Multicriteria Feasibility Assessment of BioSuccinic Acid Production from Lignocellulosic Biomass

Submitted By

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It is important not to worship what is known, but to question it.

J. Bronowski

ABSTRACT

The goal of any lignocellulosic based biorefinery should be to produce a spectrum of marketable products and energy utilizing all significant components of biomass. Depending on the maturity of available technology, biorefineries can target high-value low-volume (HVLV), middle-value middle-volume (MVMV), and low-value high-volume (LVHV) outputs provided they are economically feasible. BioSuccinic Acid (BioSA), a MVMV product, has considerable potential as a candidate for biorefineries based on an analysis we carried out initially. The total world production of Succinic Acid (SA) in 2013–2014 was 38,000 tons, valued at 2.90 USD/kg SA and with predicted worldwide market demand of 94,000 tons by 2025. However, the most crucial challenge encountered with BioSA production is the cost of production compared to its conventional fossil-based counterpart. About a decade ago, many industries were set up to produce succinic acid from starch-based renewable sources when the cost of petroleum and petroleum-based products was higher than 100 dollars a barrel. The drop-in petroleum prices have led to the closure or re-orientation of some of these industrial units.

Initial detailed feasibility assessments help to avoid economic uncertainty. Techno-Economic Analysis (TEA) followed by Life Cycle Analysis (LCA) are standard methodologies used to ascertain the technical, economic, and environmental sustainability of BioSA production. However, achieving balance among these sustainability domains (economic, environmental, and social) is a challenging task. Improvement in one domain's performance, say the economic criteria, can decrease the performance of another domain, such as the environmental, or vice versa. This is

considered as a trade-off or burden shifting (from one domain to another). Also, comparison of processes based on TEA and LCA together is difficult as the final results are usually in different units. TEA results are in a monetary unit, whereas LCA results are presented by using different environmental indicators. Thus, it is important to develop a holistic framework that combines all domains of sustainability in a single monetary unit and then compares it with the conventional fossil resources route. The evaluation of all aspects of sustainability in monetary units is the basis of this study.

A conceptual multiproduct biorefinery utilizing 1000 kg/hr corn stover as a feedstock was designed to produce BioSA as a main product and furfural and electricity as coproducts in three different scenarios. In scenario 1, after the pretreatment of corn stover, both C-6 and C-5 sugar streams are diverted to the fermentation section for the BioSA production, whereas in scenario 2, the C-5 sugar stream is diverted for furfural production and BioSA produced from C-6 sugar only. In scenario 3, the C-5 sugar stream is diverted to a Wastewater Treatment Plant (WWTP) for biogas generation. The generated biogas is consumed in a Combined Heat and Power (CHP) unit for electricity and steam production, while the C-6 sugar stream was used for BioSA production. The value addition of the lignin stream is done by producing electricity and steam in a CHP unit for all three scenarios. A cradle-to-gate LCA was performed for all three scenarios using the production of 1 kg BioSA as the functional unit. ReCiPe midpoint and endpoint were used as the impact assessment methods. The environmental impacts were addressed in the form of damages to the areas of protection (AOP), such as human health, ecosystem, and resources. The evaluated environmental impacts or damages to AOPs were converted in the form of the monetary unit (dollar unit) and Minimum Selling Price (MSP) was evaluated for each scenario based on the

respective TEA study. These biorefining scenarios were then compared to the fossil-based succinic acid production route.

TEA studies indicated that the production of BioSA using both C-6 and C-5 sugars and electricity from lignin (scenario 1) was found to be the most economical, with an MSP of 2.28 USD/ kg BioSA and an 8-year payback period. The biorefinery also produced electricity and steam required to run the biorefinery operations. In scenario 2, the production of furfural is an energy-intensive process because of the high pressure and temperature conditions for the conversion of C-5 sugars. This makes the process (scenario 2) economically less favorable. The purchase of steam for biorefinery operations adds to the operating cost and eventually leads to a higher MSP of BioSA. However, the economic performance of this scenario could be enhanced by heat integration. Scenario 3, with the production of biogas with the C-5 stream is found to be the second-best option with an MSP of 3.19 USD/kg BioSA and an 8-year payback period.

The midpoint impact LCA results demonstrated that feedstock production, transportation, and pretreatment stages greatly influence all three scenarios. Endpoint impacts and monetary valuation indicated that scenario 1 shows the best performance, followed by scenario 3, the fossil resources-based route, and scenario 2. The calculated environmental costs are 1.48, 3.05, 2.04, and 2.24 USD/kg BioSA for scenarios 1 to 3 and the fossil route, respectively. Sensitivity analysis for monetary valuation suggested that the environmental costs are highly sensitive to damage to human health, and variations in damage to resources have minimum impact on the environmental cost. Cradle-to-gate midpoint LCA considering 18 impact categories reveals that scenario 1 and fossil route show the best performance with the least value in midpoint and endpoint impact categories. The MSP values for the combined techno-economic and environmental cost derived from LCA were 3.76 and 4.54 USD/kg SA for scenario 1 and fossil resource route, respectively.

Process improvements are needed in the BioSA process to bring additional benefits to BioSA production route. More specifically, improvement in areas like feedstock plantation and harvesting, transportation, and pretreatment will help to improve the environmental performance of the bio route. These results can further be integrated with process economics and social policy tools like Cost-Benefit Analysis (CBA) and Social Cost of Carbon (SCC), respectively, during the decision-making stage.

In addition, the selection of the SA production route based on multiple criteria, i.e., techno-economics, environment and social aspects are challenging. It is a Multi-Criteria Decision Analysis (MCDA) problem. Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) with the involvement and inputs of real experts working in an area of biorefining and bioprocessing was evaluated. The hierarchical model with two main criteria (techno-economics and environment) and seven sub-criteria, namely MSP, waste, raw material input, energy requirement, damage to human health, damage to the ecosystem, and damage to resources, and four alternatives AL-1, AL-2, AL-3 and AL-4 identical to scenario 1, scenario 2, scenario 3, and fossil resource route, respectively, was developed. The results indicate that with a slightly more influence of techno-economic criteria than environmental criteria, AL-1 (scenario 1) has the highest preference, followed by AL-2 (scenario 2), AL-3 (scenario 3), and AL-4 (fossil resource route). The sensitivity analysis results demonstrate that these preferences are less sensitive to variations in the weightage given to main criteria.

Based on the results obtained in this thesis, it is apparent that for the production of SA from renewable resources, utilization of all major components of biomass, TEA, and LCA followed by the monetary valuation of assessed environmental impacts, decision-making based on multiple criteria with involvement of real experts is essential. The contribution of such assessment, if bolted

before commercialization, can make the bioroute for SA production more sustainable and helps to avoid economic failure. It is recommended that this type of evaluation can be extended to similar biorefining processes.

Keywords: Biochemicals, Biosuccinic acid, Fossil based succinic acid, Corn stover, Multi-product biorefinery, Techno-Economic Assessment, Life Cycle Assessment, Monetary Valuation, Environmental cost, Multi-Criteria Decision Analysis, Hesitant Fuzzy Analytical Hierarchy Process

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I dedicate this thesis to my supervisors,

Dr. Sudip Kumar Rakshit and Dr. Arturo Sanchez

--- असतोमा सद्गमय, तमसोमा ज्योतिर्गमया ---

(From untruth, lead me to truth; From darkness, lead me to light)

List of Abbreviations

Acronym	Abbreviation
AOP	Area of Protection
AHP	Analytical Hierarchy Process
AHI	Absolutely High Importance
ALI	Absolutely Low Importance
A. succiniciproducens	*Anaerobiospirillum succiniciproducens*
A. succinogenes	*Actinobacillus succinogenes*
BAHY	Biodiversity Adjusted Hector Year
BioSA	BioSuccinic Acid
CHP	Combined Heat and Power
CAGR	Compound Annual Growth Rate
CAPEX	Capital Expenditure
CBA	Cost Benefit Analysis
DCF	Discounted Cash Flow
DALY	Disability Adjusted Life Year
DOE	Department of Energy
ESHI	Essentially High Importance
EHI	Equally High Importance
EE	Exactly Equal
ELI	Equally Low Importance
ESLI	Essentially Low Importance

E. coli	*Escherichia coli*
F. succinogenes	*Fibrobacter succinogenes*
FOC	Fixed Operating Cost
FCI	Fixed Capital Investment
GHG	Green House Gas
GWP	Global Warming Potential
GDP	Gross Domestic Product
GHP	Gross Household Production
HVLV	High Volume-Low Value
HFAHP	Hesitant Fuzzy Analytical Hierarchy Process
IPCC	Intergovernmental Panel on Climate Change
IRR	Internal Rate of Return
ISBL	Inside Battery Limit
LEP	Lacking Economic Production
LVHV	Low Volume-High Value
LCA	Life Cycle Assessment
MOC	Material of Construction
MCDA	Multi-Criteria Decision Analysis
MVMV	Middle Volume-Middle Value
MSP	Minimum Selling Price
M. succiniciproducens	*Mannheimia succiniciproducens*
NPV	Net Present Value
NREU	Non-Renewable Energy Use

OPEX	Operating Expenditure
OPEC	Organization of Petroleum Exporting Countries
PPP	Purchasing Power Parity
PEP	Potential Annual Economic Production
QALY	Quality Adjusted Life Year
SA	Succinic Acid
SCC	Social Cost of Carbon
TCI	Total Capital Investment
THF	Tetrahydrofuran
TEA	Techno-Economic Analysis
USD	United States Dollar
VOC	Variable Operating Cost
WWTP	Waste Water Treatment Plant

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Outline of the Thesis

Chapter 1 *Introduction*

This chapter presents an introduction about Succinic Acid production from biomass and its latest market trends. The rationale of the work and the overall and specific research objectives of the thesis are also presented.

Chapter 2 *Literature review*

This chapter discusses recent developments in the area of biochemical production from lignocellulosic biomass. The key features of the pretreatment process and their limitations are also highlighted. The trends in market demand and market prices for potential bioproducts was reviewed. The importance of sustainability assessment for bioproducts commercialization and limitations in available methodologies are discussed. Recommendations have been made to overcome these limitations. The incorporation of a multiproduct biorefinery concept for the value addition of C-5 sugar and lignin in addition to the use of C-6 sugars is suggested. A novel holistic framework for the sustainability assessment of bioproduct synthesis is developed. The importance of key features of the model, i.e., Techno-Economic Analysis (TEA), Life Cycle Assessment (LCA) followed by monetary valuation of environmental impacts highlighted. The feasibility of biorefining systems has to be compared to the conventional fossil resource route simultaneously. A large part of the content of this review chapter has been published in a peer-reviewed journal **Fuel (Elsevier)**: "**Perspectives for scale-up of biorefineries using biochemical conversion**

pathways: technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022). https://doi.org/10.1016/j.fuel.2022.124532".

Chapter 3 *Scenario-based techno-economics and heat integration feasibility assessment of integrated multiproduct biorefineries with biosuccinic acid as the main product and various byproduct options.*

This chapter reports the TEA analysis of BioSA production from corn stover. Three scenario-based analyses were performed to identify the best design scenario for BioSA production as a main product from a technical and economical point of view. Co-products generation, i.e., furfural and electricity from C-5 sugar and CHP based energy from lignin were also assessed. Each design scenario was assessed by evaluating the TOC, VOC, utility requirements, NPV, and MSP of BioSA. Heat integration feasibility was also calculated for all three design scenarios. The analysis results are discussed with reference to previous studies and emphasize the benefits of the proposed design configuration for BioSA production. This work has been reported in the **Springer Nature journal,** "**Biomass Conversion and Biorefinery",** published online, 22 June, 2022. https://doi.org/10.1007/s13399-022-02945-9

Chapter 4 *Scenario-based life cycle assessment and environmental monetary valuation of biosuccinic acid production from lignocellulosic biomass.*

This chapter reports the Life Cycle Assessment followed by a monetary valuation of assessed environmental impacts of BioSA production from corn stover. Three scenario-based analyses are performed to identify the best design scenario for BioSA production as the main product from the environmental point of view. Conventional fossil-based SA production is also compared with all

three scenarios. This work has been submitted to the **Elsevier** journal **"Industrial Crops and Products"** in March 2023.

Chapter 5 *Multi-criteria decision analysis of succinic acid production options using hesitant fuzzy analytical hierarchy process.*

This chapter reports Multi-Criteria Decision Analysis (MCDA) for BioSA production based on weighed options provided by experts working in the field among available alternatives. TEA and LCA were considered the main criteria followed by seven sub-criteria and ranks are given for four alternatives routes of SA production. Hesitant Fuzzy Analytical Hierarchy Process used to perform MCDA. A paper based on this study will be submitted to **Elsevier** "**Journal of Cleaner Production**" in May 2023.

Chapter 6 *Summary and recommendations*

The general conclusion drawn from the entire study is presented in this chapter. Recommendations for future work are also suggested.

CHAPTER 1
INTRODUCTION

1 Introduction

A rapid increase in energy and chemical demand and need to improve the worlds carbon foot print has placed immense pressure on consumer prices and is prompting researchers to look for sustainable and consistent energy resources. Biomass is a very good renewable resource from which various chemicals and fuels can be produced. The synthesis of these products from agricultural and woody biomass have been studied for few decades. Ideal biorefineries can be set up at locations where biomass is abundantly available and can serve as the starting material to produce multiple products using complex processing methods and technologies [1].

The oil embargo by OPEC countries in 1973 resulted in considerable efforts to look for an alternative liquid fuel for transportation. Research on the production of ethanol from lignocellulosic biomass was initiated at that time. The rationale for these efforts were further strengthened by considerations such as finite nature of fossil fuels, availability of renewable biomass and more recently to mitigate climate change. However, the geo-politics of crude oil availability pricing has made it difficult to make ethanol an economically competitive product especially when crude process are very low.

Oil prices are determined by supply and demand, which is closely in relation to economic activity, market expectations, geopolitical dominance, and the monopoly adopted by countries to achieve these goals. Rapid developments in biorefining and bioprocessing has been driven by mandates, climate change concerns, emissions targets and energy security. For example, between 2004 and 2006, the market for bioethanol and biodiesel grew by 26 % and 127 %, respectively [2]. The attractiveness and competitiveness of biorefining is lost when the oil prices are reduced [3]. There are numerous uncertainties in oil prices due to OPEC supply, non-OPEC supply tariffs, embargoes,

and demands. The competitiveness of biorefining is reduced when the prices of crude oil was 55 USD/barrel and 57 USD/barrel in the year of 2017 and 2018 and even it is questioned at 100 USD/barrel too [4]. The fluctuating prices of crude oil makes it difficult for industry to invest on low value products as profits become unpredictable and is dependent on fossil resource prices. Taking this into account some a comparison has been made between High Volume-Low Value (HVLV), Middle Volume-Middle Value (MVMV), and Low Volume-High Value (LVHV) outputs [5], as shown in **Figure 1.1**. Based on this it has been suggested that MVMV products be chosen for biorefining industry.

Succinic Acid (SA) is considered as one such product with tremendous potential as a MVMV candidate for biorefineries. The Department of Energy (DoE) USA has considered it as a compound of strategic importance in the near future based on renewable material. It is a niche product due to its potential application in food additives, detergents, cosmetics, pigments, toners, cement additives, and pharmaceutical intermediates [6,7].

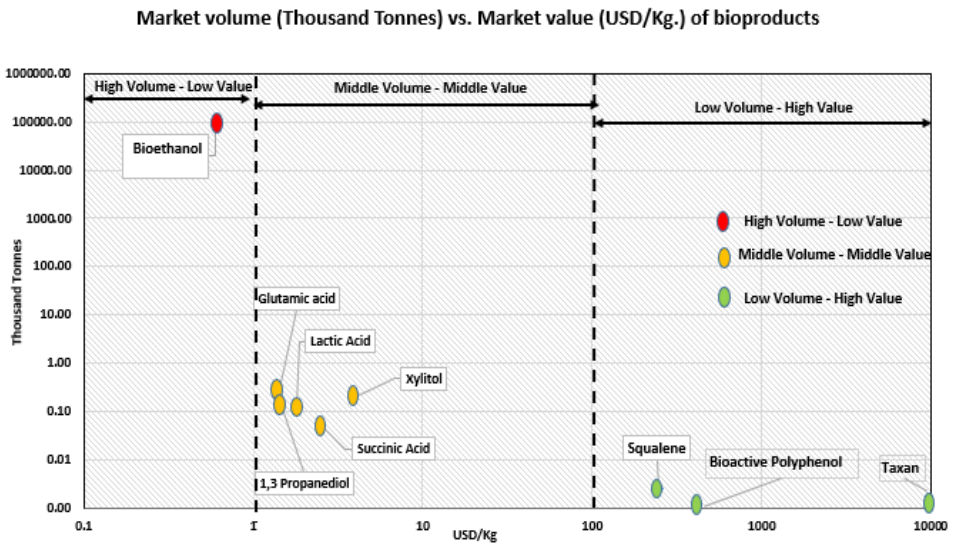

Figure 1. 1 Market volume vs. market values of bioproducts [5]

The total world production of SA in 1990 was between 16,000 to 18,000 metric tons (MT), the potential market will reach up to 1.8 billion USD in 2025 with a compound annual growth rate (CAGR) of 27.4% [8].

The conventional synthesis route for SA production is the catalytic hydrogenation of maleic anhydride to succinic anhydride, followed by hydration to SA. The reaction occurs at a temperature of 120 to 180 °C and 0.5 to 4.0 MPa hydrogen pressure [5,8]. Other processes like carbonylation, starting from ethylene glycol, ethylene, acetylene, and an unsaturated carboxylic acid, are also promising routes for SA production [9]. The price of SA derived by this route is directly influenced by crude oil prices.

Due to increasing petroleum prices at the beginning of the last decade and improvements in fermentation and purification technologies, the production of a SA from renewable feedstocks has been projected to have the considerable potential [10,11]. *Anaerobiosprillum succiniciproducens* and *Actinobacillus succinogenes* are the potential microorganisms to produce SA on a larger scale [12,13]. Genetically engineered *E. coli* can be applied for the various feedstock, i.e., sugarcane, cassava, corn stalk, and algae, for BioSA synthesis [14–17]. It exhibits immense potential for the production of SA under aerobic and anaerobic conditions [18–20]. The fast growth rate, standard cultivation techniques, inexpensive media, and comprehensive knowledge make it a promising BioSA producer.

Around 2010, SA was considered a good choice for biorefining investment. The price of petroleum crude was high, making BioSA competitive compared to SA produced chemically. A number of BioSA companies started up simultaneously around the years 2012-13 [5]. Most of the ventures opened when the average crude oil price was between 93 to 98 USD/barrel, and when the prices plunged to between 43 to 65 USD/barrel, the companies started shutting down or changed their

corporate goals. The trend between crude oil prices and their impacts on BioSA production companies is shown in **Figure 1.2**.

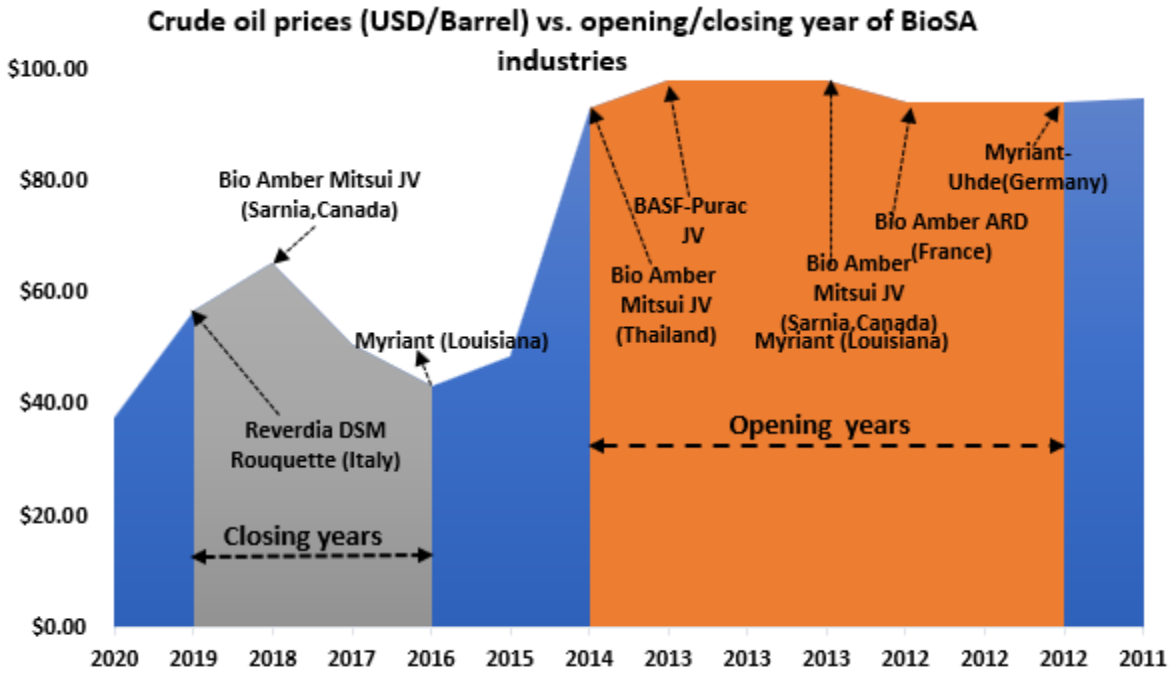

Figure 1. 2 Crude oil prices vs. opening and closing years for commercial scale BioSA producing industries

The BioSA industries mentioned used first-generation biomass like starch and sucrose sugar as a raw material. These substrates can be fermented easily and do not require costly pretreatment. Inspite of this they were not competitive when crude oil is cheap. In addition, the use of starch-based resources results in the food vs. fuel debate.

Lignocellulosic biomass can serve as a potential solution to end the debate, even they associated with some limitations and obstacles. The availability of lignocellulosic biomass is quite abundant from agricultural and industrial resources. The total potential generation of lignocellulosic biomass from cereal crops, plantation crops and oil seed crops are is 2900 million tons, 540 million tons

and 14 million tons, respectively [21]. The worldwide production of lignocellulosic biomass is 180 million tons annually. An estimate saw that 1.3 x 10^{10} metric tons/year of wood generated from terrestrial plants meets two-thirds of the world's energy requirement [22]. Agricultural residue like corn stover, sugar cane bagasse, and rice and wheat straws are very promising cellulosic feedstock that can be derived from plant residues. However, the recalcitrant nature of lignocellulosic biomass leads to higher capital and intensive labor costs. All lignocellulosic biomass is composed of three major units, i.e., cellulose, hemicellulose, and lignin. Agricultural lignocellulosic biomass generally comprises 10-25 % lignin, 20-30 % hemicellulose, and 40-50 % cellulose [23,24]. Utilization of all the components of lignocellulosic biomass, i.e., C-6 sugars derived from cellulose, C-5 sugars derived from hemicellulose, and lignin in an integrated biorefinery with a main product and several co-products reducing the overall processing cost can be the best solution. The potential for such multi-product biorefineries has been evaluated in this thesis.

For the production of SA from lignocellulosic biomass, several challenges must be considered to make it competitive with its counterpart. The challenges range from feedstock production to development of energy-efficient technologies for pretreatment, enzymatic hydrolysis and microbial fermentation, co-product development to environmental impact minimization and societal acceptance [25–28].

The concept of biorefinery is often associated with increased sustainability. However, this needs to be validated by developing a holistic sustainability assessment models which combines all aspects of sustainability, i.e., technical, economic, environmental and social impacts before lab scaled results are scaled up to industrial production. Again, strategic decisions are difficult to make as most often TEA is done in terms of money(dollar) value while environmental impacts are reported in terms of GHG emissions and number of other parameters [5]. In order to overcome this

hurdle, the monetization of the environmental impacts has been carried out in this thesis as pictorially shown in **Figure 1.3**.

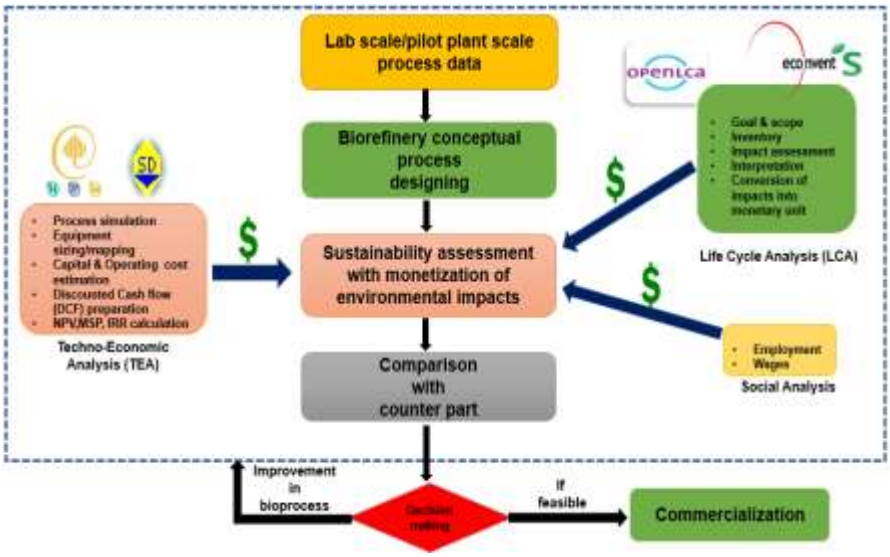

Figure 1. 3 Biorefinery sustainability assessment framework with the monetization of environmental impacts [5]

1.1 The rationale of the thesis

This thesis aims to demonstrate a novel holistic sustainability assessment of BioSA production from lignocellulosic biomass corn stover as a raw material input. A conceptual biorefinery design utilizing all three major components of lignocellulosic biomass for the production of BioSA and co-products was developed. It was decided to assess the technical, economic, social, and environmental performance of such processes. The rationale for carrying out this study are as follows:

i. Most lab-based bioprocesses related to BioSA indicate that environmental factors will make BioSA competitive with its conventional fossil-based counterpart. However, there is

a need to validate and quantify these environmental benefits associated with BioSA production.

ii. The sustainability assessment of BioSA production from first-generation feedstock like starch is widely studied and the process has already been commercialized. However, these assessments were limited to either TEA or LCA.

iii. The results of these assessments were presented in different units specific to their domains. The results of LCA studies, are presented in environmental impact categories in different units like kg CO_2 equivalent while the results of TEA studies are presented in the form of economic parameters such as minimum selling price (MSP), revenue, and profitability. These results need to be in a single score or in the same monetary units in order to make comparisons easier and allowing strategic decisions to be taken.

iv. The feasibility assessment of BioSA production from second-generation biomass is much needed by considering integrated multiproduct biorefinery, which utilizes all the major components of biomass.

v. Comparison with fossil-based SA production route is also essential as this will help make decisions regarding setting up such biorefineries.

vi. Beyond TEA and LCA, even after the latter is monetized, the experience and knowledge of experts in the field need to be taken into account before scale up and commercial implementation. Improvement in one domain's performance, i.e. economic criteria, can decrease the performance of another, i.e. the environmental domain, or vice versa. This is considered a trade-off or burden-shifting. Selection of a SA production route should be made by balancing multiple aspects, in this case. These are Multi-Criteria Decision

Analysis (MCDA) problems and is needed to facilitate decision-makers and in selection of recommended SA production route.

1.2 Objectives of the study

Based on the above rationale, the overall objective of this thesis is to perform a sustainability assessment in a single score or monetary unit for the technical, economic, and environmental aspects of BioSA production from lignocellulosic biomass (corn stover) in a multiproduct biorefinery design where all the major components of biomass (cellulose, hemicellulose, and lignin) are utilized.

The specific objectives of the thesis are as follows:

i. To perform TEA of BioSA production from corn stover based on three conceptually derived biorefinery design scenarios.
ii. To perform LCA followed by monetization of assessed environmental impacts for all three design scenarios and to perform a critical comparison with fossil-based SA production route.
iii. To develop a decision-making tool using Multi-Criteria Decision Analysis (MCDA) that facilitates decision-makers and stakeholders in the selection of production routes for platform chemicals like succinic acid by considering technical, economic, and environmental criteria.

The visual presentation of the objectives can be found in **Figure 1.4**.

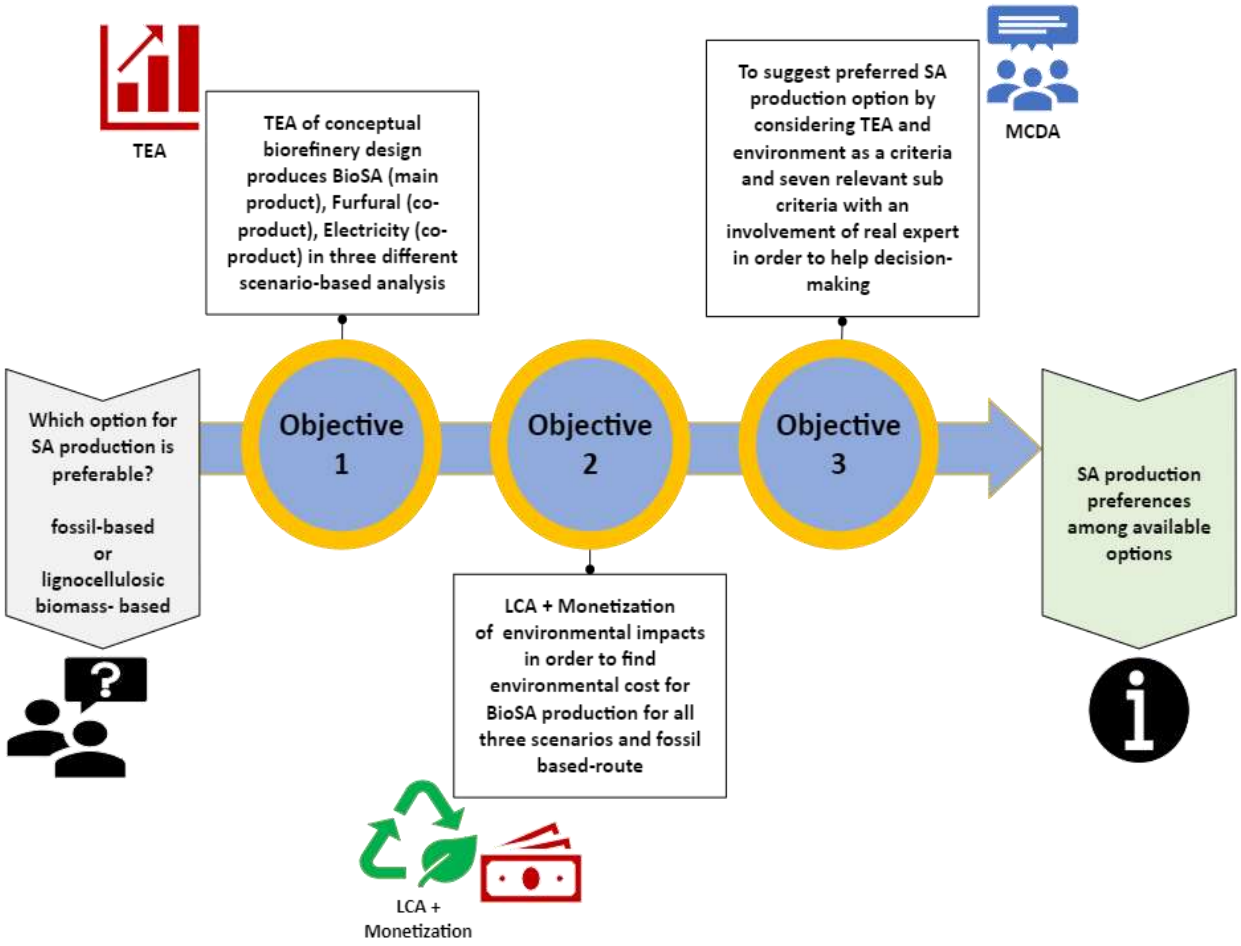

Figure 1. 4 Graphical representation of objectives for the thesis

1.3 References

[1] S. Fernando, S. Adhikari, C. Chandrapal, N. Murali, Biorefineries: current status, challenges, and future direction, Energy & Fuels. 20 (2006) 1727–1737.

