



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

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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 ($\text{C}_2\text{H}_5\text{OH}$)), 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:

- $\tau_{ij} = \frac{g_{ij} - g_{ij}^0}{RT}$ 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 C₂H₆O/water (H₂O) using H₂SO₄ 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 C₂H₆O and H₂O at a 70:30 %v/v ratio, with H₂SO₄ at a concentration of 2% w/v based on the solvent (This study).

Scenario 2: the flowsheet setup for organosolv fractionation with CH₂O₂ 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 H₂O/C₂H₆O/ethyl acetate (C₄H₈O₂)/CH₂O₂ in a ratio of 43:20:16:21% v/v, respectively [10].

Scenario 3: process flow configuration for organosolv fractionation using CH₃ONa 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 CH₃ONa 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.

$$TAC = \frac{CC}{n} + UC + ChemC + RM \quad (2)$$

Table 1: Feedstock, chemicals, and utilities prices.

Input	Unit	Price	Ref.
Bagasse	USD/ton	14.00	[30]
C ₂ H ₆ O	USD/L	~0.80	[31]
H ₂ O	USD/L	~0.00028	[32]
H ₂ SO ₄	USD/L	~0.16	[31]
CH ₂ O ₂	USD/L	~0.49	[31]
C ₄ H ₈ O ₂	USD/L	~1.30	[31]
CH ₃ ONa	USD/kg	~0.60	[31]
CH ₃ OH	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 H₂SO₄. 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 H₂SO₄ 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 H₂SO₄ 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 CH₂O₂ 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.

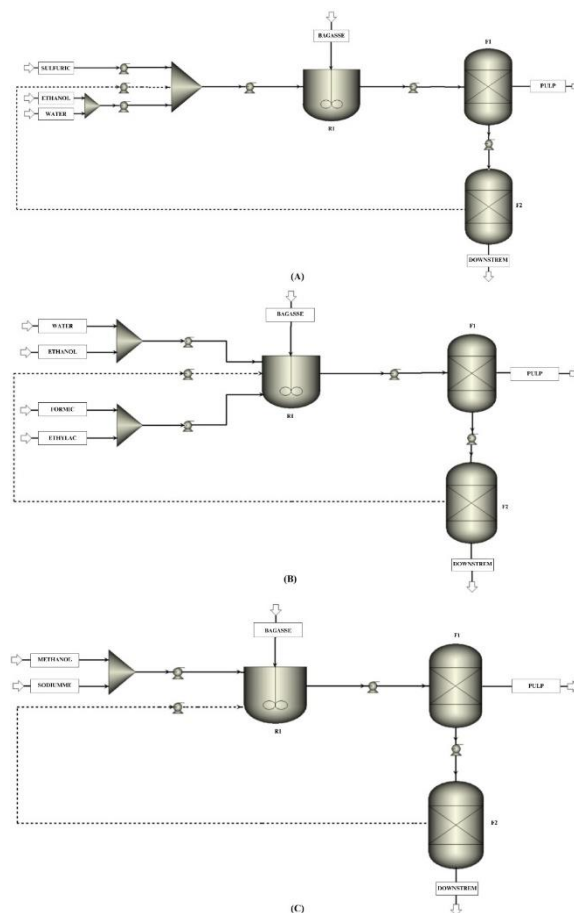
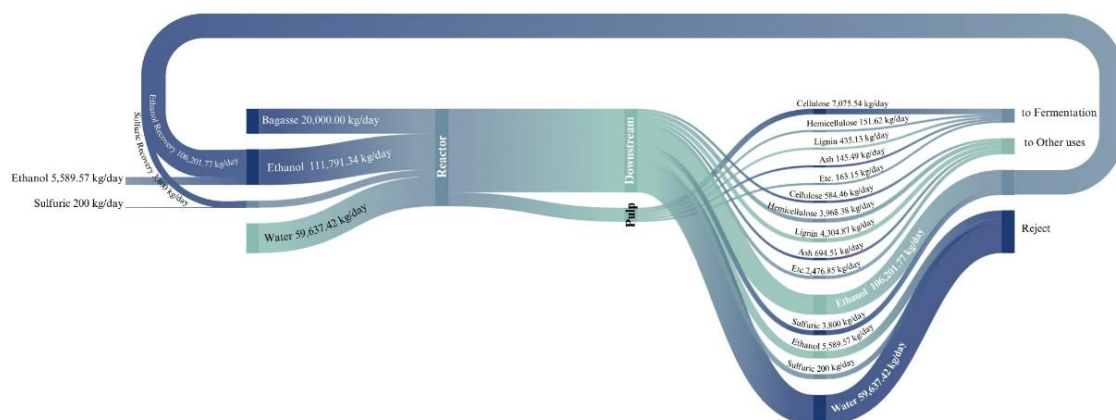


