_8O_2$**	**Pulp**	**Downstream**
Phase		Solid	Liquid	Liquid	Liquid	Liquid	Solid	
Temperature	°C	25.00	25.00	25.00	25.00	25.00	159.00	159.00
Pressure	bar	1.01	1.01	1.01	1.01	1.01	20.00	20.00
Mass Flows	kg/day	20,000.00	85,480.30	1,597.02	1,941.58	1,883.44	9,180.25	101,722.09
Cellulose	kg/day	7,660.00	-	-	-	-	7,240.23	419.77
Hemicellulose	kg/day	4,120.00	-	-	-	-	419.83	3,700.17
Lignin	kg/day	4,740.00	-	-	-	-	900.13	3,839.87
Ash	kg/day	840.00	-	-	-	-	360.02	479.98
Etc.	kg/day	2,640.00	-	-	-	-	260.04	2,379.96
C_2H_6O	kg/day	-	-	1,597.02	-	-	-	1,597.02
H_2O	kg/day	-	85,480.30	-	-	-	-	85,480.30
CH_2O_2	kg/day	-	-	-	1,941.58	-	-	1,941.58
$C_4H_8O_2$	kg/day	-	-	-	-	1,883.44	-	1,883.44
Scenario 3; Organosolv fractionation by CH_3ONa								
			CH_3OH		**CH_3ONa**		**Pulp**	**Downstream**
Phase		Solid	Liquid		Solid		Solid	
Temperature	°C	25.00	25.00		25.00		150.00	150.00
Pressure	bar	1.01	1.01		1.01		20.00	20.00
Mass Flows	kg/day	20,000.00	7,929.21		1,000.00		12,399.89	16,529.32
Cellulose	kg/day	7,660.00	-		-		7,060.22	599.78
Hemicellulose	kg/day	4,120.00	-		-		2,959.81	1,160.19
Lignin	kg/day	4,740.00	-		-		639.90	4,100.10
Ash	kg/day	840.00	-		-		600.01	239.99
Etc.	kg/day	2,640.00	-		-		1,139.95	1,500.05
CH_3OH	kg/day	-	7,929.21		-		-	7,929.21
CH_3ONa	kg/day	-	-		1,000.00		-	1,000.00



(a)

(b)

(c)

Figure 2: Mass balance for organosolv fractionation experiments into 3 Scenarios by Sankey diagram (a) Scenario 1; Organosolv fractionation by H_2SO_4 catalyst, (b) Scenario 2; Organosolv fractionation by CH_2O_2 catalyst and (c) Scenario 3; Organosolv fractionation by CH_3ONa catalyst.

In summary, based on the mass balance in Figure 2, Scenario 2 achieved the highest cellulose yield at 94.52%, but had the lowest lignin removal efficiency at 81.01%. In contrast, Scenario 1 exhibited the highest lignin removal efficiency at 90.82%, while Scenario 3 demonstrated the highest hemicellulose recovery at 2,959.81 kg/day and a cellulose yield of 92.17%, which is comparable to Scenario 1. Therefore, the selection of the Organosolv fractionation process should be based on the intended objective of biomass fractionation. If maximizing cellulose yield is the priority, Scenario 2 is the most suitable choice. If efficient lignin removal is the primary goal, Scenario 1 should be selected. However, if a balanced approach between cellulose production and hemicellulose recovery is desired, Scenario 3 is the optimal option.

3.1 *Economic evaluation*

Table 3 shows the main equipment costs for the fractionation of organosolv with different scenarios. It was found that scenario 1 has the highest total capital cost (2,454,980 USD) and total operating cost (3,044,100 USD) among the three scenarios.

Table 3: TAC breakdown for the organosolv fractionation processes.

	Unit	Scenario 1	Scenario 2	Scenario 3
Total Capital Cost	USD	2,454,980.00	2,347,960.00	2,314,070.00
Total Operating Cost	USD/Year	3,044,100.00	2,873,240.00	2,238,160.00
Total Raw Materials Cost	USD/Year	1,962,760.00	1,803,810.00	1,225,150.00
Total Utilities Cost	USD/Year	88,854.10	89,186.70	78,994.90
P.O. Period [Year]	Year	5	5	5
Equipment Cost	USD	87,200.00	93,300.00	108,400.00
Total Installed Cost	USD	444,300.00	419,400.00	416,300.00
Electricity rate	kW	74.79	75.07	66.49
Electricity cost	USD/H	11.22	11.26	9.97
TAC	USD	5,586,710.10	5,235,828.70	4,005,118.90
TAC	million USD	5.59	5.24	4.01

Scenarios 2 and 3 have slightly lower capital costs compared to scenario 1. This suggests that the process optimization in this scenario reduces resource consumption and operational demands. Utility costs are relatively similar across scenarios but slightly higher in scenario 2 (89,186.70 USD) compared to scenario 1 (88,854.10 USD) and scenario 3 (78,994.90 USD). The variation could be linked to energy-intensive steps in the process or differences in temperature and pressure requirements. Total installed costs are comparable across all scenarios, suggesting a similar scale and infrastructure. According to TAC, scenario 3 offers the most cost-efficient process overall, primarily due to reduced operating costs. Scenario 2 presents a moderate reduction in costs, while scenario 1 is the most expensive due to higher raw material and operating expenses.

Figure 3 shows the main contributions for the TACs in different organosolv fractionations. The cost distribution analysis reveals that the operating cost is the most significant contributor to TAC across all scenarios, followed by the capital cost and raw materials cost, while the utilities cost has the least influence on the overall TAC. In this study, the capital cost accounts for approximately 32.51% to 39.51% of the TAC, depending on the scenario. In comparison, Cheng *et al*., [38] reported that liquid hot water pretreatment of sugarcane bagasse for second-generation ethanol production had a capital cost contribution of 28.17% of the total process cost. Similarly, Sganzerla *et al*., [39] found that in subcritical water hydrolysis, about 35% of the fixed capital investment was specifically associated with the reactor system. Additionally, for organosolv pretreatment of olive leaves, a capital cost contribution of 34.7% was previously reported [40], which is consistent with the range observed in this study. Regarding operating costs, this study shows a contribution of 38.22% to 40.39% of the TAC, whereas previous research on organosolv pretreatment reported a higher operating cost contribution of 54.78% [40]. For raw material costs, the results from this study are in line with earlier reports, which estimated raw material contributions to be approximately 30% of the total cost [41].

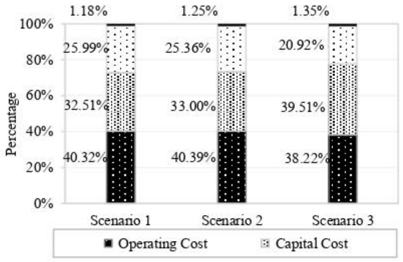


Figure 3: TAC contributions from each fractionation method.

3.2 *Sensitivity analysis*

A sensitivity analysis was done to investigate the effects of future technological improvements for organosolv fractionation and how they affect the TAC of the process. The acceptable percentage of cost variation in sensitivity analysis depends on the objective and scope of the study; however, generally accepted ranges such as ±10–30% for operating and utility costs, ±15–40% for capital investment, and up to ±50% for raw material and product prices. These are commonly used in industrial process modeling to evaluate economic robustness and uncertainty [41], [42]. In this study, a fixed variation of ±10% was applied across all cases to allow for a straightforward and consistent comparison of the economic impact among the different fractionation scenarios. Several process improvements and price fluctuations were evaluated regarding their impacts on the economic aspects of the process of the three scenarios, as shown in Table 4 and Figure 4. Cases 1–6 are related to costs and general chemical consumption in the process and reflect directly in the TAC calculations and are related to technological process improvements. The effects on the TAC in Case 1, changes in the cost of raw material, decreasing and increasing by 10% of total raw material usage, caused the TAC of scenario 1, scenario 2, and scenario 3, change by 0.03%, 0.03%, and 0.04% respectively. Case 2 changes the cost of chemicals in process, decreasing and increasing by 10% of total chemicals usage, causing the TAC of scenario 1, scenario 2, and scenario 3, change by 9.81%, 9.79%, and 9.70% respectively. Case 3, changes the cost of utilities in process decreasing and increasing in 10% of total utilities usage caused TAC of scenario 1, scenario 2, and scenario 3, change of 0.01%, 0.01%, and 0.02% respectively and Case 4, changes the usage of utilities consumption in process decreasing and increasing in 10% of total utilities consumption usage caused TAC of scenario 1, scenario 2, and scenario 3, change of 0.01%, 0.01%, and 0.02% changes in the project's costs. In this regard, the organosolv fractionation processes for sugarcane, using the accelerators from all three groups, were found to have minimal changes. Further study of the final products, specifically product prices, is necessary to conduct a comprehensive analysis of the overall production costs and future returns, respectively. However, cases 5–6 are related to technological process improvements or changes in TAC. The evaluation of TAC is merely an assessment of the impacts that will occur due to the results. Chemical costs have the most significant impact on TAC in the organosolv fractionation process, as indicated by the sensitivity analysis results. Specifically, H_2SO_4 and CH_2O_2 contribute to the highest TAC variations, reaching ±0.39% and ±0.36%, respectively, surpassing the effects of raw material and energy costs. These findings are consistent with the study by Parascanu *et al.* [43], which identified energy and chemical costs as the primary factors influencing the economic viability of bioethanol production. Additionally, Gadkari *et al.*, [44] reported that chemical costs have a moderate to high impact on profitability, particularly in cases where sugarcane bagasse must be purchased and when enzyme or chemical costs are significantly high in the production process. Notably, Scenario 1 and Scenario 5 exhibit the lowest chemical costs, making them more economically viable compared to other plant configurations. Furthermore, reducing chemical costs helps lower the minimum selling price of BDO, thereby enhancing its market competitiveness. The most effective strategies for improving profitability include utilizing free sugarcane bagasse, optimizing chemical usage efficiency, and scaling up the plant to reduce unit costs [44]. Table 5 and Figure 5, which present the cost assessment in the process of separating lignocellulose into the main product of cellulose, with the co-product of lignin. It was found that scenario 1 had a cost of 2.39$/kg for cellulose products and 3.93$/kg for lignin products. Scenario 2 had a cost of cellulose products and lignin products of 2.19$ and 4.13$/kg, respectively. Scenario 3 had a cost of cellulose products and lignin products of 1.72$ and 2.96$ per kg, respectively. Based on the results, scenario 3 required the lowest cost for producing the desired products in the fractionation process. Additionally, the cost of product separation is closely linked to the efficiency of the fractionation process. This highlights that scenario 3 is the most suitable option for producing cellulose and lignin at the lowest cost.

Table 4: Sensitivity analysis of price fluctuations on TAC across different scenarios.

Parameter Changed	Case	Min	Baseline	Max	Unit	TAC (million US$/year) Min	Change (%)	Baseline	Max	Change (%)
Scenario 1; Organosolv fractionation by H_2SO_4 catalyst										
Raw material cost	Case 1	12.84	14.27	15.70	US$/ton	5.57	-0.02	5.59	5.60	0.02
Chemicals cost	Case 2	different for C_2H_6O, and H_2SO_4				5.20	-0.39	5.59	5.97	0.39
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	5.57	-0.01	5.59	5.60	0.01
Utilities consumption	Case 4	70.86	78.73	86.60	KW	5.59	0.00	5.59	5.59	0.00
Temperature change	Case 5	153.00	170	187.00	°C	5.59	0.00	5.59	5.59	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	5.58	-0.01	5.59	5.60	0.01
Scenario 2; Organosolv fractionation by CH_2O_2 catalyst										
Raw material cost	Case 1	12.84	14.27	15.70	US$/ton	5.21	-0.03	5.24	5.27	0.03
Chemicals cost	Case 2	different for C_2H_6O, CH_2O_2, and $C_4H_8O_2$				4.88	-0.36	5.24	5.60	0.36
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	5.22	-0.02	5.24	5.26	0.02
Utilities consumption	Case 4	67.57	75.07	82.58	KW	5.24	0.00	5.24	5.24	0.00
Temperature change	Case 5	143.10	159.00	174.90	°C	5.24	0.00	5.24	5.24	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	5.23	-0.01	5.24	5.25	0.01
Scenario 3; Organosolv fractionation by CH_3ONa catalyst										
Raw material cost	Case 1	12.84	14.27	15.70	US$/ton	3.98	-0.03	4.01	4.04	0.03
Chemicals cost	Case 2	different for CH_3OH, and CH_3ONa				3.77	-0.24	4.01	4.25	0.24
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	3.99	-0.02	4.01	4.03	0.02
Utilities consumption	Case 4	59.84	66.49	73.14	KW	4.01	0.00	4.01	4.01	0.00
Temperature change	Case 5	135.00	150.00	165.00	°C	4.01	0.00	4.01	4.01	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	4.00	-0.01	4.01	4.02	0.01

Table 5: Summarizes the overall efficiency and cost of separating components using different reaction accelerators in organosolv fractionation processes of bagasse.

Scenarios	Cellulose (kg/year)	[1]CFE (%)	Lignin (kg/year)	[2]LRE (%)	[3]TAC (US$/year)	[4]CoC (US$/kg)	5 CoL (US$/kg)
1	2,334,928.86	92.37	1,420,606.44	90.82	5,586,710.10	2.39	3.93
2	2,389,276.56	94.52	1,267,158.42	81.01	5,235,828.70	2.19	4.13
3	2,329,873.26	92.17	1,353,033.00	86.50	4,005,118.90	1.72	2.96

[1]CFE; Cellulose fractionation efficiency, [2]LRE; Lignin removal efficiency, [3]TAC; Total annual cost, [4]CoC; Cost of Cellulose fractionation, [5]CoL; Cost of Lignin fractionation.

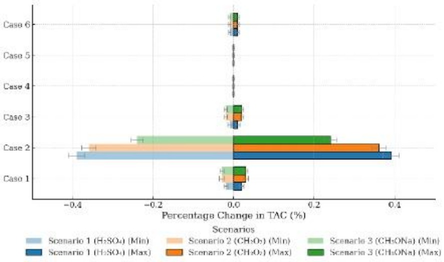


Figure 4: Sensitivity analysis of price fluctuations on TAC across different scenarios.

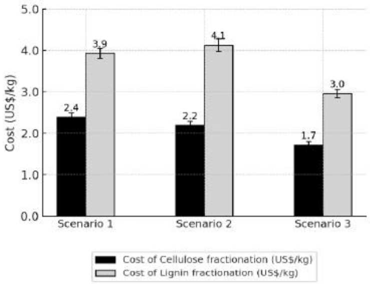


Figure 5: Cost of component separation in the organosolv process of bagasse.

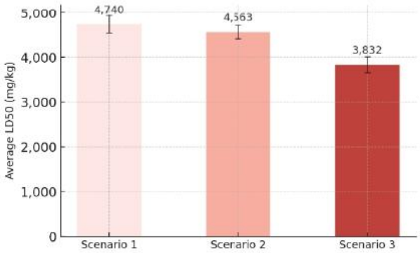


Figure 6: Comparison of average LD50 in each scenario.