[2] G.R. Timilsina, A. Shrestha, An overview of global markets and policies, The Impacts of Biofuels on the Economy, Environment, and Poverty. (2014) 1–14.

[3] J. Baffes, M.A. Kose, F. Ohnsorge, M. Stocker, The great plunge in oil prices: Causes, consequences, and policy responses, Consequences, and Policy Responses (June 2015). (2015).

[4] F.H. Reboredo, F.C. Lidon, J.C. Ramalho, M.F. Pessoa, The forgotten implications of low oil prices on biofuels, Biofuels, Bioproducts and Biorefining. 11 (2017) 625–632.

[5] N.M. Kosamia, M. Samavi, K. Piok, S.K. Rakshit, Perspectives for scale up of biorefineries using biochemical conversion pathways: Technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022). https://doi.org/10.1016/j.fuel.2022.124532.

[6] T. Werpy, G. Petersen, Top Value-Added Chemicals from Biomass Volume I, Us Nrel. (2004) Medium: ED; Size: 76 pp. pages. https://doi.org/10.2172/15008859.

[7] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic acid: Technology development and commercialization, Fermentation. 3 (2017). https://doi.org/10.3390/fermentation3020026.

[8] N.M. Kosamia, A. Sanchez, S.K. Rakshit, Scenario-based techno-economics and heat integration feasibility assessment of integrated multiproduct biorefineries with biosuccinic acid as the main product and various byproduct options, Biomass Convers Biorefin. (2022). https://doi.org/10.1007/s13399-022-02945-9.

[9] Y. Feng, H. Yin, A. Wang, T. Xie, T. Jiang, Selective hydrogenation of maleic anhydride to succinic anhydride catalyzed by metallic nickel catalysts, Appl Catal A Gen. 425 (2012) 205–212.

[10] J.J. Beauprez, M. de Mey, W.K. Soetaert, Microbial succinic acid production: natural versus metabolic engineered producers, Process Biochemistry. 45 (2010) 1103–1114.

[11] H. Song, S.Y. Lee, Production of succinic acid by bacterial fermentation, Enzyme Microb Technol. 39 (2006) 352–361.

[12] P.C. Lee, S. Lee, S.H. Hong, H.N. Chang, Batch and continuous cultures of Mannheimia succiniciproducens MBEL55E for the production of succinic acid from whey and corn steep liquor, Bioprocess Biosyst Eng. 26 (2003) 63–67.

[13] M. v Guettler, D. Rumler, M.K. Jain, Actinobacillus succinogenes sp. nov., a novel succinic-acid-producing strain from the bovine rumen, Int J Syst Evol Microbiol. 49 (1999) 207–216.

[14] S. Chan, S. Kanchanatawee, K. Jantama, Production of succinic acid from sucrose and sugarcane molasses by metabolically engineered Escherichia coli, Bioresour Technol. 103 (2012) 329–336.

[15] C. Chen, S. Ding, D. Wang, Z. Li, Q. Ye, Simultaneous saccharification and fermentation of cassava to succinic acid by Escherichia coli NZN111, Bioresour Technol. 163 (2014) 100–105.

[16] M. Jiang, Q. Wan, R. Liu, L. Liang, X. Chen, M. Wu, H. Zhang, K. Chen, J. Ma, P. Wei, Succinic acid production from corn stalk hydrolysate in an E. coli mutant generated by atmospheric and room-temperature plasmas and metabolic evolution strategies, J Ind Microbiol Biotechnol. 41 (2014) 115–123.

[17] B. Bai, J. Zhou, M. Yang, Y. Liu, X. Xu, J. Xing, Efficient production of succinic acid from macroalgae hydrolysate by metabolically engineered Escherichia coli, Bioresour Technol. 185 (2015) 56–61.

[18] G.N. Vemuri, M.A. Eiteman, E. Altman, Succinate production in dual-phase Escherichia coli fermentations depends on the time of transition from aerobic to anaerobic conditions, J Ind Microbiol Biotechnol. 28 (2002) 325–332.

[19] H. Lin, G.N. Bennett, K.-Y. San, Metabolic engineering of aerobic succinate production systems in Escherichia coli to improve process productivity and achieve the maximum theoretical succinate yield, Metab Eng. 7 (2005) 116–127.

[20] H. Lin, G.N. Bennett, K. San, Genetic reconstruction of the aerobic central metabolism in Escherichia coli for the absolute aerobic production of succinate, Biotechnol Bioeng. 89 (2005) 148–156.

[21] S. Rajaram, A. Varma, Production and characterization of xylanase from Bacillus thermo alkalophilus grown on agricultural wastes, Appl Microbiol Biotechnol. 34 (1990) 141–144.

[22] A.L. Demain, M. Newcomb, J.H.D. Wu, Cellulase, clostridia, and ethanol, Microbiology and Molecular Biology Reviews. 69 (2005) 124–154.

[23] R.C. Pettersen, The chemical composition of wood, The Chemistry of Solid Wood. 207 (1984) 57–126.

[24] J.R. Mielenz, Ethanol production from biomass: technology and commercialization status, Curr Opin Microbiol. 4 (2001) 324–329.

[25] S.K. Hoekman, Biofuels in the US–challenges and opportunities, Renew Energy. 34 (2009) 14–22.

[26] V. Menon, M. Rao, Trends in bioconversion of lignocellulose: biofuels, platform chemicals & biorefinery concept, Prog Energy Combust Sci. 38 (2012) 522–550.

[27] L. Luo, E. van der Voet, G. Huppes, Biorefining of lignocellulosic feedstock–Technical, economic and environmental considerations, Bioresour Technol. 101 (2010) 5023–5032.

[28] E. Ximenes, Y. Kim, N. Mosier, B. Dien, M. Ladisch, Inhibition of cellulases by phenols, Enzyme Microb Technol. 46 (2010) 170–176.

CHAPTER 2

LITERATURE REVIEW*

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2 Literature review

2.1 Succinic acid, application, and conventional production route

Succinic acid (SA) ($C_6H_6O_4$), also known as dicarboxylic acid, amber acid, or butanedioic acid, is a 4-carbon dicarboxylic acid and is one of the most studied platform chemicals. Due to the linear structure and presence of the bifunctional carboxyl group, SA has a high level of reactivity which in turn makes it an excellent precursor for the synthesis of butanediol, butyrolactone, tetrahydrofuran, fatty acids, linear aliphatic esters, and biodegradable polymers [1]. SA has application in food additives, detergents, cosmetics, pigments, toners, cement additives, soldering fluxes, and pharmaceutical intermediates. As an ion chelator it is also used to prevent corrosion and pitting in the metal industry. The food industry uses it as an acidulate, pH regulator, antimicrobial and flavoring agent. **Figure 2.1** shows the potential application of SA for manufacturing specialty chemicals, commodity chemicals, and additives. Conventionally SA is produced by catalytic hydrogenation of maleic anhydride into succinic anhydride followed by hydration of the latter to SA. The hydrogenation reaction for SA production occurs in the liquid phase at a temperature ranging from 120 to 180 °C and under the hydrogen pressure of 0.5 to 4.0 MPa and in the presence of Ni or Pd-based redox catalysts [2]. The current market price for the SA ranges from 2.5 to 3.00 USD/kg, However, this range fluctuates based on the price of maleic anhydride that is derived from crude oil [3].

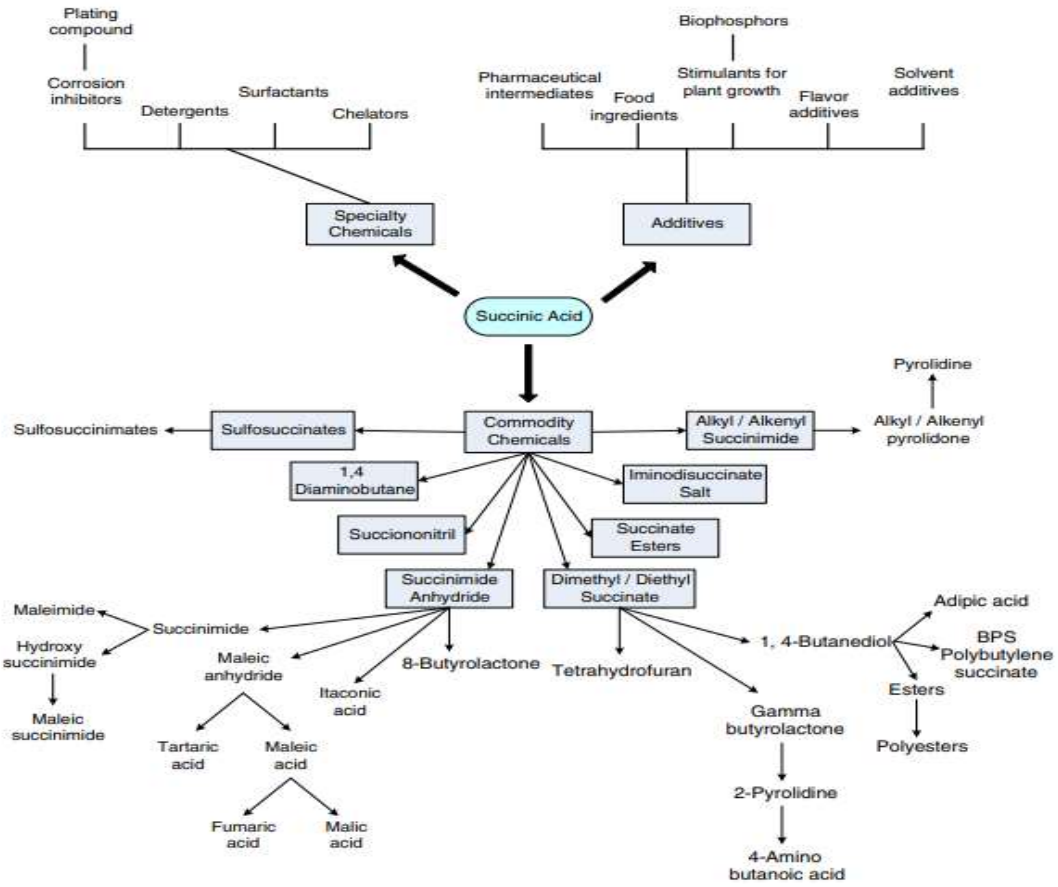

Figure 2. 1 Schematic representation of SA application to produce various products [4]

2.2 Biobased succinic acid and commercial scale industries

The fluctuating prices of crude oil due to geopolitical issues including embargos by oil producing countries, sanctions imposed on certain countries, etc. has resulted in the search for an alternative method for production of platform chemicals like SA from renewable feedstock. The production of SA by microorganisms is promising as it is a part of main metabolic pathway of aerobic respiration cells. This pathway is known as the Krebs or citric acid or tricarboxylic acid (TCA) cycle (**Figure 2.2**) which is a series of chemical reactions to release stored energy through the oxidation of acetyl-CoA derived from carbohydrates, fats, and proteins.

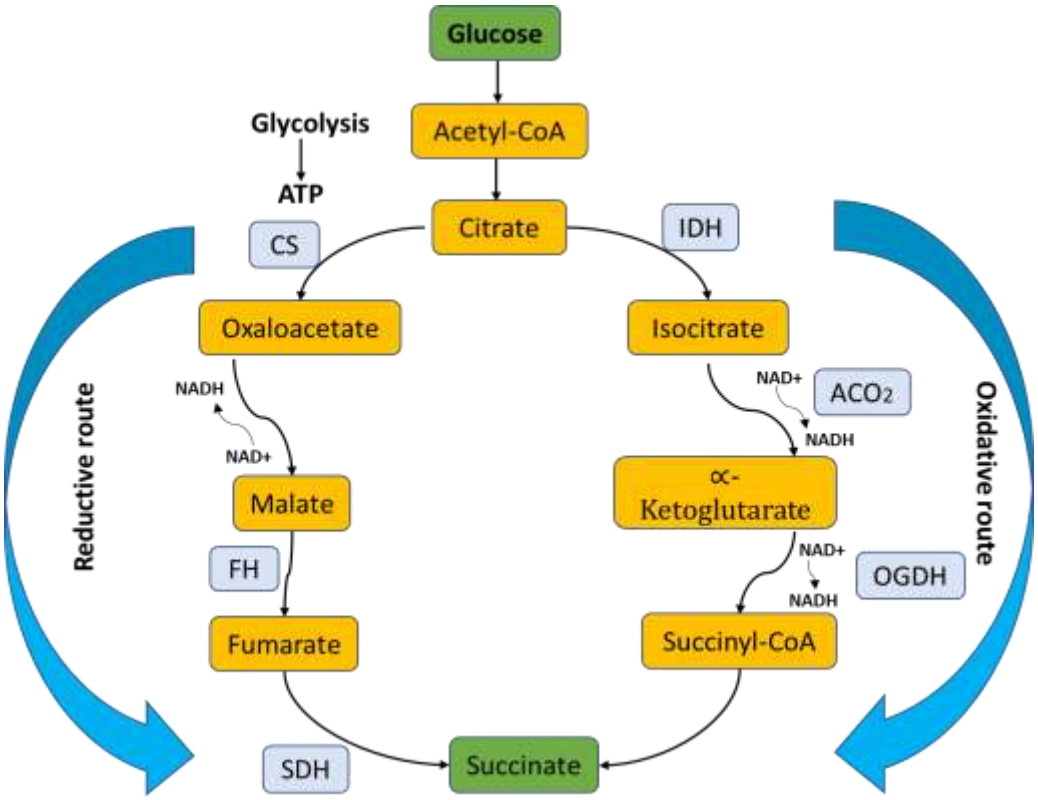

Figure 2. 2 TCA cycle and its oxidative and reductive route for BioSA production; adapted and redrawn from [5]

SA is a metabolite of the reductive route of the TCA cycle and can theoretically produce two molecules of SA from each molecule of C-6 sugar. In addition, an important advantage of this process is that it consumes carbon dioxide as a raw material. The stoichiometry for BioSA production from C-6 sugar can be presented below

$$7\ C_6H_{12}O_6 + 6\ CO_2 \rightarrow\ 12\ C_4H_6O_4 + 6\ H_2O$$

The theoretical molar yield of SA from C-6 sugar and carbon dioxide via the reductive route is 1.71 mole/mole of sugar [5]. This potential of BioSA using microorganism led to the setup of many commercial-scale BioSA production units worldwide from the first-generation feedstock like starch and sucrose sugar. For example, Bio Amber started commercial scale production in

Canada with an annual capacity of 34,000 tons from sorghum grit as a starting material. Myriant in the USA commissioned a BioSA production unit with an annual capacity of 13,600 tons using commodity sugars as a starting material. In 2012, Reverdia in Italy also started commercial-scale production of BioSA with an annual capacity of 10,000 tons using commodity sugars derived from first-generation feedstock [6]. The utilization of first-generation feedstock which serve as food for the production of biochemicals always results in food versus fuel debate. The desired alternative thus is the production of BioSA from second-generation feedstock like lignocellulosic biomass like woody and agricultural residues [4].

2.3 Constraints associated with the use of lignocellulosic biomass for the production of BioSA

The availability of lignocellulosic biomass worldwide is 180 million tons annually. It is estimated that 1.3 x 10^{10} metric tons/year of wood generated from terrestrial plants could meet two-thirds of the world's energy requirements [7]. Lignocellulosic biomass is also abundant from agricultural and industrial resources. It has been reported that cereal crops generate 2900 million tons, plantation crops 540 million tons, and oil seed crops 14 million tons of lignocellulosic biomass [8]. Corn stover, sugar cane bagasse, rice, and wheat straws are the most promising cellulosic feedstock derived from agricultural residues. However, the complex nature of lignocellulosic biomass and recalcitrant of cellulose leads to high capital and intensive labor costs. All lignocellulosic biomass is composed of three significant units, namely cellulose, hemicellulose, and lignin. In general, agricultural lignocellulosic biomass comprises 10-25 % lignin, 20-30 % hemicellulose, and 40-50 % cellulose [9,10].

The sugars present in lignocellulosic biomass are difficult to access due to the rigid structure of biomass and require pretreatment to separate the main components of the substrate followed by

hydrolysis to release the sugars from cellulose, and hemicellulose. During the pretreatment step, degradation products and impurities like acetate, format, furfural, 5-hydroxy methyl furfural, and soluble lignin products, are formed. These in many cases inhibit further processing of biomass [11]. In addition, the cost of the pretreatment needs to be low and environmentally friendly. Pretreatment processes can be divided into physical (milling and grinding), physicochemical (steam pretreatment, wet oxidation), chemical (alkali, dilute acid, oxidizing agent, and biological), or a combination of these [12].

The major bottlenecks in these processes include the development of an effective, low-cost pretreatment method, the cost of enzymes for the hydrolysis of cellulose, and the utilization of hemicellulose and lignin. Many pretreatment methods have been tried to make lignocellulosic sugars more accessible to enzymes. The varied nature and composition of the lignocellulosic biomass, and the complex interaction between the cellulosic fibers and lignin, which helps the tree or plant to withstand differences in temperature and environments, make their pretreatment difficult. **Table 2.1** indicates a list of pretreatment methods tried and the advantages and disadvantages associated with each method. Most of the pretreatment methods reported are either not effective enough or too costly to implement in large-scale industrial process. An example is the use of ionic liquids which are very effective as they are able to solubilize cellulose making it easy to separate cellulose from lignin. However, these solvents are very costly. The cost of the solvents is certainly too high for the usage on an industrial scale, even after it is recycled [25].

The degree of separation of the three components depends on the type of biomass used. The cellulose and hemicellulose streams after pretreatment often contain impurities that eventually results in a decrease in enzymatic hydrolysis. In many severe treatment processes, the production of cyclic and other compounds limits product yields. In addition, the production cost of bio-based

chemicals and fuels from lignocellulosic biomass is still less economically attractive than its counterpart petroleum route on an energy equivalent basis due to more energy consumption in pretreatment steps [26]. Thus, selecting an appropriate pretreatment is one of the key decisions to make for successful commercialization of bioprocess.

Table 2. 1 Advantages, disadvantages, and critical comments on different pretreatment methods for lignocellulosic biomass

Type of pretreatment	Key advantages	Hurdles associated with processes	Critical comment	Ref
Milling	Handling of biomass becomes easy due to particle size reduction of biomass, and the crystallinity of biomass is also drastically reduced.	Higher energy consumption due to intensive energy requirement for size reduction of biomass. Insufficient separation of components is the major drawback of this method.	This process is applied to a wide range of biomass, generation of toxic by-products are low; however, improvement in the energy efficiency of this process is still required.	[13]
Dilute acid	Lower enzymes are needed for hydrolysis, the presence of acid	Most commonly used pretreatment, however, the formation of inhibitors i.e., 5-HMF,	Lower solid recovery is still a challenging issue with this	[14–16]

	itself hydrolyses biomass and converts it into fermentable sugar during the pretreatment step.	phenolic acid, and aldehydes, make it less attractive. The usage of acids during the pretreatment requires specific materials for building a reactor that can sustain corrosive conditions. Excessive washing of biomass after pretreatment demands a higher amount of water.	pretreatment method, recycling of used acidic solution is still under exploration for the economic viability of this process.	
Mild alkali	Lower sugar degradation than acid treatment, performed at ambient temperature and pressure.	Higher downstream processing cost because of the excessive amount of water usage for the removal of salt from biomass after the pretreatment process. In addition, long residence time and the formation of irrecoverable salt are also the main constraints associated with this process.	The method is effective for lignin removal and partial hemicellulose solubilization.	[16–18]
Ozonolysis	Efficient for lignin removal with minimal degradation of	The effectiveness of pretreatment depends on the moisture content of biomass, higher	Higher costs of ozone generation and effective handling of ozone	[18]

	hemicellulose and cellulose.	moisture content hampers the oxidation of lignin, and a higher amount of ozone requirement makes this process expensive.	are the critical aspects associated with this method.	
Organosolv	Efficient lignin extraction, presence of lesser lignin substrate as a result of efficient enzymatic hydrolysis.	Utilization of organic solvents, which are highly flammable, removal of solvents after pretreatment demands evaporation and condensation, which makes this process more complex.	Solvent recycling is the most important aspect of the economic viability of this process.	[19]
Ionic liquid	Mild reaction condition is the prime advantage, higher fractionation efficiency of lignin and hemicellulose.	Challenges associated with higher cost, difficulty in recycling and reuse, and formation of inhibitors.	Ionic liquid pretreatment is considered environmentally friendly, however, the costs details of processing lignocellulosic biomass with ionic liquids are still under investigation.	[18]

Steam explosion	Limited usage of chemicals, no recycling cost, and environment friendly.	The formation of inhibitors due to high temperature and pressure reaction conditions are the prime disadvantages associated with this process.	Issues related to fermentation inhibitor formation and incomplete digestion of lignin-carbohydrate metrix are being studied, however, the addition of catalysts such as H_2SO_4 effectively enhances the efficiency of the process.	[20,21]
Liquid hot water	Effective removal of soluble lignin and hemicellulose.	Insoluble lignin remains in high quantities, and the removal of a large amount of water in the downstream process results in higher energy-intensive downstream processes.	As no chemical catalysts are used, this method is considered a green technique for biomass valorization. However, the presence of lignin can have issues in subsequent sugar processing	[22]
Wet oxidation	More suitable for biomass with	Due to the high cost of hydrogen peroxide and the combustible nature	Applicability of this method is limited to higher lignin	[20]

	higher lignin content.	of oxygen, the two main reactants of this process make this process infeasible for commercialization.	content biomass only, more studies are required for a wider range of biomass and subsequent processing effects.	
Ammonia Fiber Explosion (AFEX)	Effective for the herbaceous plant, agricultural residue, higher efficiency, and selectivity with lignin.	The effectiveness of the pretreatment process depends on the lignin content of biomass, which is not favorable for higher lignin content biomass, higher process cost, and environmental issue due to ammonia.	Apart from the effectiveness of this method, the application of AFEX is not reported beyond the lab scale due to environmental concerns with ammonia.	[18,22]
Oxidative pretreatment	Effective for the removal of lignin and hemicellulose, the presence of hydrogen peroxide forms hydroxyl radicals which degrade the lignin.	Adverse impact on hemicellulose fraction of biomass and makes it inaccessible for fermentation makes it not a preferable option	Significant damage to the hemicellulose fraction restricts its applicability on a commercial scale.	[23]
Biological pretreatment	Efficient, environmentally safe, low-energy consumption.	The slow hydrolysis rate of lignocellulosic biomass makes it less favorable for	The slower rate and requirement of a large amount of space are the	[24]

commercial-scale biorefinery application, the poor performance of naturally produced enzymes, i.e., specificity for a fixed temperature, pH, and substrate, demands higher amounts of enzymes which creates an extra burden on bioprocess economy.	limiting factor for the commercial application of this method.

Other challenges that must be considered to make the bioconversion competitive with its chemical counterpart, are enzymatic hydrolysis microbial fermentation, co-product development, and societal acceptance [27–29].

The cost of enzymes for the breakdown of cellulose to glucose is a key constraint in the use of lignocellulosic residues for bioproducts. This is because the production of cellulase enzyme uses an insoluble substrate as inducer, long fermentation times of fungal enzyme producers, low yields and conversion rates [6]. In a chapter in the "**Handbook of Biorefinery Research and Technology**" by **Springer (Edited by: Virendra Bisariya, in press,** https://doi.org/10.1007/978-94-007-6724-9) we highlighted the types and properties of cellulase enzyme required for biorefineries. In addition, we reviewed the required process strategies, constraints associated with scaling up the cellulase enzyme production and its feasibility from Techno-Economic Assessment (TEA) and Life Cycle Assessment (LCA) point of view.

2.4 BioSA producing microorganisms and downstream processing

Fermentation can be carried out with both C-6 and C-5 sugars which often leads to low yields for fermentative products like ethanol. However, many organisms can produce BioSA from both types of sugars. Various researchers studied the synthesis of succinic acid production from lignocellulosic biomass as shown in **Table 2.2**.

Table 2. 2 Various studies for BioSA production by using various lignocellulosic biomass

Sr.no	Feedstock	Microbes	Succinic acid yield (g/g)	Concentration (g/l)	Ref
1	Corn fiber hydrolysate	*A. succinogenes*	0.96	70.3	[30]
2	Corn Stover	*A. succinogenes*	0.73	56.4	[31]
3	Cane molasses	*A. succinogenes*	0.81	55.2	[32]
4	Wood hydrolysate	*A. succinogenes*	0.88	24.0	[33]
5	Rapeseed	*A. succinogenes*	0.12	23.4	[34]
6	Orange peel	*F. succinogenes*	0.044	1.75	[35]
7	Softwood	*E. coli*	0.72	42.2	[36]
8	Wheat straw	*F. succinogenes*	0.05	1.55	[35]
9	Whey	*M. succiniciproducens*	0.71	13.4	[37]
10	Wood hydrolysate	*M. succiniciproducens*	0.56	11.7	[38]

Sr.no	Feedstock	Microbes	Succinic acid yield (g/g)	Concentration (g/l)	Ref
11	whey	*A. succinogenes*	0.91	34.7	[39]

Various microorganisms have been screened for the BioSA production. This includes bacteria such as *A. succiniciproducens, A. succinogenes, M. succiniciproducens, E. coli, Corynebacterium glutamicum* and fungi such as *S. cerevisiae, Yarrowia lipolytica.* Most SA-producing microorganisms produce SA as the primary fermentation product. Natural producers of SA isolated from a rumen fluid which requires control of pH for a fast and efficient fermentation. *A. succiniciproducens* was one of the first gram-negative bacteria isolated from the bovine rumen and identified as a SA producer. Fermentation with this strict anaerobe reached titers of 50 g/l SA [39,40]. *M. succiniciproducens* was isolated from the rumen of a Korean cow and referred to as a mixed acid producer as it produces formic and acetic acid along with BioSA. The most important feature of this microorganism is it can effectively produce BioSA from substrates like glycerol, xylose, sucrose, fructose, and maltose. However, it is not able to convert sorbitol, xylan, or cellulose to SA. In nitrogen or yeast-containing medium, this microorganism showed a high succinate production rate [41]. Among all available options*, A. succinogenes* is known as the best organism for BioSA production. The most promising characteristic of *A. succinogenes* is that it can convert C-6 and C-5 sugar into BioSA. In addition, higher production capability, robustness, and low aeration requirement makes it the most promising strain. The highest BioSA concentration of 105.8 g/l was recorded for *A. succinogenes* when corn steep liquor and yeast extract were used [42]. Using *Basfia succiniciproducens*, successful production of BioSA was achieved in continuous mode, and crude glycerol was derived from biodiesel as a substrate [43]. *E. coli* can grow in high cell densities in defined mineral media without losing BioSA production capabilities.

In addition, due to the robustness of this strain, there is less need for complex nutrients, which makes the downstream process easier. On the contrary, its performance is hampered in the presence of acetate, the most common inhibitor in the cellulosic mixed sugar stream. Thus, it is not the best choice for the lignocellulosic biomass substrates. In addition, in the presence of various sugars, *E. coli* prefers glucose, which is considered a limitation. *Corynebacterium glutamicum* is a fast-growing gram-positive bacterium capable of producing SA, acetic acid, and lactic acid using a broad range of carbon sources. Under the fed-batch condition, it can grow aerobically and anaerobically, in addition with an engineered strain of this bacterium, high SA titer has been reached up to 23.0 g/l [44].

One of the prime limitations of BioSA-producing microorganisms is that it requires neutral pH conditions (not too acidic or basic) for the best conversion of sugars to SA during fermentation reaction. To overcome such issues, slightly low pH tolerance hosts such as *Yarrowia lipolytica* and *S. cerevisiae* developed. One advantage associated with *S. cerevisiae* is that it is an industrial strain that also tolerates higher substrate concentration, thrive under slightly acidic conditions and capable to produce SA aerobically and anaerobically.

The recovery of BioSA from the fermentation broth is challenging, complex, and expensive. Acetic acid and formic acid are the two most common impurities generated during the fermentation process. However, the impurities can depend on the type of microorganism used, type of feedstock used, type of nutrients used during the fermentation stage etc. [5].

The downstream purification operation alone accounts for more than 60 % of the total production cost [5]. Hence, selecting an optimum purification process is an essential consideration while designing the process. In addition, observed purity of succinic acid was much lower due to the inefficiency of removal of acetic acid by this end process in their electrodialysis studies. The higher

cost of membranes limits their application on a commercial scale. Succinic acid also precipitates in the form of calcium succinate by adding calcium hydroxide to the broth. The filtration of calcium succinate, followed by the addition of sulfuric acid, facilitates higher recovery of succinic (nearly 95 %). The generation of gypsum limits the application of this technology [45]. Reactive distillation followed by vacuum distillation and crystallization also shows promising results with almost 73% succinic acid recovery with 99.8 % purity [46,47]. Reactive extraction followed by crystallization and drying is considered the most effective method for the BioSA separation and purification from the fermentation broth from a process economic point of view as the recyclability of extraction solvents are more than 98% [48].

2.5 Sustainability assessment of biorefining processes and inclusion of monetary cost of environmental effects

Several publications analyzed the early stage technical and economical sustainability [49-51], environmental sustainability [52-54], and social sustainability [55] of biofuels and biochemicals production from biomass. Some of these studies included two domains (economic and environmental) of sustainability [56-58]. In addition, frameworks for the overall sustainability evaluation were also developed for specific regions, which target three domains (economical, environmental, social) together using sustainability matrixes and Multicriteria Decision Analysis (MCDA) [59,60]. Multi-criteria decision making also enables the conglomeration of main aspects named economic, environmental, and social sustainability from the stakeholder's point of view [61,62]. Various methods of MCDA i.e., multi attributional utility theory (MAUT), analytical hierarchy process (AHP), elimination and choice expressing the reality (ELECTRE), preference ranking organization method for enrichment of evolutions (PROMETHEE), dominance-based rough set approach (DRSA) are used for to manage the mixed data from the different sustainability

criteria and spheres [61]. The MCDA also facilitates the sustainability assessment from the stakeholder's perspective. However, the existing multi-criteria decision analysis methods are considered steady-state methods and are unable to provide future trends or projections [62]. In addition, very few attempts have been made in the direction of monetization of impacts for getting a single score (monetary units) value for economic and environmental domains to identify and overcome the prevailing obstacles in the development of biochemical production processes [63]. In this section, different approaches for the sustainability assessment of biofuels and biochemical production from biomass will be highlighted. The premise of our discussion is that biorefining processes will become competitive.