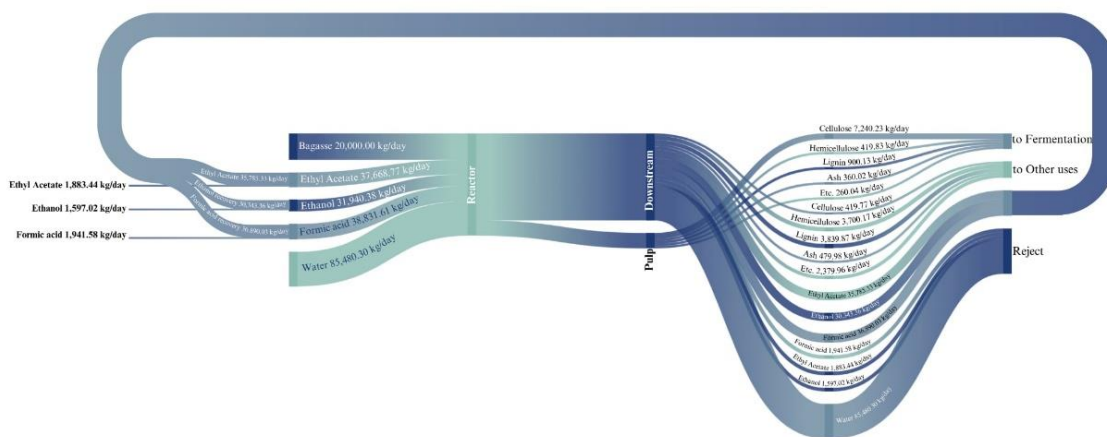
Figure 1: Flowsheet setup for organosolv fractionation experiments into 3 scenarios. (a) Scenario 1: organosolv fractionation by H_2SO_4 catalyst, (b) Scenario 2: organosolv fractionation by CH_2O_2 catalyst and (c) Scenario 3: organosolv fractionation by CH_3ONa catalyst.

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

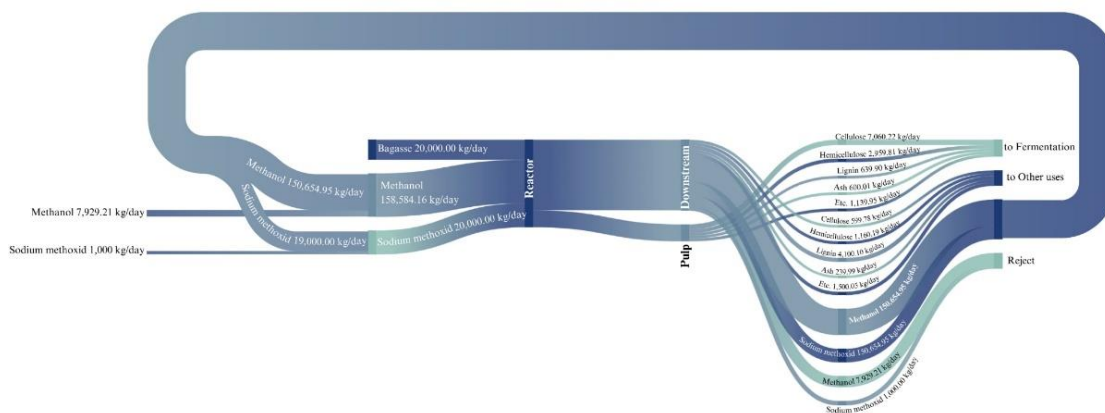
Scenario 1; Organosolv fractionation by H₂SO₄							
	Units	Bagasse	H₂SO₄	C₂H₆O	H₂O	Pulp	Downstream
Phase		Solid	Liquid	Liquid	Liquid	Solid	
Temperature	°C	25.00	25.00	25.00	25.00	170.00	170.00
Pressure	bar	1.01	1.01	1.01	1.01	20.00	20.00
Mass Flows	kg/day	20,000.00	200.00	5,589.57	59,637.42	7,970.93	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 ₂ H ₆ O	kg/day	-	-	5,589.57	-	-	5,589.57
H ₂ O	kg/day	-	-	-	59,637.42	-	59,637.42
H ₂ SO ₄	kg/day	-	200.00	-	-	-	200.00
Scenario 2; Organosolv fractionation by CH₂O₂							
		H₂O	C₂H₆O	CH₂O₂	C₄H₈O₂	Pulp	Downstream
Phase		Solid	Liquid	Liquid	Liquid	Solid	
Temperature	°C	25.00	25.00	25.00	25.00	159.00	159.00
Pressure	bar	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	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 ₂ H ₆ O	kg/day	-	-	1,597.02	-	-	1,597.02
H ₂ O	kg/day	-	85,480.30	-	-	-	85,480.30
CH ₂ O ₂	kg/day	-	-	-	1,941.58	-	1,941.58
C ₄ H ₈ O ₂	kg/day	-	-	-	-	1,883.44	1,883.44
Scenario 3; Organosolv fractionation by CH₃ONa							
		CH₃OH	CH₃ONa			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 ₃ OH	kg/day	-	7,929.21		-	-	7,929.21
CH ₃ ONa	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].