3.3 *Toxicity evaluation*

The LD50, or Median Lethal Dose, is a measurement standard used in the field of toxicology to assess the quantity of a substance that causes death in 50% of a population exposed to it. Generally, it is expressed in terms of the amount of the substance administered per unit of body weight, such as milligrams of substance per kilogram of body weight (mg/kg). The LD50 value is determined through experiments conducted on animals, commonly rodents such as rats. In these experiments, different doses of a substance are administered, and the responses of the animals are observed. The quantity that results in 50% mortality within a specified time frame is identified as the LD50 [45]. In this study, toxicity assessments have been conducted on the group of chemicals used in the organosolv fractionation process. Table 6 summarizes the results of toxicity assessments based on the Globally Harmonised System for Classification and Labeling of Chemicals (GHS) and the hazard classification of chemicals used according to the World Health Organization (WHO).

The WHO hazard classification, or the categorization of hazards by the WHO, is a system used to classify the risks and dangers of chemicals to human health and the environment. This system aids in the assessment and ranking of the risks posed by various substances, ensuring the highest level of safety for individuals and the environment. The WHO hazard classification consists of four risk levels: Class I: extremely hazardous to human health and the environment. Class II: highly hazardous substances with a high risk to human health and the environment. Class III: moderately hazardous substances with a moderate risk to human health and the environment. Class IV: slightly hazardous substances with a very low risk to human health and the environment [46]. This classification system provides individuals who need to use or manage chemicals with sufficient information to make decisions that prioritize maximum safety for both human health and the environment. The assessment reveals that in Scenarios 1 and 3, the substances are classified as Class IV (unlikely to cause harm when used safely), while in the group of Scenario 2, there are chemicals classified at a higher risk level of Class III (slightly hazardous). For example, CH_2O_2 with an LD50 value (for rats: Oral) of 730 mg/kg. Therefore, the evaluation of all three scenarios indicates that Scenarios 1 and 3 are the safest for use, both in terms of human safety and environmental impact.

To assess the hazard level of chemicals in each scenario, the average LD50 value is used as an indicator, as LD50 is a standard measure of acute toxicity, with lower values indicating higher toxicity. Figure 6 shows a decreasing trend in the average LD50 from Scenario 1 (4,740 mg/kg) to Scenario 3 (3,832 mg/kg), suggesting that the chemicals used in Scenario 3 exhibit the highest toxicity, while those in Scenario 1 are the least toxic. This finding is significant for risk assessment and the informed selection of chemicals to ensure safety. It serves as a criterion for selecting appropriate chemicals to minimize health and environmental risks. Furthermore, this trend may reflect the chemical characteristics of the substances used in each scenario, such as molecular structure, degradation rate, or toxicity mechanisms, all of which are crucial factors that warrant further investigation. Understanding the factors influencing LD50 values can contribute to designing safer and more environmentally friendly chemical processes. This, in turn, supports the development of a sustainable and safe industrial sector, benefiting both workers and the broader ecosystem.

As organosolv fractionation scales up to industrial levels, effective and sustainable wastewater treatment becomes critical. Each catalyst–solvent system presents unique challenges and opportunities for treatment and recovery. For scenario 1, the primary concern is the acidic effluent. Acid recovery techniques, such as freezing-thawing concentration or membrane separation, can minimize H_2SO_4 waste and enable reuse. Neutralization followed by biological treatment ensures environmentally compliant discharge. In scenario 2, this generates solvent-rich wastewater, with azeotropic challenges. Azeotropic or extractive distillation is recommended for efficient solvent recovery, while CH_2O_2 can be separated via liquid-liquid extraction. These recovery methods improve process sustainability and reduce effluent load. Scenario 3 contains alkaline species and CH_3OH. Distillation allows for CH_3OH recovery, while pH adjustment and ion exchange can remove residual sodium ions, making the water suitable for reuse or safe discharge. Integrating wastewater treatment with solvent and catalyst recovery not only aligns with environmental regulations but also contributes to the economic feasibility of the organosolv biorefinery. Future industrial designs should incorporate closed-loop systems and life cycle-based assessments to optimize both environmental and economic performance.

Table 6: The toxicity of chemicals in the processes of all three scenarios.

Scenarios	**LD50 (mg/kg) (for the rat: Oral)**	**WHO Hazard classification [46]**	**Formula**	**The National Fire Protection Association system (NFPA)**			**Globally Harmonised System for Classification and Labeling of Chemicals (GHS)**
				Health	**Flammability**	**Reactivity**	
Scenario 1;							
Ethanol	7,340	Class IV (unlikely if used safely)	C_2H_6O	2	3	0	Highly flammable liquid and vapour. Causes serious eye irritation.
Sulfuric acid	2,140	Class IV (unlikely if used safely)	H_2SO_4	3	0	0	Corrosive to Metals, Skin corrosion, Serious eye damage.
Scenario 2;							
Ethanol	7,340	Class IV (unlikely if used safely)	C_2H_6O	2	3	0	Highly flammable liquid and vapour. Causes serious eye irritation.
Formic acid	730	Class III (unlikely if used safely)	CH_2O_2	3	2	0	Flammable liquid, Acute toxicity (oral), Acute toxicity (inhal.), Skin corrosion/ irritation, Serious eye damage/eye irritation, Specific target organ toxicity single exposure.
Ethyl Acetate	5,620	Class IV (unlikely if used safely)	$C_4H_8O_2$	1	3	0	Flammable liquid 2, Specific Target Organ Toxicity, Single Exposure 3, Eye irritation.
Scenario 3;							
Methanol	5,628	Class IV (unlikely if used safely)	CH_3OH	1	3	0	Flammable liquids, Acute toxicity (Oral, dermal, inhalation), Specific target organ toxicity following single exposure.
Sodium methoxide	2,037	Class IV (unlikely if used safely)	CH_3NaO	3	2	2	Flammable liquids, Corrosive to metals, Acute oral toxicity, Acute dermal toxicity, Acute Inhalation Toxicity - Vapors, Skin Corrosion/Irritation, Serious Eye Damage/Eye Irritation, Specific target organ toxicity (single exposure).

4 Conclusions

This study focuses on the techno-economic analysis of the fractionation process of sugarcane bagasse using the organosolv method, comparing three different catalysts: H_2SO_4, CH_2O_2, and CH_3ONa. The process simulation was conducted using Aspen Plus to evaluate the yields of cellulose, lignin, and hemicellulose, as well as to assess production costs. The results indicate that Scenario 2 achieved the highest cellulose yield at 94.52% and the highest lignin yield at 900.13 kg/day, while Scenario 1 exhibited the highest lignin removal efficiency at 90.82%, and Scenario 3 achieved the highest hemicellulose recovery at 2,959.81 kg/day.

In terms of cost assessment, Scenario 3 was identified as the most cost-effective option, as it had the lowest operational costs, along with lower raw material and chemical costs compared to the other scenarios. Sensitivity analysis further revealed that chemicals are the most significant factor affecting total expenses. Regarding chemical safety, Scenario 1 and Scenario 3 were found to be safer for industrial applications due to their lower toxicity levels compared to CH_2O_2, which is classified as a hazardous substance under the WHO and GHS classification systems. This study was based on laboratory-scale experimental data and mathematical modeling to simulate the process and assess the feasibility of scaling up to an industrial level. The analysis of mass balance, cost, and safety for each process helped identify the most efficient and economically viable approach. Therefore, the findings of this study provide valuable insights for designing scalable and sustainable biomass fractionation processes that align with the goals of developing a sustainable bioindustry.

Acknowledgments

Nopparat Suriyachai was financially supported by Unit of Excellence (UOE220/2567) from the University of Phayao.

Author Contributions

S.K.: writing - original draft, formal analysis, methodology, software, data curation; N.S.: conceptualization, validation, writing - review & editing, visualization, Funding acquisition; S.C.: validation, investigation, supervision; S.I.: methodology, supervision, visualization; K.S.: resources, data curation; T.K.: conceptualization, methodology, investigation, writing - review & editing, Project administration, validation.

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

References

[1] EPPO, "Energy Statistics of Thailand 2023," EPPO, Bangkok, Thailand, 2024.

[2] Preethi, M. Gunasekaran, G. Kumar, O. P. Karthikeyan, S. Varjani, and B. J. Rajesh, "Lignocellulosic biomass as an optimistic feedstock for the production of biofuels as valuable energy source: Techno-economic analysis, environmental impact analysis, breakthrough and perspectives," *Environmental Technology & Innovation*, vol. 24, 2021, Art. no. 102080, doi: 10.1016/j.eti.2021.102080.

[3] M. Jayakumar, G. T. Gindaba, K. B. Gebeyehu, S. Periyasamy, A. Jabesa, G. Baskar, B. I. John, and A. Pugazhendhi, "Bioethanol production from agricultural residues as lignocellulosic biomass feedstocks waste valorization approach: A comprehensive review," *Science of The Total Environment,* vol. 879, 2023, Art. no. 163158, doi: 10.1016/j.scitotenv.2023.163158.

[4] DEDE, "Alternative Energy Development Plan: AEDP2015 (B.E. 2558–2579): Ministry of Energy, 2015, Bangkok, Thailand, 2024.

[5] A. Devi, S. Bajar, H. Kour, R. Kothari, D. Pant, and A. Singh, "Lignocellulosic biomass valorization for bioethanol production: A circular bioeconomy approach," *Bioenergy Research*, vol. 15, no. 4, pp. 1820–1841, 2022, doi: 10.1007/s12155-022-10401-9.

[6] N. Raina, S. Sharma, A. K. Sharma, R. Rana, V. Sharma, and M. Kumar, "Process performance evaluation of different chemical pretreatments of lignocellulosic biomass for bioethanol production," *Industrial Crops and Products*, vol. 211, 2024, Art. no. 118207, doi: 10.1016/ j.indcrop.2024.118207.

[7] A. M. Joseph, Y. Tulasi, D. Shrivastava, and B. Kiran, "Techno-economic feasibility and exergy analysis of bioethanol production from waste," *Energy Conversion and Management: X*, vol. 18, 2023, Art. no. 100358, doi: 10.1016/j.ecmx. 2023.100358.

[8] H. A. Ruiz, W. G. Sganzerla, V. Larnaudie, R. J. Veersma, G. van Erven, S. Rios-Gonzalez, R. M. Rodriguez-Jasso, G. Rosero-Chasoy, M. D. Ferrari, M. A. Kabel, T. Forster-Carneiro, and C. Lareo, "Advances in process design, techno-economic assessment and environmental aspects for hydrothermal pretreatment in the fractionation of biomass under biorefinery

concept," *Bioresource Technology*, vol. 369, 2023, Art. no. 128469, doi: 10.1016/j.biortech.2022.128469.

[9] K. Weerasai, N. Laosiripojana, S. Imman, T. Kreetachat, and N. Suriyachai, "Reusable alkaline catalyzed organosolv pretreatment and delignification of bagasse for sugar platform biorefinery," *Biomass Conversion and Biorefinery*, vol. 13, 2023, pp. 1751–1761, doi: 10.1007/s13399-020-01269-w.

[10] N. Suriyachai, V. Champreda, N. Kraikul, W. Techanan, and N. Laosiripojana, "Fractionation of lignocellulosic biopolymers from sugarcane bagasse using formic acid-catalyzed organosolv process," *3 Biotech*, vol. 8, 2018, Art. no. 221, doi: 10.1007/s13205-018-1244-9.

[11] E. J. Panakkal, M. Sriariyanun, J. Ratanapoompinyo, P. Yasurin, K. Cheenkachorn, W. Rodiahwati, and P. Tantayotai, "Influence of sulfuric acid pretreatment and inhibitor of sugarcane bagasse on the production of fermentable sugar and ethanol," *Applied Science and Engineering Progress*, vol. 15, 2022, Art. no. 5238, doi: 10.14416/j.asep.2021.07.006.

[12] S. Gutierrez, F. Mangone, P. Vergara, V. Gonzalez, J. P. Ferreira, J. C. Villar, and F. Garcia-Ochoa, "Lignocellulosic biomass pre-treatments by diluted sulfuric acid and ethanol-water mixture: A comparative techno-economic analysis," *Bioresource Technology Reports*, vol. 23, 2023, Art. no. 101514, doi: 10.1016/j.biteb.2023.101514.

[13] B. Liu, L. Liu, B. Deng, C. Huang, J. Zhu, L. Liang, X. He, Y. Wei, C. Qin, C. Liang, S. Liu, and S. Yao, "Application and prospect of organic acid pretreatment in lignocellulosic biomass separation: A review," *International Journal of Biological Macromolecules*, vol. 222, pp. 1400–1413, 2022, doi: 10.1016/j.ijbiomac.2022.09.270.

[14] N. R. Baral and A. Shah, "Comparative techno-economic analysis of steam explosion, dilute sulfuric acid, ammonia fiber explosion and biological pretreatments of corn stover," *Bioresource Technology*, vol. 232, pp. 331–343, 2017, doi: 10.1016/j.biortech.2017.02.068.

[15] A. R. Gurgel da Silva, A. Giuliano, M. Errico, B.-G. Rong, and D. Barletta, "Economic value and environmental impact analysis of lignocellulosic ethanol production: Assessment of different pretreatment processes," *Clean Technologies and Environmental Policy*, vol. 21, pp. 637–654, 2019, doi: 10.1007/s10098-018-01663-z.

[16] S. Areeya, E. J. Panakkal, M. Sriariyanun, T. Kangsadan, A. Tawai, S. Amornraksa, U. W. Hartley, and P. Yasurin, "A review on chemical pretreatment of lignocellulosic biomass for the production of bioproducts: Mechanisms, challenges and applications," *Applied Science and Engineering Progress*, vol. 16, 2023, Art. no. 6767, doi: 10.14416/j.asep.2023.02.008.

[17] R. Fu, L. Kang, C. Zhang, and Q. Fei, "Application and progress of techno-economic analysis and life cycle assessment in biomanufacturing of fuels and chemicals," *Green Chemical Engineering*, vol. 4, no. 2, pp. 189–198, 2023, doi: 10.1016/j.gce.2022.09.002.

[18] M. Abdou Alio, A. Marcati, A. Pons, and C. Vial, "Modeling and simulation of a sawdust mixture-based integrated biorefinery plant producing bioethanol," *Bioresource Technology*, vol. 325, 2021, Art. no. 124650, doi: 10.1016/j.biortech.2020.124650.

[19] F. Bisotti, M. Gilardi, O. T. Berglihn, R. Tschentscher, L. D. Hansen, S. J. Horn, A. Várnai, and B. Wittgens, "From laboratory scale to innovative spruce-based biorefinery. Note I: Conceptual process design and simulation," *Computer Aided Chemical Engineering*, vol. 53, pp. 2449–2454, 2024, doi: 10.1016/B978-0-443-28824-1.50409-9.

[20] J. C. Solarte-Toro, C. A. Rueda-Duran, M. Ortiz-Sanchez, and C. A. C. Alzate, "A comprehensive review on the economic assessment of biorefineries: The first step towards sustainable biomass conversion," *Bioresource Technology Reports*, vol. 15, 2021, Art. no. 100776, doi: 10.1016/j.biteb.2021.100776.

[21] T. Y. Chong, S. A. Cheah, C. T. Ong, L. Y. Wong, C. R. Goh, I. S. Tan, H. C. Y. Foo, M. K. Lam, and S. Lim, "Techno-economic evaluation of third-generation bioethanol production utilizing the macroalgae waste: A case study in Malaysia," *Energy*, vol. 210, 2020, Art. no. 118491, doi: 10.1016/j.energy.2020.118491.