2.5.1 Techno-Economic Analysis (TEA) as a tool for assessing the economic sustainability of bioprocesses

TEA enables decision-makers to access the data related to technical and economic domains for the intended bioprocess. It includes process design, simulation, capital and operating cost calculation, and equipment installation cost for scaled commercial biorefinery [64]. The analysis starts with preparing a conceptual process flow of biorefinery which contains information related to unit processes and unit operations involved during the bioconversion. Process simulation tools, including Aspen plus and SuperPro designer, backed by empirical equations, are used to solve mass and energy balance, which is subsequently used for calculating equipment sizes and utilities for the bioprocess [65–67]. Quantification of capital and operating cost is done by considering various parameters. These include material of construction (MOC) of equipment, raw material cost, utility cost, operational time, product yield, project life, etc. [68]. In addition, the preparation of discounted cash flow (DCF) facilitates other important detailed processes economic related data. These data include project revenue, taxes, IRR, NPV, payback period, and minimum selling price

[69]. In order to address uncertainties, Monte Carlo simulation is often used in TEA analysis of biorefineries [70,71]. TEA also facilitates some social sustainability parameters related to employment, like job creation and wages [68]. Some recent studies on TEA for biorefining products are given in **Table 2.3**. The results of TEA studies are presented in the form of economic parameters such as MSP, revenue, and profitability. These are expressed in terms of a dollar value.

Table 2. 3 List of TEA studies on biorefining products

Bioproduct Name	Sustainability assessment tool	Remarks	Ref
Bioethanol	TEA	This study entails the TEA study for bioethanol production from different lignocellulosic biomass i.e., sugar cane bagasse, coffee cut-stems, rice husk, and empty fruit brunches. The results of the study are presented in terms of production cost per liter of bioethanol. The separation and dehydration stages were identified as the second highest energy-consuming stage after the detoxification and sugar concentration stage. Results show considerable savings in production costs when the ethanol production process is coupled with a cogeneration system.	[72]
Lactic acid	TEA	TEA study for the production of lactic acid from corn stover was performed by using Aspen plus as simulation software. The minimum selling price (MSP) of 0.523 USD/kg was evaluated for lignocellulosic biomass-based lactic acid. Feedstock, enzyme, and non-enzyme conversion contribution in minimum selling price calculated at 0.23 USD/kg	[73]

Bioproduct Name	Sustainability assessment tool	Remarks	Ref
1,3-Propanediol	TEA	product, 0.130 USD/kg product, and 0.192 USD/kg product, respectively. Economic feasibility was assessed by choosing crude glycerol as a feedstock and *Clostridium diolis* DSM 15410 as a microorganism. The effect of the selling price on purchase cost and through output was also studied. The study presented that 45% of operating costs corresponded to utilities. Downstream operations like distillation and evaporation had a major contribution to the higher utility consumption.	[74]
Succinic acid	TEA	This study assesses the techno economics of BioSA production from sugarcane bagasse hemicellulose hydrolysate. The production cost of 2.32 USD/kg was calculated. Downstream processing, which contains adsorption, evaporation, centrifuge, crystallization, and dryer units, contributes 17 % of the total investment.	[75]
Xylitol	TEA	Production of xylitol from lignocellulosic sugarcane biomass performs along with electricity as a co-product. The minimum selling price (MSP) of 3000 USD/tonne was calculated by performing TEA analysis, and Aspen Plus was used for the calculation of mass and energy balance. In the downstream operation, the evaporation step accounted for 55.4 % of the total steam requirement. Crystallization and	[76]

Bioproduct Name	Sustainability assessment tool	Remarks	Ref
		drying in downstream operations also accounted for 79% of the total electricity requirement.	
Microbial Oil	TEA	Microbial oil production in the presence of oleaginous yeast from wheat straw and distillery waste was studied. The minimum selling price of 14 €/kg was evaluated for microbial oil at a plant capacity of 100 t/year.	[77]
PHB	TEA	This TEA study calculates the production feasibility of PHB from sugarcane bagasse along with electricity as a co-product. Minimum selling price (MSP) 2.06 USD/kg evaluated. 15 % contribution calculated for PHB fermentation and downstream processing section in total installed equipment cost.	[49]

For example, 0.49 USD/L and 0.58 USD/L production costs were assessed for ethanol in standalone and combined with cogeneration plant configurations [72]. The contribution of enzyme cost (0.724 USD/kg lactic acid) in the minimum selling price of lactic acid was identified as the area of concern for lactic acid production from corn stover [73]. Production of succinic acid from sugarcane bagasse also shows a higher probability (84.6%) of getting an internal rate of return (IRR) of more than 12% [75]. A total capital investment (TCI) of 320.2 USD was calculated for PHB production from sugarcane bagasse [49]. It is important to carry out TEA and monetization of environmental contributions after successful laboratory-scale experiments and before scaling up to industrial-level processes.

2.5.2 Life Cycle Assessment (LCA) as a tool for assessing environmental sustainability and social sustainability of bioprocesses

LCA is a standard methodology for the assessment of environmental sustainability. This is done in four stages, starting from the definition of goal and scope, followed by life cycle inventory analysis, impact assessment, and finally, the interpretation stage. The first stage examines the input and output of material within the specified system boundaries for a studied functional unit. Compilation and quantification of input and output for a product system are done in the inventory analysis stage. In the impact assessment stage, process inventories are converted into environmental impacts [78]. Environmental impacts can be evaluated up to the midpoint or endpoint. The midpoint impacts are problem-oriented and include global warming, fossil fuel depletion, human toxicity, acidification, and eutrophication, whereas the endpoint impacts include damage-oriented like human health, ecosystem quality, etc. Different methods like CML 2002, Eco indicator, ReCiPe, LIME, Lucas, and TRACI are often used for the impact assessment [79,80]. LCA can be costly and time-consuming, depending on the boundary conditions set for the study. This can be from the cradle to the grave (biomass extraction to end of life and waste handling, including manufacturing and use stage), cradle to gate (excluding use stage and waste handling), or gate to gate (involve only manufacturing stage only) [81]. Employment, education and training, knowledge management, and innovation potential can also be incorporated into LCA to evaluate the social sustainability of bioprocess [82,83]. A list of some LCA studies on biorefinery products is given in **Table 2.4**.

Table 2. 4 List of LCA studies on biorefining products

Bioproduct name	Sustainability assessment tool	Remarks	Ref
Bioethanol	LCA	This study contains LCA of bioethanol production from vetiver (perennial grass) leaves and compares the environmental impacts with conventional fossil counterparts. The results of the study are represented in terms of greenhouse gas emission (CO_2 eq).	[84]
Lactic acid	LCA	The study illustrates the production of lactic acid from sugarcane bagasse and its environmental impacts. The results of the study are global warming potential, human toxicity potential, ionizing radiation potential, ecotoxicity potential and acidification potential.	[85]
1,3-Propanediol	LCA	Environmental impacts comparison between fossil-based 1, 3-propanediol and biobased 1, 3-Propanediol carried out. NO_X emission, nonrenewable energy, and CO_2 emission are compared with its counterpart.	[86]
Succinic acid	LCA	Environmental impacts of biobased succinic acid and fossil-based succinic acid compared. Environmental indicators, i.e., global warming potential assessed.	[54]
Xylitol	LCA	Environmental impacts were evaluated for the production of xylitol by using corn cob. Study results	[87]

Bioproduct name	Sustainability assessment tool	Remarks	Ref
		highlighted environmental sustainability in terms of climate change, fossil fuel depletion, ozone layer depletion, ecotoxicity, eutrophication and photochemical oxidation.	
Microbial Oil	LCA	Environmental indicators like eutrophication, greenhouse gas emission, and acidification potential were evaluated.	[88]
PHA	LCA	Life cycle assessment for PHA production from rapeseed oil studied. Endpoint analysis of environmental impacts like human health, ecosystems, and natural resources damage evaluated using impact assessment method ReCiPe.	[89]
PHB	LCA	A life cycle assessment was performed to integrate co-product manufacturing in the African sugar industry. The studied environmental impacts are abiotic depletion, global warming, human toxicity, terrestrial ecotoxicity, acidification, eutrophication, and ozone layer depletion. Multicriteria decision analysis (MCDA) for an optimum choice of co-product has also been performed.	[90]

The results of LCA studies are presented in different environmental impact categories in different units like kg CO_2 equivalent, which does not represent dollar value. This makes it difficult to quantify and compare different processes. For example, the impact on climate change by the production of ethanol and furfural from vetiver leaves was calculated to be -0.003 kg CO_2 equivalent [84]. Replacing one ton of fossil-based lactic acid production with bio-based lactic acid means potential savings of 3925.65 kg CO_2 equivalent, 1296.16 kg 1,4-DB equivalent., 397.79 kBq U_{235} equivalent obtained in global warming, human toxicity, and ionizing radiation [85]. In addition, environmental impact assessment results of PHA production are reported by 17 impact categories with different units like DALY and species * yr [89]. Furthermore, the global warming potential of 4.2 kg CO_2 equivalent was reported for PHB production from sugarcane bagasse [90]. Such studies will be crucial for moving to a bio-based economy and proving that it would be monetarily beneficial.

2.5.3 Monetization of environmental impacts as a need for sustainability assessment of bioprocesses

For successful commercialization of bioproducts, it is essential that the bioproduct must be sustainable in all domains, i.e., economic, environmental, and social. However, it is challenging to make a balance between these parameters. Improvement in one domain's performance, like economic criteria, can decrease the performance of another, like the environmental domain, or vice versa. This is considered a trade-off or burden shifting (from one domain to another). Implementing TEA and LCA individually does not help identify tradeoffs, as the final results are more specific and in different units [91]. It is very important to combine the results from TEA and LCA to address such tradeoffs [92,93]. However, the results from both domains are in different units. TEA results are in a monetary unit, whereas LCA results are not in monetary units. Life

cycle impact assessment (LCIA) results are presented using different indicators with different units. Most of the reported work in these areas employs one of the approaches, either technical-economical or environmental assessment only. Available information from these approaches is limited and needs to be studied critically. In addition, calculations related to mass, energy balance, and cost calculation depend on initial lab-scale experimental results, the selection of process model in simulation software, and their reliability on a commercial scale, the accuracy of raw material prices, equipment prices, the assumption made for equipment's material of construction (MOC) and consideration of appropriate margins for uncertainty analysis [94]. Furthermore, the assumption of "conceptualized nth plant" is often made to make the analysis possible, which does not reflect the pioneering process plant. Instead, it is assumed that the technology has a mature future in commercialization [95–98]. Thus, a holistic framework for biorefinery sustainability assessment involving TEA and LCA is necessary.

It has been observed that many biorefining processes are not found to be economically feasible compared to the well-established fossil fuel industry. Research publications often conclude by mentioning that biorefining products can become economically feasible if the environmental benefits are considered. Hence, it is necessary to convert the LCA results to a monetary (dollar) valuation and combine it with the economic costs. For example, the volume of carbon dioxide emissions and accumulation of whole processes can be evaluated in dollar terms by factors that are available in equivalent terms. For example, in Canada, the Social Cost of Carbon (SCC) is estimated to be 50 USD per tCO_2 and is expected to increase with time [99].

A clear comparison of the two routes (biorefining to fossil resources) can then be used to determine feasibility. Pizzol et al. [100] studied monetary valuation approaches and suggested a budget constraint method that is related to human well-being as the best approach for LCA impacts

monetization. Some studies also suggested a step-by-step method for calculating the monetary values of greenhouse gases in three LCIA methods like LIME, ReCiPe, and EPS [101]. Other literature studies also proposed a sustainability assessment framework in which indicators for economic, environmental, and social domains are calculated and converted into the monetary unit by using the dimensional function or scaling factor for a specific region [102].

In present work, we proposed a new approach (**as shown in Figure 1.3 - Chapter 1**) which combines all the domains of sustainability with the monetization of environmental impacts to be considered before lab scaled results are scaled up to industrial production.

2.6 Integrated lignocellulosic biorefining and determination of profitable scenarios

The previous sections stressed the need for monetization of environmental effects along with TEA analysis to determine process feasibility.

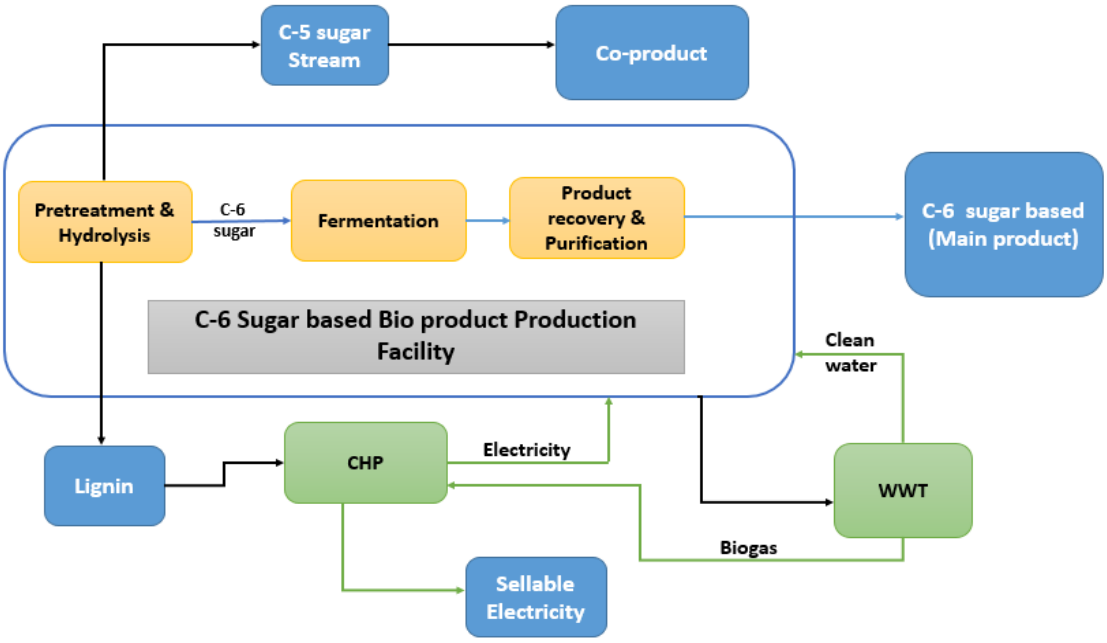

Figure 2. 3 Integrated biorefinery for utilizing all three main components of lignocellulosic biomass [6]

However, the economics of biorefineries that utilizes lignocellulosic residue as substrates are seldom going to be better than fossil resources routes if only one component of biomass is utilized. In order to be competitive, all three components of lignocellulosic residues need to be used in a single plant. The flow diagram of an integrated BioSA plant is given below in **Figure. 2.3**.

In the case of such a refinery, the potential products that can be obtained along with the main C-6 sugar-based products will involve using the C-5 sugars of hemicellulose and the lignin stream simultaneously. Some suggestions for such products are given in **Table 2.5**.

Table 2. 5 List of potential co-products from C-5 and lignin stream

Sr. no.	Stream name	Potential co-product	Remarks	Ref
1	C-5 Stream	PHA	Production of this compostable biopolymer on an industrial scale is still expensive, but production from hemicellulose hydrolysate seems an attractive option.	[103–105]
2	C-5 Stream	Acetic acid	Myriad of applications in chemical, food, and medical industries. Microorganism i.e., *Moorella thermoacetica* and *Clostridium thermoaceticum* converts monosaccharaides to acetic acid in anaerobic conditions.	[106–108]
3	C-5 Stream	Furfural	Chemo catalytic conversion from C-5 sugar is a promising option.	[109]
4	C-5 Stream	Xylitol	Conversion of C-5 sugar to Xylitol via a catalytic route or biological route is a promising option.	[110]

5	C-5 Stream	Lactic acid	Hetero fermentative lactic acid bacteria (LAB) show tremendous potential for the production of lactic acid from hemicellulose hydrolysate from various lignocellulosic biomass. Biopolymers, i.e., Polylactic acid derived from lactic acid, is an appealing alternative to petroleum-based plastics.	[111–114]
6	Lignin	As a fuel for the CHP (Combined Heat and Power generation)	Possibility for integration in the same bioprocessing facility. A good revenue generation source by selling excess electricity.	[115]
7	Lignin	Vanillin production	Potential to compete for counterpart petroleum route by value addition of lignin stream.	[116,117]

The choice of such products will depend on the type and species of lignocellulosic biomass used. The combined TEA and LCA monetized values for each set of products or "scenarios" need to be studied in detail before a decision to scale up the process for potential use as an industrial product is planned. This could also guide biorefining research direction as scenarios that do not result in sufficient profit over fossil fuel routes should not be pursued. The utilization of all three components of biomass in one industry also saves the cost of transportation or disposal of the components not used in the premises. For example, the utilization of lignin in paper mills as a source of heat energy not only brings down the cost of disposal but also brings down the energy bills of many such industries [6].

2.7 Multi-criteria Decision Analysis (MCDA) of biochemicals productions

Multicriteria Decision Analysis (MCDA) methods have become a popular and helpful tool for decision making used by stakeholders and policymakers when the problems are complex and demand consideration of multiple aspect [118]. MCDA methods have been widely applied to social, economic, environmental, and industrial systems in addition to biofuel and bioenergy production from biomass [119-123]. The MCDA problem is structured in a hierarchical model starting with goal, criteria, sub-criteria, and alternatives. Once the model is formed by selecting relevant criteria, sub-criteria, and alternatives, the weights of individual criteria, sub-criteria, and alternatives are determined to show their relative importance [118]. Usually, in bioenergy and biofuel production from renewable sources, technical, economic, social, and environmental aspects are considered [124-127]. In earlier published works, process efficiency, safety, process maturity, and waste generation are considered as sub-criteria for the technical aspect [127-129]. Investment costs, payback period, Net Present Value (NPV), service life, and operational and maintenance cost are considered as a sub-criteria to address the economic aspect [129-133]. For the environmental aspect NO_x emission, CO_2 emission, land use, and particle emission are considered as a sub-criteria by earlier published articles [124,126,128,133]. Social acceptability, job creation, and social benefits are reported as sub-criteria for the social aspects [129]. There are several methods, such as TOPSIS, VIKOR, ANP, MAUT, AHP, ELECTRE, and PROMETHEE used to solve MCDA problems in different areas. However, each method has its advantages and disadvantages [134]. In addition, the most challenging issue with all these methods is that they do not involve the opinions of actual experts from the relevant areas. Earlier, HFAHP was used by Acar et al. [135] to identify the most suitable option for hydrogen production by considering a total of five criteria (economic performance, environmental performance, social performance, technical

performance, and availability) and 17 sub-criteria. In the present work, two criteria (techno-economic and environment) and seven sub-criteria were considered to identify the best succinic acid production route among four available alternatives (three from corn stover and one from a fossil-based route). Colak and Kaya [136], used HFAHP for the selection of energy storage technologies for Turkey among nine available alternatives by considering technical, economic, environmental and socio-political as a main criteria. Candan and Toklu [137], investigated most preferred location for solar power plant in Turkey using HFAHP. This work considered energy cost, safety, solar energy potential, and logistics facilities as a main criteria for the analysis. Kheybari et al. [138] reported preferred energy production technology from biomass for Iran by choosing technical, economic, environmental and social criteria. In this analysis as a sub criteria technology reliability, cleaning system, biomass availability, skilled personal, flexibility, incentives and subsidies, waste, required floor space, social acceptability were considered. There are very few attempts have been made to use HFAHP for an area like biofuel and biochemical production from lignocellulosic biomass. Thus, in this thesis, Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) is used as an MCDA method that considers the opinions of the real experts for the evaluation of weights of criteria, sub-criteria, and alternatives for a preferred succinic acid production route selection.

2.8 Reported works on BioSA production's sustainability assessment

Many research papers have studied the sustainability of BioSA production by performing TEA and LCA. The cluster networks (**Figure 2.4 and Figure 2.5**) shown below reviews the important papers in the area of BioSA sustainability assessment in TEA and LCA respectively. For building these literature review networks key words such as Succinic acid, Techno-Economic Analysis, Life Cycle Assessment used in the Connected papers software -https://www.connectedpapers.com.

The bunching of some articles published between 2010 to 2022 indicate most relevant works (dark blue nodes) and derivative works (light blue nods) which are slightly away from the context of the present thesis. The size of the node represents the impact of an article. Bigger node size represents high impact and smaller node size represents less impact of an article.

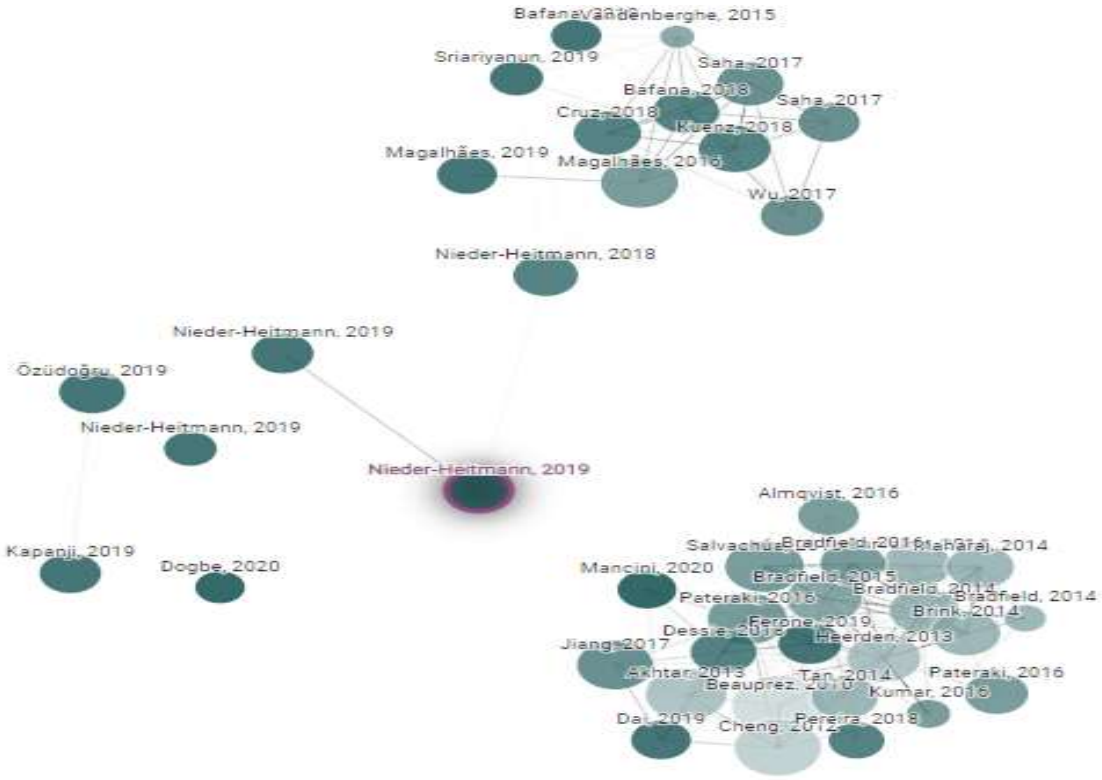

Figure 2. 4 Literature network for succinic acid's TEA-related studies

(Network created by using connected papers)

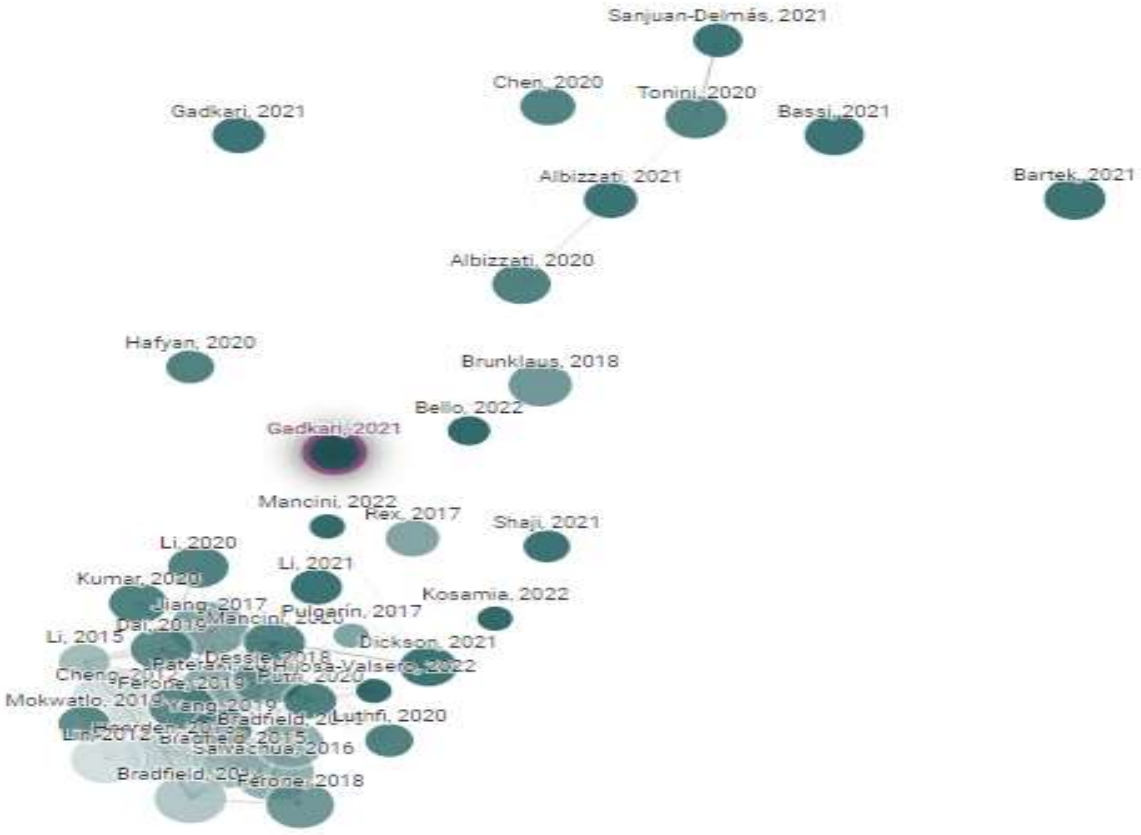

Figure 2. 5 Literature network for succinic acid's LCA-related studies

(Network developed by using connected papers)

Most articles in this area address only one aspect of sustainability, i.e., TEA or LCA. Very few attempts have been made to address the overall sustainability of BioSA production. To our knowledge, no article addresses the sustainability (TEA and LCA) assessment of BioSA production from lignocellulosic biomass by considering the monetary valuation of environmental impacts in a multiproduct biorefinery design, as shown in **Table 2.6**. In addition, no article addresses the MCDA analysis of BioSA production route issue while making a decision to select succinic acid production route between fossil and renewable routes with the involvement of real

experts. In this work all, these aspects have been considered for the production of succinic acid from lignocellulosic biomass.