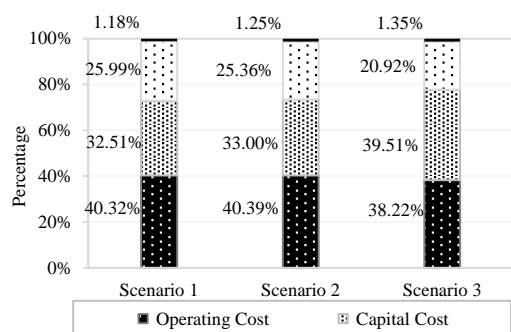


Figure 3: TAC contributions from each fractionation method.

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 $\pm 50\%$ 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 $\pm 10\%$ 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 $\pm 0.39\%$ and $\pm 0.36\%$, 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.

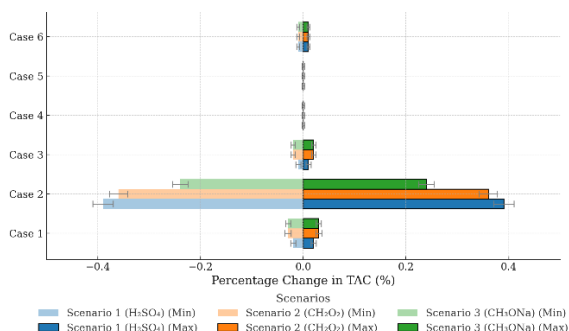
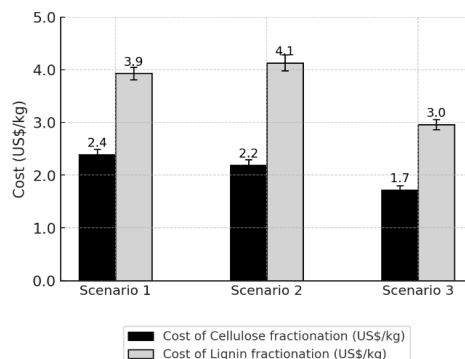
Table 4: Sensitivity analysis of price fluctuations on TAC across different scenarios.

Parameter Changed	Case	Min	Baseline	Max	Unit	TAC (million US\$/year)				
						Min	Change (%)	Baseline	Max	Change (%)
Scenario 1; Organosolv fractionation by H ₂ SO 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 ₂ H ₆ O, and H ₂ SO 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 ₂ O 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 ₂ H ₆ O, CH ₂ O ₂ , and C ₄ H ₈ O 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 ₃ ONa 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 ₃ OH, and CH ₃ ONa				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

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

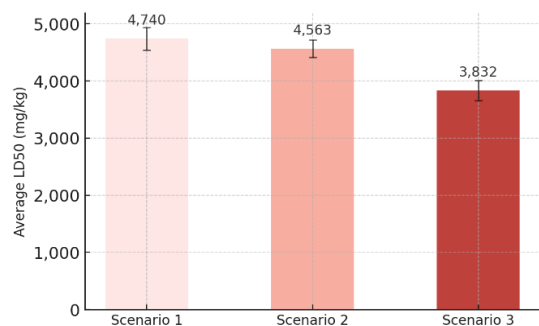


Figure 6: Comparison of average LD50 in each scenario.

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 ₂ H ₆ O	2	3	0	Highly flammable liquid and vapour. Causes serious eye irritation.
Sulfuric acid	2,140	Class IV (unlikely if used safely)	H ₂ SO ₄	3	0	0	Corrosive to Metals, Skin corrosion, Serious eye damage.
Scenario 2;							
Ethanol	7,340	Class IV (unlikely if used safely)	C ₂ H ₆ O	2	3	0	Highly flammable liquid and vapour. Causes serious eye irritation.
Formic acid	730	Class III (unlikely if used safely)	CH ₂ O 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 ₄ H ₈ O 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 ₃ OH	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 ₃ NaO	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.

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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.

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