[22] T. Y. Chong, S. A. Cheah, C. T. Ong, L. Y. Wong, C. R. Goh, I. S. Tan, H. C. Y. Foo, M. K. Lam, and S. Lim, "Techno-economic evaluation of third-generation bioethanol production utilizing the macroalgae waste: A case study in

Malaysia," *Energy*, vol. 210, 2020, Art. no. 118491, doi: 10.1016/j.energy.2020.118491.

[23] H. Chen, D. Zhou, G. Luo, S. Zhang, and J. Chen, "Macroalgae for biofuels production: Progress and perspectives," *Bioresource Technology*, vol. 320, 2021, Art. no. 124533, doi: 10.1016/j.biortech.2021.124533.

[24] L. Ansaloni, D. Fabbri, and G. Spigno, "Valorization of macroalgal biomass for the production of renewable chemicals: A review," *Industrial Crops and Products*, vol. 159, 2021, Art. no. 113051, doi: 10.1016/j.indcrop.2020.113051.

[25] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton, and D. Dudgeon, "Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: Dilute-acid pretreatment and enzymatic hydrolysis of corn stover," *National Renewable Energy Laboratory*, NREL/TP-5100-47764, 2011, doi: 10.2172/1013269.

[26] H. W. Oh, S. C. Lee, H. C. Woo, and Y. H. Kim, "Energy-efficient recovery of fermented butyric acid using octyl acetate extraction," *Biotechnology for Biofuels and Bioproducts*, vol. 15, no. 1, 2022, Art. no. 46, doi: 10.1186/s13068-022-02146-6.

[27] J. Viell, A. Harwardt, J. Seiler, and W. Marquardt, "Is biomass fractionation by Organosolv-like processes economically viable? A conceptual design study," *Bioresource Technology*, vol. 150, pp. 89–97, 2013, doi: 10.1016/j.biortech.2013.09.078.

[28] A. R. G. da Silva, M. Errico, and B.-G. Rong, "Solvent recycle and impurity purge evaluation for organosolv pretreatment method for bioethanol production from lignocellulosic biomass," *Computer Aided Chemical Engineering*, vol. 40, pp. 1141–1146, 2017, doi: 10.1016/B978-0-444-63965-3.50192-6.

[29] G. Towler and R. Sinnott, *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*, 3rd ed. Oxford, UK: Butterworth-Heinemann, 2021.

[30] P. Peerapong, "Renewable energy strategies for sustainable development in Thailand," Ph.D. dissertation, Sirindhorn International Institute of Technology, Thammasat University, Pathum Thani, Thailand, 2019.

[31] Echemi. "Weekly chemical prices." Echemi.com. https://www.echemi.com/weekly-price (accessed Mar. 26, 2025).

[32] P. W. Authority. "Provincial Waterworks Authority website." PWA.co.th. https://www.pwa.co.th (accessed Mar. 26, 2024).

[33] E. G. A. of Thailand. "EGAT Price." EGAT.co.th. https://www.egat.co.th/home/egat-price (accessed Mar. 26, 2024).

[34] K. L. Lim, W. Y. Wong, N. J. Rubinsin, S. K. Loh, and M. T. Lim, "Techno-economic analysis of an integrated bio-refinery for the production of biofuels and value-added chemicals from oil palm empty fruit bunches," *Processes*, vol. 10, no. 10, 2022, Art. no. 1965, doi: 10.3390/pr10101965.

[35] R. H. Hafyan, J. M. Miskolczi, M. U. Uddin, V. K. Kamarudin, V. N. Nguyen, and S. K. Mohapatra, "Integrated biorefinery for bioethanol and succinic acid co-production from bread waste: Techno-economic feasibility and life cycle assessment," *Energy Conversion and Management*, vol. 301, 2024, Art. no. 118033, doi: 10.1016/j.enconman.2023.118033.

[36] S. S. Wirawan, M. D. Solikhah, P. T. Widiyanti, N. P. D. Nitamiwati, R. Romelan, Y. Heryana, A. Nurhasanah, and A. Sugiyono, "Unlocking Indonesia's sweet sorghum potential: A techno-economic analysis of small-scale integrated sorghum-based fuel grade bioethanol industry," *Bioresource Technology Reports*, vol. 25, 2024, Art. no. 101706, doi: 10.1016/j.biteb.2023.101706.

[37] L. G. Nair, K. Agrawal, and P. Verma, "Organosolv pretreatment: An in-depth purview of mechanics of the system," *Bioresources and Bioprocessing*, vol. 10, no. 1, 2023, Art. no. 50, doi: 10.1186/s40643-023-00673-0.

[38] M.-H. Cheng, Z. Wang, B. S. Dien, P. J. W. Slininger, and V. Singh, "Economic analysis of cellulosic ethanol production from sugarcane bagasse using a sequential deacetylation, hot water and disk-refining pretreatment," *Processes*, vol. 7, no. 10, 2019, Art. no. 642, doi: 10.3390/pr7100642.

[39] W. G. Sganzerla, D. Lachos-Perez, L. S. Buller, G. L. Zabot, and T. Forster-Carneiro, "Cost analysis of subcritical water pretreatment of sugarcane straw and bagasse for second-generation bioethanol production: A case study in a sugarcane mill," *Biofuels, Bioproducts and*

Biorefining, vol. 16, no. 2, pp. 435–450, 2022, doi: 10.1002/bbb.2332.

[40] J. M. Romero-García, J. C. Solarte-Toro, Á. Galán-Martín, E. Ruiz, E. Castro, M. Ortiz-Sánchez, and C. A. Cardona Alzate, "Olive leaves upgrading applying a novel two-stage organosolv pretreatment: Techno-economic and environmental assessment," *Biochemical Engineering Journal*, vol. 207, 2024, Art. no. 109317, doi: 10.1016/j.bej.2024.109317.

[41] J. Peng, H. Xu, W. Wang, Y. Kong, Z. Su, and B. Li, "Techno-economic analysis of bioethanol preparation process via deep eutectic solvent pretreatment," *Industrial Crops and Products*, vol. 172, 2021, Art. no. 114036, doi: 10.1016/j.indcrop.2021.114036.

[42] R. Turton, J. A. Shaeiwitz, D. Bhattacharyya, and W. B. Whiting, *Analysis, Synthesis, and Design of Chemical Processes*. Hoboken, NJ: Pearson Education, 2018.

[43] M. M. Parascanu, N. Sanchez, F. Sandoval-Salas, C. M. Carreto, G. Soreanu, and L. Sanchez-Silva, "Environmental and economic analysis of bioethanol production from sugarcane molasses and agave juice," *Environmental Science and Pollution Research*, vol. 28, no. 45, pp. 64374–64393, 2021, doi: 10.1007/s11356-021-15471-4.

[44] S. Gadkari, V. Narisetty, S. K. Maity, H. G. Manyar, K. Mohanty, R. B. Jeyakumar, K. K. Pant, and V. Kumar, "Techno-economic analysis of 2,3-butanediol production from sugarcane bagasse," *ACS Sustainable Chemistry & Engineering*, vol. 11, no. 22, pp. 8337–8349, 2023, doi: 10.1021/acssuschemeng.3c01221.

[45] K. Morris-Schaffer and M. J. McCoy, "A review of the LD_{50} and its current role in hazard communication," *ACS Chemical Health & Safety*, vol. 28, no. 1, pp. 25–33, 2021, doi: 10.1021/acs.chas.0c00096.

[46] World Health Organization, *The WHO recommended Classification of Pesticides by Hazard and Guidelines to Classification*. Geneva, Switzerland: World Health Organization, 2019.

Appendix B. Sustainability

sustainability

MDPI

Article

Valorization of Sugarcane Bagasse in Thailand: An Economic Analysis of Ethanol and Co-Product Recovery via Organosolv Fractionation

Suphalerk Khaowdang [1], Nopparat Suriyachai [1], Saksit Imman [1], Nathiya Kreetachat [1], Santi Chuetor [2], Surachai Wongcharee [3], Kowit Suwannahong [4], Methawee Nukunudompanich [5] and Torpong Kreetachat [1,]*

[1] School of Energy and Environment, University of Phayao, Phayao 56000, Thailand; suphalerk.kh@up.ac.th (S.K.); nopparat.su@up.ac.th (N.S.); saksit.im@up.ac.th (S.I.); nathiya.kr@up.ac.th (N.K.)
[2] Department of Chemical Engineering, Faculty of Engineering, King Mongkut's University of Technology North Bangkok, Bangkok 10800, Thailand; santi.c@eng.kmutnb.ac.th
[3] Faculty of Engineering, Mahasarakham University, Khamriang, Mahasarakham 44150, Thailand; surachai.w@msu.ac.th
[4] Department of Environmental Health, Faculty of Public Health, Burapha University, Chonburi 20131, Thailand; kowit.su@go.buu.ac.th
[5] Department of Industrial Engineering, School of Engineering, King Mongkut's Institute of Technology, Bangkok 10520, Thailand; methawee.nu@kmitl.ac.th
* Correspondence: torpong.envi@gmail.com

Abstract

A comprehensive techno-economic assessment was undertaken to determine the viability of bioethanol production from sugarcane bagasse in Thailand through organosolv fractionation, incorporating three distinct catalytic systems: sulfuric acid, formic acid, and sodium methoxide. Rigorous process simulations were executed using Aspen Plus, facilitating the derivation of detailed mass and energy balances, which served as the foundational input for downstream cost modeling. Economic performance metrics, including the total annualized cost and minimum ethanol selling price, were systematically quantified for each scenario. Among the evaluated configurations, the formic acid-catalyzed organosolv system exhibited superior techno-economic attributes, achieving the lowest unit production costs of 1.14 USD/L for ethanol and 1.84 USD/kg for lignin, corresponding to an estimated ethanol selling price of approximately 1.14 USD/L. This favorable outcome was attained with only moderate capital intensity, indicating a well-balanced trade-off between operational efficiency and investment burden. Conversely, the sodium methoxide-based process configuration imposed the highest economic burden, with a TAC of 15.27 million USD/year, culminating in a markedly elevated MESP of 5.49 USD/kg (approximately 4.33 USD/L). The sulfuric acid-driven system demonstrated effective delignification performance. Sensitivity analysis revealed that reagent procurement costs exert the greatest impact on TAC variation, highlighting chemical expenditure as the key economic driver. These findings emphasize the critical role of solvent choice, catalytic performance, and process integration in improving the cost-efficiency of lignocellulosic ethanol production. Among the examined options, the formic acid-based organosolv process stands out as the most economically viable for large-scale implementation within Thailand's bioeconomy.

Keywords: lignocellulosic biomass; organosolv pretreatment; process simulation; co-product utilization; economic feasibility

check for updates

Academic Editors: Sabino De Gisi, Carmen Teodosiu, Giovanni Gadaleta and George Barjoveanu

Received: 12 June 2025
Revised: 24 July 2025
Accepted: 4 August 2025
Published: 7 August 2025

Citation: Khaowdang, S.; Suriyachai, N.; Imman, S.; Kreetachat, N.; Chuetor, S.; Wongcharee, S.; Suwannahong, K.; Nukunudompanich, M.; Kreetachat, T. Valorization of Sugarcane Bagasse in Thailand: An Economic Analysis of Ethanol and Co-Product Recovery via Organosolv Fractionation. *Sustainability* **2025**, *17*, 7145. https://doi.org/10.3390/su17157145

1. Introduction

The global energy crisis is intensifying due to the depletion of non-renewable fossil fuels such as petroleum and crude oil. This challenge is aggravated by rising energy demand across all sectors, leading to a growing supply–demand imbalance. In Thailand, commercial energy consumption in 2022 averaged 1.52 million barrels of crude oil equivalent per day, an increase of 9.3% from the previous year. Refined petroleum products accounted for 53% of total consumption, while refined oil usage reached 137 million liters per day. Notably, oil imports surged by 123.9% to 12 million liters per day [1].

Heavy reliance on fossil fuels threatens energy security and contributes to environmental issues such as greenhouse gas emissions and air pollution. In response, countries including Thailand are increasingly turning to renewable energy. Among various options, lignocellulosic biomass from agricultural residues has emerged as a promising and sustainable feedstock, offering both environmental and energy benefits [2,3].

In agricultural countries such as Thailand, the widespread cultivation of economic crops generates a substantial amount of biomass waste. This has attracted significant research interest in utilizing such waste materials, particularly for the production of bioethanol, a clean and sustainable alternative energy source that can effectively replace fossil fuels [4]. Agricultural biomass residues are typically rich in carbohydrates, making them a low-cost and suitable feedstock for bioethanol production through fermentation processes. Yeast, a type of microorganism, functions as an enzymatic biocatalyst in these processes, facilitating the conversion of sugars into ethanol through fermentation.

The sugar industry is a key contributor to Thailand's economy, supporting both domestic consumption and exports. As the world's second-largest sugar exporter, Thailand generated an average annual value of USD 3222 million between 2011 and 2015. In addition to sugar, by-products such as bagasse serve as valuable feedstock for renewable energy applications, including electricity and ethanol production. Consequently, sugarcane is regarded as a high-potential biomass resource. According to the Department of Alternative Energy Development and Efficiency (DEDE), Thailand had a sugarcane surplus of 44.69 million tons in 2023, with bagasse volume projected to reach 52.70 million tons by 2027 [5]. This underscores the increasing availability of biomass for future energy production.

The production of bioethanol from biomass generally involves four key steps: (1) biomass fractionation, (2) hydrolysis, (3) fermentation, and (4) purification. Most research efforts to date have focused primarily on laboratory-scale investigations, whereas process design, synthesis, and industrial-scale simulation remain relatively underexplored [6]. Among these stages, biomass fractionation is recognized as the most energy-intensive step in the bioethanol production process. Consequently, it has emerged as a critical target for optimization, particularly in the context of scaling up to commercial-level operations [7].

The conducted study addresses knowledge gaps by evaluating the techno-economic feasibility of industrial-scale biomass fractionation. A key determinant of economic viability is the efficiency of bioenergy production from biomass feedstocks [8,9]. Among available technologies, organosolv fractionation has gained attention for its ability to deconstruct lignocellulosic structures through solvent penetration into the biomass matrix. Organic solvents such as alcohols (e.g., methanol (CH_3OH) and ethanol (C_2H_6O)), esters, and ketones have been explored for their effectiveness in disrupting biomass and separating key components. The success of lignin and hemicellulose removal largely depends on the solvent type used.

Furthermore, the ability to efficiently isolate cellulose from the lignocellulosic structure directly affects the amount of glucose that can be obtained during the subsequent hydrolysis step, which is a key precursor for ethanol production through fermentation. The amount of ethanol produced is directly correlated with the amount of glucose fed into the process. Theoretically, 1 g of glucose can yield a maximum of approximately 0.51 g of ethanol, equivalent to 51% of the glucose mass [10]. Therefore, the more effectively lignin and hemicellulose are removed, the more accessible the cellulose becomes to enzymatic hydrolysis, resulting in more complete saccharification and higher ethanol yields, potentially approaching the theoretical maximum. These factors are critical for evaluating the technical and economic viability of the process at an industrial scale.