Table 2. 6 List of literature studies on simultaneous BioSA sustainability assessments

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
Pulp logs	✓	**X**	**X**	✓	**X**	TEA of a conceptual biorefinery design treated 650000 metric tons of pulp log to produce BioSA, acetic acid, and dimethyl ether performed. Calculated CPAEX and OPEX for biorefinery were 635,000,000 and 180,000,000 Australian dollars.	[103]
Waste apple pomace	✓	**X**	**X**	✓	**X**	TEA for BioSA production under two different scenarios-wise designs performed for a biorefinery produces 10 to 30 k tones BioSA. As co-products, Biogas and electricity were also assessed in the analysis. The study demonstrates the economic viability of BioSA production with MSP of 0.73 and 0.33 USD/kg BioSA for scenario-1 and scenario-2, respectively.	[50]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
Sugarcane bagasse	✓	**X**	**X**	✓	**X**	These work asses the economic impacts of integrating the production of BioSA within the optimized sugarcane biorefinery along with the production of first-generation ethanol and electricity. The estimated production cost for BioSA was 2.32 USD/kg BioSA. In addition, the analysis suggested that BioSA-producing biorefinery presented slightly lower IRR compared to ethanol distillery.	[75]
Sugar cane-derived C-6 sugar	✓	**X**	**X**	**X**	**X**	TEA was performed for a conceptually derived plant located in Brazil with an annual capacity of 30 k tons. The evaluated selling price for BioSA from the analysis was 2.26 USD/kg BioSA. In addition, it was suggested that process improvement can reduce the MSP up to 1 USD/kg BioSA.	[139]
Sugarcane bagasse	✓	**X**	**X**	**X**	**X**	The economic feasibility of BioSA production was assessed by considering	[140]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
						various pretreatment options for sugar cane bagasse. It was recommended from the analysis that the steam explosion was the most profitable pretreatment, which demands a total capital investment of 384.2 million USD and IRR of 28.04 % for a biorefinery processing 3000 tons of bagasse per hour.	
Dextrose derived from corn	**X**	✓	**X**	**X**	**X**	This analysis addresses the environmental aspect of BioSA production by performing LCA. GHG emissions and NREU from cradle-to-gate in Europe. The analysis suggested that from an environmental perspective, Low pH yeast fermentation with direct crystallization is the most beneficial process for BioSA production.	[141]
C-6 sugar and Lignocellulosic biomass	**X**	✓	**X**	**X**	**X**	In this analysis, a comparison between BioSA and petroleum-derived was made by performing LCA from a cradle-to-gate approach. The process inventory data for the	[54]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
						analysis was adapted from a real BioSA manufacturing facility in Louisiana. The results suggested that BioSA has lower GWP and non-ren CED values than petroleum-based SA.	
Bread waste	**X**	✓	**X**	**X**	**X**	The environmental performance of BioSA production was performed by considering "1 kg BioSA" as a functional unit. The scope of the analysis span from cradle to production gate. The analysis indicated that the waste bread-based BioSA shows better environmental performance compared to fossil-based SA; however, GHG emissions were 50 % higher compared to processes using biomass such as sorghum grit or wet corn mill. In addition, steam and heating oil requirements during the biorefinery operations were identified as the process hotspots.	[142]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
Corn wet mill	**X**	✓	**X**	**X**	**X**	The analysis shows that BioSA production at low pH with direct crystallization for product recovery showed lower GWP and resource depletion impacts, resulting in higher impacts in land use and particulate matter formation categories.	[143]
Apple pomace	**X**	✓	**X**	**X**	**X**	The outcome of the analysis suggested that extraction and distillation operation for BioSA recovery and purification from fermentation broth contributes the most to environmental impacts. The analysis suggested that the GWP of the design was found to be highest compared to the process designed from the first-generation feedstocks and even fossil-based SA production.	[144]
Mixed food waste	**X**	✓	**X**	**X**	**X**	Cradle-to-gate LCA study to perform comparable LCA analysis for the production of BioSA and Biogas from mixed food waste was performed. The outcome of the analysis	[145]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
						demonstrates that the GWP for BioSA production is 2340 kg CO_2 eq/ton BioSA	
Sugarcane bagasse	✓	✓	X	X	X	Both TEA and LCA of BioSA production for a plant processing 4t/hr sugar cane bagasse suggest that the production cost for BioSA was 1.61 USD/kg BioSA and calculated MSP was 2.37 USD/kg BioSA. Furthermore, 1.39 kg of CO_2 eq/kg BioSA GHG is estimated.	[146]
Glucose derived from first-generation feedstock	X	X	X	X	X	Sustainability assessment of BioSA production evaluated by applying various matrixes. The calculated MSP of BioSA from this analysis was 1.04 €/kg BioSA and energy efficiency performance was also better than fossil-based SA. The material efficiency of petroleum-based SA was higher than BioSA.	[2]
Sugarcane bagasse	X	✓	X	✓	✓	In this study, both LCA and MCDA for BioSA production were performed. As co-products, PHB and electricity	[90]

Feedstock	TEA	LCA	Monetary valuation	Multiproduct biorefinery design	MCDA	Remark	Ref
						were also evaluated along with BioSA from sugar cane bagasse. The geographical scope of the study was South Africa, and the LCA parameter was normalized to find the most sustainable scenario among the six studied scenarios.	
Corn stover	✓	✓	✓	✓	✓	Present work addressed all the aspects of sustainability assessment for BioSA production. Monetary valuation of environmental impacts also assessed in this work. Integrated biorefinery concept incorporated by producing furfural, electricity as a co-products. MCDA analysis performed in order to select preferred succinic acid production route.	Present work

2.9 Summary of literature review

BioSA is a platform chemical with increasing market demand as it is used in a host of different industries. This chapter reviewed the conventional and biobased resource routes of SA production. In addition, the potential feedstocks and microorganisms for the production of BioSA were also

reviewed. For utilizing lignocellulosic biomass as a feedstock for the production of biochemicals like BioSA, the effectiveness of pretreatment and the costs associated with the enzymes used for the hydrolysis of biomass were identified as key constraints. Furthermore, the importance of comprehensive TEA and LCA of biochemicals production were highlighted. The limitations and gaps in research associated with the use of these tools were also identified. Moreover, the need for monetization of the environmental outputs of LCA was also rationalized. In order to improve the economics of biorefineries the value addition of hemicellulose and lignin in integrated plants is highly recommended and potential co-products from these biomass components were also reviewed. MCDA and its application for biochemicals production are briefly covered in this chapter. Published studies on the sustainability assessment of BioSA production and their key findings were also compared and critically analyzed. Based on the thorough literature review, the following major research gaps were identified:

- The value addition of hemicellulose and lignin for co-product generation along with the main product BioSA from cellulose in an integrated biorefinery needed to be evaluated based on techno-economic basis.
- TEA and monetization of environmental effects based on LCA need to be quantified in a common unit and compared with the conventional fossil-based SA production. route.
- Before a decision on setting up a succinic acid production plant is taken multiple criteria analysis along with TEA and LCA needs to be carried out. MCDA based on methods like Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) that involves inputs from experts in the field will help in making realistic comprehensive choices based on all three pillars of sustainable processes.

2.10 References

[1] G. Du, L. Liu, J. Chen, White biotechnology for organic acids, in: Industrial Biorefineries & White Biotechnology, Elsevier, 2015: pp. 409–444.

[2] J.M. Pinazo, M.E. Domine, V. Parvulescu, F. Petru, Sustainability metrics for succinic acid production: A comparison between biomass-based and petrochemical routes, Catal Today. 239 (2015) 17–24.

[3] M. Morales, M. Ataman, S. Badr, S. Linster, I. Kourlimpinis, S. Papadokonstantakis, V. Hatzimanikatis, K. Hungerbühler, Sustainability assessment of succinic acid production technologies from biomass using metabolic engineering, Energy Environ Sci. 9 (2016) 2794–2805.

[4] J. Akhtar, A. Idris, Recent advances in production of succinic acid from lignocellulosic biomass, Appl Microbiol Biotechnol. 98 (2014) 987–1000.

[5] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic acid: Technology development and commercialization, Fermentation. 3 (2017). https://doi.org/10.3390/fermentation3020026.

[6] N.M. Kosamia, M. Samavi, K. Piok, S.K. Rakshit, Perspectives for scale up of biorefineries using biochemical conversion pathways: Technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022). https://doi.org/10.1016/j.fuel.2022.124532.

[7] A.L. Demain, M. Newcomb, J.H.D. Wu, Cellulase, clostridia, and ethanol, Microbiology and Molecular Biology Reviews. 69 (2005) 124–154.

[8] S. Rajaram, A. Varma, Production and characterization of xylanase from Bacillus thermoalkalophilus grown on agricultural wastes, Appl Microbiol Biotechnol. 34 (1990) 141–144.

[9] R.C. Pettersen, The chemical composition of wood, The Chemistry of Solid Wood. 207 (1984) 57–126.

[10] J.R. Mielenz, Ethanol production from biomass: technology and commercialization status, Curr Opin Microbiol. 4 (2001) 324–329.

[11] X. Wang, L.P. Yomano, J.Y. Lee, S.W. York, H. Zheng, M.T. Mullinnix, K.T. Shanmugam, L.O. Ingram, Engineering furfural tolerance in Escherichia coli improves the fermentation of lignocellulosic sugars into renewable chemicals, Proceedings of the National Academy of Sciences. 110 (2013) 4021–4026.

[12] P. Kumar, D.M. Barrett, M.J. Delwiche, P. Stroeve, Methods for pretreatment of lignocellulosic biomass for efficient hydrolysis and biofuel production, Ind Eng Chem Res. 48 (2009) 3713–3729.

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

[14] L.J. Jönsson, C. Martín, Pretreatment of lignocellulose: formation of inhibitory by-products and strategies for minimizing their effects, Bioresour Technol. 199 (2016) 103–112.

[15] B.C. Saha, L.B. Iten, M.A. Cotta, Y.V. Wu, Dilute acid pretreatment, enzymatic saccharification, and fermentation of rice hulls to ethanol, Biotechnol Prog. 21 (2005) 816–822.

[16] V. Ashokkumar, R. Venkatkarthick, S. Jayashree, S. Chuetor, S. Dharmaraj, G. Kumar, W.-H. Chen, C. Ngamcharussrivichai, Recent advances in lignocellulosic biomass for biofuels and value-added bioproducts-A critical review, Bioresour Technol. 344 (2022) 126195.

[17] J.S. Kim, Y.Y. Lee, T.H. Kim, A review on alkaline pretreatment technology for bioconversion of lignocellulosic biomass, Bioresour Technol. 199 (2016) 42–48.

[18] A.K. Kumar, S. Sharma, Recent updates on different methods of pretreatment of lignocellulosic feedstocks: a review, Bioresour Bioprocess. 4 (2017) 1–19.

[19] K. Zhang, Z. Pei, D. Wang, Organic solvent pretreatment of lignocellulosic biomass for biofuels and biochemicals: a review, Bioresour Technol. 199 (2016) 21–33.

[20] P. Bajpai, Pretreatment of lignocellulosic biomass, in: Pretreatment of Lignocellulosic Biomass for Biofuel Production, Springer, 2016: pp. 17–70.

[21] N. Mosier, C. Wyman, B. Dale, R. Elander, Y.Y. Lee, M. Holtzapple, M. Ladisch, Features of promising technologies for pretreatment of lignocellulosic biomass, Bioresour Technol. 96 (2005) 673–686.

[22] X. Zhuang, W. Wang, Q. Yu, W. Qi, Q. Wang, X. Tan, G. Zhou, Z. Yuan, Liquid hot water pretreatment of lignocellulosic biomass for bioethanol production accompanying with high valuable products, Bioresour Technol. 199 (2016) 68–75.

[23] M. Lucas, S.K. Hanson, G.L. Wagner, D.B. Kimball, K.D. Rector, Evidence for room temperature delignification of wood using hydrogen peroxide and manganese acetate as a catalyst, Bioresour Technol. 119 (2012) 174–180.

[24] R. Liguori, V. Faraco, Biological processes for advancing lignocellulosic waste biorefinery by advocating circular economy, Bioresour Technol. 215 (2016) 13–20.

[25] I.G. Audu, N. Brosse, L. Desharnais, S.K. Rakshit, Investigation of the effects of ionic liquid 1-butyl-3-methylimidazolium acetate pretreatment and enzymatic hydrolysis of Typha capensis, Energy & Fuels. 27 (2013) 189–196.

[26] M.A. Carriquiry, X. Du, G.R. Timilsina, Second generation biofuels: Economics and policies, Energy Policy. 39 (2011) 4222–4234.

[27] S.K. Hoekman, Biofuels in the US–challenges and opportunities, Renew Energy. 34 (2009) 14–22.

[28] V. Menon, M. Rao, Trends in bioconversion of lignocellulose: biofuels, platform chemicals & biorefinery concept, Prog Energy Combust Sci. 38 (2012) 522–550.

[29] L. Luo, E. van der Voet, G. Huppes, Biorefining of lignocellulosic feedstock–Technical, economic and environmental considerations, Bioresour Technol. 101 (2010) 5023–5032.

[30] K.-Q. Chen, J. Li, J.-F. Ma, M. Jiang, P. Wei, Z.-M. Liu, H.-J. Ying, Succinic acid production by Actinobacillus succinogenes using hydrolysates of spent yeast cells and corn fiber, Bioresour Technol. 102 (2011) 1704–1708.

[31] J. Li, X.-Y. Zheng, X.-J. Fang, S.-W. Liu, K.-Q. Chen, M. Jiang, P. Wei, P.-K. Ouyang, A complete industrial system for economical succinic acid production by Actinobacillus succinogenes, Bioresour Technol. 102 (2011) 6147–6152.

[32] Y.-P. Liu, P. Zheng, Z.-H. Sun, Y. Ni, J.-J. Dong, L.-L. Zhu, Economical succinic acid production from cane molasses by Actinobacillus succinogenes, Bioresour Technol. 99 (2008) 1736–1742.

[33] P.C. Lee, S. Lee, S.H. Hong, H.N. Chang, S.C. Park, Biological conversion of wood hydrolysate to succinic acid by Anaerobiospirillum succiniciproducens, Biotechnol Lett. 25 (2003) 111–114.

[34] K. Chen, H. Zhang, Y. Miao, P. Wei, J. Chen, Simultaneous saccharification and fermentation of acid-pretreated rapeseed meal for succinic acid production using Actinobacillus succinogenes, Enzyme Microb Technol. 48 (2011) 339–344.

[35] Q. Li, J.A. Siles, I.P. Thompson, Succinic acid production from orange peel and wheat straw by batch fermentations of Fibrobacter succinogenes S85, Appl Microbiol Biotechnol. 88 (2010) 671–678.

[36] D.B. Hodge, C. Andersson, K.A. Berglund, U. Rova, Detoxification requirements for bioconversion of softwood dilute acid hydrolyzates to succinic acid, Enzyme Microb Technol. 44 (2009) 309–316.

[37] P.C. Lee, S. Lee, S.H. Hong, H.N. Chang, Batch and continuous cultures of Mannheimia succiniciproducens MBEL55E for the production of succinic acid from whey and corn steep liquor, Bioprocess Biosyst Eng. 26 (2003) 63–67.

[38] D.Y. Kim, S.C. Yim, P.C. Lee, W.G. Lee, S.Y. Lee, H.N. Chang, Batch and continuous fermentation of succinic acid from wood hydrolysate by Mannheimia succiniciproducens MBEL55E, Enzyme Microb Technol. 35 (2004) 648–653.

[39] N.S. Samuelov, R. Lamed, S. Lowe, J.G. Zeikus, Influence of CO2-HCO3− levels and pH on growth, succinate production, and enzyme activities of Anaerobiospirillum succiniciproducens, Appl Environ Microbiol. 57 (1991) 3013–3019.

[40] M. v Guettler, M.K. Jain, Method for making succinic acid, Anaerobiospirillum succiniciproducens variants for use in process and methods for obtaining variants, (1996).

[41] S.Y. Lee, J.M. Kim, H. Song, J.W. Lee, T.Y. Kim, Y.-S. Jang, From genome sequence to integrated bioprocess for succinic acid production by Mannheimia succiniciproducens, Appl Microbiol Biotechnol. 79 (2008) 11–22.

[42] Z. Dai, F. Guo, S. Zhang, W. Zhang, Q. Yang, W. Dong, M. Jiang, J. Ma, F. Xin, Bio-based succinic acid: an overview of strain development, substrate utilization, and downstream purification, Biofuels, Bioproducts and Biorefining. 14 (2020) 965–985.

[43] E. Scholten, T. Renz, J. Thomas, Continuous cultivation approach for fermentative succinic acid production from crude glycerol by Basfia succiniciproducens DD1, Biotechnol Lett. 31 (2009) 1947–1951.

[44] S. Okino, R. Noburyu, M. Suda, T. Jojima, M. Inui, H. Yukawa, An efficient succinic acid production process in a metabolically engineered Corynebacterium glutamicum strain, Appl Microbiol Biotechnol. 81 (2008) 459–464.

[45] R. Datta, S.-P. Tsai, P. Bonsignore, S.-H. Moon, J.R. Frank, Technological and economic potential of poly (lactic acid) and lactic acid derivatives, FEMS Microbiol Rev. 16 (1995) 221–231.

[46] Y.S. Huh, Y.-S. Jun, Y.K. Hong, H. Song, S.Y. Lee, W.H. Hong, Effective purification of succinic acid from fermentation broth produced by Mannheimia succiniciproducens, Process Biochemistry. 41 (2006) 1461–1465.

[47] S.Y. Lee, J.M. Kim, H. Song, J.W. Lee, T.Y. Kim, Y.-S. Jang, From genome sequence to integrated bioprocess for succinic acid production by Mannheimia succiniciproducens, Appl Microbiol Biotechnol. 79 (2008) 11–22.

[48] T. Kurzrock, S. Schallinger, D. Weuster-Botz, Integrated separation process for isolation and purification of biosuccinic acid, Biotechnol Prog. 27 (2011) 1623–1628. https://doi.org/10.1002/btpr.673.

[49] M. Nieder-Heitmann, K. Haigh, J.F. Görgens, Process design and economic evaluation of integrated, multi-product biorefineries for the co-production of bio-energy, succinic acid, and polyhydroxybutyrate (PHB) from sugarcane bagasse and trash lignocelluloses, Biofuels, Bioproducts and Biorefining. 13 (2019) 599–617.

[50] O.V. Okoro, A. Shavandi, An assessment of the utilization of waste apple slurry in bio-succinic acid and bioenergy production, International Journal of Environmental Science and Technology. (2021) 1–12.

[51] J.A. Quintero, C.A. Cardona, E. Felix, J. Moncada, Ó.J. Sánchez, L.F. Gutiérrez, Techno-economic analysis of bioethanol production in Africa: Tanzania case, Energy. 48 (2012) 442–454.

[52] A. de Azevedo, F. Fornasier, M. da Silva Szarblewski, R. de C. de Souza Schneider, M. Hoeltz, D. de Souza, Life cycle assessment of bioethanol production from cattle manure, J Clean Prod. 162 (2017) 1021–1030.

[53] B. Khoshnevisan, M. Tabatabaei, P. Tsapekos, S. Rafiee, M. Aghbashlo, S. Lindeneg, I. Angelidaki, Environmental life cycle assessment of different biorefinery platforms valorizing municipal solid waste to bioenergy, microbial protein, lactic and succinic acid, Renewable and Sustainable Energy Reviews. 117 (2020) 109493.

[54] H.I. Moussa, A. Elkamel, S.B. Young, Assessing energy performance of bio-based succinic acid production using LCA, J Clean Prod. 139 (2016) 761–769. https://doi.org/10.1016/j.jclepro.2016.08.104.

[55] M. Lehtonen, Social sustainability of the Brazilian bioethanol: power relations in a centre-periphery perspective, Biomass Bioenergy. 35 (2011) 2425–2434.

[56] L. Luo, E. van der Voet, G. Huppes, Biorefining of lignocellulosic feedstock–Technical, economic and environmental considerations, Bioresour Technol. 101 (2010) 5023–5032.

[57] M. Morales, M. Ataman, S. Badr, S. Linster, I. Kourlimpinis, S. Papadokonstantakis, V. Hatzimanikatis, K. Hungerbühler, Sustainability assessment of succinic acid production technologies from biomass using metabolic engineering, Energy Environ Sci. 9 (2016) 2794–2805.

[58] A. Sanchez, G. Magaña, D. Gomez, M. Solís, R. Banares-Alcantara, Bidimensional sustainability analysis of lignocellulosic ethanol production processes. Method and case study, Biofuels, Bioproducts and Biorefining. 8 (2014) 670–685.

[59] T. Silalertruksa, S.H. Gheewala, P. Pongpat, Sustainability assessment of sugarcane biorefinery and molasses ethanol production in Thailand using eco-efficiency indicator, Appl Energy. 160 (2015) 603–609.

[60] T.F. Cardoso, M.D.B. Watanabe, A. Souza, M.F. Chagas, O. Cavalett, E.R. Morais, L.A.H. Nogueira, M. Leal, O.A. Braunbeck, L.A.B. Cortez, A regional approach to determine economic, environmental and social impacts of different sugarcane production systems in Brazil, Biomass Bioenergy. 120 (2019) 9–20.

[61] M.G. López-Ortega, Y. Guadalajara, T.L. Junqueira, I.L.M. Sampaio, A. Bonomi, A. Sánchez, Sustainability Analysis of Bioethanol Production in Mexico by a Retrofitted Sugarcane Industry based on the Brazilian Expertise, Energy. (2021) 121056.

[62] M. Cinelli, S.R. Coles, K. Kirwan, Analysis of the potentials of multi criteria decision analysis methods to conduct sustainability assessment, Ecol Indic. 46 (2014) 138–148.

[63] A. Halog, Y. Manik, Advancing integrated systems modelling framework for life cycle sustainability assessment, Sustainability. 3 (2011) 469–499.

[64] T.R. Brown, R.C. Brown, Techno-economics of advanced biofuels pathways, RSC Adv. 3 (2013) 5758–5764.

[65] D. Klein-Marcuschamer, P. Oleskowicz-Popiel, B.A. Simmons, H.W. Blanch, Technoeconomic analysis of biofuels: a wiki-based platform for lignocellulosic biorefineries, Biomass Bioenergy. 34 (2010) 1914–1921.

[66] M. Yang, K.A. Rosentrater, Techno-economic analysis of the production process of structural bio-adhesive derived from glycerol, J Clean Prod. 228 (2019) 388–398.

[67] A.A. Koutinas, A. Chatzifragkou, N. Kopsahelis, S. Papanikolaou, I.K. Kookos, Design and techno-economic evaluation of microbial oil production as a renewable resource for biodiesel and oleochemical production, Fuel. 116 (2014) 566–577.

[68] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover, National Renewable Energy Lab.(NREL), Golden, CO (United States), 2011.

[69] F.K. Kazi, J. Fortman, R. Anex, G. Kothandaraman, D. Hsu, A. Aden, A. Dutta, Techno-economic analysis of biochemical scenarios for production of cellulosic ethanol, National Renewable Energy Lab. (NREL), Golden, CO (United States), 2010.

[70] J.F.O. Granjo, B.P.M. Duarte, N.M.C. Oliveira, Integrated production of biodiesel in a soybean biorefinery: modeling, simulation and economical assessment, Energy. 129 (2017) 273–291.

[71] E. Hytönen, P. Stuart, Techno-economic assessment and risk analysis of biorefinery processes, in: Computer Aided Chemical Engineering, Elsevier, 2011: pp. 1376–1380.

[72] J.A. Quintero, J. Moncada, C.A. Cardona, Techno-economic analysis of bioethanol production from lignocellulosic residues in Colombia: a process simulation approach, Bioresour Technol. 139 (2013) 300–307.

[73] G. Liu, J. Sun, J. Zhang, Y. Tu, J. Bao, High titer L-lactic acid production from corn stover with minimum wastewater generation and techno-economic evaluation based on Aspen plus modeling, Bioresour Technol. 198 (2015) 803–810.

[74] S. Espinel-Ríos, J.E. Ruiz-Espinoza, Production of 1, 3-propanediol from crude glycerol: Bioprocess design and profitability analysis, Rev Mex Ing Quim. 18 (2019) 831–840.

[75] B.C. Klein, J.F.L. Silva, T.L. Junqueira, S.C. Rabelo, P. v Arruda, J.L. Ienczak, P.E. Mantelatto, J.G.C. Pradella, S.V. Junior, A. Bonomi, Process development and techno-economic analysis of bio-based succinic acid derived from pentoses integrated to a sugarcane biorefinery, Biofuels, Bioproducts and Biorefining. 11 (2017) 1051–1064.

[76] H.M.R. Özüdoğru, M. Nieder-Heitmann, K.F. Haigh, J.F. Görgens, Techno-economic analysis of product biorefineries utilizing sugarcane lignocelluloses: Xylitol, citric acid and glutamic acid scenarios annexed to sugar mills with electricity co-production, Ind Crops Prod. 133 (2019) 259–268.

[77] S. Parsons, F. Abeln, M.C. McManus, C.J. Chuck, Techno-economic analysis (TEA) of microbial oil production from waste resources as part of a biorefinery concept: assessment at multiple scales under uncertainty, Journal of Chemical Technology & Biotechnology. 94 (2019) 701–711.

[78] M. Finkbeiner, A. Inaba, R. Tan, K. Christiansen, H.-J. Klüppel, The new international standards for life cycle assessment: ISO 14040 and ISO 14044, Int J Life Cycle Assess. 11 (2006) 80–85.

[79] M. Owsianiak, A. Laurent, A. Bjørn, M.Z. Hauschild, IMPACT 2002+, ReCiPe 2008 and ILCD's recommended practice for characterization modelling in life cycle impact assessment: a case study-based comparison, Int J Life Cycle Assess. 19 (2014) 1007–1021.

[80] R.K. Rosenbaum, M.Z. Hauschild, A.-M. Boulay, P. Fantke, A. Laurent, M. Núñez, M. Vieira, Life cycle impact assessment, in: Life Cycle Assessment, Springer, 2018: pp. 167–270.

[81] M.Z. Hauschild, Assessing environmental impacts in a life-cycle perspective, (2005).

[82] E. Heinzle, A.P. Biwer, C.L. Cooney, Development of sustainable bioprocesses: modeling and assessment, John Wiley & Sons, 2007.

[83] S.V. Hjuler, S.B. Hansen, LCA of biofuels and biomaterials, in: Life Cycle Assessment, Springer, 2018: pp. 755–782.

[84] J.K. Raman, E. Gnansounou, LCA of bioethanol and furfural production from vetiver, Bioresour Technol. 185 (2015) 202–210.

[85] A.G. Daful, K. Haigh, P. Vaskan, J.F. Görgens, Environmental impact assessment of lignocellulosic lactic acid production: Integrated with existing sugar mills, Food and Bioproducts Processing. 99 (2016) 58–70.

[86] R.J. Hanes, N.B. Cruze, P.K. Goel, B.R. Bakshi, Allocation games: addressing the ill-posed nature of allocation in life-cycle inventories, Environ Sci Technol. 49 (2015) 7996–8003.

[87] D. Dasgupta, A. Sidana, P. Ghosh, T. Sharma, J. Singh, A. Prabhune, S. More, T. Bhaskar, D. Ghosh, Energy and life cycle impact assessment for xylitol production from corncob, J Clean Prod. 278 (2021) 123217.

[88] N. Bonatsos, C. Marazioti, E. Moutousidi, A. Anagnostou, A. Koutinas, I.K. Kookos, Techno-economic analysis and life cycle assessment of heterotrophic yeast-derived single cell oil production process, Fuel. 264 (2020) 116839.

[89] T. Nitkiewicz, M. Wojnarowska, M. Sołtysik, A. Kaczmarski, T. Witko, C. Ingrao, M. Guzik, How sustainable are biopolymers? Findings from a life cycle assessment of polyhydroxyalkanoate production from rapeseed-oil derivatives, Science of The Total Environment. 749 (2020) 141279.

[90] M. Nieder-Heitmann, K.F. Haigh, J.F. Görgens, Life cycle assessment and multi-criteria analysis of sugarcane biorefinery scenarios: Finding a sustainable solution for the South African sugar industry, J Clean Prod. 239 (2019). https://doi.org/10.1016/j.jclepro.2019.118039.

[91] S. Dutta, F. Neto, M.C. Coelho, Microalgae biofuels: A comparative study on techno-economic analysis & life-cycle assessment, Algal Res. 20 (2016) 44–52.

[92] J.D. Kern, A.M. Hise, G.W. Characklis, R. Gerlach, S. Viamajala, R.D. Gardner, Using life cycle assessment and techno-economic analysis in a real options framework to inform the design of algal biofuel production facilities, Bioresour Technol. 225 (2017) 418–428.

[93] A. Levasseur, O. Bahn, D. Beloin-Saint-Pierre, M. Marinova, K. Vaillancourt, Assessing butanol from integrated forest biorefinery: A combined techno-economic and life cycle approach, Appl Energy. 198 (2017) 440–452.

[94] R. Mahmud, S.M. Moni, K. High, M. Carbajales-Dale, Integration of techno-economic analysis and life cycle assessment for sustainable process design–A review, J Clean Prod. 317 (2021) 128247.

[95] N.A. Boakye-Boaten, L. Kurkalova, S. Xiu, A. Shahbazi, Techno-economic analysis for the biochemical conversion of Miscanthus x giganteus into bioethanol, Biomass Bioenergy. 98 (2017) 85–94.

[96] P. Sassner, M. Galbe, G. Zacchi, Techno-economic evaluation of bioethanol production from three different lignocellulosic materials, Biomass Bioenergy. 32 (2008) 422–430.

[97] F.K. Kazi, J.A. Fortman, R.P. Anex, D.D. Hsu, A. Aden, A. Dutta, G. Kothandaraman, Techno-economic comparison of process technologies for biochemical ethanol production from corn stover, Fuel. 89 (2010) S20–S28.

[98] L. Zhao, X. Zhang, J. Xu, X. Ou, S. Chang, M. Wu, Techno-economic analysis of bioethanol production from lignocellulosic biomass in China: Dilute-acid pretreatment and enzymatic hydrolysis of corn stover, Energies (Basel). 8 (2015) 4096–4117.

[99] F.L. Stewart, S. Carrière, The Greenhouse Gas Pollution Pricing Act and The Interaction of Federal and Provincial Enforcement Efforts, SSRN Electron. J. (2019).

[100] M. Pizzol, B. Weidema, M. Brandão, P. Osset, Monetary valuation in life cycle assessment: a review, J Clean Prod. 86 (2015) 170–179.

[101] Y. Dong, M. Hauschild, H. Sørup, R. Rousselet, P. Fantke, Evaluating the monetary values of greenhouse gases emissions in life cycle impact assessment, J Clean Prod. 209 (2019) 538–549.

[102] A. Sanchez, G. Magaña, M.I. Partida, S. Sanchez, Bi-dimensional sustainability analysis of a multi-feed biorefinery design for biofuels co-production from lignocellulosic residues and agro-industrial wastes, Chemical Engineering Research and Design. 107 (2016) 195–217.

[103] M.S.G. Lopes, J.G.C. Gomez, M.K. Taciro, T.T. Mendonça, L.F. Silva, Polyhydroxyalkanoate biosynthesis and simultaneous remotion of organic inhibitors from sugarcane bagasse hydrolysate by Burkholderia sp, J Ind Microbiol Biotechnol. 41 (2014) 1353–1363.

[104] W. Pan, J.A. Perrotta, A.J. Stipanovic, C.T. Nomura, J.P. Nakas, Production of polyhydroxyalkanoates by Burkholderia cepacia ATCC 17759 using a detoxified sugar maple hemicellulosic hydrolysate, J Ind Microbiol Biotechnol. 39 (2012) 459–469.

[105] K. Dietrich, M.-J. Dumont, L.F. del Rio, V. Orsat, Producing PHAs in the bioeconomy—Towards a sustainable bioplastic, Sustain Prod Consum. 9 (2017) 58–70.

[106] N. Balasubramanian, J.S. Kim, Y.Y. Lee, Fermentation of xylose into acetic acid by Clostridium thermoaceticum, Appl Biochem Biotechnol. 91 (2001) 367–376.

[107] M. Ehsanipour, A.V. Suko, R. Bura, Fermentation of lignocellulosic sugars to acetic acid by Moorella thermoacetica, J Ind Microbiol Biotechnol. 43 (2016) 807–816.

[108] A. Ghayur, T.V. Verheyen, E. Meuleman, Techno-economic analysis of a succinic acid biorefinery coproducing acetic acid and dimethyl ether, J Clean Prod. 230 (2019) 1165–1175. https://doi.org/10.1016/j.jclepro.2019.05.180.

[109] H. Kobayashi, A. Fukuoka, Synthesis and utilisation of sugar compounds derived from lignocellulosic biomass, Green Chemistry. 15 (2013) 1740–1763.

[110] A.D. Mountraki, K.R. Koutsospyros, B.B. Mlayah, A.C. Kokossis, Selection of biorefinery routes: the case of xylitol and its integration with an organosolv process, Waste Biomass Valorization. 8 (2017) 2283–2300.

[111] E. Cubas-Cano, C. González-Fernández, M. Ballesteros, E. Tomás-Pejó, Lactobacillus pentosus CECT 4023 T co-utilizes glucose and xylose to produce lactic acid from wheat straw hydrolysate: Anaerobiosis as a key factor, Biotechnol Prog. 35 (2019) e2739.

[112] R.A. de Oliveira, C.E.V. Rossell, J. Venus, S.C. Rabelo, R. Maciel Filho, Detoxification of sugarcane-derived hemicellulosic hydrolysate using a lactic acid producing strain, J Biotechnol. 278 (2018) 56–63.

[113] A. Garde, G. Jonsson, A.S. Schmidt, B.K. Ahring, Lactic acid production from wheat straw hemicellulose hydrolysate by Lactobacillus pentosus and Lactobacillus brevis, Bioresour Technol. 81 (2002) 217–223.

[114] D. Wischral, J.M. Arias, L.F. Modesto, D. de França Passos, N. Pereira Jr, Lactic acid production from sugarcane bagasse hydrolysates by Lactobacillus pentosus: integrating xylose and glucose fermentation, Biotechnol Prog. 35 (2019) e2718.

[115] F. Starfelt, E. Thorin, E. Dotzauer, J. Yan, Performance evaluation of adding ethanol production into an existing combined heat and power plant, Bioresour Technol. 101 (2010) 613–618.

[116] M. Fache, B. Boutevin, S. Caillol, Vanillin production from lignin and its use as a renewable chemical, ACS Sustain Chem Eng. 4 (2016) 35–46.

[117] R.A. Sheldon, H. van Bekkum, Fine chemicals through heterogeneous catalysis, John Wiley & Sons, 2008.

[118] J.-J. Wang, Y.-Y. Jing, C.-F. Zhang, J.-H. Zhao, Review on multi-criteria decision analysis aid in sustainable energy decision-making, Renewable and Sustainable Energy Reviews. 13 (2009) 2263–2278.

[119] N.-B. Chang, G. Parvathinathan, J.B. Breeden, Combining GIS with fuzzy multicriteria decision-making for landfill siting in a fast-growing urban region, J Environ Manage. 87 (2008) 139–153.

[120] X.-S. Qin, G.H. Huang, A. Chakma, X.H. Nie, Q.G. Lin, A MCDM-based expert system for climate-change impact assessment and adaptation planning–A case study for the Georgia Basin, Canada, Expert Syst Appl. 34 (2008) 2164–2179.

[121] C.-C. Chou, A fuzzy MCDM method for solving marine transshipment container port selection problems, Appl Math Comput. 186 (2007) 435–444.

[122] R.Z. Farahani, N. Asgari, Combination of MCDM and covering techniques in a hierarchical model for facility location: A case study, Eur J Oper Res. 176 (2007) 1839–1858.

[123] N.K. Kwak, C.W. Lee, J.H. Kim, An MCDM model for media selection in the dual consumer/industrial market, Eur J Oper Res. 166 (2005) 255–265.

[124] M. Jovanović, N. Afgan, P. Radovanović, V. Stevanović, Sustainable development of the Belgrade energy system, Energy. 34 (2009) 532–539.

[125] H.C. Doukas, B.M. Andreas, J.E. Psarras, Multi-criteria decision aid for the formulation of sustainable technological energy priorities using linguistic variables, Eur J Oper Res. 182 (2007) 844–855.

[126] J.-J. Wang, Y.-Y. Jing, C.-F. Zhang, G.-H. Shi, X.-T. Zhang, A fuzzy multi-criteria decision-making model for trigeneration system, Energy Policy. 36 (2008) 3823–3832.

[127] J.-J. Wang, Y.-Y. Jing, C.-F. Zhang, X.-T. Zhang, G.-H. Shi, Integrated evaluation of distributed triple-generation systems using improved grey incidence approach, Energy. 33 (2008) 1427–1437.

[128] M.S. Mohsen, B.A. Akash, Evaluation of domestic solar water heating system in Jordan using analytic hierarchy process, Energy Convers Manag. 38 (1997) 1815–1822.

[129] F. Cavallaro, L. Ciraolo, A multicriteria approach to evaluate wind energy plants on an Italian island, Energy Policy. 33 (2005) 235–244.

[130] D. Diakoulaki, F. Karangelis, Multi-criteria decision analysis and cost–benefit analysis of alternative scenarios for the power generation sector in Greece, Renewable and Sustainable Energy Reviews. 11 (2007) 716–727.

[131] J. Burton, K. Hubacek, Is small beautiful? A multicriteria assessment of small-scale energy technology applications in local governments, Energy Policy. 35 (2007) 6402–6412.

[132] A. Papadopoulos, A. Karagiannidis, Application of the multi-criteria analysis method Electre III for the optimisation of decentralised energy systems, Omega (Westport). 36 (2008) 766–776.

[133] D.A. Haralambopoulos, H. Polatidis, Renewable energy projects: structuring a multi-criteria group decision-making framework, Renew Energy. 28 (2003) 961–973.

[134] D.E. Ighravwe, S.A. Oke, A multi-criteria decision-making framework for selecting a suitable maintenance strategy for public buildings using sustainability criteria, Journal of Building Engineering. 24 (2019) 100753.

[135] C. Acar, A. Beskese, G.T. Temur, Sustainability analysis of different hydrogen production options using hesitant fuzzy AHP, Int J Hydrogen Energy. 43 (2018) 18059–18076.

[136] M. Colak, İ. Kaya, Multi-criteria evaluation of energy storage technologies based on hesitant fuzzy information: A case study for Turkey, J Energy Storage. 28 (2020) 101211.

[137] G. Candan, M.C. TOKLU, Determining solar power plant location using hesitant fuzzy ahp method, Alphanumeric Journal. 9 (2021) 25–34.

[138] S. Kheybari, F.M. Rezaie, S.A. Naji, F. Najafi, Evaluation of energy production technologies from biomass using analytical hierarchy process: The case of Iran, J Clean Prod. 232 (2019) 257–265.

[139] Ç. Efe, L.A.M. van der Wielen, A.J.J. Straathof, Techno-economic analysis of succinic acid production using adsorption from fermentation medium, Biomass Bioenergy. 56 (2013) 479–492.

[140] M. Nieder-Heitmann, K. Haigh, J. Louw, J.F. Görgens, Economic evaluation and comparison of succinic acid and electricity co-production from sugarcane bagasse and trash lignocelluloses in a biorefinery, using different pretreatment methods: dilute acid (H2SO4), alkaline (NaOH), organosolv, ammonia fibre expa, Biofuels, Bioproducts and Biorefining. 14 (2020) 55–77.

[141] B. Cok, I. Tsiropoulos, A.L. Roes, M.K. Patel, Succinic acid production derived from carbohydrates: An energy and greenhouse gas assessment of a platform chemical toward a bio-based economy, Biofuels, Bioproducts and Biorefining. 8 (2014) 16–29. https://doi.org/10.1002/bbb.1427.

[142] S. Gadkari, D. Kumar, Z. hao Qin, C.S.K. Lin, V. Kumar, Life cycle analysis of fermentative production of succinic acid from bread waste, Waste Management. 126 (2021) 861–871. https://doi.org/10.1016/j.wasman.2021.04.013.

[143] Jo Dewulf, S. de Meester, R.A.F. Alvarenga, M. Smidt, J. den Hollander, H. Bosch, Y. Xiang, M. van der Graaf, A. Lambin, J.-P. Duda, Sustainability Assessment of Renewables-Based Products: Methods and Case Studies, First Edition. Edited Life Cycle Assessment of Biobased and Fossil-Based Succinic Acid of Succinic Acid 20.1.1 Succinic Acid, A Key Biobased Building Block, (n.d.).

[144] S. González-García, L. Argiz, P. Míguez, B. Gullón, Exploring the production of bio-succinic acid from apple pomace using an environmental approach, Chemical Engineering Journal. 350 (2018) 982–991. https://doi.org/10.1016/j.cej.2018.06.052.

[145] B. Brunklaus, E. Rex, E. Carlsson, J. Berlin, The future of Swedish food waste: An environmental assessment of existing and prospective valorization techniques, J Clean Prod. 202 (2018) 1–10. https://doi.org/10.1016/j.jclepro.2018.07.240.

[146] A. Shaji, Y. Shastri, V. Kumar, V. v. Ranade, N. Hindle, Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse, ACS Sustain Chem Eng. 9 (2021) 12738–12746. https://doi.org/10.1021/acssuschemeng.1c02483.

CHAPTER 3

OBJECTIVE 1*

Scenario-based techno-economics and heat integration feasibility assessment of integrated multiproduct biorefineries with biosuccinic acid as the main product and various byproduct options

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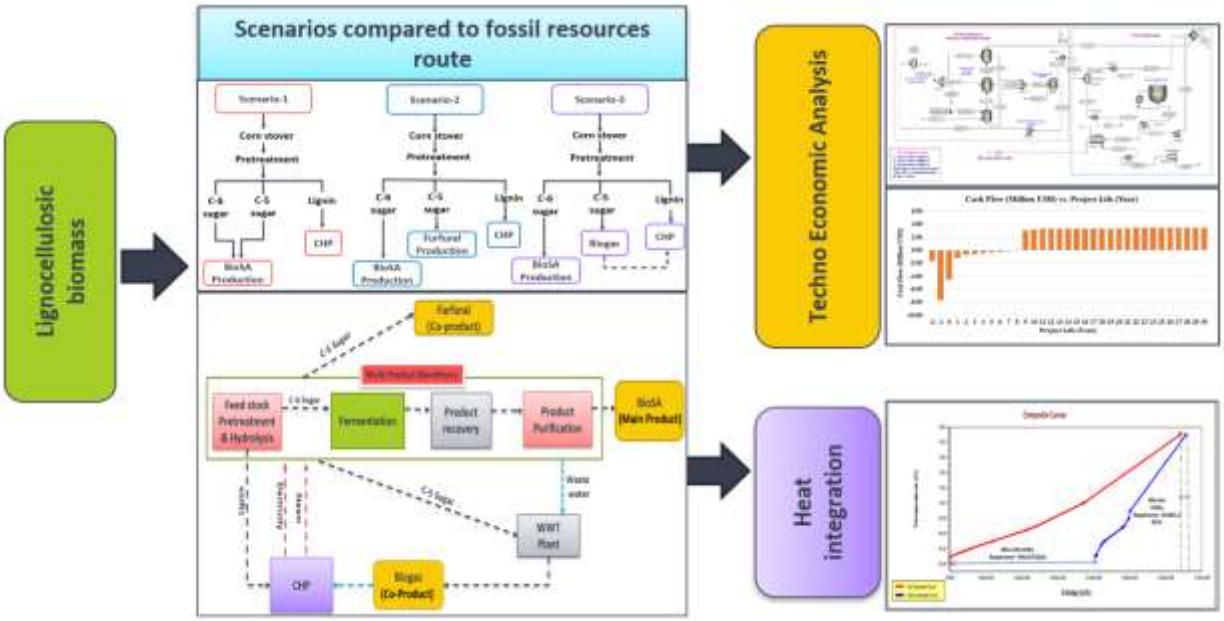
3 Techno-economic analysis of BioSA production along with coproduct synthesis in multiproduct biorefinery

3.1 Abstract



Synthesis of biochemicals from lignocellulosic biomass in a multiproduct biorefinery has considerable potential benefits over that obtained from conventional fossil-based resources. The benefits are enhanced from an economic perspective when all three major components of such biomass are utilized simultaneously. This study investigates the best economically viable configuration to produce BioSuccinic Acid (BioSA) from C-6 sugars obtained on hydrolysis of cellulose from corn stover in an integrated plant. Value addition of C-5 sugars was also assessed for furfural and biogas production, while lignin was evaluated for electricity generation as co-products. Three scenarios of multi-product biorefineries were compared using Aspen Plus® design simulation software. Scenario 1 investigates the production of BioSA from C-6 and C-5 sugars and electricity from lignin. Scenario 2 involves the production of BioSA from C-6 sugar, furfural

from C-5 sugar, and electricity from lignin. Scenario 3 assesses the production of BioSA from C-6, biogas from C-5 sugars which is diverted to a Combined Heat and Power (CHP) unit for electricity production, and electricity from lignin. Heat integration feasibility was also studied by preparing composite curves. The results indicate that the production of BioSA from C-6 and C-5 sugars and utilization of lignin as a solid fuel in a CHP unit is the most economically viable configuration with a Minimum Selling Price (MSP) of 2.28 USD/kg BioSA and a payback period of 8 years on investment. Maximum heat recovery feasibility was obtained with scenario 2. However, because of the higher operating costs for furfural production, this configuration had the highest MSP and payback period of 3.33 USD/kg BioSA and 9 years, respectively. Scenario 3 has the advantage of low capital investment requirements and a payback period of 8 years. However, lower production of BioSA results in a higher MSP of 3.19 USD/kg BioSA. Overall, this study confirms that utilization of all three components of a lignocellulosic residue and proper choice of co-products using detailed techno-economic evaluation can make the production of the important platform chemical BioSA economically feasible and competitive with fossil-based Succinic Acid (SA).

Keywords: Techno-economic assessment, Biosuccinic acid, Multiproduct biorefinery, Furfural, Biogas

3.2 Introduction

The continued rapid increase in energy and chemical demands has placed immense pressure on consumer prices and the environment. This has prompted researchers to look for renewable, sustainable, and consistent resources. Biomass is an excellent resource from which various chemicals and fuels can be produced. Ideal biorefineries need to be integrated systems where biomass can serve as the starting material to produce multiple products using complex processing

methods and technologies [1]. The goal of any biorefinery should be to provide a spectrum of marketable products and energy by processing all components of biomass. Depending on the maturity of available technology, biorefineries can target High-Value Low-Volume (HVLV), Middle- Value Middle–Volume (MVMV), and Low-Value High-Volume (LVHV) outputs [2,3]. BioSA, a MVMV product, has considerable potential as a candidate for biorefineries. The Department of Energy (DoE) USA has considered it as a compound of strategic importance in the chemical industry based on renewable materials [4]. The total world production of SA in 2013-2014 was 38,000 tons, valued at 2.90 USD/kg SA and increased to 50,000 tons in 2016. In addition, BioSA was reported to be the fastest-growing bio-based product in 2015, with predicted market demand of 94,000 tons by 2025 [5–7]. In another report, the potential market of SA is expected to reach 1.8 billion USD in 2025 with a Compound Annual Growth Rate (CAGR) of 27.4% [8]. BioSA is a niche platform product as it has potential applications in food additives, detergents, cosmetics, pigments, toners, cement additives, and pharmaceutical intermediates. The pharmaceutical industry uses SA to produce antibiotics, amino acids, and vitamins [9]. Commodity products like 1,4 butanediol, γ-butyrolactone, and 2-pyrrolidinone are also made from SA. Derivatives of SA such as 1, 4 butanediols, and tetrahydrofuran make possible the synthesis of bio-based polybutylene terephthalate for casing application and spandex production [10]. Hence, it is no surprise that there is so much focus on its production. In the last few years, many ventures have been initiated for BioSA production using first-generation feedstock [11]. Even with the first-generation feedstock (like starch), which has easier and cheaper pretreatment steps, some industries have either closed or remain suspended due to alternate corporate plans, bankruptcy, and economic loss, including loss of taxpayer funds [12]. Recently, the BioAmber chemical

industry, located in Sarnia, Canada, has been taken over by LCY Bioscience and has started producing BioSA again after a transient period [13].

It is important to utilize all three components of lignocellulosic substrates to make biorefining economically feasible in competition with fossil resources. Furfural is the best-described and most widely used platform chemical that can be produced from the dehydration of C-5 sugar of lignocellulosic biomass [14]. Furfural's CAGR is projected to be 5%, with a market volume and size of 4.2 million tons and 896 million USD, respectively, from 2020 to 2027 [15]. In oil refineries, it is primarily used as a solvent for the synthesis of a broad range of chemicals. In addition, the pharmaceutical, agrochemical, and plastic industries are also major consumers of this valuable chemical platform [16]. There are several experiment-based studies for the production of furfural from various available biomass resources [17–21], but very few studies have carried out process simulations and performed Techno-Economic Assessment (TEA) of this bioproduct [22–24]. There is no industrial chemical synthesis route used to produce furfural from fossil fuel. Furfural is produced exclusively by the hydrolysis of C-5 sugars obtained from lignocellulosic biomass. Currently, China produces more than 70% of commercial furfural, followed by the Dominican Republic and South Africa [25].

To access early-stage feasibility and avoid economic failure, researchers adopt various methodologies. TEA, followed by Life Cycle Analysis (LCA), is the standard methodology used to ascertain technical, economic, and environmental sustainability. Numerous studies have been performed to evaluate the TEA of stand-alone SA biorefineries from various feedstocks [26–29]. González-García et al. [30] assessed the production of BioSA from an environmental perspective to identify the most environmental impact contributing areas in the BioSA refinery by performing LCA. To resolve the apple pomace waste management issue and for the creation of an additional

source of revenue for apple farmers and the related processing industry, the production of BioSA from apple pomace was studied by Okoro et al. [31]. Shaji et al. [32] performed TEA and LCA simultaneously for BioSA production from sugarcane bagasse and identified pretreatment and fermentation as the biggest contributors to production costs. In addition, they suggested that the evaluation of heat integration feasibility for BioSA biorefinery is essential. However, to date, to our knowledge, only two studies [31,33] considered the multiproduct configuration in their assessment by using all major components (C-6 sugar, C-5 sugar, and lignin) of biomass to produce BioSA along with co-products. No study is available that assessed the heat integration feasibility for a multiproduct biorefinery that produces BioSA as the main product, furfural or biogas, and electricity as a co-product. These factors have been considered in this assessment to develop a novel corn stover-based BioSA biorefinery that has economic and technical competitiveness over the conventional fossil-based SA production route.

In this study, three scenarios are compared to maximize the value addition of lignocellulosic biomass using all main components of biomass (cellulose, hemicellulose, and lignin) to produce the main product (BioSA) and different combinations of co-products (furfural, biogas, or combustion electrical energy). Scenario 1 considered the production of BioSA and electricity, whereas scenario 2 was designed to produce BioSA, furfural, and electricity, and scenario 3 for BioSA and biogas for electricity production. This paper also presents a BioSA biorefinery design that exploits the use of alternate energy sources for the generation of electricity to make the process self-sufficient in electricity. This includes on-site usage of lignin and biogas generated from the Waste Water Treatment Plant (WWTP) to produce electricity in CHP. In addition, heat integration is also evaluated to add potential savings in utility for BioSA refineries to reduce the MSP further.

3.3 Methodology

3.3.1 Framework of this work

The framework of this work was to evaluate the economic outcome of a biorefinery that uses corn stover as the substrate and produces BioSA as a main product and furfural or biogas as a co-product from hemicellulose and electricity from lignin. Three different product scenario combinations were studied. The objective of this study was to identify the scenario which gives the best economic performance with BioSA as the main product. Calculation of economic performance parameters, namely, Operating Expenditure (OPEX), Capital Expenditure (CAPEX), MSP, and payback period for each scenario, is included in this evaluation. In the second part of this study, heat integration was performed to calculate potential savings in process utility for each scenario. The results obtained from these two studies were then consolidated to propose the best industrial-scale option for an economically competitive BioSA production process from lignocellulosic biomass like corn stover.

3.3.2 Design basis

The basis of all calculations in this study was a BioSA biorefinery that treats 1000 kg/hr corn stover as a lignocellulosic feedstock operating for 8410 hr per year with 96 % uptime. The average composition of corn stover was assumed to be 37.4 % cellulose, 21.1 % of hemicellulose, and 18.0 % of lignin, and the rest 23.5 % extractives, ash, protein, acetate, unknown soluble solids, arabinan, galactan, and mannan on the dry mass basis [34,35]. For the value addition of hemicellulose and lignin, multiproduct biorefinery was investigated in three scenarios, as shown in **Figure 3.1**.

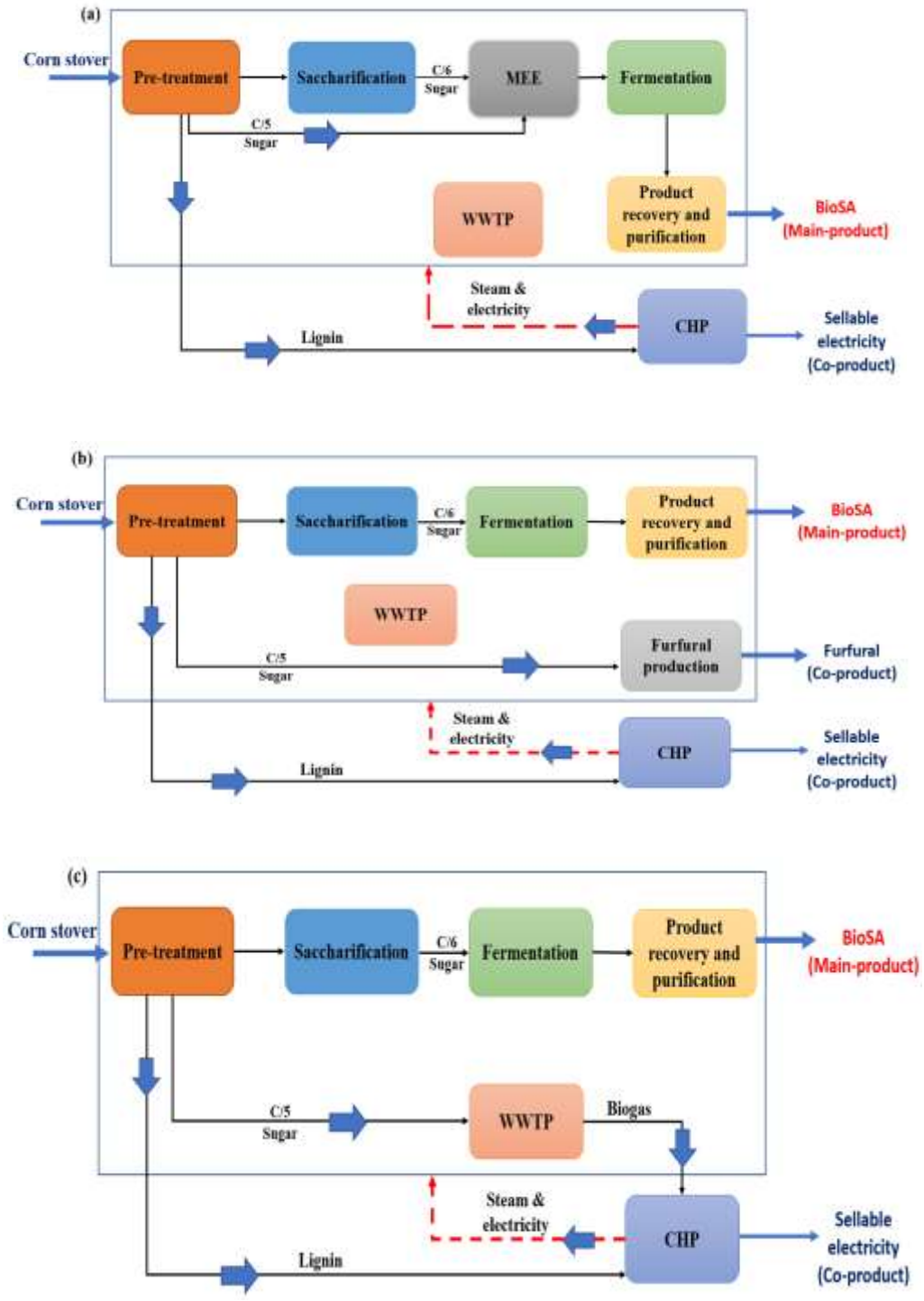


Figure 3. 1 General overview of biorefinery scenarios compared in this study (a) scenario 1 (b) scenario 2 (c) scenario 3

In scenario 1, after the pretreatment of corn stover, both C-6 and C-5 sugar streams are diverted to the fermentation section for the BioSA production, whereas in scenario 2, the C-5 sugar stream is diverted for furfural production and BioSA produced from C-6 sugar only. In scenario 3, the C-5 sugar stream is diverted to a WWTP for biogas generation. The generated biogas is consumed in a CHP unit for electricity and steam production along with the combustion of lignin, while the C-6 sugar stream is used for BioSA production. In this study, the value addition of the lignin stream is done by producing electricity and steam in a CHP unit for all three scenarios.

3.3.3 Process simulation

Thermodynamic properties of lignocellulosic biomass have been studied previously [36]. The three scenarios mentioned were simulated using Aspen Plus ® V.11.0 (Bedford USA), available at the Chemical Engineering Department of Lakehead University. The thermodynamic property method selected for this case was non-random two-liquid (NRTL), which is also recommended by the guidelines for predicting the corresponding phase equilibrium compositions of chemicals at low pressure (lesser than 10 bar) and moderate temperature (2- 200 °C) [37,38]. The pretreatment, saccharification, and fermentation reactions were simulated using the R-stoic reactor model. For the downstream processing, reactive extraction, crystallization, and drying operation were simulated using Aspen Plus's separation, crystallizer, and dryer models, respectively. Pumps and compressors were considered minor equipment that operated at 75 % mechanical efficiency. Heater and cooler models were used to simulate heat exchangers in biorefinery design. For heat integration, the initial data required, including mass flows and incoming and outgoing temperature for hot and cold streams, were taken from the simulation, and a 10 °C approach temperature (ΔT_{min}) was set. Composite curves were prepared for hot and cold utility by using the integration tool Aspen Energy Analysis®.

3.3.4 Process economy

Process economic analysis is reported in terms of US dollars (USD) for the year 2021. Equipment cost estimates were taken from the National Renewable Energy Laboratory's (NREL) report [39]. Equipment prices were indexed up to 2021. The installed cost of equipment was calculated by using Aspen Process Economic Analyzer® and sourced from literature after adjusting it for the desired capacity and cost year by using the Chemical Engineering Plant Cost Index (CEPCI). The values of CEPCI for the reference year (2007) and estimation year (2021) were assumed to be 525 and 607, respectively [34,40]. Estimated capital costs were considered as a preliminary estimate with an accuracy range of $\pm$ 30%, typically used to decide between design choices, such as the different scenarios investigated [41,42]. Fixed Capital Investment (FCI) is calculated by adding Total Direct Cost (TDC) and Total Indirect Cost (TIC) and includes warehouse, site development, and piping costs. For the Total Capital Investment (TCI), a working capital of 5% of FCI and land costs are also considered [43]. Fixed Operating Costs (FOC) and Variable Operating Costs (VOC) are determined based on biorefinery operations and raw materials requirements. VOC includes the raw materials, byproducts, feedstock, and process utilities, whereas labor, labor overhead, plant maintenance, property taxes, and insurance are covered under FOC. General expenses related to product distribution, research and development, and administration costs were excluded from the Total Operating Cost (TOC) [39]. At a 10 % discount rate, Discounted Cash Flow Analysis (DCFA) was performed to determine the Net Present Value (NPV) and MSP of BioSA. Project life was assumed to be 30 years with a 3-year construction period (8 % TCI used in year 2, 60% spent in year 1, and 32 % spent in year -0). The straight-line depreciation method is used with an 8 % interest and 35 % income tax rate. All processes in the biorefinery are assumed in Inside Battery Limits (ISBL) for all the scenarios.

3.4 Biorefinery process description

A detailed description of the biorefinery, along with their process flow diagrams are described in this section. Many of the sections are similar for all three scenarios. However, the Multi-Effect Evaporation (MEE) and furfural production section are additional units in scenario 1 and scenario 2, respectively. For scenario 3, the C-5 sugar stream is diverted to WWTP for biogas production. The entire biorefinery is modeled in seven sections which include pretreatment and detoxification (Section-101), saccharification (Section-201), MEE (Section -301), fermentation (Section-401), product recovery and purification (Section-501), WWTP (Section -601) and CHP (Section -701). For scenario 2, furfural production (Section-801) was also simulated. For this assessment, as a cooling and heating utility, cooling water and hot water are used, respectively. It was assumed that process temperatures as low as 25 °C were achieved using cooling water, whereas for process temperatures up to 60 °C hot water is used. High-pressure steam (13 bar) and low-pressure steam (2.6 bar) are used for the higher process (more than 60 °C) temperature requirements.

3.4.1 Pretreatment and detoxification (Section-101)

As a feedstock, corn stover is subjected to pretreatment to make the lignocellulosic components available for further processing. Composition of corn stover can be found in **Table 3.1**. Corn stover is crushed to 80 mm in size in a crusher (C-101-1).

Table 3. 1 Composition of lignocellulosic biomass-corn stover [34]

Component	Composition (% Dry basis)
Cellulose	37.4
Hemicellulose	21.1
Lignin	18.0
Ash	5.2
Protein	3.1
Extractives	4.7
Arabinan	2.9
Mannan	1.6
Galactan	2.0
Unknown soluble solids	1.1
Acetate	2.9
Moisture	15

Crushed stover is directed to acid impregnation in a mixing unit (M-101-2), which enhances the solid recovery during the steam explosion pretreatment [44]. Acid-impregnated corn stover undergoes steam explosion pretreatment in a reactor (R-101-1) at 190 °C and 1.15 MPa (15 bar) for 7.5 min. In order to limit the usage of chemicals, higher process maturity, and profitability on

a commercial scale [45], the steam explosion pretreatment method is preferred over the other available pretreatment methods. The pretreated reaction mass is flashed into a tank (T-101-1) and the vapor is condensed in a cooler (Co-101-2) and sent to the WWTP (Section-601). The solid fraction is removed by filtration (F-101-1), and the liquid hemicellulose hydrolysate (F-1Liquid) is sent to the detoxification reactor (R-101-2), which operates at 50 °C for 45 min residence time. This is followed by a neutralization reactor (R-101-3). The detoxification or over-liming by-product gypsum is separated from the reaction mass by hydro cyclone (SS-101-2). Cellulose and lignin from the filter (F-1solid) are separated by employing alkali treatment (T-101-2) followed by black liquor treatment with sulfuric acid in a mixing tank (M-101-4). The three major product streams from this section are the cellulose stream (20 % solid concentration), lignin stream, and hemicellulose hydrolysate (C-5 sugar) **(Figure 3.2).**

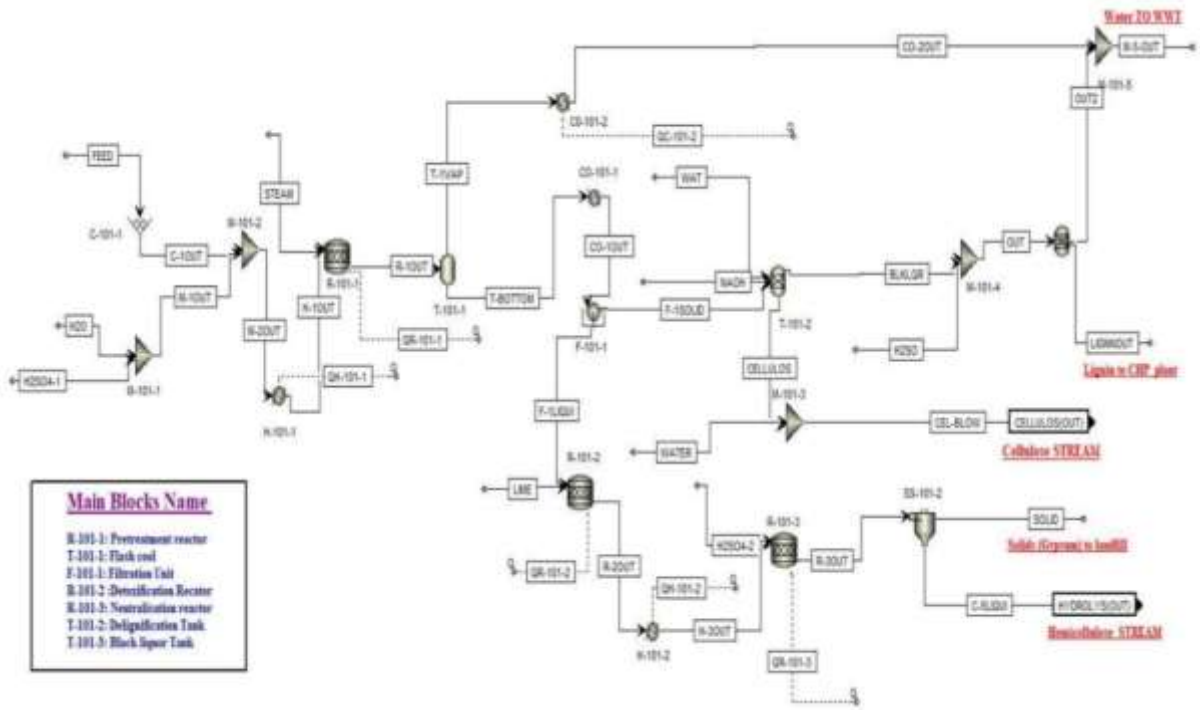


Figure 3. 2 Section-101 including pretreatment and detoxification processes

The conversion of hemicellulose to xylose is 84 %, which is corroborated by studies using steam explosion pretreatment of corn stover [46]. The information related to pretreatment and detoxification reaction stoichiometries and conversion factor can be found in **Table 3.2**.