Biomass fractionation is a critical step in reducing the recalcitrance of lignocellulosic structures, with the primary objective of removing lignin and hemicellulose. This structural deconstruction enhances cellulose accessibility to enzymes, thereby improving hydrolysis efficiency and increasing the yield of fermentable sugars and ethanol. Numerous studies have investigated various solvent–catalyst systems to evaluate process performance and industrial applicability. For instance, Weerasai et al. [11] reported that using CH_3ONa in CH_3OH as a basic catalyst in the organosolv process resulted in lignin removal of 86.5% and a glucose yield of 83.9%, although the process is constrained by high chemical costs and the need for precise reaction control. Alternatively, Suriyachai et al. [12] demonstrated that formic acid (CH_2O_2)-based organosolv pretreatment improved cellulose purity and hydrolysis efficiency. CH_2O_2 also offers advantages in terms of recyclability and environmental friendliness, though improper reaction conditions may lead to cellulose degradation. Panakkal et al. [13] investigated sulfuric acid (H_2SO_4) hydrolysis of sugarcane bagasse and identified optimal conditions at 3.50% acid concentration, 136.08 °C, and 75.36 min, yielding a maximum reducing sugar output of 180.15 mg/g, 3.06 times higher than that of untreated biomass. While H_2SO_4 is cost-effective and widely available, it poses challenges such as inhibitor formation, corrosiveness, and the requirement for intensive wastewater treatment. In addition, Kreetachat et al. [14] studied H_2SO_4-catalyzed Liquid Hot Water (LHW) pretreatment combined with Simultaneous Saccharification and Fermentation (SSF) for ethanol production from sweet sorghum stalk. Using the Response Surface Methodology (RSM), the optimal pretreatment conditions were determined to be 110 °C, 90 min, and 0.9% H_2SO_4, resulting in a glucose yield of 91.09% and a maximum ethanol concentration of 23.1 g/L after 72 h of fermentation.

In conventional organosolv processes, H_2SO_4 is widely used for its strong catalytic effect in disrupting lignocellulosic structures [14]. However, its corrosiveness and the high cost of wastewater treatment limit its industrial viability [15]. As a greener alternative, organic acids like CH_2O_2 are less corrosive, recyclable, and gentler on equipment. Yet, their lower acidity can reduce lignin and hemicellulose removal efficiency [16]. Among alkaline catalysts, CH_3ONa has shown strong potential for improving cellulose purity and offers cost benefits, making it a promising substitute for conventional NaOH in specific fractionation applications [11]. In summary, biomass fractionation using various solvents and catalysts offers both benefits and challenges that require thorough technical and economic evaluation [17,18]. The choice of solvent system, i.e., acidic, alkaline, organosolv-based, or ionic liquids, should balance deconstruction efficiency with solvent recovery and reuse potential [19]. Among these, organosolv fractionation stands out for effectively removing lignin while preserving cellulose and hemicellulose. Its ability to recover and recycle solvents helps reduce both operational costs and environmental impact, making it a promising and economically viable approach for large-scale biomass processing [19].

Previous research on the use of various solvents for biomass fractionation has highlighted both advantages and limitations in terms of process efficiency, cost, and environmental impact. Therefore, process simulation at the industrial scale is essential for evaluating the techno-economic feasibility of biomass fractionation, providing a comprehensive understanding of both technical and economic aspects [20–24]. Process simulation not only facilitates process optimization and cost reduction but also serves as a valuable tool for assessing the economic viability of bioethanol production. By analyzing the overall system, it is possible to identify cost-intensive steps and explore alternative strategies to minimize total expenses. Furthermore, selecting the most appropriate approach should also account for environmental impacts to ensure the long-term sustainability of biomass fractionation processes [24–26].

This study investigates the development of organosolv-based fractionation of sugarcane bagasse, an agricultural residue from Thailand's sugar industry, for bioethanol production. The main objective is to evaluate the economic feasibility of the process using laboratory-scale data. Experiments compared catalytic systems (H_2SO_4, CH_2O_2, and CH_3ONa) and optimized operating conditions for each. The resulting data and key assumptions were scaled up to estimate industrial performance. Mathematical modeling was then applied to assess both technical and economic viability, supporting decision-making for potential commercial-scale implementation.

2. Materials and Methods

2.1. Process Synthesis and Design

The present study applied mathematical modeling and process simulation using Aspen Plus v11 (Aspen Technology, Inc., Bedford, MA, USA) to examine the fractionation of sugarcane bagasse, a key agricultural residue in Thailand. Aspen Plus is an industry-standard tool widely used by institutions like the National Renewable Energy Laboratory (NREL) for biorefinery design. Its strong thermodynamic features, especially the Non-Random Two-Liquid (NRTL) model, support accurate simulation of non-ideal liquid systems in biomass pretreatment. The software's extensive property database, unit operations, and flexible modeling environment allow for scalable process development and detailed techno-economic analysis, enhancing the reliability of the results. The chemical composition (Table 1) with comparison of sugarcane bagasse in different countries was analyzed based on prior studies conducted by Suriyachai et al. [12] and Weerasai et al. [11]. This case study was divided into three categories according to the type of catalyst used in the organosolv fractionation process: (1) H_2SO_4-based organosolv (Industrial-grade, Qingdao Hisea Chem Co., Ltd., Qingdao, China), (2) CH_2O_2-based organosolv (Industrial-grade, Feicheng Acid Chemicals, Feicheng, China), and (3) CH_3ONa-based organosolv (CH_3ONa-based organosolv (Zhengzhou Clover Chemical Co., Ltd., Zhengzhou, China). All simulations were performed using the NRTL thermodynamic model for phase equilibrium calculations. Component property data were sourced from the Aspen Plus database and supplemented with information from NREL to ensure greater simulation accuracy [27].

Table 1. Comparison of chemical compositions of sugarcane bagasse from different countries.

Composition	Brazil [28]	China [29]	Thailand [11] *
Cellulose	42.19	39.52	38.30
Xylan	27.60	25.63	20.70
Lignin	21.56	30.36	23.70
Ash	2.84	1.45	4.20
Other	5.63	1.72	13.00

Note: * This research is based on the following data.

The Non-Random Two-Liquid (NRTL) model is commonly applied to estimate activity coefficients, especially in liquid–liquid (LLE) and vapor–liquid equilibrium (VLE) systems [30]. Its strength lies in capturing non-ideal behavior by accounting for molecular interactions and the uneven distribution of molecules within the liquid phase. This makes it particularly effective for systems with strong polar interactions or non-random mixing. The activity coefficient of each component in a multicomponent mixture is calculated using the NRTL equations, as illustrated in Equation (1).

$$ln\gamma_i = \sum_{j=1}^{N} \frac{\tau_{ji} G_{ji} x_j}{\sum_{k=1}^{N} G_{ki} x_k} + \sum_{j=1}^{N} \frac{x_j G_{ij}}{\sum_{l=1}^{N} G_{li} x_l} \left[\tau_{ij} - \frac{\sum_{m=1}^{N} \tau_{mj} G_{mj} x_m}{\sum_{k=1}^{N} G_{kj} x_k} \right] \quad (1)$$

where

- $\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT}$ is the interaction parameter between components i and j;
- $G_{ij} = e^{-\alpha_{ij}\ \tau_{ij}}$ is a weighting factor;
- x_j is the mole fraction of component j;
- α_{ij} is a non-randomness parameter (typically between 0.2 and 0.47).

In the NRTL equation provided, k and m are dummy indices used for summation over components in the system:

- k typically indexes all components in the denominators to normalize the interactions with respect to component i or j;
- m is used similarly to k but specifically for summing interactions between component j and all other components m (inside the inner bracket) in the second term of the equation.

Roles:

k appears in

- $\sum_{k=1}^{N} G_{ki}\ x_k$: Denominator of the first term (normalizing interaction contributions to component i);
- $\sum_{k=1}^{N} G_{kj}\ x_k$: Denominator inside the brackets in the second term (normalizing interactions related to component j).

m appears in

- $\sum_{m=1}^{N} \tau_{mj}\ G_{mj}\ x_m$: Numerator inside the bracket (weighted average interaction toward j from all m).

In essence, k and m are used to iterate over all components in the mixture, similar to j, but serve distinct roles depending on where they appear in the formula.

2.2. Process Setup for Organosolv Fractionation

The biomass feed rate was set at 20,000.00 kg/day, and the solvent recycling efficiency was assumed to be 95%. Figure 1a,b presents the process flowsheet for biomass fractionation using the organosolv technique, employing sugarcane bagasse an agricultural residue from Thailand's sugar industry as the primary feedstock.

The diagram outlines the ethanol production process from sugarcane bagasse, involving a series of integrated unit operations. The process starts with the introduction of sugarcane bagasse (BAG) and catalysts into reactor R1, a Recirculating Continuous Stirred-Tank Reactor (RCSTR), which ensures uniform mixing and enhances reaction efficiency. The output from R1 proceeds to unit F1, a membrane filter press, for solid–liquid separation. The resulting cellulose pulp (PULP) is transferred to the HYDRO unit, an agitated hydrolysis reactor with temperature and pH control, where water (WT-RH) is added to depolymerize cellulose into glucose. The glucose solution is then sent to the FERMEN unit for anaerobic fermentation with yeast (YEAST), converting glucose into ethanol and CO_2. Ethanol is collected in the END unit, while the liquid stream from F1 goes to the distillation column (F2) for solvent recovery. Recovered ethanol is partially recycled (S-RCY), and the residue is processed in the PRECIP unit to extract primary solids (P-SOLID). The remaining liquid is concentrated in the EVAP unit to recover additional solids (RE-SOLIDs), followed by filtration (FILTER) to isolate lignin (LIGNIN) as a by-product. The leftover sugar solution is directed to the SUGAR unit for further use. In the HYDRO unit, cellulose $(C_6H_{10}O_5)n$ is hydrolyzed with water to produce glucose $(C_6H_{12}O_6)$, as represented in Equation (2).

$$(C_6H_{10}O_5)_n + nH_2O \rightarrow nC_6H_{12}O_6 \tag{2}$$

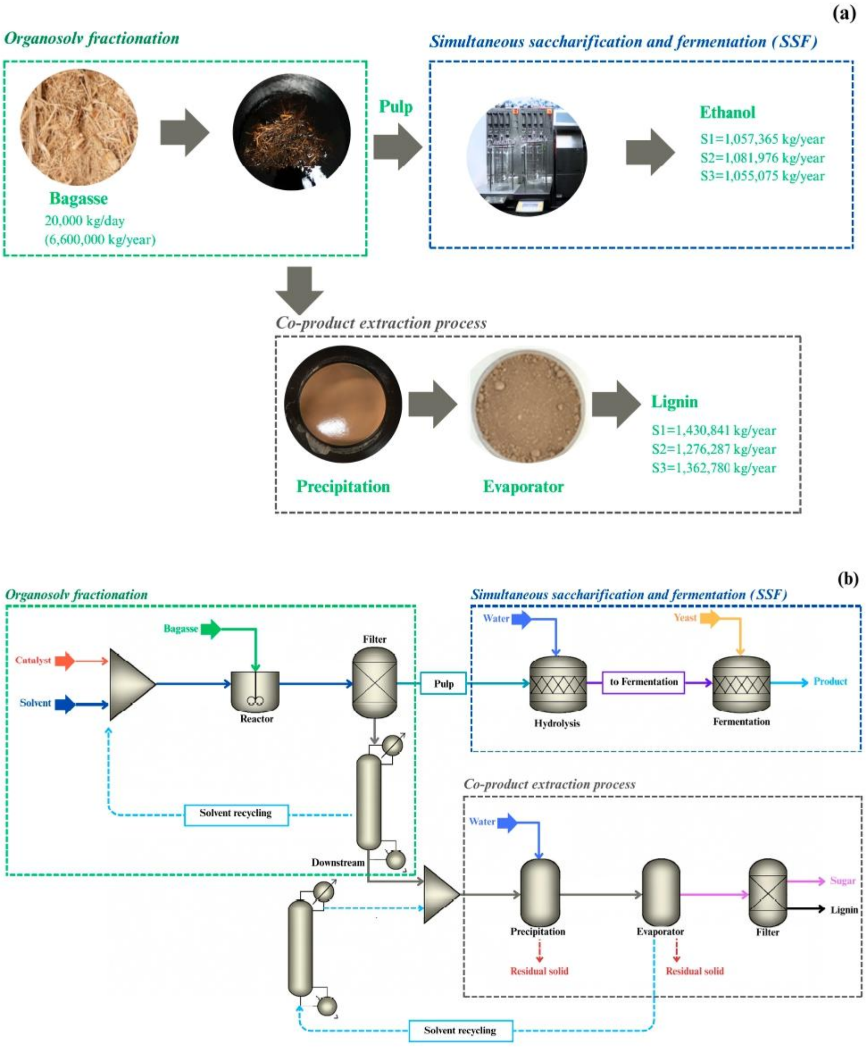


Figure 1. Flowsheet setup for ethanol production from sugarcane bagasse via the organosolv process; (**a**) feed rate per day and (**b**) scenario for organosolv fractionation.

From the hydrolysis process, 1 g of cellulose can theoretically produce around 1.11 g of glucose due to water incorporation during the reaction. However, actual yields typically range between 80% and 95%, influenced by the catalyst type and operating conditions. The glucose-rich hydrolysate is then fed into the FERMEN unit, an anaerobic fermentation reactor operating at 30–35 °C. Yeast is added to convert glucose into ethanol and carbon dioxide, as shown in Equation (3).

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2 + ATP \tag{3}$$

The final product obtained from the ENDPRO unit is ethanol, which is ready for subsequent separation and purification processes.

Scenario 1 involves organosolv fractionation using a 70:30% v/v ethanol–water solvent mixture, with 2% w/v H_2SO_4 as the catalyst. The process was carried out at 170 °C, 20 bar, and a 60-min residence time. Scenario 2 depicts organosolv fractionation using CH_2O_2 as the catalyst. The reactor conditions were 159 °C, 20 bar, and a 40-min residence time. The solvent mixture comprised water, ethanol, ethyl acetate, and CH_2O_2 in a 43:20:16:21% v/v ratio [12]. Scenario 3 describes organosolv fractionation using 5.1% w/v CH_3ONa as the catalyst. The process runs at 150 °C, 20 bar, with a residence time of 63.9 min [11]. The current study assumes 7920 h of annual plant operation and a 95% solvent recycling rate, a common value in Organosolv processes. Reported recycling efficiencies vary, with studies noting values as high as 99% [31] and as low as 68.9% [32]. Efficient solvent recycling is vital for lowering costs and environmental impact, though repeated use may degrade performance. Thus, advancing solvent regeneration methods and improving biomass preparation are key to enhancing process efficiency and economic viability.