Table 3. 2 Pretreatment and detoxification (Section -101) main reaction stoichiometries and conversion factors

Reaction	Conversion Factor	Reference
R-101-1		
Cellulose (Solid) + H_2O → Glucose	0.07	[46]
Hemicellulose (Solid) + H_2O → Xylose	0.84	[34]
Arabinan (Solid) + H_2O → Arabinos	0.90	[34]
Mannan (Solid) + H_2O → Mannose	0.90	[34]
Hemicellulose (Solid) → Furfural + 2 H_2O	0.005	[34]
Mannan (Solid) → HMF+ 2 H_2O	0.05	[34]
R-101-2		
H_2SO_4 + Ca $(OH)_2$ → Gypsum (Solid)	1.00	[34]
R-101-3		
H_2SO_4 + Ca $(OH)_2$ → Gypsum (Solid)	1.00	[34]

3.4.2 Saccharification (Section-201)

Most of the polysaccharides like cellulose remain unconverted or hydrolyzed in the pretreatment stage and are transformed into glucose in this section (**Figure 3.3**).

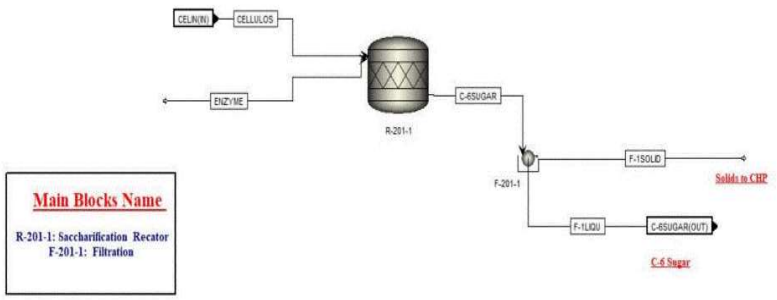


Figure 3. 3 Section-201 involving the enzymatic saccharification process

In the saccharification reactor (R-201-1), the reaction takes place at 32 °C and 96 hr with an enzyme loading rate of 20 mg/g dry mass. The conversion of cellulose to glucose at the end of enzymatic hydrolysis has been taken to be 90 % [34]. Detailed information related to process stoichiometries and conversion factor for saccharification and fermentation (Section-401) can be found in **Table 3.3**.

Table 3. 3 Saccharification (Section-201) and BioSA fermentation (Section -401) main reaction stoichiometries and conversion factors

Reaction	Conversion Factor	Reference
R-201-1		
Cellulose (Solid) + H_2O → Glucose	0.90	[34]
2Cellulose (Solid) + H_2O → Cellobiose	0.012	[34]
R-401-1S and R-401-2S (Seed reactors)		
Glucose + 1.1 NH_3 → 5.7 Biomass + 3 H_2O + 0.2 CO_2	0.30	[47]
Xylose + 0.9 NH_3 → 4.7 Biomass + 2.5 H_2O + 0.2CO_2	0.30	[47]
R-401-3F		
Glucose + 1.1 NH_3 → 5.7 Biomass + 3 H_2O + 0.2 CO_2	0.085	[47]
Xylose + 0.9 NH_3 → 4.7 Biomass + 2.5 H_2O + 0.2CO_2	0.043	[47]
Glucose + 0.85 CO_2 → 1.71 BioSA+ 0.85 H_2O	0.67	[48]
3 Glucose + 2 CO_2 → 4 BioSA+ 2 H_2O + 2 Acetic acid	0.16	[49]
7 Xylose + 5 CO_2 → 10 BioSA+ 5 H_2O	0.30	[47]
3 Xylose + 2 CO_2 → 4 BioSA+ 2 H_2O + 0.5 Acetic acid	0.26	[47]
7 Arabinose + 5 CO_2 → 10 BioSA+ 5 H_2O	0.20	[50]
Cellobiose + CO_2 → 2 BioSA+ 2.5 Acetic acid	0.97	[51]

3.4.3 Multi Effect Evaporator (MEE) (Section-301)

For scenario 1 only, where both C-6 and C-5 sugar are used for the SA fermentation, the MEE unit is used to concentrate the sugar stream from 110 g/l to the required concentration of 200 g/l to serve as the substrate for the fermentation microorganism *A. succinogenes*. A preheater (H-301-1) provides sensible heat to the sugar mixture stream. Excess water is evaporated by three calandria (CAL-1, CAL-2, CAL-3) and the cooler arrangement (**Figure 3.4**). Condensed water from the cooler (CO-301-3) is transferred to the WWTP, and concentrated sugar is directed to the fermentation section by a transfer pump (P-301-1).

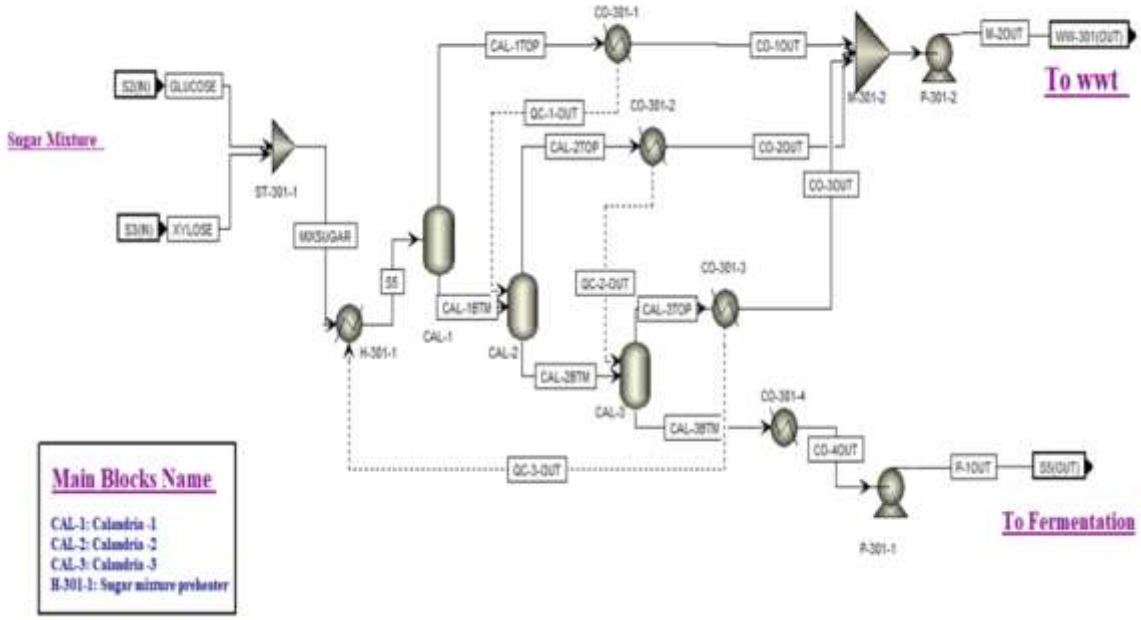


Figure 3. 4 Section-301 involving MEE

3.4.4 Fermentation (Section-401)

The *A. succinogenes* strain, which is capnophilic (CO_2 loving) in nature and requires CO_2 feed to maintain oxygen-free conditions in the fermentation reactor, is considered for the BioSA

fermentation to convert both C-6 and C-5 sugars as it has been reported to have high yield and productivity [52,53]. *A. succinogenes* has been reported to be among the best biocatalysts for industrial succinate fermentation [54,55]. 10 % by volume of the total sugars is diverted to the seed culture reactors (R-401-1S, R-401-2S) to minimize the microorganism's lag phase **(Figure 3.5),** and the remaining 90 % sugar volume is sent to the main fermentation reactor (R-401-3F) via the preheater (H-401-1) and the cooler (Co-401-1) arrangement.

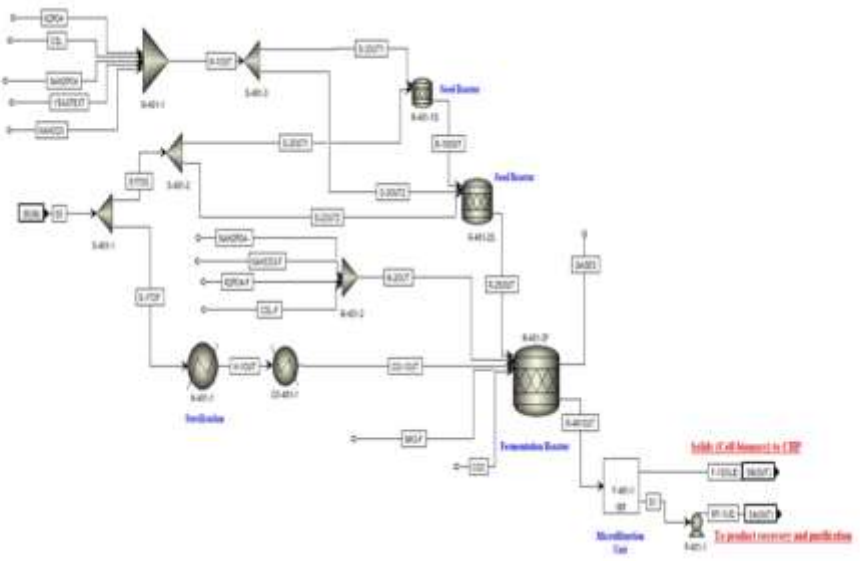


Figure 3. 5 Section-401used for the fermentation section

Temperature and residence time for the fermentation reaction is considered 37°C and 38 hr, respectively. The strain of *A. succinogenes* has an optimum sugar concentration of ≤100 g/l (when C-6 is used) and 200 g/ l (when both C-6 and C-5 were used) was introduced intermittently for replenishing the sugar concentration into the fermenter. For better performance and to avoid inhibition of microorganisms fed-batch configuration was used [56–58]. A microfiltration unit (F-401-1) is used for cell removal, and the filtrate is transferred for product recovery and purification section by a pump (P-401-1).

3.4.5 Product recovery and purification (Section-501)

In this process stage, BioSA is recovered and purified by reactive extraction (C-1, C-2, C-3), back extraction (BCEX), followed by crystallization (CRY-501), and drying (D-501-1). Each reactive extractive column has a separation efficiency of 86 %. A mixture of 1-octanol (87 % wt) and triethylamine (13 % wt) is used as the extractant. BioSA is back-extracted from the organic solvent by a mixture of trimethylamine (25% wt) and water (75 % wt) in the back-extraction column [59]. Extracted BioSA undergoes crystallization at 20 °C [60]. This is followed by filtration (F-501-1) and drying for moisture removal **(Figure 3.6)**.

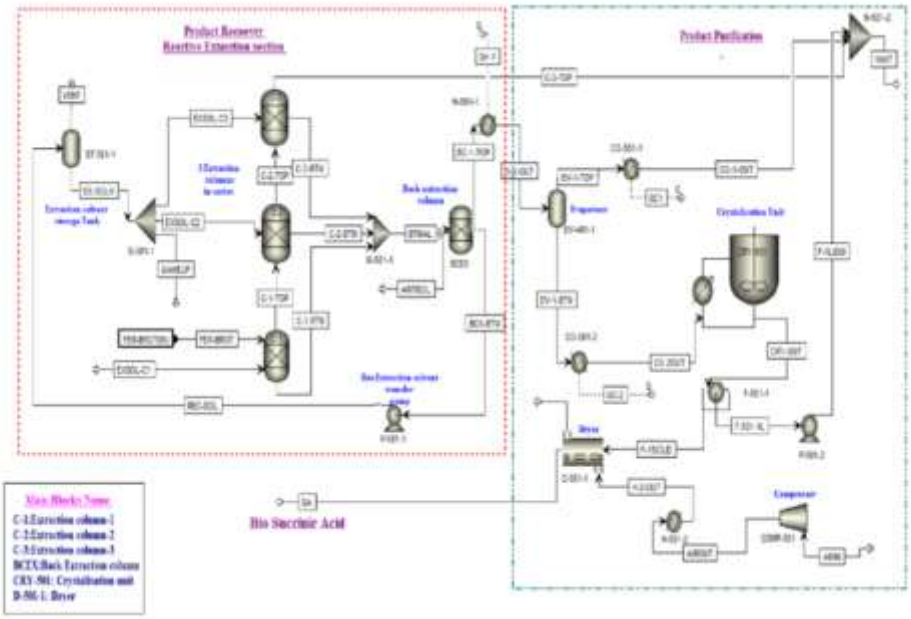


Figure 3. 6 Section-501 used for product recovery and purification

3.4.6 Waste Water Treatment Plant (WWTP) (Section-601)

All the liquid waste streams from the biorefinery are collected in the WWTP. This is modeled by using the R-stoic reactor involving a mesophilic anaerobic digestion unit (R-601-H, R-601-A, R-

601-M). Hydrolysis, acidogenesis, and acetogenesis followed by methanogenesis **(Figure 3.7)** are modeled individually by R-stoic reactor that produces biogas and sludge.

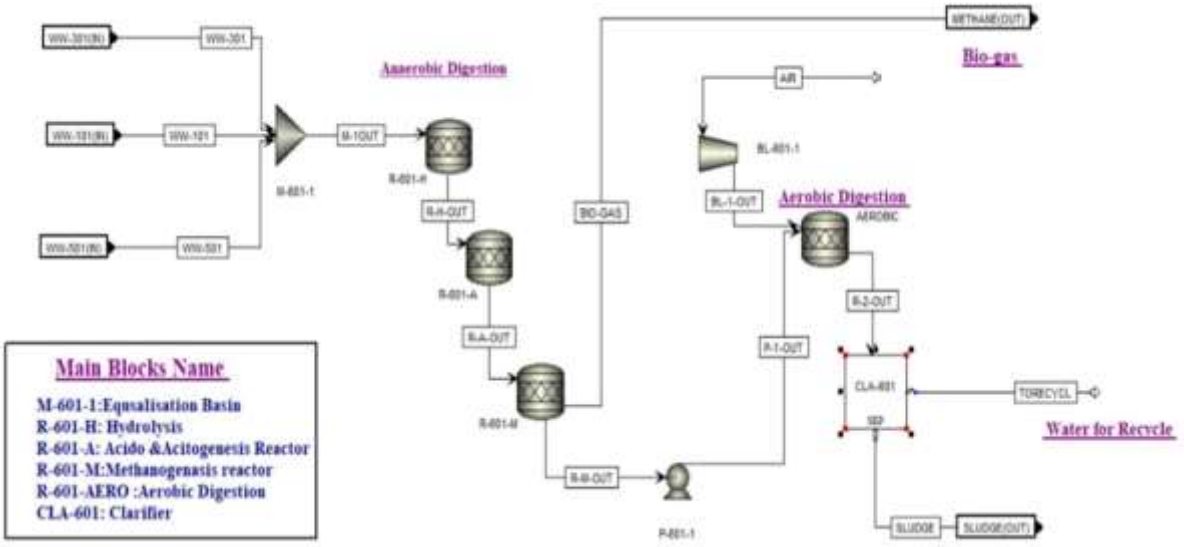


Figure 3. 7 Section-601 used for the Waste Water Treatment Plant (WWTP)

The sludge is pumped into the aerobic digestion unit (R-601-2), followed by the clarification unit (CLA-601). The concentrated sludge from the clarifier is directed to the CHP. The overflow water is reused for other biorefinery operations after purification. Biogas generated from the WWTP is diverted to the CHP unit. The process stoichiometry and fractional conversion for the anaerobic and aerobic digestion processes are based on a National Renewable Energy Laboratory (NREL) report [34].

3.4.7 Combined Heat and Power (CHP) generation (Section-701)

The required energy for BioSA production can be obtained from the CHP plant. Different streams from the biorefinery, including lignin, biogas, sludge, cell mass from saccharification, and fermentation, can be burned in the boiler **(Figure 3.8)**. Generated vapors were introduced into two

high- and low-pressure turbines (TUR-1, TUR-2). The output from this section is high-pressure steam (13 bar), low-pressure steam (4 bar), and electricity. The electricity produced and the steam generated will depend on the scenario under consideration. The boiler economizer (H-701-2) and superheater (FL-701-1) are modeled using the heater and flash model respectively.

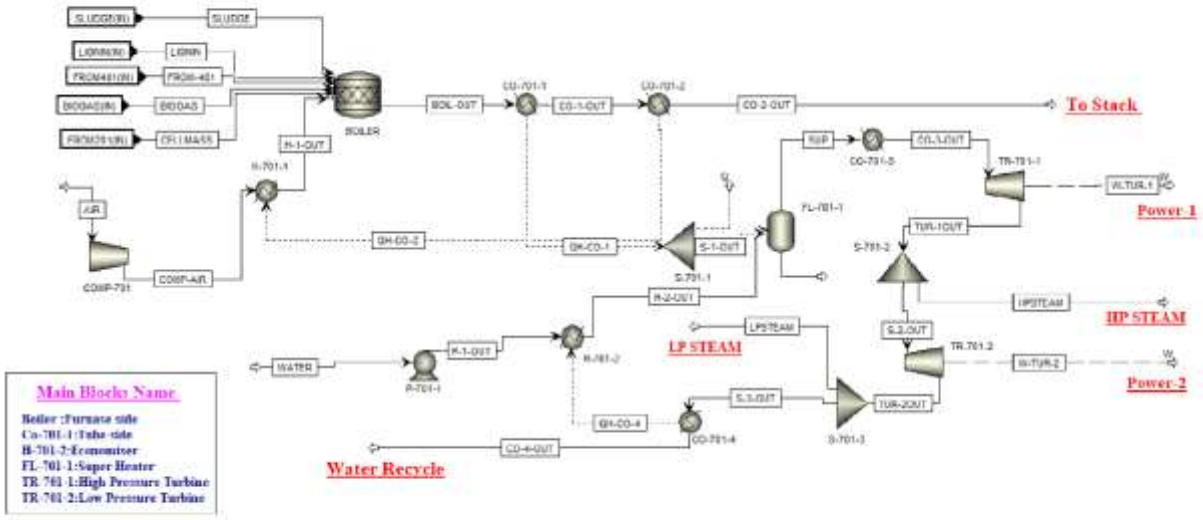


Figure 3. 8 Section-701 representing the Combined Heat and Power (CHP) unit

3.4.8 Furfural production (Section-801)

For scenario 2, C-5 sugar (10.8 % wt/wt) from the pretreatment and detoxification section-101 is diverted to Section-801. The furfural production process consists of a bi-phasic reactor (R-801-1) followed by a decanter (SE-801-1) and two columns (C-1-FUR, C-2-FUR) for product separation. The addition of NaCl improves the saturation of water, which reduces the solubility of tetrahydrofuran (THF) in water and results in reduced solvent losses. Detailed information related to process stoichiometries and conversion factor for furfural production (Section-801) and Waste

Water Treatment Plant (Section-601) can be found in **Table 3.4**. Reactor R-801-1 operates at 200 °C and 15 bar pressure, which is modeled based on a study conducted by Rong Xing et al. [61].

Table 3. 4 Wastewater treatment plant (Section-601) and furfural production (Section-801) main reaction stoichiometries and conversion factors

Reaction	Conversion Factor	Reference
Anaerobic reactions		
2 Ethanol → $3CH_4 + CO_2$	0.90	[34]
Acetic acid → 2.43 Biomass	0.03	[34]
1.12 Acetic acid → 2.2 CH_4 + 0.73CO_2	0.90	[34]
Aerobic reactions		
3 O_2 + Ethanol → 3 Water + 2 CO_2	0.61	[34]
2O_2 + Acetic acid → 2 Water + 2 CO_2	0.68	[34]
Acetic acid → 2.43 Biomass	0.22	[34]
Ethanol → 1.8704 Biomass	0.22	[34]

R-801-1		
Xylose → Furfural + 3 H_2O	0.90	[61]
Xylose → Acetic acid + 5 H_2O	0.10	[61]
Arabinos → Furfural + 3 H_2O	0.90	[61]

Organic solvent recovered from C-1-FUR from the top and bottom product is transferred to C-2- for the recovery of furfural as shown in **Figure 3.9**.

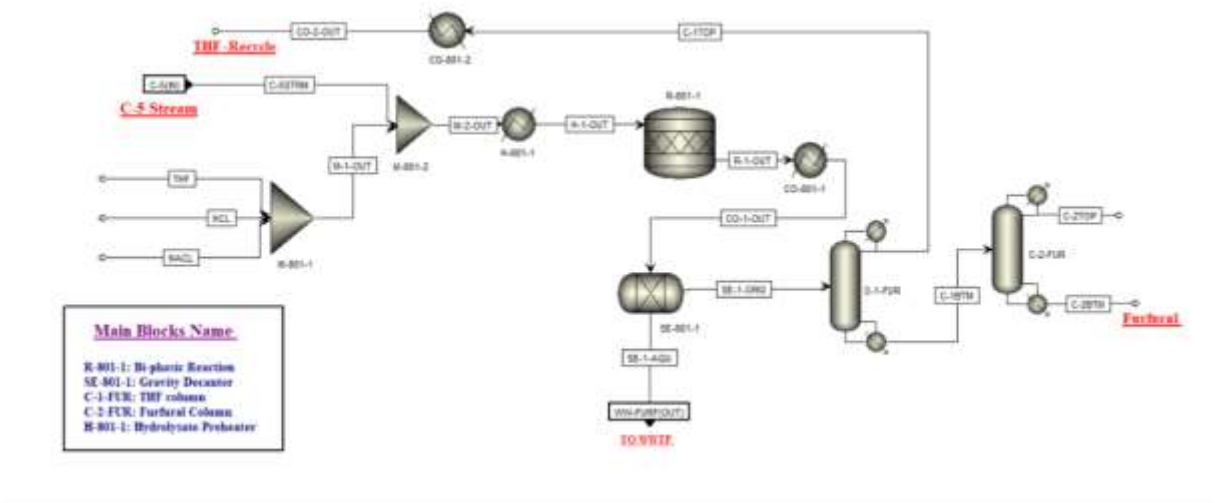


Figure 3. 9 Section-801used for furfural production

3.5 Results and discussion

Detailed information of simulation, equipment sizing and mapping can be found in **Table 3.5**. In addition, equations used for the calculation of process economy also tabulated in **Table 3.6**.

Table 3. 5 Detailed information of simulation and equipment cost calculation for main equipments

***Note:** Equipment costs are scaled based on the NREL report by Humbird et al. [34] as a reference cost. CEPCI (Chemical Engineering Plant Cost Index) value for the year 2007 (reference year) taken 525 and for the scaled year (2021) taken 607. Equipment sizes are determined by the mass flow rate of individual equipment in the BioSA refinery.

Reaction block	Simulation details	Sizing and costing details
Pretreatment reactor (R-101-1)	To simulate steam explosion pretreatment reaction temperature 190 °C and pressure 1.15 MPa (15 bar) set for reactor R-101-1. stoichiometry reactor (R-stoic) model used to replicate conversion processes for pretreatment reaction. After the acid impregnation step and before pretreatment, stream M-2OUT is heated by preheater H-101-1 up to pretreatment temperature. As a base method, NRTL was selected for the simulation of the process.	Scaled from the base cost of (6604133 USD) with scaling exponential 0.6 and CEPIC values (525 for 2007 and 607 for 2020). The preferred material for the reactor chosen during costing is Hastelloy due to higher pressure and temperature reaction conditions in acidic pH. Costing performance based on Humbird et al. [34].
Saccharification rector (R-201-1)	Reaction temperature 50 °C and 1 atm pressure. Total residence time for the saccharification operation is considered 96 hours. For	Sized based on volumetric flow rate. Total volume = residence time x volumetric flowrate. Number of tanks = total volume/30 m^3. A Stainless steel-304 (SS-304) saccharification

Reaction block	Simulation details	Sizing and costing details
	cleaning 6 hours were considered for the calculation. As a base method, NRTL was selected for the simulation of the process.	tank was considered and scaled to the required size by using 0.7 as a scaling factor.
Seed train reactors	To produce a sufficient number of microorganisms for fermenters, the seed train was simulated by using the R-stoic model at a temperature of 38 °C and 1 atm pressure. The size and numbers of reactors in the train were decided based on a sugar stream flow rate to seed train reactors. 10 % of the total sugar streamflow was diverted to seed reactors. As a base method, NRTL was selected for the simulation of the process.	Sized based on volumetric flow rate. The seed train contains a total of 10 reactors. For costing purposes stainless steel (SS-316) is considered.
Fermenter	*A. Succinogenes* *m*icroorganism used for the conversion of sugar to succinic acid at 38°C and 1 atm at neutral pH conditions. To maintain an anaerobic	Sized based on volumetric flow rate. Total volume = residence time x volumetric flowrate. Number of tanks = total volume/30 m3

Reaction block	Simulation details	Sizing and costing details
	condition continuous supply of CO_2 was considered. As a base method, NRTL was selected for the simulation of the process.	Total installation cost = no of fermentation unit x installed cost per unit The cost calculated by the aspen process economic analyzer is used for the costing.
Extraction and back extraction columns	Each column was simulated considering 86 % separation efficiency. Three extraction columns in a series and one back extraction column with separation efficiency of 99 % succinic acid simulated based on Kurzrock et al. [59]. As a base method, UNIFAC was selected for the simulation of the process.	All columns were mapped as a DVT CYLINDER and cost was calculated by using an aspen process economic analyzer.
Anaerobic basin	R-STOIC reactor model was used to simulate the conversion of organic constituents into biogas. Hydrolysis, Acidogenesis and acetogenesis, and methanogenesis stage were simulated in three different reactors. As a base method,	Costing is performed by scaling the process by using 0.6 as a scaling factor from the base cost (6750000 USD). Concrete was considered as a material of construction during costing. Costing is performed based on Humbird et al [34].

Reaction block	Simulation details	Sizing and costing details
	NRTL was selected for the simulation of the process.	
Clarifier	Sludge removal efficiency selected 0.90 % by keeping a solid to solid outlet ratio of 0.9 infiltration unit. As a base method, NRTL was selected for the simulation of the process.	Equipment cost calculated by Aspen Process economizer
Boiler	To replicate the combustion reaction, the R-stoic reaction model was used, and the cooler unit was used to replicate the tube side of the boiler. For economizer and superheating operating heater model used. As a base method, NRTL was selected for the simulation of the process.	Baghouse cost is also considered during the costing. Costing is performed by scaling the process by using 0.6 as a scaling factor from base cost (28550000USD) and with a 1.8 installation factor. Costing performance based on Humbird et al. [34].
Turbine	Two turbines simulated for higher- and low-pressure steam and electricity production.	Cost also covers the generator cost. Costing is performed by scaling the process by using 0.6 as a scaling factor from base cost (9500000USD) and with a 1.8 installation

Reaction block	Simulation details	Sizing and costing details
		factor. Costing is performed based on Humbird et al [34].
Bi-phasic Reactor	Biphasic reactor for xylose to furfural conversion simulated using R-stoic model. The conversion process was simulated at a temperature of 200 °C and a pressure of 15 atm. UNIFAC property method used to simulate phase separation.	Costing is performed by scaling the process by using 0.6 as a scaling factor from base cost (6604133USD) and with a 1.5 installation factor. Costing is performed based on Humbird et al. [34].
Distillation columns	For the separation of furfural from organic solvent two distillation columns were simulated for the separation of THF and furfural respectively. Column-1 was simulated in 18 stages and column-2 was simulated in 23 stages. As a base method, NRTL was selected for the simulation of the process.	Equipment cost calculated by Aspen Process economizer

Table 3. 6 Important equations used for economic analysis

Sr. No	Equation used for	Equation
1	Equipment cost	$\text{Cost} = \text{Cost ref} * \left(\frac{\text{Capacity}}{\text{Capacity ref}}\right)^{\text{scaling factor}} * \left(\frac{\text{CEPCI}}{\text{CEPCIref}}\right)$
2	Cash flow for the project	Cash flow= Net Profit + Depreciation
3	Total income tax annually	$\text{Income tax} = (\text{Revenue} - \text{All expenses}) * \text{Tax rate}$
4	Net profit before paying income tax	$\text{Net profit before tax} = (\text{Revenue} - \text{All expenses})$
5	Net profit after paying income tax	$\text{Net profit after tax} = (\text{Revenue} - \text{All expenses} - \text{Income tax})$
6	Payback period for the project	$\text{Payback period} = \frac{\text{Total investment}}{\text{Average annual cashflow}}$
7	Minimum selling price (MSP)	$\text{MSP} = \frac{\text{Annualized Capital cost+ Operating cost}}{\text{BioSA production capacity of the biorefinery}}$

3.5.1 Process simulation results

Process simulation results for utility and power requirements are presented in **Figure 3.10**. Scenario 2 consumed the highest hot and cold utilities compared to the other scenarios. Bi-phasic reactor (R-801-1) is the highest consumer of energy with 1051 kW hot utility demand. The requirement of high pressure and temperature conditions makes the furfural production process energy-intensive. Scenario 3 demands the least amount of hot and cold utility due to the diversion of C-5 sugar for biogas generation. In addition, it has the highest electricity production of 207 kW compared to the other two scenarios. However, it also has a higher load on WWT and requires 131 kW of electricity to treat the higher load of wastewater.

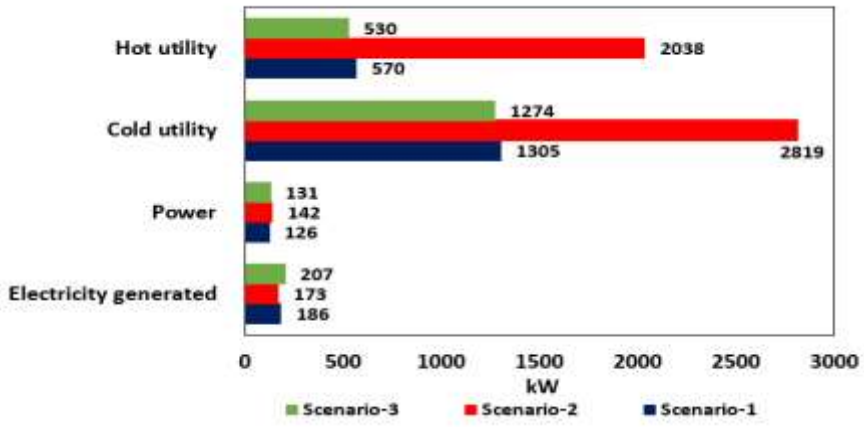


Figure 3. 10 Scenario wise comparison of utility and power requirement

The need for MEE (Section-301) to concentrate sugar stream for fermentation results in scenario 1 requiring higher utility compared to scenario 3. However, 60 kW of excess electricity is also available for sale from this configuration. From scenario 3, a maximum of 76 kW of excess electricity is available for sale. **Table 3.7** represents the mass flow of products, co-products, and sellable electricity produced in each scenario.

Table 3. 7 Product/co-product mass flow in each scenario

Product/co-product mass flow	Scenario 1	Scenario 2	Scenario 3
BioSA (kg/hr)	383.16	258.19	258.19
Furfural (kg/hr)	-	99.98	-
Sellable electricity (kW)	60	31	76

3.5.2 Process economy results

Table 3.8 shows a comparison of TDC, TIC, FCI, and TCI for all scenarios. The observed difference in process economy parameters is due to the difference in process steps for each scenario. The detailed information equipment purchase and installation cost can be found in **Table 3.9**.

Table 3. 8 Total Capital Investment (TCI) and other process economy parameter comparison for the three scenarios

Cost components	Scenario 1 (million USD)	Scenario 2 (million USD)	Scenario 3 (million USD)
Pretreatment and detoxification (Section -101)	6.08	6.08	6.08
Saccharification (Section-201)	0.75	0.75	0.75

Cost components	**Scenario 1 (million USD)**	**Scenario 2 (million USD)**	**Scenario 3 (million USD)**
Multi Effect Evaporation (MEE) (section-301)	0.60	-	-
Fermentation (Section-401)	1.44	1.49	1.48
Product recovery and purification (Section-501)	1.10	1.03	1.03
Waste Water Treatment Plant (WWTP) (Section-601)	1.37	1.20	1.36
Combine Heat and Power (CHP) unit (Section-701)	2.92	2.92	3.28
Furfural production (Section-801)	-	2.80	-
Installed equipment cost	**14.26**	**16.27**	**13.98**
Warehouse (4% of Inside Battery Limit (ISBL))	0.40	0.49	0.37
Site development (9% of ISBL)	0.90	1.09	0.84
Piping (4.5 % of ISBL)	0.45	0.55	0.42

Cost components	Scenario 1 (million USD)	Scenario 2 (million USD)	Scenario 3 (million USD)
Total Direct Costs (TDC)	**16.01**	**18.39**	**15.61**
Portable expenses (10% of TDC)	1.60	1.84	1.56
Field expenses (10% of TDC)	1.60	1.84	1.56
Office and construction (20% of TDC)	3.20	3.68	3.12
Project contingency (10% of TDC)	1.60	1.84	1.56
Other costs (startup and permits) (10% of TDC)	1.60	1.84	1.56
Total Indirect Costs (TIC)	**9.60**	**11.04**	**9.37**
Fixed capital investment (TDC+TIC)	25.61	20.24	24.99
Working capital (5% FCI)	1.28	1.47	1.25
Land	0.48	0.55	0.47
Total Capital Investment (TCI)	**27.37**	**31.46**	**26.71**

Table 3. 9 Detailed information of equipment purchase and installation cost

***Note:** The equipment costs are indexed from the reference cost by using Chemical Engineering Plant Cost Index (CEPCI) value for the year of calculation. The reference year is 2007 for which the CEPCI value 525 is considered. The calculation year is 2021 with 607 as a CEPCI value.

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
Pre-treatment (Section-101)	H-101-1	Calculated using CEPCI	3309.33	7280.53	3309.33	7280.53	3309.33	7280.53
	R-101-1	Calculated using CEPCI	850781.60	1276172.39	850781.60	1276172.39	850781.59	1276172.39
	Flash Drum	Calculated using CEPCI	12495.76	24991.52	12495.76	24991.52	12495.75	24991.51
	CO-101-1	Calculated using CEPCI	2925.57	6436.25	2925.57	6436.25	2925.56	6436.24

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
	CO-101-2	Calculated using CEPCI	17721.34	38986.94	17721.34	38986.94	17721.33	38986.94
	P-101-1	Calculated using CEPCI	411.47	946.37	411.47	946.37	411.46	946.37
	F-101-1	Calculated using CEPCI	2235058.13	3799598.82	2235058.13	3799598.82	2235058.12	3799598.81
	R-101-2	Calculated using CEPCI	99600.00	164800.00	99600.00	164800.00	99600	164800
	R-101-2 AGITATOR	Calculated using CEPCI	1622.02	2433.04	1622.02	2433.04	1622.02	2433.035
	CO-101-3	Calculated using CEPCI	99600.00	164800.00	99600.00	164800.00	99600	164800
	R-101-3	Calculated using CEPCI	99600.00	164800.00	99600.00	164800.00	99600	164800

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
	R-101-3 Agitator	Calculated using CEPCI	1653.50	2480.26	1653.50	2480.26	1653.50	2480.25
	F-101-2	Calculated using CEPCI	140200.00	186900.00	140200.00	186900.00	140200	186900
	P-101-3	Calculated using CEPCI	1385.50	3186.65	1385.50	3186.65	1385.49	3186.64
	SP-101-1	Calculated using CEPCI	2094.49	4188.97	2094.49	4188.97	2094.48	4188.97
	SP-101-2	Calculated using CEPCI	140200.00	186900.00	140200.00	186900.00	140200	186900
	C-5 stream storage tank	Calculated using CEPCI	6209.13	18627.40	6209.13	18627.40	6209.13	18627.39
	Cellulose storage tank	Calculated using CEPCI	6598.86	19796.58	6598.86	19796.58	6598.86	19796.58

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
Saccharification (Section-201)	Screw conveyer - 1 (for corn stover)	Calculated using CEPCI	872.34	872.34	872.34	872.34	872.34	872.34
	Screw conveyer - 2 (Lignin to CHP)	Calculated using CEPCI	391.09	391.09	391.09	391.09	391.08	391.08
	P-101-4	Calculated using CEPCI	3463.55	7966.17	3463.55	7966.17	3463.55	7966.17
	H-201-1	Calculated using CEPCI	3216.72	7076.77	3216.72	7076.77	3216.72	7076.77
	R-201-1	Calculated using CEPCI	266996.27	533992.54	266996.27	533992.54	266996.27	533992.54
	CO-201-1	Calculated using CEPCI	5498.34	12096.34	5498.34	12096.34	5498.34	12096.34
	F-201-1	Calculated using CEPCI	140200.00	186900.00	140200.00	186900.00	140200.00	186900.00

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
MEE (Section-301)	P-201-1	Calculated using CEPCI	2667.08	6134.28	2667.08	6134.28	2667.08	6134.28
	M-301-1 (Storage tank)	Calculated using CEPCI	14185.14	42555.43				
	H-301-1	Calculated using CEPCI	15952.57	35095.64				
	CAL-1	Aspen Plus	19100.00	129200.00				
	CAL-2	ASPEN Plus	19100.00	129200.00				
	CAL-3	Aspen Plus	16500.00	125200.00				
	CO-301-1	Calculated using CEPCI	13467.14	29627.71				
	CO-301-2	Calculated using CEPCI	14657.67	32246.88				
	CO-301-3	Calculated using CEPCI	15952.57	35095.65				

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
Fermentation (Section-401)	CO-301-4	Calculated using CEPCI	5660.50	12453.10				
	P-301-1	Calculated using CEPCI	2249.36	5173.53				
	M-301-2 (Storage tank)	Calculated using CEPCI	8038.78	24116.33				
	P-301-2	Calculated using CEPCI	1859.90	4277.77				
	H-401-1	Calculated using CEPCI	2627.52	5780.55	5488.58	12074.88	5488.58	12074.88
	CO-401-1	Calculated using CEPCI	3755.04	8261.09	4850.60	10671.32	4850.60	10671.32
	Micro filtration	Calculated using CEPCI	16500.00	117700.00	16500.00	117700.00	16500.00	117700.00

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
	Seed reactors	Calculated using CEPCI	17406.20	34812.41	24190.32	48380.65	20158.60	40317.20
	Fermenters	Calculated using CEPCI	309822.79	1051816.46	309822.79	1051816.46	309822.79	1051816.46
	Fermentation broth storage tank	Calculated using CEPCI	121387.65	218497.77	134829.86	242693.75	134829.86	242693.75
	P-401-1	Calculated using CEPCI	2284.67	5254.74	2706.75	6225.54	2706.75	6225.54
	Multistage compressor	Calculated using CEPCI	1677.21	2683.54	1677.21	2683.54	1677.21	2683.54
	ST-501-1	Calculated using CEPCI	4449.40	13348.21	4449.40	13348.21	4449.40	13348.21
	C-1	Aspen Plus	16500.00	117700.00	16500.00	117700.00	16500.00	117700.00
	C-2	Aspen Plus	16500.00	117700.00	16500.00	117700.00	16500.00	117700.00
	C-3	Aspen Plus	16500.00	117700.00	16500.00	117700.00	16500.00	117700.00
	BCEX	Aspen Plus	16500.00	117700.00	16500.00	117700.00	16500.00	117700.00

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
Product recovery and purification (Section-501)	P-501-1	Calculated using CEPCI	843.75	1940.63	591.07	1359.45	591.07	1359.45
	H-501-1	Calculated using CEPCI	4130.83	9087.84	3143.36	6915.40	3143.36	6915.40
	EV-501-1	Calculated using CEPCI	16500.00	125200.00	16500.00	125200.00	16500.00	125200.00
	CO-501-2	Calculated using CEPCI	3128.36	6882.39	2370.24	5214.53	2370.24	5214.53
	CO-501-1	Calculated using CEPCI	14965.74	32924.63	11398.86	25077.49	11398.86	25077.49
	CRY-501	Calculated using CEPCI	146300.00	225000.00	111700.00	176100.00	111700.00	176100.00
	F-501-1	Calculated using CEPCI	140200.00	186900.00	140200.00	186900.00	140200.00	186900.00

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
WWTP (Section-601)	DRY-501	Calculated using CEPCI	12400.00	20100.00	11300.00	18400.00	11300.00	18400.00
	H-501-2	Calculated using CEPCI	322.99	710.57	322.99	710.57	322.99	710.57
	COMP-501	Calculated using CEPCI	1677.21	2683.54	1677.21	2683.54	1677.21	2683.54
	M-601-1 (Equalization basin)	Calculated using CEPCI	117990.70	117990.70	120386.02	120386.02	117724.06	117724.06
	Anaerobic reactor	Calculated using CEPCI	884914.98	884914.98	902895.17	902895.17	882930.45	882930.45
	P-601-1	Calculated using CEPCI	6114.15	14062.55	6269.20	14419.16	6164.93	14179.34
	Aerobic reactor	Calculated using CEPCI	117988.66	117988.66	119211.56	119211.56	117724.06	117724.06

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
CHP (Section-701)	Clarification	Calculated using CEPCI	81500.00	232300.00	20700.00	43500.00	81500.00	232300.00
	Boiler, Comp 1-701, H-701-1, Co-701-1	Calculated using CEPCI	1257887.11	2264196.80	1257887.11	2264196.80	1396476.44	2513657.60
	TR-1-701 and TR-2-701	Calculated using CEPCI	341925.53	615465.96	341925.53	615465.96	388741.63	699734.93
	P-701-1	Calculated using CEPCI	969.33	2229.46	969.33	2229.46	1114.28	2562.84
	P-701-2 (Condensate pump)	Calculated using CEPCI	194.14	446.51	194.14	446.51	194.14	446.51
	CO-701-2	Calculated using CEPCI	6463.04	14218.68	6463.04	14218.68	7070.24	15554.53
	CO-701-3	Calculated using CEPCI	4562.16	10036.75	4562.16	10036.75	8102.68	17825.90

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
Furfural production (Section-801)	CO-701-4	Calculated using CEPCI	533.50	1173.69	533.50	1173.69	3393.86	7466.49
	Economizer	Calculated using CEPCI	4562.16	10036.75	4562.16	10036.75	8101.22	17822.69
	M-FUR-1	Calculated using CEPCI			792.21	792.21		
	M-FUR-2	Calculated using CEPCI			1093.71	1093.71		
	R-FUR-1	Calculated using CEPCI			1117491.24	1676236.86		
	CO-FUR-1	Calculated using CEPCI			26632.50	58591.51		
	SEP-FUR	Aspen Plus			16500.00	117700.00		
	C-1-FUR	Aspen Plus			112800.00	430400.00		
	C-2-FUR	Aspen Plus			145200.00	494500.00		

			Scenario 1		Scenario 2		Scenario 3	
Area	**Equipment Id**	**Cost calculation source**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**	**Purchase cost (USD 2021)**	**Installation cost (USD 2021)**
	CO-FUR-2	Calculated using CEPCI			1815.50	3994.09		
	H-FUR-1	Calculated using CEPCI			7295.23	16049.50		
Total (million USD)				**14.26**		**16.27**		**13.986**

These figures will have a net contribution to the overall profitability of the scenarios, as will be discussed later. For all three scenarios, TOC and FOC for 1 kg BioSA production were calculated as shown in **Table 3.10**.

Table 3. 10 Total Operating Cost (TOC) and Fixed Operating Cost (FOC) details for three scenarios

Description	**TOC (USD/kg BioSA)**	**FOC (USD/kg BioSA)**
Scenario 1	1.44	0.53
Scenario 2	2.47	0.82
Scenario 3	1.90	0.70

For the calculation of Operating cost considered prices for raw material can be found in **Table 3.11**.

Table 3. 11 Raw materials prices considered in this study [62,63]

Raw material	**Quoted price (USD/tones)**
Corn stover	53.1
Sulfuric acid	89
NAOH	270
Lime	150

Raw material	Quoted price (USD/tones)
Corn steep liquor	200
Ammonia	530
Enzyme	15000
1-octanol	2000
Trimethyl amine (TME)	6000
K_2HPO_4	990
NaH_2PO_4	3500
$NaHCO_3$	280

The obtained value of TOC is the sum of VOC and FOC. The contribution of each raw material to VOC is shown in **Figure 3.11**. Co-product generation and raw material prices have a great impact on TOC. For scenario 1, minimum TOC was obtained as it has a higher amount of BioSA production compared to the other two cases. Enzyme cost is the highest contributing factor in VOC for all scenarios. Extraction solvents for the BioSA recovery are the second-highest contributor in all scenarios. For scenario 2 purchased steam and furfural recovery solvents contribute an additional 16 % and 12 %, respectively to VOC. The selling price of sellable electricity and furfural is considered as a credit during the discount cash flow preparation.

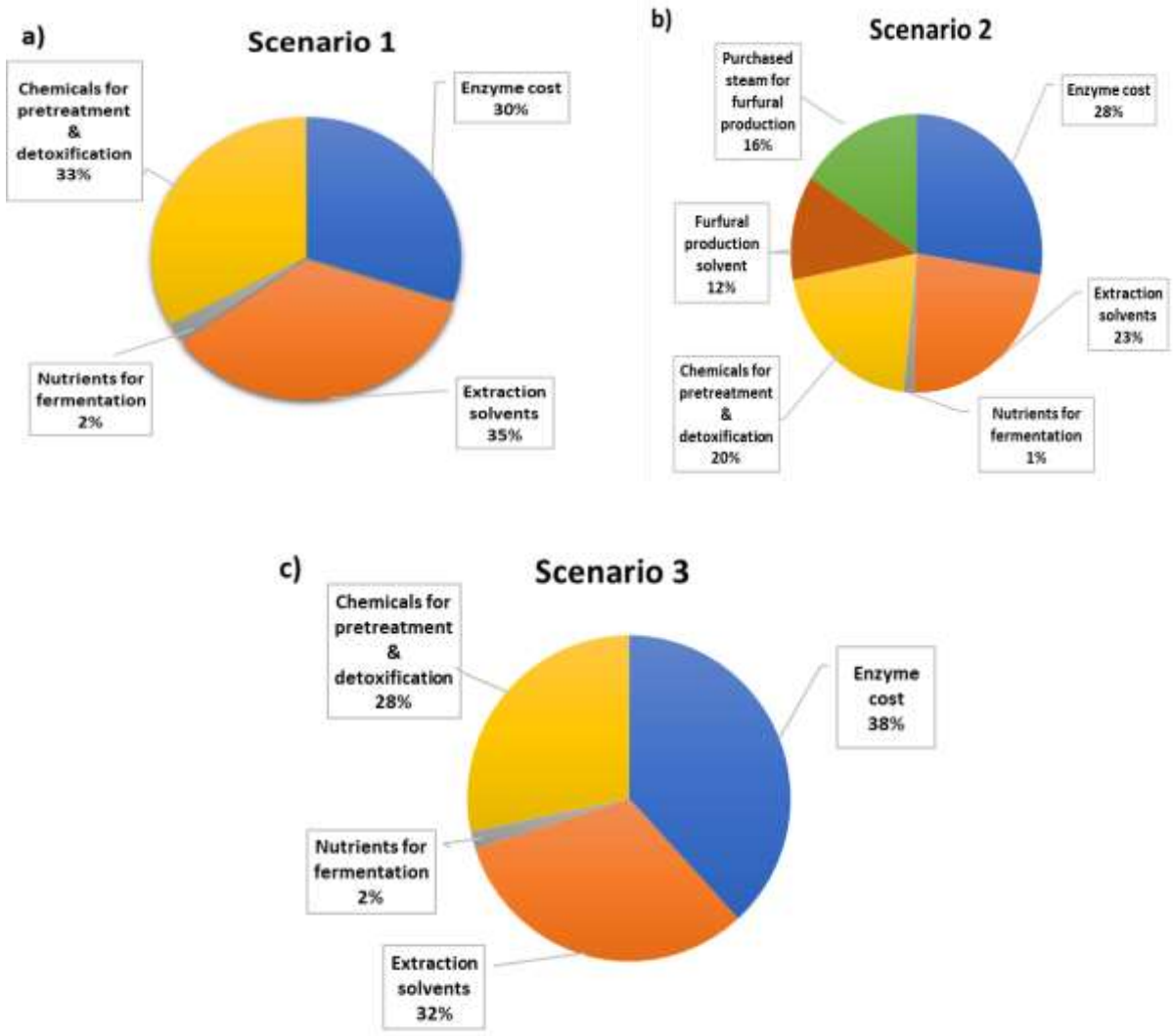


Figure 3. 11 Scenario wise Variable Operating Cost (VOC) comparison (a) scenario 1 (b) scenario 2 and (c) scenario 3

3.5.3 Sensitivity analysis of TOC with respect to raw material prices and various economic parameters to NPV

Variation in raw material prices also affects the variable operating cost. Variations in enzyme cost, extraction solvent cost, and feedstock prices and their impact on total operating cost were also studied by performing sensitivity analysis with a ±50 % variation in prices. From **Figure 3.12 (a)**,

it is observed that a 50% reduction in enzyme cost decreases the TOC up to 1.29 USD/kg BioSA, whereas 1.59 USD/kg BioSA TOC is observed at a 50% increment in enzyme price for scenario 1. Feedstock price and extraction solvent also had a notable influence on TOC.

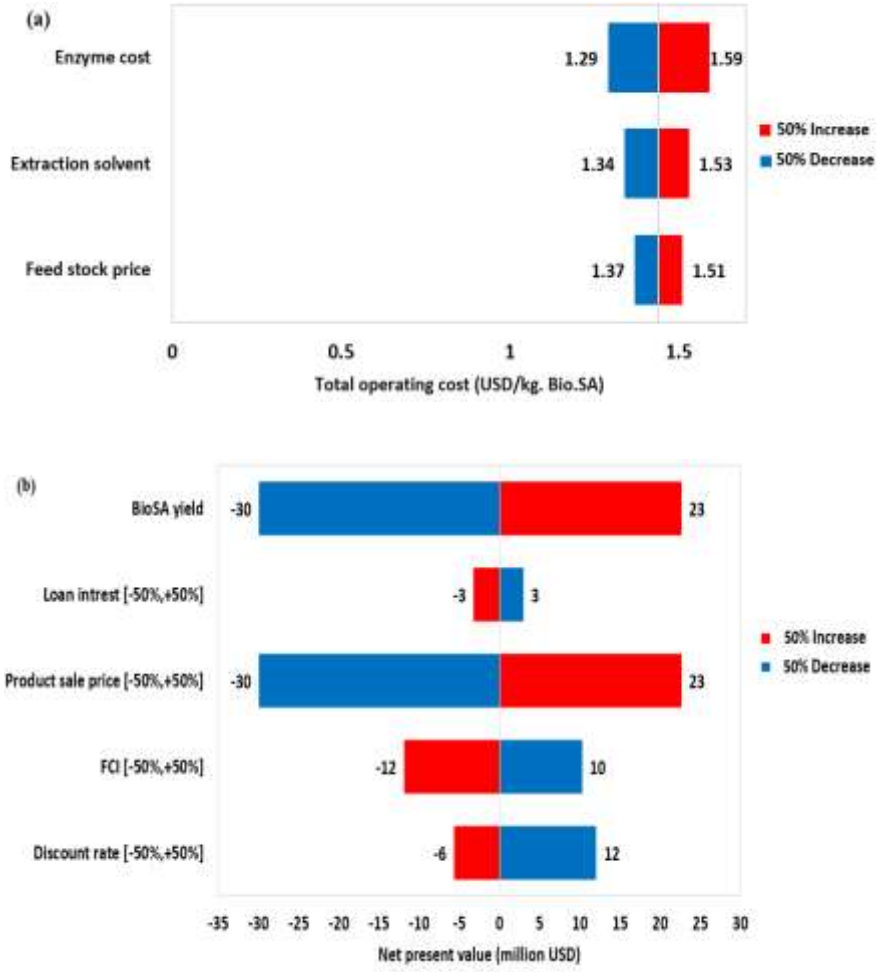


Figure 3. 12 Sensitivity analysis for scenario 1 showing the effects of several parameters on (a) total operating cost and (b) net present value

For a 50% reduction in extraction solvent price, TOC is reduced to 1.34 USD/kg, whereas, with a 50 % increase, TOC rises to 1.53 USD/kg. For ±50 % change in feedstock price, ±4.86 % variations in TOC were observed. Thus, onsite enzyme production and the development of a less

costly extraction solvent with higher extraction efficiency needs to be explored for the improvement of the process economy of BioSA. A sensitivity analysis was also carried out for Scenario 1 to understand the effect of various factors on NPV, as shown in **Figure 3.12 (b)**. It was observed that the product sale price has the biggest impact on NPV. For instance, when product sale price increased by 50 %, an increment of 23 % was observed in NPV, whereas FCI, discount rate, and loan interest had the opposite impact on NPV. Variations in loan interest rates had a comparatively smaller influence on NPV. In addition, NPV was also highly influenced by the BioSA yield. Hence the development of efficient SA-producing microorganisms and better fermentation strategies need to be explored for the improvement of BioSA yield and eventually the overall process economy. Moreover, the governments also have to introduce lower interest rate loans for the establishment of green projects. Such incentives help to improve the bioprocess economy and make them competitive with its conventional fossil resource counterpart.

3.5.4 Payback period and probability distribution of MSP for BioSA

DCFA was performed for all the scenarios at a 10 % discount rate for 30 years of plant life. MSP and payback period data are indicated in **Table 3.12**.

Table 3. 12 Comparison of Minimum Selling Price (MSP) and payback period for the three scenarios studied

Description	MSP (USD/kg BioSA)	Payback period (years)
Scenario 1	2.28	8
Scenario 2	3.33	9
Scenario 3	3.19	8

Scenario 1 shows the best performance for MSP and the payback period compared to other scenarios. Scenario 1 and scenario 3 have the same payback period of 8 years, but a considerable difference in MSP was observed between them. For the payback period of scenario 1, cash flow as a function of project life can be found in the **Figure 3.13**.

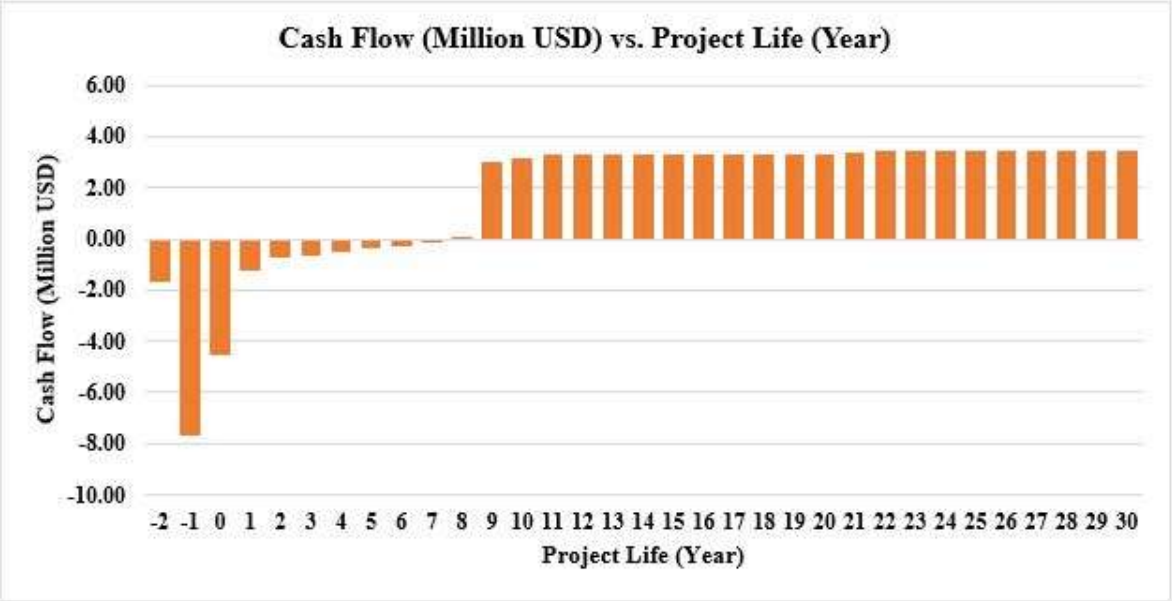


Figure 3. 13 Cash flow vs project life for scenario 1

In this calculation, three years for the construction and site establishment is also considered. For addressing uncertainties, a multi-variant Monte-Carlo analysis was also carried out based on revenue parameters with a -50 % and +100% limit. All revenue prices, including feedstock price and discount cashflow rate are used as key parameters for the analysis. Triangular probability distribution of determinants was applied [64] and stochastic results of MSP after 1000 iterations are presented in **Figure 3.14**. From the figure, it is observed that the mean value of MSP of BioSA for scenario 1 is 2.44 USD/kg with a standard deviation of 0.2624. The calculated MSP of BioSA from the present study was also compared to earlier studies as well as fossil-based SA. For

instance, Shaji et al. [32] calculated MSP of 2.37 USD/kg from sugarcane bagasse, which is slightly higher than scenario 1 and less than scenario 2 and scenario 3. The study undertaken by Stylianou et al. [65] estimated 2.5 USD/kg BioSA from organic waste source hydrolysates. Okoro et al. [31] calculated a very low MSP (0.77 USD/kg) for BioSA production from waste apple slurry. However, in their waste stream-based study zero feedstock price was assumed. In the present study, Scenario 1 shows the best potential as compared to the fossil-based route, which has an MSP of 2.3 USD/kg [8].

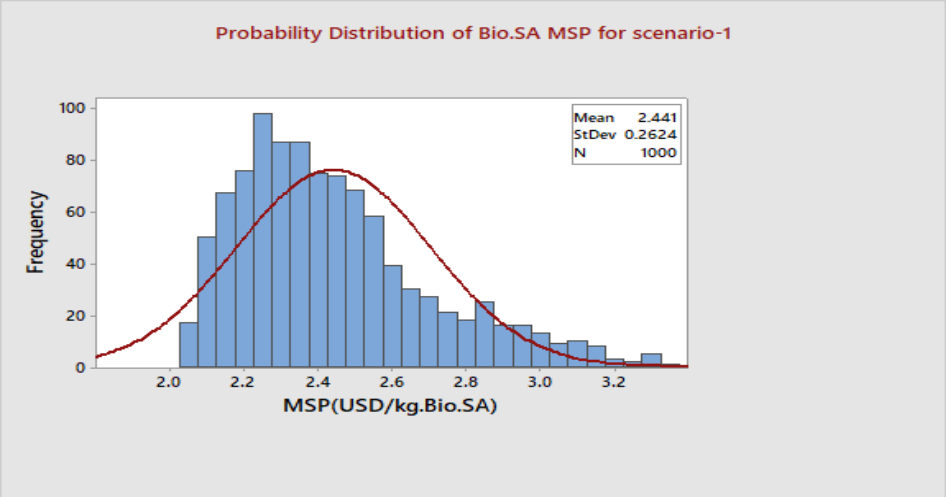


Figure 3. 14 Probability distribution of BioSA Minimum Selling Price (MSP) for scenario 1

3.5.5 Heat integration

Heat integration, an important aspect of green chemistry also studied for all three scenarios. **Figure 3.15** illustrates the composite curve for scenario 1, scenario 2, and scenario 3, respectively. Maximum possible heat recovery for all scenarios presented by the difference between minimum cold and hot utility requirements. It was observed that scenario 2 had the highest potential for heat recovery of 616694 kJ/hr or 1714.341 kW. Bi-phasic reactor (R-801-1) consumes the highest hot utility due to higher reaction temperature demand for the conversion of C-5 sugar to furfural. For

scenario 1 and Scenario 3, the calculated potential for heat recovery is 2510676 kJ/hr (697.39 kW) and 2562347 kJ/hr (711.74 kW) respectively. For scenario 1 and scenario 3 pretreatment reactors (R-101-1) were identified as the most energy-intensive process equipment.