In the Organosolv process, lignin is efficiently extracted from lignocellulosic biomass through the use of organic solvents such as ethanol, methanol, or formic acid in combination with water and either acidic or alkaline catalysts. This process facilitates the cleavage of lignin–carbohydrate linkages within the plant cell wall matrix, particularly targeting the β-O-4 ether bonds, which are the most abundant interunit linkages in native lignin. Under acidic conditions, the chemical mechanism of lignin depolymerization begins with the protonation of the hydroxyl group at the α-position (α-OH), leading to the formation of a stable benzylic carbocation intermediate. This intermediate plays a crucial role in promoting the cleavage of the β-O-4 ether bond. The representative reaction mechanism is shown as follows (Equation (4)):

$$\text{Ar–CH(OH)–CH}_2\text{–O–Ar}' + H^+ \rightarrow \text{Ar–CH}^+\text{–CH}_2\text{–O–Ar}' \rightarrow \text{Ar–CHO} + \text{HO–CH}_2\text{–Ar}' \tag{4}$$

In this equation, Ar and Ar′ represent aromatic rings in the lignin polymer; CH(OH) denotes the hydroxyl group at the α-position; and CH_2–O corresponds to the β-O-4 ether linkage. The products Ar–CHO and HO–CH_2–Ar′ are aromatic aldehydes and alcohols, respectively, indicating the effective depolymerization of lignin. Once dissolved into the solvent phase, lignin can be recovered by precipitation through water addition or solvent evaporation. The resulting lignin is characterized by its sulfur-free composition, low ash content, and low molecular weight, making it highly suitable for the production of high-value bioproducts such as resins, carbon fibers, and bio-based composite materials. Nevertheless, the Organosolv process presents economic limitations, primarily due to the high cost of organic solvents and the need for efficient solvent recovery systems to ensure the process's overall economic and environmental sustainability [33].

2.3. Economic Analysis

The factorial estimation method, utilizing parameters specified by Gavin and Ray [34], was employed to calculate the costs associated with both liquid and solid processing systems in this analysis. All cost calculations were conducted using United States dollars as the base currency as shown in Table 2.

Table 2. Feedstock, chemicals, and utilities prices.

Input	Unit	Price	Reference
Bagasse	USD/ton	14.00	[35]
C_2H_6O	USD/L	~0.80	[36]
H_2O	USD/L	~0.00028	[37]
H_2SO_4	USD/L	~0.16	[36]
CH_2O_2	USD/L	~0.49	[36]
$C_4H_8O_2$	USD/L	~1.30	[36]
CH_3ONa	USD/kg	~0.60	[36]
CH_3OH	USD/L	~0.28	[36]
Electricity	USD/KV	2.1	[38]

The total annual cost (TAC), calculated using the Capital Recovery Factor (CRF), is a common method in techno-economic analysis (TEA) to estimate the annualized cost of industrial-scale processes, as outlined in Equation (5).

$$TAC = (TCI \times CRF) + OC \tag{5}$$

where TCI is Total Capital Investment, which includes the cost of plant construction, equipment, and installation. OC refers to the Operating Cost, which encompasses annual expenses such as raw materials, chemicals, energy, and labor. The Capital Recovery Factor (CRF) serves to convert a one-time initial investment into an equivalent annual cost that accounts for the time value of money or the expected rate of return (e.g., 10% per year), as shown in Equation (6).

$$CRF = \frac{i(1+i)^{n}}{(1+i)^{n} - 1} \tag{6}$$

where

- i = interest rate or desired rate of return (per year);
- n = project lifetime or payback period (years).

2.4. Sensitivity Analysis

Sensitivity analysis helps assess a project's robustness by examining how cost and performance respond to changes in key variables. This includes evaluating the economic impact of variations in biomass characteristics and catalyst reaction rates, with a particular focus on the effects of process parameter shifts. The analysis also considers future technological developments, focusing on factors like raw material properties, chemical prices, and utility costs. The key variables tested include solvent type, catalyst amount, temperature, and pressure, with each adjusted independently to determine its specific influence on system performance [39–41].

3. Results

3.1. Scenario

Based on an initial sugarcane bagasse feedstock of 20,000.00 kg/day (6,600,000 kg/year), the simulation results from the organosolv fractionation process across three scenarios demonstrate the distribution of chemical components within the product stream. Sugarcane bagasse consists of 38.30% cellulose (2,527,800 kg/year), 20.70% hemicellulose (1,359,600 kg/year), 23.70% lignin (1,564,200 kg/year), 4.20% ash (277,200 kg/year), and 13.00% other components (871,200 kg/day). The chemical composition of sugarcane bagasse (Table 1) influences the techno-economic performance of the biorefinery process. Variations in cellulose, hemicellulose, and lignin contents affect conversion yields, utility requirements, and co-product value. Higher cellulose content enhances fermentable sugar yield and product revenue, while increased lignin may contribute to energy recovery or elevate residue management costs. Although moderate, these compositional differences impact mass balances, equipment sizing, and operating costs. Accordingly, TEA outcomes must be evaluated in the context of the specific compositional characteristics of the feedstock used in each scenario.

For Scenario 1, Table 3 presents the mass balance of the organosolv fractionation process using H_2SO_4 as the catalyst. From the sugarcane bagasse conditioning step, it was found that the solid stream (Pulp), which proceeds to hydrolysis and fermentation for ethanol production, contained 2,584,341.72 kg/year of cellulose, 55,377.74 kg/year of hemicellulose (xylan), 158,931.96 kg/year of lignin, 53,139.49 kg/year of ash, and small amounts of other components. Based on these figures, the organosolv process using H_2SO_4 achieved a cellulose recovery efficiency of 92.37% and a lignin removal rate of 90.82%. When compared to the laboratory-scale results reported by [42], which documented cellulose recovery as high as 99%, the simulation results showed slightly lower performance. However, the lignin removal rate in this simulation exceeded the reported 86.4% in the same study. These differences highlight the inherent variability between laboratory-scale experiments and industrial-scale simulations, which can arise from variations in operating conditions, process scale, and technical limitations affecting biomass fractionation efficiency.

Table 3. Mass balance for organosolv fractionation experiments in three scenarios.

	Units	Bagasse	Downstream	Lignin	Sugar	Pulp	to Fermentation	Product
				Scenario 1; Organosolv Fractionation by H_2SO_4				
Cellulose	kg/year	2,797,815.00	213,473.28	196,395.42	17,077.86	2,584,341.72	516,868.34	516,868.34
Xylan	kg/year	1,504,830.00	1,449,452.26	246,406.88	1,203,045.37	55,377.74	55,377.74	55,377.74
Lignin	kg/year	1,731,285.00	1,572,353.04	1,430,841.26	141,511.77	158,931.96	158,931.96	158,931.96
Ash	kg/year	306,810.00	253,670.51	-	253,670.51	53,139.49	53,139.49	53,139.49
Extractives	kg/year	964,260.00	904,668.73	-	904,668.73	59,591.27	59,591.27	59,591.27
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	2,041,590.44	-	3583.91	-	-	1,057,365.16
Co_2	kg/year	-	-	-	-	-	-	1,010,101.99
Glucose	kg/year	-	-	-	-	-	2,297,087.79	229,708.78
Water	kg/year	-	1,089,128.38	-	155,788.26	-	8,536,287.65	10,603,698.80
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,823,742.37
H_2SO_4	kg/year	-	73,050.00	-	73,048.73	-	-	-
CH_2O_2	kg/year	-	-	-	-	-	-	-
CH_3OH	kg/year	-	-	-	-	-	-	-

Table 3. *Cont.*

	Units	Bagasse	Downstream	Lignin	Sugar	Pulp	to Fermentation	Product
Scenario 2; Organosolv fractionation by CH_2O_2								
Cellulose	kg/year	2,797,815.00	153,320.26	141,054.64	12,265.62	2,644,494.74	528,898.95	528,898.95
Xylan	kg/year	1,504,830.00	1,351,487.82	229,752.93	1,121,734.89	153,342.18	153,342.18	153,342.18
Lignin	kg/year	1,731,285.00	1,402,513.98	1,276,287.72	126,226.26	328,771.02	328,771.02	328,771.02
Ash	kg/year	306,810.00	175,311.23	-	175,311.23	131,498.77	131,498.77	131,498.77
Extractives	kg/year	964,260.00	869,280.39	-	869,280.39	94,979.61	94,979.61	94,979.61
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	583,311.56	-	-	-	-	1,081,976.34
Co_2	kg/year	-	-	-	-	-	-	1,033,613.08
Glucose	kg/year	-	-	-	-	-	2,350,554.71	235,055.47
Water	kg/year	-	1,561,084.02	-	-	-	8,530,940.88	10,646,472.99
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,775,662.21
H_2SO	kg/year	-	-	-	-	-	-	-
CH_2O_2	kg/year	-	709,162.09	-	-	-	-	-
CH_3OH	kg/year	-	687,926.46	-	-	-	-	-
Scenario 3; Organosolv fractionation by CH_3ONa								
Cellulose	kg/year	2,797,815.00	219,068.91	201,543.40	17,525.51	2,578,746.09	515,749.22	515,749.22
Xylan	kg/year	1,504,830.00	423,760.13	72,039.22	351,720.91	1,081,069.87	1,081,069.87	1,081,069.87
Lignin	kg/year	1,731,285.00	1,497,561.53	1,362,780.99	134,780.54	233,723.48	233,723.48	233,723.48
Ash	kg/year	306,810.00	87,655.62	-	87,655.62	219,154.38	219,154.38	219,154.38
Extractives	kg/year	964,260.00	547,892.53	-	547,892.53	-	416,367.47	416,367.47
Enzyme	kg/year	-	-	-	-	-	-	-
Ethanol	kg/year	-	-	-	-	-	-	1,055,075.74
Co_2	kg/year	-	-	-	-	-	-	1,007,914.91
Glucose	kg/year	-	-	-	-	-	2,292,114.12	229,211.41
Water	kg/year	-	-	-	-	-	8,536,785.02	10,599,719.80
Xylose	kg/year	-	-	-	-	-	-	-
Yeast	kg/year	-	-	-	-	-	-	5,828,214.94
H_2SO_4	kg/year	-	-	-	-	-	-	-
CH_2O_2	kg/year	-	-	-	-	-	-	-
CH_3OH	kg/year	-	2,896,143.95	-	-	-	-	-
CH_3ONa	kg/year	-	365,250.00	-	-	365,250.00	-	-

In the fermentation stage, the fermentation stream received 2,297,087.79 kg/year of glucose from hydrolysis and produced 1,057,365.16 kg/year of ethanol from the Product unit. This corresponds to a glucose-to-ethanol conversion efficiency of approximately 46.04% by mass, which is lower than the theoretical value of around 51% reported by [10]. The loss of glucose may be attributed to its conversion into by-products such as organic acids or other water-soluble compounds, reduced yeast effectiveness due to fermentation inhibitors generated during the fractionation process, or ethanol losses during separation and distillation.

Although the organosolv fractionation process using H_2SO_4 demonstrated high cellulose recovery and lignin removal efficiencies, the ethanol production outcomes suggest potential areas for improvement, particularly in enhancing fermentation performance and minimizing inhibitor formation. These improvements are essential to increase the overall glucose-to-ethanol conversion efficiency in commercial-scale biorefinery systems.

For Scenario 2, Table 3 illustrates the mass balance of the organosolv fractionation process using CH_2O_2 as the catalyst. During the sugarcane bagasse conditioning step, the solid stream (Pulp) designated for subsequent hydrolysis and fermentation consisted of 2,644,494.74 kg/year of cellulose, 153,342.18 kg/year of hemicellulose (xylan), 328,771.02 kg/year of lignin, 131,498.77 kg/year of ash, and 94,979.61 kg/year of extractives. In summary, organosolv fractionation using CH_2O_2 achieved a cellulose recovery efficiency of 94.52% and a lignin removal rate of 81.01%. The simulation results indicate that the cellulose recovery rate is nearly identical to that reported in the study by [12], which observed a recovery of 94.6%. However, the lignin removal in this simulation was slightly higher, 81.01% compared to 80.4%, in the same study. These differences are likely due to process efficiency variations under simulated industrial-scale conditions.

Based on the simulation results, the fermentation unit (to Fermentation) received 2,350,554.71 kg/year of glucose from the hydrolysis stage and produced 1,081,976.34 kg/year of ethanol in the Product unit. This corresponds to a glucose-to-ethanol conversion efficiency of approximately 46.03% by mass, which is similar to that in Scenario 1 but remains below the theoretical maximum of 51.14%. The lower efficiency suggests that part of the glucose was lost during fermentation, likely due to the formation of metabolic by-products, the presence of fermentation inhibitors generated during pretreatment, or ethanol losses in downstream separation and purification processes. Notably, the solid stream (Pulp) in this scenario contained more cellulose (2,644,494.74 kg/year) compared to Scenario 1, suggesting that CH_2O_2 is more effective at preserving cellulose structure under the simulated conditions. However, the lignin content in the Pulp stream was also significantly higher (328,771.02 kg/year), indicating a lower lignin removal efficiency compared to the H_2SO_4-based process. The residual lignin may hinder enzyme accessibility and reduce hydrolysis efficiency in the subsequent steps. Therefore, while the process in Scenario 2 demonstrates improved cellulose preservation, its limitations in lignin removal and suboptimal glucose-to-ethanol conversion efficiency highlight key areas for further optimization, particularly if the process is to be scaled up for commercial biorefinery applications.

For Scenario 3, Table 3 presents the mass balance of the organosolv fractionation process using CH_3ONa as the catalyst. During the sugarcane bagasse conditioning step, the solid stream (Pulp), which proceeds to hydrolysis and fermentation for ethanol production, yielded the following component quantities: cellulose (2,578,746.09 kg/year), hemicellulose (1,081,069.87 kg/year), lignin (233,723.48 kg/year), ash (219,154.38 kg/year), and other extractive components (416,367.47 kg/year). In summary, organosolv pretreatment with CH_3ONa achieved a cellulose recovery of 92.17% and a lignin removal efficiency of 86.50%. The simulation results indicate that cellulose recovery is slightly lower than the experimental value of 93.1% reported in [11]. However, both the simulation and experimental results demonstrate the same lignin removal efficiency of 86.5%, suggestive of a consistent and stable performance of the pretreatment process under these conditions.

Based on the simulation results of Scenario 3, which utilizes CH_3ONa and methanol as the solvent system in the organosolv fractionation process, the solid stream (Pulp) contained 2,578,746.09 kg/year of cellulose and 233,723.48 kg/year of residual lignin. Notably, the hemicellulose (xylan) content reached 1,081,069.87 kg/year, which is higher than in both Scenario 1 and Scenario 2. This indicates that this solvent system offers superior preservation of total carbohydrate components, especially hemicellulose, which tends to degrade more easily in other pretreatment conditions.

Furthermore, the fermentation unit received 2,292,114.13 kg/year of glucose from the hydrolysis stage and yielded 1,055,075.74 kg/year of ethanol in the final product stream, corresponding to a glucose-to-ethanol conversion efficiency of approximately 46.04%. This value is comparable to those observed in Scenarios 1 and 2 but remains below the theoretical maximum of 51.14%, implying partial glucose loss. The reduction in fermentation efficiency could be attributed to the formation of by-products or the presence of residual chemicals, such as methanol or sodium salts, which may inhibit yeast activity during fermentation.

Overall, Scenario 3 demonstrates an effective recovery of carbohydrate components, particularly hemicellulose, while maintaining high cellulose retention. However, its lignin removal efficiency is lower compared to Scenario 1. Nevertheless, the potential impact of chemical residues on fermentation and downstream ethanol separation must be carefully evaluated if this system is to be developed for industrial-scale applications.

Simulation outcomes from the three organosolv fractionation scenarios—using H_2SO_4 (Scenario 1), CH_2O_2 (Scenario 2), and CH_3ONa with methanol (Scenario 3)—revealed distinct trade-offs in biomass recovery and ethanol production. Scenario 1 achieved the highest lignin removal (90.82%) but had lower hemicellulose retention. Scenario 2 yielded the highest cellulose recovery (2.64 million kg/year), though with slightly reduced lignin removal (81.01%). Scenario 3 offered the most balanced recovery, with the highest hemicellulose retention (1.08 million kg/year), high cellulose yield, and 86.50% lignin removal. Despite these differences, all scenarios achieved similar glucose-to-ethanol conversion efficiencies (~46%), indicating that fermentation performance may be more constrained by inhibitors than by pretreatment differences. Optimization should thus target both carbohydrate recovery and inhibitor minimization. Each scenario presents specific advantages: Scenario 1 in lignin removal, Scenario 2 in cellulose yield, and Scenario 3 in overall carbohydrate preservation.

3.2. Economic Evaluation

Table 4 presents the detailed costs of major equipment and operational expenses for ethanol production via the organosolv process under each scenario. It was found that Scenario 1 had the highest overall costs compared to the other scenarios, with a total capital cost of USD 4,358,930.00 and a total operating cost of USD 3,368,230.00 per year. The total raw materials cost was USD 1,957,890.00, which is slightly higher than that of Scenario 2 but significantly lower than Scenario 3. These figures suggest that the process in Scenario 1 may be more complex or require more energy-intensive equipment and a larger amount of raw materials than the other scenarios.

Table 4. TAC breakdown for the organosolv fractionation processes.

Cost Analysis	Unit	Scenario 1	Scenario 2	Scenario 3
Total Capital Cost	USD	4,358,930	3,671,550	3,640,210
Total Operating Cost	USD/Year	3,368,230	3,183,650	14,526,300
Total Raw Materials Cost	USD/Year	1,957,890	1,791,750	12,292,500
Total Product Sales	USD/Year	43,710,900	43,291,000	43,950,800
Total Utilities Cost	USD/Year	94,615	92,066	92,288
Desired Rate of Return	Year	20	20	20
Equipment Cost	USD	295,500	242,900	262,300
Total Installed Cost	USD	1,391,500	1,066,700	1,079,100
Electricity rate	kW	79.64	77.49	77.68
Electricity cost	USD/H	11.94	11.62	11.65
TAC	USD	4,263,365	3,927,396	15,273,841
TAC	million USD	4.26	3.92	15.27

Scenario 2 exhibits slightly lower overall costs compared to Scenario 1, with raw materials and operating costs of USD 1,791,750.00 and USD 3,183,650.00, respectively. The total capital cost is USD 3,671,550.00. However, Scenario 2 has the highest utility cost among the three scenarios, at USD 92,066.00, which may indicate the presence of more energy-intensive process steps or greater requirements for environmental control. Scenario 3 incurred the highest total costs among all scenarios, with substantially elevated values across key cost categories. Specifically, the raw materials cost was USD 12,292,500.00, the operating cost reached USD 14,526,300.00, the capital investment cost amounted to USD 3,640,210.00, and the utilities cost was USD 92,288.00. As a result, TAC for this scenario was USD 15,273,841.00, equivalent to 15.27 million USD, representing the highest TAC among the three scenarios. Although Scenario 3 generated the highest total product sales at USD 43,950,800.00 per year, the notably high raw material and operating costs suggest a lower economic viability. This may be attributed to the use of costly chemicals or more resource-intensive process steps compared to the other scenarios.

Based on the data in Table 4, Scenario 2 demonstrates the lowest TAC, making it the most economically favorable option, despite having the highest utilities cost. Scenario 1 shows the highest capital investment, indicating a more complex process. In contrast, Scenario 3 has the highest TAC due to significantly higher raw material and operating costs, even though it yields the highest total product revenue.

Figure 2 illustrates the percentage contributions of each cost component to TAC for the three organosolv fractionation scenarios. The analysis shows that the capital cost is the largest contributor in Scenarios 1 and 2, accounting for 44.6% and 42.0%, respectively, while it is significantly lower in Scenario 3 at only 11.9%. In contrast, the operating cost becomes the dominant component in Scenario 3 (47.5%) and also contributes substantially in Scenarios 1 and 2 at 34.4% and 36.4%, respectively. The raw materials cost is highest in Scenario 3 at 40.2%, compared to 20.0% and 20.5% in Scenarios 1 and 2, respectively. The utilities cost has the least impact in all scenarios, contributing less than 1.1% across the board.

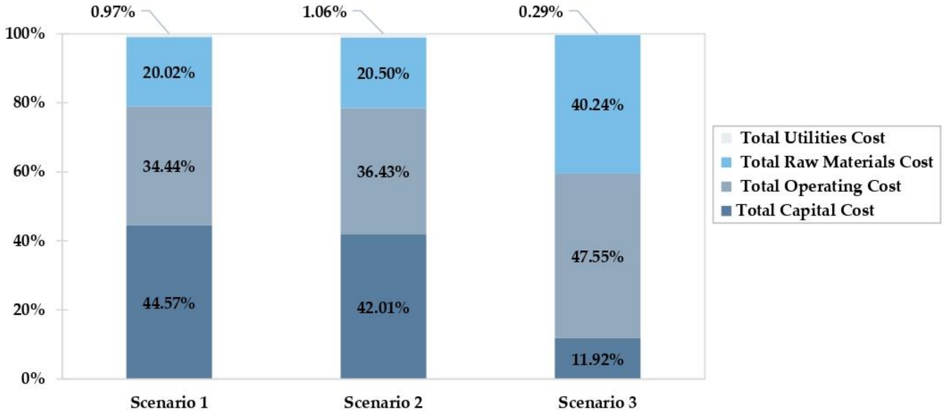


Figure 2. TAC contributions from each fractionation method.

These findings confirm that operating and raw materials costs are significant contributors to TAC. Notably, the capital cost contribution observed in this work varies significantly among the scenarios, ranging from 11.9% in Scenario 3 to 44.6% in Scenario 1. In comparison, previous studies reported relatively consistent and higher capital cost shares. For example, Cheng et al. reported a capital cost share of 28.17% for the Liquid Hot Water pretreatment of sugarcane bagasse [43]. Similarly, Sganzerla et al. noted that approximately 35% of the fixed capital investment in subcritical water hydrolysis was attributed to the reactor system [44], and a 34.7% capital cost share was reported for organosolv pretreatment of olive leaves [45]. These comparisons suggest that the capital intensity in the organosolv processes evaluated in this study can vary widely depending on the specific process configuration, solvent system, and plant design, with Scenario 3 demonstrating a notably lower capital burden.

Regarding operating costs, the results show a substantial share ranging from 34.4% to 47.5%, which is slightly lower than the 54.78% previously reported for organosolv pretreatment [45]. In contrast, the raw material costs are notably higher, accounting for 20.0% to 40.2%, compared to approximately 30% reported in earlier research [46]. The increased share may be attributed to variations in solvent systems, process design, or cost assumptions applied in the simulation. In particular, the high raw material cost in Scenario 3 reflects the greater influence of input chemical prices and usage rates in that configuration.

3.3. Assessment of Sensitivity Parameters

A sensitivity analysis was conducted to evaluate the potential impacts of future technological changes on the economic viability of the organosolv biomass fractionation process, with a particular focus on TAC, which serves as a key indicator of economic feasibility at the industrial scale. In general, sensitivity analyses in process simulation commonly adopt variation ranges of ±10–30% for operating and utility costs, ±15–40% for capital investment, and up to ±50% for raw material and product prices [46,47]. However, to ensure a consistent and comparable assessment across all scenarios, a fixed variation of ±10% was uniformly applied.

As shown in Table 5 and Figure 3, changes in chemical costs (Case 2) exerted the most substantial influence on TAC. Scenario 2, which utilized CH_2O_2, showed the highest TAC fluctuation at ±0.18%, followed by Scenario 3 (CH_3ONa) at ±0.12% and Scenario 1 (H_2SO_4) at ±0.01%. In contrast, fluctuations in raw material costs (Case 1), utility costs (Case 3), utility consumption (Case 4), operating temperature (Case 5), and pressure (Case 6) resulted in negligible changes in TAC, typically within ±0.01% or even 0.00% in several cases. Among the scenarios, Scenario 1 exhibited the highest cost stability, as all parameters resulted in TAC variation of no more than ±0.01%. These results confirm that the chemical cost is the most sensitive and economically influential parameter in organosolv fractionation, particularly when employing CH_2O_2 and CH_3ONa as catalysts.

Table 5. Sensitivity analysis of price fluctuations on TAC across different scenarios.

Parameter Changed		Min	Baseline	Max	Unit	TAC (Million US$/Year)				
						Min	Change (%)	Baseline	Max	Change (%)
Scenario 1; Organosolv fractionation by H_2SO_4 catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	4.25	−0.01	4.26	4.27	0.01
Chemicals cost	Case 2	different for water, ethanol and H_2SO_4				4.25	−0.01	4.26	4.27	0.01
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	4.25	−0.01	4.26	4.27	0.01
Utilities consumption	Case 4	75.71	84.12	92.53	KW	4.26	0.00	4.26	4.26	0.00
Temperature change	Case 5	153.00	170.00	187.00	°C	4.26	0.00	4.26	4.26	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	4.26	0.00	4.26	4.26	0.00
Scenario 2; Organosolv fractionation by CH_2O_2 catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	3.91	−0.01	3.92	4.02	0.01
Chemicals cost	Case 2	different for water, ethanol and CH_2O_2				3.74	−0.18	3.92	4.10	0.18
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	3.91	−0.01	3.92	3.93	0.01
Utilities consumption	Case 4	69.74	77.49	85.24	KW	3.92	0.00	3.92	3.92	0.00
Temperature change	Case 5	143.10	159.00	174.90	°C	3.92	0.00	3.92	3.92	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	3.91	−0.01	3.92	3.93	0.01

Table 5. *Cont.*

Parameter Changed		Min	Baseline	Max	Unit	TAC (Million US$/Year)				
						Min	Change (%)	Baseline	Max	Change (%)
Scenario 3; Organosolv fractionation by CH_3ONa catalyst										
Raw material cost	Case 1	12.84	14.00	15.70	US$/ton	15.26	−0.01	15.27	15.28	0.01
Chemicals cost	Case 2	different for water, ethanol and CH_3ONa				15.15	−0.12	15.27	15.15	0.12
Utilities Cost	Case 3	0.14	0.15	0.17	US$/kWhr	15.26	−0.01	15.27	15.28	0.01
Utilities consumption	Case 4	69.91	77.68	85.45	KW	15.27	0.00	15.27	15.27	0.00
Temperature change	Case 5	135.00	150.00	165.00	°C	15.27	0.00	15.27	15.27	0.00
Pressure change	Case 6	18.00	20.00	22.00	bar	15.27	0.00	15.27	15.27	0.00

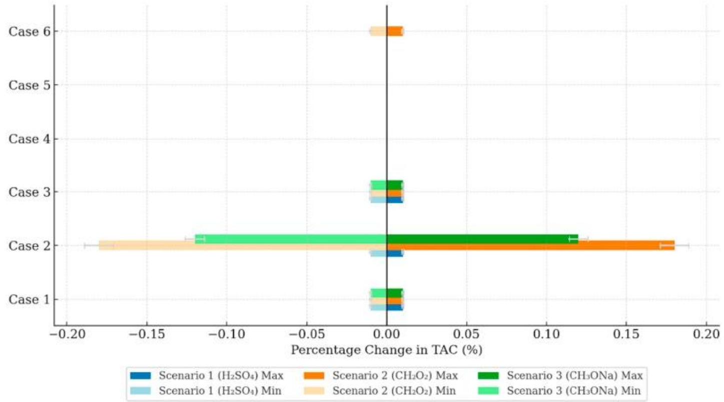


Figure 3. Sensitivity analysis of price fluctuations on TAC across different scenarios.

These findings align with previous studies such as Parascanu et al. [48], who identified chemical and energy inputs as key cost drivers in lignocellulosic biorefineries, and Gadkari et al. [49], who emphasized the significance of chemical cost control in reducing the minimum product selling price. To improve the economic viability of organosolv-based biorefineries, it is recommended to adopt strategies such as low-cost or free lignocellulosic feedstock sourcing, solvent recovery optimization, and scaling up production capacity to exploit economies of scale.

Table 6 presents the annual ethanol production, TAC, total product sales, and fractionation costs of cellulose, lignin, and ethanol across three organosolv process scenarios. Among these, Scenario 2 demonstrates the most favorable economic performance. It achieves the highest ethanol yield at 977,555.63 kg/year and the greatest total product sales revenue of 88,138,800.00 USD/year. Although TAC of Scenario 2 (23,493,394.47 USD/year) is slightly higher than that of Scenario 3, it remains lower than Scenario 1, resulting in a competitive ethanol unit cost.

The value-based allocation approach was applied to distribute TAC between the main products, ethanol and lignin. This method allocates costs according to the economic value of each product rather than their mass proportions (as in mass-based allocation). The economic value of each product was first calculated by multiplying its annual production quantity (kg/year) by its respective market price (USD/kg). The total value was then used to determine each product's value fraction, which was subsequently multiplied by TAC to derive the allocated cost for each product. Finally, the allocated cost was divided by the product's annual production to obtain the unit production cost. This method improves economic accuracy, especially in cases where the co-products differ significantly in market value. It has been widely recognized in techno-economic assessments, such as the work by [50], and in life cycle analysis (LCA) studies, including that of [51], as a standard and appropriate method for cost allocation in biorefinery systems and product life cycle evaluations [52].

Table 6. Value-based distribution of TAC for ethanol and lignin recovery.

Scenario	Ethanol Production	Lignin Production	TAC	Total Product Sales	Cost of Lignin Production	Cost of Ethanol Production	
	(kg/Year)	**(kg/Year)**	**(USD/Year)**	**(USD/Year)**	**(USD/kg)**	**(USD/kg)**	**(USD/L) ***
1	1,057,365	1,430,841	4,263,365	43,710,900	1.88	1.49	1.20
2	1,081,976	1,276,287	3,927,396	43,291,000	1.84	1.45	1.14
3	1,055,075	1,362,780	15,273,841	43,950,800	6.96	5.49	4.33

Note: * Data are calculated based on an ethanol density of 0.789 kg/L [27].

Table 6 presents the value-based allocation of TAC for ethanol and lignin production across three scenarios. Scenario 2 exhibits the lowest production costs for both ethanol (1.45 USD/kg) and lignin (1.84 USD/kg), while maintaining comparable total product sales to the other scenarios, indicating superior economic performance. In contrast, Scenario 3, despite achieving the highest total product sales, incurs a significantly higher TAC, resulting in markedly elevated unit production costs. Scenario 1 shows intermediate values in terms of both costs and revenues. Overall, the value-based allocation approach highlights Scenario 2 as the most cost-effective option, offering the lowest unit production costs for both primary products.

Priadi et al. [53] reported an ethanol production cost of ~1.11 USD/L using enzymatic hydrolysis, notably lower than the 1.14–4.32 USD/L range observed in Table 6. The discrepancy likely arises from differences in feedstock, process scale, and regional costs. Similarly, Gubicza et al. [54] and Kautto et al. [55] achieved lower MESPs (~1.03 and 0.81 USD/L, respectively) through optimized organosolv pretreatment and lignin valorization. These findings emphasize the impact of feedstock type, pretreatment efficiency, and co-product recovery on production economics. Using a value-based cost allocation approach, Scenario 2 showed the highest economic feasibility, with the lowest ethanol 1.14 USD/L (1.45 USD/kg) and lignin costs (1.84 USD/kg). Further cost reductions could be achieved through lignin valorization (e.g., eugenol production) and the fermentation of residual sugars such as xylose, enhancing overall resource utilization and process viability in the Thai context.

A strategic evaluation of ethanol production efficiency under the three proposed scenarios was conducted using Normalized 3D Vector Analysis in combination with heatmap visualization. This integrated approach serves as a systematic method for assessing multi-dimensional process performance. It applies Min–Max normalization to rescale variables with differing units into a common range (0–1), enabling equitable comparisons. The normalized values are then represented as three-dimensional vectors, $\vec{v} = (\acute{x},\acute{y},\acute{z})$, typically corresponding to ethanol yield, TAC, and total product sales. The direction and magnitude of each vector reflect the overall efficiency and balance among key indicators. Simultaneously, the heatmap visualizes the normalized values using a color gradient to highlight the strengths and weaknesses of each scenario. Together, these tools facilitate a comprehensive techno-economic comparison, supporting strategic decision-making in complex biorefinery systems.

Figure 4 presents a comparative techno-economic analysis of ethanol production from sugarcane bagasse under three scenarios (Scenario 1–3). The assessment incorporates both normalized three-dimensional vector plots (ranging from 0 to 1) and heatmaps to evaluate strategic indicators, including ethanol and lignin yields, TAC, total sales revenue, lignin production cost, and ethanol production cost per unit. Based on the 3D vector analysis, Scenario 2 demonstrates the most outstanding performance, characterized by the longest vector length, indicating an optimal balance between high ethanol yield and reasonable production cost. In contrast, Scenario 1, while achieving the highest lignin output, exhibits a higher TAC and ethanol cost. Scenario 3, although offering the lowest TAC, yields minimal ethanol output, resulting in the weakest overall economic performance. The heatmap further corroborates this trend. Scenario 2 achieves superior values in key performance indicators (e.g., ethanol production, revenue, and low unit costs), whereas Scenario 3 records the lowest values in several critical dimensions. From a strategic perspective, Scenario 2 emerges as the most favorable option for ethanol production from sugarcane bagasse using the organosolv process.

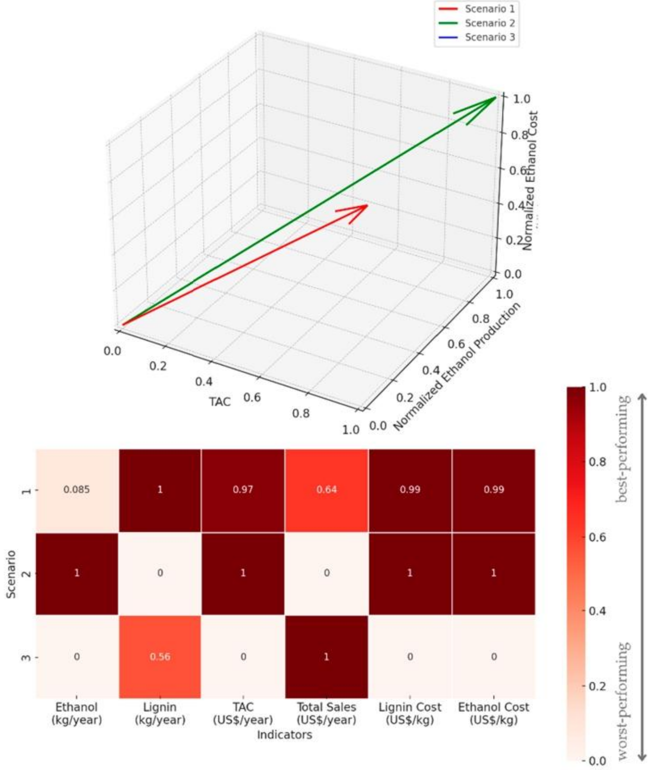


Figure 4. Comparative analysis of techno-economic performance for ethanol production from sugarcane bagasse via the organosolv process using normalized 3D vectors and heatmaps.

4. Discussion

The evaluation of organosolv fractionation for ethanol production from sugarcane bagasse underscores the pivotal influence of catalyst and solvent selection on biomass deconstruction efficiency, ethanol yield, and overall process economics at an industrial scale. Among the three catalytic scenarios examined, distinct trade-offs were observed in terms of biomass component recovery, conversion efficiency, and economic performance.

Scenario 1, employing sulfuric acid (H_2SO_4), achieved the highest lignin removal efficiency at 90.82%, alongside a glucose-to-ethanol conversion efficiency of 46.04%, which was comparable to the other scenarios. However, the corrosive nature of H_2SO_4 and the associated environmental burdens, including intensive wastewater treatment, contributed to elevated operational and maintenance costs, resulting in a higher TAC. In contrast, Scenario 2, utilizing formic acid (CH_2O_2), demonstrated superior cellulose preservation with the highest recovery rate of 94.52%. When evaluated using a value-based cost allocation approach, Scenario 2 yielded the most economically favorable outcome, with unit production costs of 1.45 USD/kg for ethanol and 1.84 USD/kg for lignin, corresponding to approximately 1.14 USD/L of ethanol. These results, combined with moderate capital requirements, position Scenario 2 as the most viable candidate for large-scale deployment. Scenario 3, based on sodium methoxide (CH_3ONa) in methanol, exhibited the strongest performance in retaining total carbohydrates, particularly hemicellulose. Nevertheless, its economic viability was undermined by the highest TAC of 15.27 million USD/year, primarily driven by elevated chemical and operational expenditures, despite achieving the greatest total revenue from product sales.

Parametric sensitivity analysis revealed that chemical costs were the most influential drivers of TAC variability across all configurations, particularly in Scenarios 2 and 3. In contrast, other factors such as feedstock price, reaction temperature, and pressure exerted minimal economic impact. These insights reinforce the necessity of stringent chemical cost management to improve process economics. Strategic performance benchmarking using Normalized 3D Vector Analysis and heatmap visualization further validated Scenario 2 as the most balanced and robust configuration. It excelled across key performance indicators, including ethanol yield, revenue generation, and production cost minimization, thus affirming its suitability for industrial-scale implementation within Thailand's emerging bioeconomy.

A comparative analysis (Table 7) with the existing literature highlights the variation in minimum ethanol selling price (MESP) across different studies, shaped by feedstock type, pretreatment strategy, and co-product valorization potential. This work emphasizes the economic impact of catalyst selection in the organosolv fractionation process. The catalyst CH_2O_2 yielded the most favorable MESP at 1.14 USD/L, followed by H_2SO_4 at 1.20 USD/L and CH_3ONa at 4.33 USD/L. These findings indicate that organic acids present a more cost-effective pathway for lignocellulosic ethanol production in Thailand. Gubicza et al. [54] and Martínez-Hernandez et al. [50] reported MESPs as low as 0.50–0.63 USD/L through advanced fermentation techniques and lignin valorization. Kautto et al. [55] demonstrated further cost reduction with assumptions of high lignin market prices. Conversely, Correia et al. [56] reported higher MESPs (2.41–2.70 USD/L) due to less favorable biomass and lower conversion yields. Within this context, the MESP achieved in Scenario 2 (1.14 USD/L) is competitive, while Scenario 3 reflects cost limitations despite technical strengths. In conclusion, the findings emphasize that the integration of optimal catalyst-solvent systems, effective co-product recovery (particularly lignin valorization), mitigation of fermentation inhibitors, and comprehensive process optimization are essential for enhancing the economic sustainability of lignocellulosic biorefineries. Such strategic advancements are imperative for the successful transition of Thailand toward a high-value, bio-based economy.

Table 7. Comparison of minimum ethanol selling price from various biomass feedstocks and conversion technologies.

Biomass	Main Process	Technical Notes	MESP (USD/L)	Reference
Sugarcane bagasse	Liquefaction + SSF + Co-Ferm	*Recombinant E. coli (LY01);* pH 6.0; no detoxification required	0.50–0.63	[54]
Hardwood (generic)	Organosolv + enzymatic hydrolysis	Ethanol-water 50:50; no catalyst or organic solvent recovery reported	0.81 (base), 0.53 (lignin @1000 USD/t)	[55]
Wheat straw	Organosolv + lignin valorization (eugenol)	H_2SO_4 used as catalyst in organosolv; lignin valorized into eugenol	0.53	[50]
Eucalyptus residues	Steam explosion + enzymatic hydrolysis + fermentation	Steam explosion at 200 °C for 10 min; enzyme: Cellic CTec2; fed-batch fermentation	2.37	[56]
Corn stover	Steam explosion + enzymatic hydrolysis + fermentation	Similar to eucalyptus; low yield from corn stover contributes to high MESP	2.65	[56]
Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by H_2SO_4	1.20	The current research (Scenario 1)
Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by CH_2O_2	1.14	The current research (Scenario 2)
Sugarcane bagasse	Organosolv + value-based allocation	Organosolv fractionation by CH_3ONa	4.33	The current research (Scenario 3)

5. Conclusions

A comprehensive techno-economic evaluation was conducted to determine the industrial viability of ethanol production from sugarcane bagasse via organosolv fractionation, utilizing three catalytic systems: sulfuric acid (H_2SO_4), formic acid (CH_2O_2), and sodium methoxide (CH_3ONa). Each catalytic configuration exhibited specific advantages with respect to biomass deconstruction, ethanol and lignin recovery, and cost efficiency. Among the evaluated scenarios, the CH_2O_2-catalyzed process demonstrated superior performance, achieving the highest cellulose recovery (94.52%), a competitive ethanol output of 1,081,976 kg/year, and the lowest production costs—1.14 USD/L for ethanol and 1.84 USD/kg for lignin. Capital investment remained moderate at 3.67 million USD, while TAC was the lowest among all scenarios at 3.93 million USD/year. Despite a slightly lower lignin removal efficiency (81.01%) compared to the H_2SO_4-based configuration (90.82%), the CH_2O_2 pathway maintained higher cellulose integrity and more favorable economic indices, which offset its minor limitations. In contrast, the CH_3ONa-based system retained a larger proportion of hemicellulose but incurred substantial raw material and reagent expenses, resulting in the highest ethanol (4.33 USD/L) and lignin (6.96 USD/kg) production costs and TAC exceeding 15 million USD/year. Chemical input costs emerged as the dominant sensitivity parameter, particularly for CH_2O_2 and CH_3ONa configurations, while variations in feedstock prices, temperature, and pressure had negligible impacts on overall cost structure. The sulfuric acid route, though efficient in delignification, was constrained by corrosion risks and the need for extensive wastewater treatment, thereby raising operating and maintenance costs. Strategic performance evaluation using normalized 3D vector analysis and heatmap visualization revealed that the CH_2O_2-based process offered the most balanced and economically viable solution, with favorable alignment across ethanol yield, revenue, and unit cost metrics. These findings underscore the potential of formic acid-catalyzed organosolv pretreatment as a scalable and sustainable approach for lignocellulosic ethanol production in Thailand. To enhance long-term viability, future process development should prioritize solvent recovery optimization, inhibitor mitigation during fermentation, and lignin valorization into higher-value bio-based chemicals. Such advancements will further strengthen the role of sugarcane bagasse valorization in supporting Thailand's transition toward a circular, bio-based economy.

Author Contributions: Conceptualization, methodology, software, writing—original draft preparation, S.K.; visualization, investigation, writing—review and editing, N.S.; software, validation, S.I.; validation, supervision, N.K.; software, validation, supervision, S.C.; supervision, K.S.; project administration, S.W.; conceptualization, methodology, investigation, validation, M.N.; conceptualization, methodology, formal analysis, resources, supervision, T.K. All authors have read and agreed to the published version of the manuscript.

Funding: Nopparat Suriyachai was supported by the Thailand Science Research and Innovation Fund and the University of Phayao (Grant No. 5041/2567).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Energy Statistics of Thailand 2023, Energy Policy and Planning Office (EPPO), Ministry of Energy, Thailand. Available online: https://www.eppo.go.th/index.php/th/component/k2/item/19566-energy-statistics-2566 (accessed on 1 June 2025).
2. Preethi, M.G.; Kumar, G.; Karthikeyan, O.P.; Varjani, S.; Rajesh, B.J. Lignocellulosic biomass as an optimistic feedstock for the production of biofuels as valuable energy source: Techno-economic analysis, Environmental Impact Analysis, Breakthrough and Perspectives. *Environ. Technol. Innov.* **2021**, *24*, 102080. [CrossRef]
3. Wang, C.; Zhang, W.; Qiu, X.; Xu, C. Hydrothermal treatment of lignocellulosic biomass towards low-carbon development: Production of high-value-added bioproducts. *EnergyChem* **2024**, *6*, 100133. [CrossRef]
4. Jayakumar, M.; Gindaba, G.T.; Gebeyehu, K.B.; Periyasamy, S.; Jabesa, A.; Baskar, G.; John, B.I.; Pugazhendhi, A. Bioethanol production from agricultural residues as lignocellulosic biomass feedstock's waste valorization approach: A comprehensive review. *Sci. Total Environ.* **2023**, *879*, 163158. [CrossRef]
5. Alternative Energy Development Plan: AEDP2015, Department of Renewable Energy Development and Energy Efficiency, Ministry of Energy, Thailand. 2015. Available online: https://www.eppo.go.th/images/POLICY/ENG/AEDP2015ENG.pdf (accessed on 11 June 2025).
6. Devi, A.; Bajar, S.; Kour, H.; Kothari, R.; Pant, D.; Singh, A.A.-O. Lignocellulosic Biomass Valorization for Bioethanol Production: A Circular Bioeconomy Approach. *BioEnergy Res.* **2022**, *15*, 1820–1841. [CrossRef] [PubMed]
7. Raina, N.; Boonmee, R.; Kirdponpattara, S.; Narasingha, M.; Sriariyanun, M.; Phitsuwan, P.; Chuetor, S. Process performance evaluation of different chemical pretreatments of lignocellulosic biomass for bioethanol production. *Ind. Crops Prod.* **2024**, *211*, 118207. [CrossRef]
8. Joseph, A.M.; Tulasi, Y.; Shrivastava, D.; Kiran, B. Techno-economic feasibility and exergy analysis of bioethanol production from waste. *Energy Convers. Manag. X* **2023**, *18*, 100358. [CrossRef]
9. Ruiz, H.A.; Sganzerla, W.G.; Larnaudie, V.; Veersma, R.J.; van Erven, G.; Shiva; Ríos-González, L.J.; Rodríguez-Jasso, R.M.; Rosero-Chasoy, G.; Ferrari, M.D.; et al. Advances in process design, techno-economic assessment and environmental aspects for hydrothermal pretreatment in the fractionation of biomass under biorefinery concept. *Bioresour. Technol.* **2023**, *369*, 128469. [CrossRef]
10. Varriale, L.; Geib, D.; Ulber, R. Short-term adaptation as a tool to improve bioethanol production using grass press-juice as fermentation medium. *Appl. Microbiol. Biotechnol.* **2024**, *108*, 393. [CrossRef]
11. Weerasai, K.; Laosiripojana, N.; Imman, S.; Kreetachat, T.; Suriyachai, N. Reusable alkaline catalyzed organosolv pretreatment and delignification of bagasse for sugar platform biorefinery. *Biomass Convers. Biorefin.* **2023**, *13*, 1751–1761. [CrossRef]
12. Suriyachai, N.; Champreda, V.; Kraikul, N.; Techanan, W.; Laosiripojana, N. Fractionation of lignocellulosic biopolymers from sugarcane bagasse using formic acid-catalyzed organosolv process. *3 Biotech* **2018**, *8*, 221. [CrossRef] [PubMed]
13. Panakkal, E.J.; Sriariyanun, M.; Ratanapoompinyo, J.; Yasurin, P.; Cheenkachorn, K.; Rodiahwati, W.; Tantayotai, P. Influence of Sulfuric Acid Pretreatment and Inhibitor of Sugarcane Bagasse on the Production of Fermentable Sugar and Ethanol. *Appl. Sci. Eng. Prog.* **2021**, *15*. [CrossRef]
14. Kreetachat, T.; Suriyachai, N.; Khongchamnan, P.; Suwannahong, K.; Wongcharee, S.; Sakulthaew, C.; Chokejaroenrat, C.; Imman, S. Optimization of Acid-Catalyzed Hydrolysis and Simultaneous Saccharification and Fermentation for Enhanced Ethanol Production from Sweet Stalk Sorghum. *Catalysts* **2025**, *15*, 379. [CrossRef]

15. Gutierrez, S.; Mangone, F.; Vergara, P.; Gonzalez, V.; Ferreira, J.P.; Villar, J.C.; Garcia-Ochoa, F. Lignocellulosic biomass pretreatments by diluted sulfuric acid and ethanol-water mixture: A comparative techno-economic analysis. *Bioresour. Technol. Rep.* **2023**, *23*, 101514. [CrossRef]
16. Liu, B.; Liu, L.; Deng, B.; Huang, C.; Zhu, J.; Liang, L.; He, X.; Wei, Y.; Qin, C.; Liang, C.; et al. Application and prospect of organic acid pretreatment in lignocellulosic biomass separation: A review. *Int. J. Biol. Macromol.* **2022**, *222*, 1400–1413. [CrossRef] [PubMed]
17. Baral, N.R.; Shah, A. Comparative techno-economic analysis of steam explosion, dilute sulfuric acid, ammonia fiber explosion and biological pretreatments of corn stover. *Bioresour. Technol.* **2017**, *232*, 331–343. [CrossRef]
18. Rodrigues Gurgel da Silva, A.; Giuliano, A.; Errico, M.; Rong, B.-G.; Barletta, D. Economic value and environmental impact analysis of lignocellulosic ethanol production: Assessment of different pretreatment processes. *Clean Technol. Environ. Policy* **2019**, *21*, 637–654. [CrossRef]
19. Areeya, S.; Jayex Panakkal, E.; Sriariyanun, M.; Kangsadan, T.; Tawai, A.; Amornraksa, S.; Hartley, U.; Yasurin, P. A Review on Chemical Pretreatment of Lignocellulosic Biomass for the Production of Bioproducts: Mechanisms, Challenges and Applications. *Appl. Sci. Eng. Prog.* **2023**, *16*, 6767. [CrossRef]
20. Fu, R.; Kang, L.; Zhang, C.; Fei, Q. Application and progress of techno-economic analysis and life cycle assessment in biomanufacturing of fuels and chemicals. *Green Chem. Eng.* **2023**, *4*, 189–198. [CrossRef]
21. Abdou Alio, M.; Marcati, A.; Pons, A.; Vial, C. Modeling and simulation of a sawdust mixture-based integrated biorefinery plant producing bioethanol. *Bioresour. Technol.* **2021**, *325*, 124650. [CrossRef]
22. Bisotti, F.; Gilardi, M.; Berglihn, O.T.; Tschentscher, R.; Hansen, L.D.; Horn, S.J.; Várnai, A.; Wittgens, B. From laboratory scale to innovative spruce-based biorefinery. Note I: Conceptual process design and simulation. In *Computer Aided Chemical Engineering*; Manenti, F., Reklaitis, G.V., Eds.; Elsevier: Amsterdam, The Netherlands, 2024; Volume 53, pp. 2449–2454.
23. Solarte-Toro, J.C.; Rueda-Duran, C.A.; Ortiz-Sanchez, M.; Cardona Alzate, C.A. A comprehensive review on the economic assessment of biorefineries: The first step towards sustainable biomass conversion. *Bioresour. Technol. Rep.* **2021**, *15*, 100776. [CrossRef]
24. Chong, T.Y.; Cheah, S.A.; Ong, C.T.; Wong, L.Y.; Goh, C.R.; Tan, I.S.; Foo, H.C.Y.; Lam, M.K.; Lim, S. Techno-economic evaluation of third-generation bioethanol production utilizing the macroalgae waste: A case study in Malaysia. *Energy* **2020**, *210*, 118491. [CrossRef]
25. Chen, H.; Zhou, D.; Luo, G.; Zhang, S.; Chen, J. Macroalgae for biofuels production: Progress and perspectives. *Bioresour. Technol.* **2021**, *320*, 124533. [CrossRef]
26. Ansaloni, L.; Fabbri, D.; Spigno, G. Valorization of macroalgal biomass for the production of renewable chemicals: A review. *Ind. Crops Prod.* **2021**, *159*, 113051. [CrossRef]
27. Humbird, D.; Davis, R.; Tao, L.; Kinchin, C.; Hsu, D. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol. *Natl. Renew. Energy Lab.* **2011**, 275–3000.
28. Rocha, G.J.d.M.; Silva, F.T.; Curvelo, A.A.d.S.; Araujo, G.T. A fast and accurate method for determination of cellulose and polyoses by HPLC. *Proceedings* **1997**. Available online: https://repositorio.usp.br/item/000929622 (accessed on 11 June 2025).
29. Tiwari, S.; Yadav, J.; Gaur, R.; Singh, R.; Verma, T.; Yadav, J.S.; Pandey, P.K.; Rath, S.K. Multistep Structural and Chemical Evaluation of Sugarcane Baggase, Pretreated With Alkali for Enhancing the Enzymatic Saccharification by Cellulase and Xylanase of the Pseudomonas sp. CVB-10 (MK443365) and Bacillus paramycoides T4 (MN370035) Mix-Culture System. *Front. Energy Res.* **2022**, *9*, 726010. [CrossRef]
30. Oh, H.W.; Lee, S.C.; Woo, H.C.; Kim, Y.H. Energy-efficient recovery of fermented butyric acid using octyl acetate extraction. *Biotechnol. Biofuels Bioprod.* **2022**, *15*, 46. [CrossRef] [PubMed]
31. Viell, J.; Harwardt, A.; Seiler, J.; Marquardt, W. Is biomass fractionation by Organosolv-like processes economically viable? A conceptual design study. *Bioresour. Technol.* **2013**, *150*, 89–97. [CrossRef] [PubMed]
32. da Silva, A.R.G.; Errico, M.; Rong, B.-G. Solvent Recycle and Impurity Purge Evaluation for Organosolv Pretreatment Method for Bioethanol Production from Lignocellulosic Biomass. In *Computer Aided Chemical Engineering*; Espuña, A., Graells, M., Puigjaner, L., Eds.; Elsevier: Amsterdam, The Netherlands, 2017; Volume 40, pp. 1141–1146.
33. Saadan, R.; Hachimi Alaoui, C.; Ihammi, A.; Chigr, M.; Fatimi, A. A Brief Overview of Lignin Extraction and Isolation Processes: From Lignocellulosic Biomass to Added-Value Biomaterials. In Proceedings of the International Electronic Conference on Forests 2024, Virtual, 23–25 September 2024.
34. Gavin, T.; Ray, S. *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*, 3rd ed.; Elsevier: London, UK, 2021.
35. Prachuab, P. *Renewable Energy Strategies for Sustainable Development in Thailand*; Thammasat University: Bangkok, Thailand, 2019.
36. Echemi. Weekly Chemical Prices. Available online: https://www.echemi.com/weekly-price.html (accessed on 20 June 2024).
37. Authority, P.W. Provincial Waterworks Authority Website. Available online: https://www.pwa.co.th (accessed on 20 June 2024).

38. Electricity Generating Authority of Thailand. Available online: https://www.egat.co.th/home/egat-price (accessed on 20 June 2024).
39. Lim, K.L.; Wong, W.Y.; James Rubinsin, N.; Loh, S.K.; Lim, M.T. Techno-Economic Analysis of an Integrated Bio-Refinery for the Production of Biofuels and Value-Added Chemicals from Oil Palm Empty Fruit Bunches. *Processes* **2022**, *10*, 1965. [CrossRef]
40. Hafyan, R.H.; Mohanarajan, J.; Uppal, M.; Kumar, V.; Narisetty, V.; Maity, S.K.; Sadhukhan, J.; Gadkari, S. Integrated biorefinery for bioethanol and succinic acid co-production from bread waste: Techno-economic feasibility and life cycle assessment. *Energy Convers. Manag.* **2024**, *301*, 118033. [CrossRef]
41. Wirawan, S.S.; Solikhah, M.D.; Widiyanti, P.T.; Nitamiwati, N.P.D.; Romelan, R.; Heryana, Y.; Nurhasanah, A.; Sugiyono, A. Unlocking Indonesia's sweet sorghum potential: A techno-economic analysis of small-scale integrated sorghum-based fuel grade bioethanol industry. *Bioresour. Technol. Rep.* **2024**, *25*, 101706. [CrossRef]
42. Nair, L.G.; Agrawal, K.; Verma, P. Organosolv pretreatment: An in-depth purview of mechanics of the system. *Bioresour Bioprocess* **2023**, *10*, 50. [CrossRef]
43. Cheng, M.-H.; Wang, Z.; Dien, B.S.; Slininger, P.J.W.; Singh, V. Economic Analysis of Cellulosic Ethanol Production from Sugarcane Bagasse Using a Sequential Deacetylation, Hot Water and Disk-Refining Pretreatment. *Processes* **2019**, *7*, 642. [CrossRef]
44. Sganzerla, W.G.; Lachos-Perez, D.; Buller, L.S.; Zabot, G.L.; Forster-Carneiro, T. Cost analysis of subcritical water pretreatment of sugarcane straw and bagasse for second-generation bioethanol production: A case study in a sugarcane mill. *Biofuels Bioprod. Biorefin.* **2022**, *16*, 435–450. [CrossRef]
45. Romero-García, J.M.; Solarte-Toro, J.C.; Galán-Martín, Á.; Ruiz, E.; Castro, E.; Ortiz-Sánchez, M.; Cardona Alzate, C.A. Olive leaves upgrading applying a novel two-stage organosolv pretreatment: Techno-economic and environmental assessment. *Biochem. Eng. J.* **2024**, *207*, 109317. [CrossRef]
46. Peng, J.; Xu, H.; Wang, W.; Kong, Y.; Su, Z.; Li, B. Techno-economic analysis of bioethanol preparation process via deep eutectic solvent pretreatment. *Ind. Crops Prod.* **2021**, *172*, 114036. [CrossRef]
47. Turton, R.; Bailie, R.C.; Whiting, W.B.; Shaeiwitz, J.A. *Analysis, Synthesis, and Design of Chemical Processes*, 5th ed.; Pearson: London, UK, 2018.
48. Parascanu, M.M.; Sanchez, N.; Sandoval-Salas, F.; Carreto, C.M.; Soreanu, G.; Sanchez-Silva, L. Environmental and economic analysis of bioethanol production from sugarcane molasses and agave juice. *Environ. Sci. Pollut. Res. Int.* **2021**, *28*, 64374–64393. [CrossRef]
49. Gadkari, S.; Narisetty, V.; Maity, S.K.; Manyar, H.; Mohanty, K.; Jeyakumar, R.B.; Pant, K.K.; Kumar, V. Techno-Economic Analysis of 2,3-Butanediol Production from Sugarcane Bagasse. *ACS Sustain. Chem. Eng.* **2023**, *11*, 8337–8349. [CrossRef]
50. Martinez-Hernandez, E.; Cui, X.; Scown, C.D.; Amezcua-Allieri, M.A.; Aburto, J.; Simmons, B.A. Techno-economic and greenhouse gas analyses of lignin valorization to eugenol and phenolic products in integrated ethanol biorefineries. *Biofuels Bioprod. Biorefin.* **2019**, *13*, 978–993. [CrossRef]
51. Liu, F.; Dong, X.; Zhao, X.; Wang, L. Life cycle assessment of organosolv biorefinery designs with the complete use of biomass. *Energy Convers. Manag.* **2021**, *246*, 114653. [CrossRef]
52. Wenger, J.; Pichler, S.; Näyhä, A.; Stern, T. Practitioners' Perceptions of Co-Product Allocation Methods in Biorefinery Development—A Case Study of the Austrian Pulp and Paper Industry. *Sustainability* **2022**, *14*, 2619. [CrossRef]
53. Priadi, H.; Awad, S.; Villot, A.; Andres, Y.; Purwanto, W.W. Techno-enviro-economic analysis of second-generation bioethanol at plant-scale by different pre-treatments of biomass from palm oil waste. *Energy Convers. Manag. X* **2024**, *21*, 100522. [CrossRef]
54. Gubicza, K.; Nieves, I.U.; Sagues, W.J.; Barta, Z.; Shanmugam, K.T.; Ingram, L.O. Techno-economic analysis of ethanol production from sugarcane bagasse using a Liquefaction plus Simultaneous Saccharification and co-Fermentation process. *Bioresour. Technol.* **2016**, *208*, 42–48. [CrossRef] [PubMed]
55. Kautto, J.; Realff, M.; Ragauskas, A.; Kässi, T. Economic Analysis of an Organosolv Process for Bioethanol Production. *Bioresources* **2014**, *9*, 6041–6072. [CrossRef]
56. Correia, B.; Matos, H.A.; Lopes, T.F.; Marques, S.; Gírio, F. Sustainability Assessment of 2G Bioethanol Production from Residual Lignocellulosic Biomass. *Processes* **2024**, *12*, 987. [CrossRef]

BIOGRAPHY

NAME	Suphalerk Khaowdang
DATE OF BIRTH	29 October 1990
PLACE OF BIRTH	Phayao Province
INSTITUTIONS ATTENDED	Master of Engineering (Environmental Engineering)
HOME ADDRESS	376 M.9, Mae Ka Subdistrict, Mueang District, Phayao Province 56000
PUBLICATION	[1] Khaowdang, S., Suriyachai, N., Imman, S., Kreetachat, T., Chuetor, S., Wongcharee, S., & Suwannahong, K. (2025). Comparative study on techno-economic analysis for various organosolv fractionation of bagasse in Thailand. Applied Science and Engineering Progress, 18(4), 7794. https://doi.org/10.14416/j.asep.2025.06.011 [2] Khaowdang, S., Suriyachai, N., Imman, S., Suwannahong, K., Wongcharee, S., & Kreetachat, T. (2025). Application of Internet of Things Technology for Ventilation and Environmental Control in Conventional Open-Air Pig Housing Systems in Thailand. AgriEngineering, 7(6), 165. https://doi.org/10.3390/agriengineering7060165 [3] Khaowdang, S.; Suriyachai, N.; Imman, S.; Kreetachat, N.; Chuetor, S.; Wongcharee, S.; Suwannahong, K.; Nukunudompanich, M.; Kreetachat, T. Valorization of Sugarcane Bagasse in Thailand: An Economic Analysis of Ethanol and Co-Product Recovery via Organosolv Fractionation. Sustainability 2025, 17, 7145. https://doi.org/10.3390/su17157145