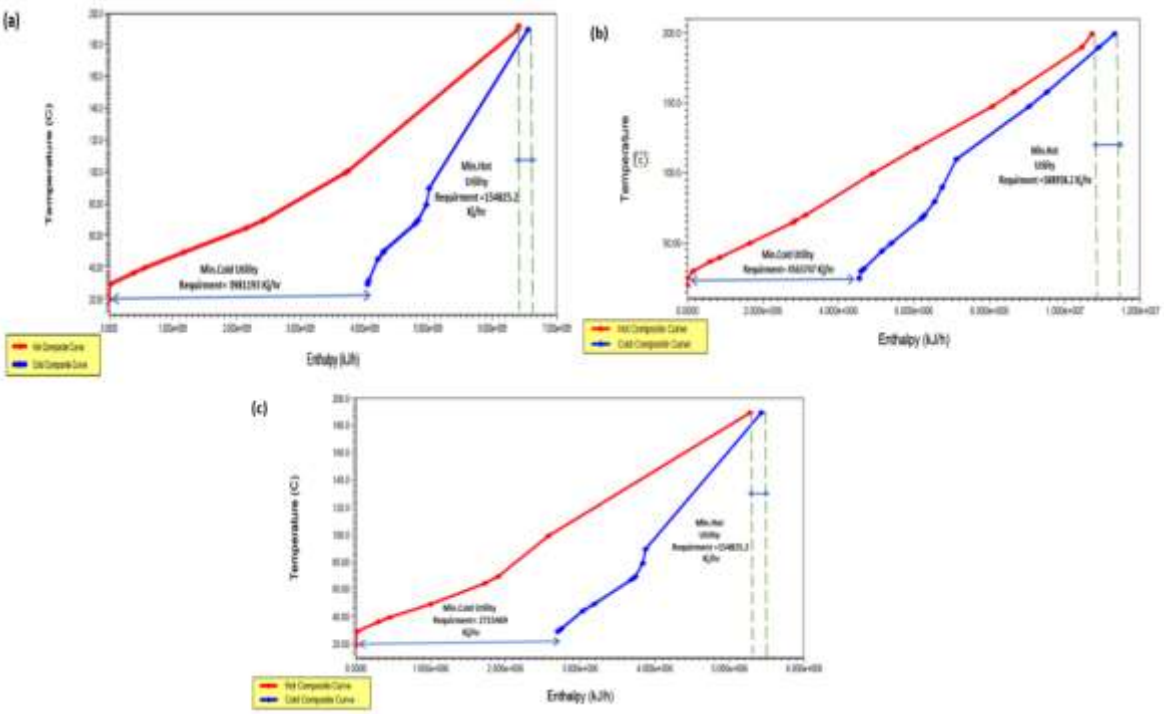


Figure 3. 15 Temperature vs. enthalpy plot for (a) scenario 1 (b) scenario 2 (c) scenario 3

3.6 Conclusion

The feasibility of multiproduct biorefinery using corn stover as a lignocellulosic biomass resource was assessed to produce BioSA, furfural, and electricity by three scenario-based studies to provide an economically sustainable BioSA biorefinery that is competitive to fossil-based SA production. Among the three scenarios studied, the production of BioSA using both C-6 and C-5 sugar and electricity from lignin (scenario 1) is the most economically viable with MSP of 2.28 USD/kg BioSA and an 8-year payback period. The biorefinery is self-dependent and can sustain itself for electricity and steam needs in this scenario. In scenario 2, the production of furfural is an energy-

intensive process because of the high pressure and temperature requirement for the conversion of C-5 sugars. This makes the process (scenario 2) economically less favorable. The purchase of steam for biorefinery operations adds to the variable operating cost and eventually leads to a higher MSP of BioSA. However, the economic performance of this scenario can be enhanced by heat integration. The composite curve for scenario 2 indicates a reduction in utility requirements. Scenario 3, with the production of biogas with the C-5 stream, is found to be the second-best option with an MSP of 3.19 USD/kg BioSA and an 8-year payback period. Value addition of biomass by using all the fractions of lignocellulosic biomass improves the process economy of biorefinery and makes them economically sustainable. However, the selection of a co-product is also an important aspect that influences the economic viability of a multiproduct biorefinery. The price of SA derived from the fossil-based route is 2.3 USD/kg [8]. However, this price is subject to fluctuation and is dependent on the geopolitics related to crude oil prices. Scenario 1 is hence competitive with the conventional counterpart. The utilization of three components of biomass and the proper selection of co-products will play a vital role in the successful growth of multiproduct biorefineries.

3.7 References

[1] S. Fernando, S. Adhikari, C. Chandrapal, N. Murali, Biorefineries: current status, challenges, and future direction, Energy & Fuels. 20 (2006) 1727–1737.

[2] B. Kamm, M. Kamm, Principles of biorefineries, Appl Microbiol Biotechnol. 64 (2004) 137–145.

[3] D.L. van Dyne, M.G. Blase, L.D. Clements, A strategy for returning agriculture and rural America to long-term full employment using biomass refineries, Perspectives on New Crops and New Uses. ASHS Press, Alexandria, Va. (1999) 114–123.

[4] T. Werpy, G. Petersen, Top value-added chemicals from biomass: volume I--results of screening for potential candidates from sugars and synthesis gas, National Renewable Energy Lab., Golden, CO (US), 2004.

[5] M. Alexandri, R. Schneider, H. Papapostolou, D. Ladakis, A. Koutinas, J. Venus, Restructuring the conventional sugar beet industry into a novel biorefinery: fractionation and bioconversion of sugar beet pulp into succinic acid and value-added coproducts, ACS Sustain Chem Eng. 7 (2019) 6569–6579.

[6] R. Dickson, E. Mancini, N. Garg, J.M. Woodley, K. v Gernaey, M. Pinelo, J. Liu, S.S. Mansouri, Sustainable bio-succinic acid production: superstructure optimization, techno-economic, and lifecycle assessment, Energy Environ Sci. (2021).

[7] R. Taylor, L. Nattrass, G. Alberts, P. Robson, C. Chudziak, A. Bauen, I.M. Libelli, G. Lotti, M. Prussi, R. Nistri, From the sugar platform to biofuels and biochemicals: final report for the European Commission Directorate-General Energy, E4tech/Re-CORD/Wageningen UR, 2015.

[8] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic acid: technology development and commercialization, Fermentation. 3 (2017) 26.

[9] Y.P. Timilsena, Bio-Succinic Acid from Lignocellulosic Materials and Its Food Application, Food Wave. 8 (2011) 22–32.

[10] J.B. McKinlay, C. Vieille, J.G. Zeikus, Prospects for a bio-based succinate industry, Appl Microbiol Biotechnol. 76 (2007) 727–740.

[11] B. Cok, I. Tsiropoulos, A.L. Roes, M.K. Patel, Succinic acid production derived from carbohydrates: An energy and greenhouse gas assessment of a platform chemical toward a bio-based economy, Biofuels, Bioproducts and Biorefining. 8 (2014) 16–29.

[12] N. Mahendrasinh Kosamia, M. Samavi, K. Piok, S. Kumar Rakshit, Perspectives for scale up of biorefineries using biochemical conversion pathways: Technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022) 124532. https://doi.org/10.1016/j.fuel.2022.124532.

[13] X. Li, E. Mupondwa, Empirical analysis of large-scale bio-succinic acid commercialization from a technoeconomic and innovation value chain perspective: BioAmber biorefinery case study in Canada, Renewable and Sustainable Energy Reviews. 137 (2021) 110587.

[14] L. Moghaddam, J. Rencoret, V.R. Maliger, D.W. Rackemann, M.D. Harrison, A. Gutierrez, J.C. del Río, W.O.S. Doherty, Structural characteristics of bagasse furfural residue and its lignin component. An NMR, Py-GC/MS, and FTIR study, ACS Sustain Chem Eng. 5 (2017) 4846–4855.

[15] C. Xu, E. Paone, D. Rodríguez-Padrón, R. Luque, F. Mauriello, Recent catalytic routes for the preparation and the upgrading of biomass derived furfural and 5-hydroxymethylfurfural, Chem Soc Rev. 49 (2020) 4273–4306.

[16] A. Mittal, S.K. Black, T.B. Vinzant, M. O'Brien, M.P. Tucker, D.K. Johnson, Production of furfural from process-relevant biomass-derived pentoses in a biphasic reaction system, ACS Sustain Chem Eng. 5 (2017) 5694–5701.

[17] C.M. Cai, T. Zhang, R. Kumar, C.E. Wyman, Integrated furfural production as a renewable fuel and chemical platform from lignocellulosic biomass, Journal of Chemical Technology and Biotechnology. 89 (2014) 2–10.

[18] X. Chen, K. Zhang, L.-P. Xiao, R.-C. Sun, G. Song, Total utilization of lignin and carbohydrates in Eucalyptus grandis: an integrated biorefinery strategy towards phenolics, levulinic acid, and furfural, Biotechnol Biofuels. 13 (2020) 1–10.

[19] N.W. Dulie, B. Woldeyes, H.D. Demsash, A.S. Jabasingh, An insight into the valorization of hemicellulose fraction of biomass into furfural: catalytic conversion and product separation, Waste Biomass Valorization. 12 (2021) 531–552.

[20] X. Lyu, G.G. Botte, Investigation of factors that inhibit furfural production using metal chloride catalysts, Chemical Engineering Journal. 403 (2021) 126271.

[21] G. Marcotullio, The chemistry and technology of furfural production in modern lignocellulose-feedstock biorefineries, (2011).

[22] A. Giuliano, D. Barletta, I. de Bari, M. Poletto, Techno-economic assessment of a lignocellulosic biorefinery co-producing ethanol and xylitol or furfural, in: Computer Aided Chemical Engineering, Elsevier, 2018: pp. 585–590.

[23] M. Morales, H. Verelst, L. Mesa, E. González, Simulation of furfural production process for revamping with ethanol technology from lignocellulosic residuals, Chem Eng Trans. 21 (2010).

[24] J.F.L. Silva, M.A. Selicani, T.L. Junqueira, B.C. Klein, S. Vaz, A. Bonomi, Integrated furfural and first-generation bioethanol production: process simulation and techno-economic analysis, Brazilian Journal of Chemical Engineering. 34 (2017) 623–634.

[25] A. Mazar, O. Ajao, M. Benali, N. Jemaa, W. Wafa Al-Dajani, M. Paleologou, Integrated Multiproduct Biorefinery for Furfural Production with Acetic Acid and Lignin Recovery: Design, Scale-Up Evaluation, and Technoeconomic Analysis, ACS Sustain Chem Eng. 8 (2020) 17345–17358.

[26] Ç. Efe, L.A.M. van der Wielen, A.J.J. Straathof, Techno-economic analysis of succinic acid production using adsorption from fermentation medium, Biomass Bioenergy. 56 (2013) 479–492. https://doi.org/10.1016/j.biombioe.2013.06.002.

[27] K.F. Lam, C.C.J. Leung, H.M. Lei, C.S.K. Lin, Economic feasibility of a pilot-scale fermentative succinic acid production from bakery wastes, Food and Bioproducts Processing. 92 (2014) 282–290. https://doi.org/10.1016/j.fbp.2013.09.001.

[28] J. Li, X.Y. Zheng, X.J. Fang, S.W. Liu, K.Q. Chen, M. Jiang, P. Wei, P.K. Ouyang, A complete industrial system for economical succinic acid production by Actinobacillus succinogenes, Bioresour Technol. 102 (2011) 6147–6152. https://doi.org/10.1016/j.biortech.2011.02.093.

[29] J.M. Pinazo, M.E. Domine, V. Parvulescu, F. Petru, Sustainability metrics for succinic acid production: A comparison between biomass-based and petrochemical routes, Catal Today. 239 (2015) 17–24. https://doi.org/10.1016/j.cattod.2014.05.035.

[30] S. González-García, L. Argiz, P. Míguez, B. Gullón, Exploring the production of bio-succinic acid from apple pomace using an environmental approach, Chemical Engineering Journal. 350 (2018) 982–991. https://doi.org/10.1016/j.cej.2018.06.052.

[31] O. v. Okoro, A. Shavandi, An assessment of the utilization of waste apple slurry in bio-succinic acid and bioenergy production, International Journal of Environmental Science and Technology. 19 (2022) 1323–1334. https://doi.org/10.1007/s13762-021-03235-z.

[32] A. Shaji, Y. Shastri, V. Kumar, V. v. Ranade, N. Hindle, Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse, ACS Sustain Chem Eng. 9 (2021) 12738–12746. https://doi.org/10.1021/acssuschemeng.1c02483.

[33] A. Ghayur, T.V. Verheyen, E. Meuleman, Techno-economic analysis of a succinic acid biorefinery coproducing acetic acid and dimethyl ether, J Clean Prod. 230 (2019) 1165–1175. https://doi.org/10.1016/j.jclepro.2019.05.180.

[34] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover, National Renewable Energy Lab. (NREL), Golden, CO (United States), 2011.

[35] D.W. Templeton, A.D. Sluiter, T.K. Hayward, B.R. Hames, S.R. Thomas, Assessing corn stover composition and sources of variability via NIRS, Cellulose. 16 (2009) 621–639.

[36] R.J. Wooley, V. Putsche, Development of an ASPEN PLUS physical property database for biofuels components, National Renewable Energy Lab., Golden, CO (United States), 1996.

[37] ASPEN (2018), ASPEN physical property system:physical property models, Aspen Tech, Cambridge, UK. (n.d.).

[38] J.E. Edwards, Process modelling selection of thermodynamic methods. www.pidesign.co.uk.

[39] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover, National Renewable Energy Lab. (NREL), Golden, CO (United States), 2011.

[40] Chemical Engineering Magazine, Chemical Engineering Plant Cost Index; 2021, (n.d.).

[41] R.K. Sinnott, J.M. Coulson, J.F. Richardson, Chemical engineering design, Elsevier Butterworth-Heinemann Oxford, 2005.

[42] G. Towler, R. Sinnott, Chemical engineering design: principles, practice and economics of plant and process design, Butterworth-Heinemann, 2021.

[43] W.D. Seider, J.D. Seader, D.R. Lewin, Product and process design principles: synthesis, analysis and evaluation, John Wiley & Sons, 2009.

[44] F. Zimbardi, E. Viola, F. Nanna, E. Larocca, M. Cardinale, D. Barisano, Acid impregnation and steam explosion of corn stover in batch processes, Ind Crops Prod. 26 (2007) 195–206.

[45] P. Bajpai, Pretreatment of lignocellulosic biomass, in: Pretreatment of Lignocellulosic Biomass for Biofuel Production, Springer, 2016: pp. 17–70.

[46] C.M.C. Morales, Strategies to increase the sugar concentration and overall sugar recovery from steam pretreated wheat straw and corn stover, 2012.

[47] Q. Yan, P. Zheng, J. Dong, Z. Sun, A fibrous bed bioreactor to improve the productivity of succinic acid by Actinobacillus succinogenes, Journal of Chemical Technology and Biotechnology. 89 (2014) 1760–1766.

[48] C.D. Van Heerden, W. Nicol, Continuous succinic acid fermentation by Actinobacillus succinogenes, Biochemical Engineering Journal. 73 (2013) 5–11.

[49] M. Jiang, W. Dai, Y. Xi, M. Wu, X. Kong, J. Ma, M. Zhang, K. Chen, P. Wei, Succinic acid production from sucrose by Actinobacillus succinogenes NJ113, Bioresource Technology. 153 (2014) 327–332.

[50] J. Li, X.-Y. Zheng, X.-J. Fang, S.-W. Liu, K.-Q. Chen, M. Jiang, P. Wei, P.-K. Ouyang, A complete industrial system for economical succinic acid production by Actinobacillus succinogenes, Bioresource Technology. 102 (2011) 6147–6152.

[51] M. Jiang, R. Xu, Y.-L. Xi, J.-H. Zhang, W.-Y. Dai, Y.-J. Wan, K.-Q. Chen, P. Wei, Succinic acid production from cellobiose by Actinobacillus succinogenes, Bioresource Technology. 135 (2013) 469–474.

[52] Z. Dai, F. Guo, S. Zhang, W. Zhang, Q. Yang, W. Dong, M. Jiang, J. Ma, F. Xin, Bio-based succinic acid: an overview of strain development, substrate utilization, and downstream purification, Biofuels, Bioproducts and Biorefining. 14 (2020) 965–985.

[53] H. Song, S.Y. Lee, Production of succinic acid by bacterial fermentation, Enzyme Microb Technol. 39 (2006) 352–361.

[54] M. v Guettler, M.K. Jain, B.K. Soni, Process for making succinic acid, microorganisms for use in the process and methods of obtaining the microorganisms, (1996).

[55] J.B. McKinlay, Y. Shachar-Hill, J.G. Zeikus, C. Vieille, Determining Actinobacillus succinogenes metabolic pathways and fluxes by NMR and GC-MS analyses of 13C-labeled metabolic product isotopomers, Metab Eng. 9 (2007) 177–192.

[56] P. Zheng, J.-J. Dong, Z.-H. Sun, Y. Ni, L. Fang, Fermentative production of succinic acid from straw hydrolysate by Actinobacillus succinogenes, Bioresour Technol. 100 (2009) 2425–2429.

[57] M. Nieder-Heitmann, K. Haigh, J. Louw, J.F. Görgens, Economic evaluation and comparison of succinic acid and electricity co-production from sugarcane bagasse and trash lignocelluloses in a biorefinery, using different pretreatment methods: dilute acid (H2SO4), alkaline (NaOH), organosolv, ammonia fibre expa, Biofuels, Bioproducts and Biorefining. 14 (2020) 55–77. https://doi.org/https://doi.org/10.1002/bbb.2020.

[58] E.O. Jokodola, V. Narisetty, E. Castro, S. Durgapal, F. Coulon, R. Sindhu, P. Binod, J.R. Banu, G. Kumar, V. Kumar, Process optimisation for production and recovery of succinic acid using xylose-rich hydrolysates by Actinobacillus succinogenes, Bioresour Technol. 344 (2022) 126224.

[59] T. Kurzrock, S. Schallinger, D. Weuster-Botz, Integrated separation process for isolation and purification of biosuccinic acid, Biotechnol Prog. 27 (2011) 1623–1628.

[60] B.P. Hogle, D. Shekhawat, K. Nagarajan, J.E. Jackson, D.J. Miller, Formation and recovery of itaconic acid from aqueous solutions of citraconic acid and succinic acid, Ind Eng Chem Res. 41 (2002) 2069–2073.

[61] R. Xing, W. Qi, G.W. Huber, Production of furfural and carboxylic acids from waste aqueous hemicellulose solutions from the pulp and paper and cellulosic ethanol industries, Energy Environ Sci. 4 (2011) 2193–2205.

[62] Jena Thompson and Wallace E. Tyner, Corn Stover for Bioenergy Production Cost Estimates and Farmer Supply Response, Corn Stover for Bioenergy Production Cost Estimates and Farmer Supply Response. (n.d.).

[63] Alibaba.com

[64] L. Ou, R. Thilakaratne, R.C. Brown, M.M. Wright, Techno-economic analysis of transportation fuels from defatted microalgae via hydrothermal liquefaction and hydro processing, Biomass Bioenergy. 72 (2015) 45–54.

[65] E. Stylianou, C. Pateraki, D. Ladakis, M. Cruz-Fernández, M. Latorre-Sánchez, C. Coll, A. Koutinas, Evaluation of organic fractions of municipal solid waste as renewable feedstock for succinic acid production, Biotechnol Biofuels. 13 (2020). https://doi.org/10.1186/s13068-020-01708-w.

CHAPTER 4

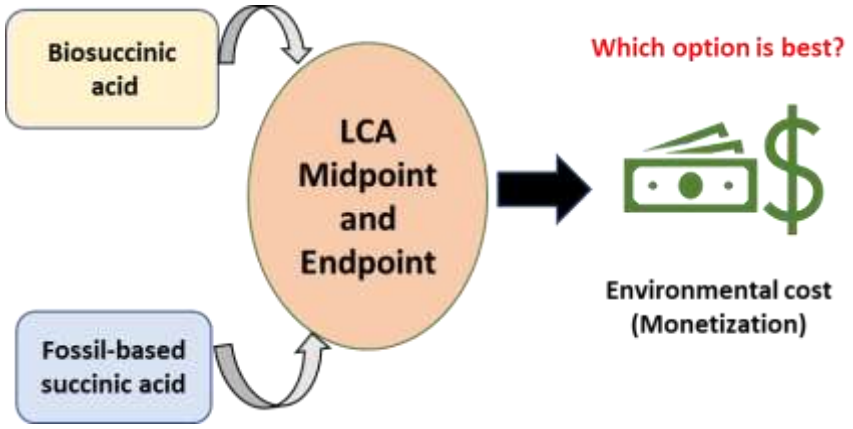
OBJECTIVE 2*

Scenario-based Life Cycle Assessment and Environmental Monetary Valuation of Biosuccinic Acid Production from Lignocellulosic Biomass

***** The whole chapter was submitted to the journal **Industrial Crops and Products** by **Elsevier** in March, 2023

4 Scenario-based life cycle assessment and environmental monetary valuation of biosuccinic acid production from lignocellulosic biomass

4.1 Abstract



A cradle-to-gate Life Cycle Assessment (LCA) followed by a monetary valuation of the environmental impacts of biosuccinic acid (BioSA) production from lignocellulosic biomass is presented in this paper. Three biorefining scenarios are studied. Scenario 1 employs C-6 and C-5 sugars to produce BioSA, while C-5 sugar is derived to produce furfural and biogas in Scenario 2 and 3, respectively. The three scenarios cogenerate electricity using the biogas produced from C-5 sugars in scenario 3 and the residual lignin in all three scenarios. These scenarios are compared against a fossil-based succinic acid production route. ReCiPe midpoint and endpoint impacts were considered in the analysis. The analysis of midpoint impact categories showed that the feedstock production and transportation stages, as well as the pretreatment process of biorefining stage, are the most important contributors to the environmental impact of BioSA production. Endpoint

impacts and monetary valuation showed that scenario 1 scored the lowest environmental cost followed by scenario 3, the fossil-based route and scenario 2 with 1.48, 2.04, 2.24 and 3.05 USD/kg BioSA, respectively. Sensitivity analysis for monetary valuation suggested that the environmental costs are highly sensitive to damage to human health, and variations in damage to resources have minimum impact on the environmental cost.

Keywords: Life cycle assessment, Biosuccinic acid, Fossil-based succinic acid, Corn stover, Monetary valuation, Multiproduct biorefinery.

4.2 Introduction

Multiproduct biorefineries using lignocellulosic residues as feedstock for producing bioproducts of interest are considered an alternative to their conventional fossil-based counterparts to reduce production costs and improve their sustainability [1,2]. Therefore, quantifying the environmental impact of these bioproducts as compared to their fossil-based alternatives is currently a major issue.

Bio-succinic acid (BioSA) is considered a bioproduct of strategic interest for speciality chemicals, pharmaceuticals, food additives, and the pigment industry [3]. The world market demand for BioSA is expected to rise at 27.4 % compound annual growth rate (CAGR) with an estimated market potential of 1.8 billion USD by 2025 [4,5]. Based on the market potential of BioSA, many commercial initiatives started production of BioSA from biomass in the last decade. However, most of them have either closed, kept in abeyance, or undergone bankruptcy due to economic failure [6,7]. To avoid such failures, doing a sustainability analysis at the design stage of the project has been suggested [8]. This should involve a comparison of economic, environmental, and social sustainability with a single score (dollar value) to the fossil-based route.

LCA has also been applied in the past to assess the environmental impacts of BioSA production in various reports [6, 9-14]. Moussa et al [15] carried out a cradle-to-gate LCA of BioSA, comparing it with the fossil-resources-derived succinic acid production route. A similar study was also performed by Smidt et al. [16] from corn-derived dextrose for a BioSA production plant located in Europe. The contribution of various process stages of BioSA production to climate change impacts with sugarcane bagasse as a feedstock has also been previously reported [17]. Nieder-Heitmann et al. [18] did LCA of multi-product scenario-based biorefinery producing BioSA, itaconic acid, PHB, and electricity from sugarcane bagasse. The detailed information of some previously published studies is presented in **Table 4.1**.

One crucial observation derived from these studies is that calculated midpoint environmental impacts (e.g., climate change and acidification) are reported with their associated units (e.g., kg CO_2 eq., kg SO_2 eq), respectively. The same situation occurs with the environmental endpoint impacts on the areas of protection (AOP) such as human health, ecosystems, and resources demanded. However, midpoint and endpoint categories do not always provide a clear-cut vision of which option is best, because of the different units employed for each category. Therefore, monetizing the environmental impacts provides a consistent base for choosing the best route of bioproduct synthesis among available options.

In addition, monetary valuation facilitates the decision-making process since techno economics and environment sustainability are reported in one comparable monetary unit [19]. Furthermore, literature often concludes by stating that BioSA production from biomass could be profitable if its environmental cost is considered. Hence, the environmental impacts of BioSA production from biomass must be monetized to compare economics and environmental aspects using the same bases [8].

Table 4. 1 Some prior studies on Life Cycle Assessment of BioSA production

Reference and overview of method used	Reported impact categories and feedback
Shaji et al. [17] Cradle-to-gate. Sugar cane bagasse as a feedstock.	Midpoint impact categories, i.e., fossil depletion (0.21 kg oil eq) and freshwater ecotoxicity (0.01 kg 1,4-DCB), similar to results obtained in this work. Impact assessment method: ReCiPe midpoint (H).
Mousa et al. [15] Energy and LCA compared against the fossil-based route. Cradle-to-gate. Dextrose (does not require a pretreatment stage) as a feedstock.	GWP lower value of non-renewable energy demand compared to fossil-based by 385% and 1045%, respectively. CHP (electricity and steam cogeneration) using lignin and residual hemicellulose. Impact assessment method: IPCC 2010 GWP 100a.
Gadkari et al. [10] GHG emissions and non-renewable energy use. Cradle-to-gate. Bread waste as a feedstock.	The analysis suggested that compared to other feedstocks, i.e., corn or sorghum grain, BioSA production using waste bread demonstrated 50.0 % higher GHG emissions. The reported value of non-renewable energy demand for BioSA derived from bread waste was 46.0 % lower than fossil-based SA. Impact assessment method: IPCC 2013 GWP 100a.
González-García et al. [13] Cradle-to-gate. Apple pomace as a feedstock.	Global warming potential, eutrophication potential, acidification potential, photochemical oxidation potential, and cumulative energy demand in their respective units. Impact assessment method: CML 2001.

Pizzol et al. [20] reviewed the key features, strengths, and weaknesses of various monetary valuation methods, such as revealed preference, abatement cost, budget constraint, and choice of experiment method. Moreover, the budget constraint was suggested as the best option among all available methods due to its higher accuracy. Dong et al. [21] also performed the LCA to evaluate greenhouse gas emissions using different impact assessment methods and converted them into monetary units. However, the study is limited to greenhouse gas emissions only.

This paper presents the LCA analysis of BioSA production with three different scenarios (i.e., biorefinery designs). The use of C-5 sugar and lignin for coproducing furfural and biogas as a fuel for electricity and steam cogeneration (CHP) are considered alternatives to improve the economics of the scenarios [22]. Midpoint and endpoint impacts were calculated, and their results discussed stressing the difficulty to choose the best scenario based on these results only. The endpoint categories for the three scenarios were monetized and compared with conventional fossil-based succinic acid production. The total production cost is also considered to identify the best scenario [22]. A sensitivity analysis of monetized endpoint categories is also presented.

4.3 Methods and Modeling

In this section, the description of biorefinery scenarios is presented first, followed by the LCA and the monetary valuation method of the calculated midpoint and endpoint environmental impacts.

4.3.1 Biorefinery and scenarios description

The biorefinery input capacity is set to 1000 kg/h of corn stover. The process comprises a standard biochemical train of four biorefining steps, starting from pretreatment, saccharification and fermentation, product recovery and purification. The CHP stage is also included using lignin and residual hemicellulose as fuel [22]. This production train is employed in all three scenarios (**Figure 4.1**):

Scenario 1: After the pretreatment and saccharification, both C-6 and C-5 sugars are fed to the fermentation stage to produce BioSA. Lignin is used in the CHP stage for electricity and steam cogeneration **(Figure 4.1 A)**.

Scenario 2: The derived C-5 sugar obtained from the steam explosion weak-acid pretreatment is used in a stage for furfural synthesis. The C-6 sugar stream is employed for BioSA production. The residual lignin stream is utilized as a fuel in the CHP stage **(Figure 4.1 B)**. The potential of other co-products, such as vanillin from lignin, has been explored elsewhere [8]. However, Due to energy requirements to operate the biorefinery, electricity is selected to be cogenerated from lignin.

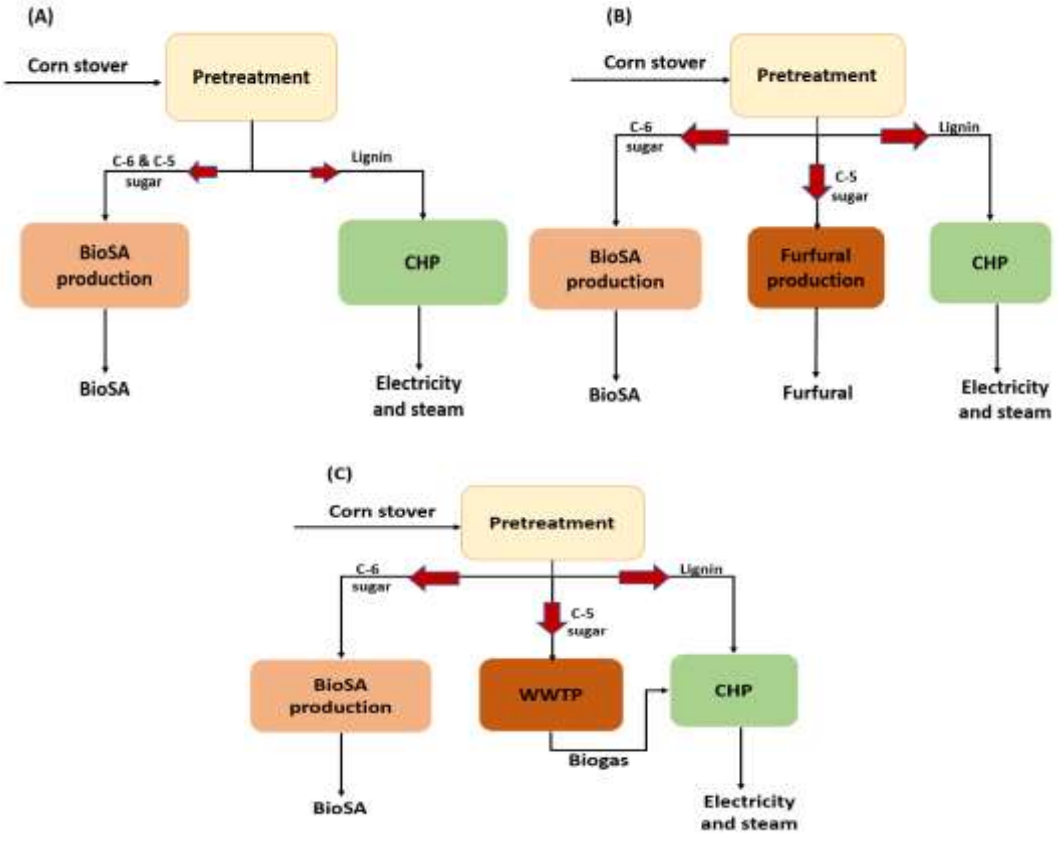


Figure 4. 1 Biorefinery design scenario

Scenario 3: C-6 sugar and lignin streams are used for BioSA and heat and electricity coproduction, respectively. The C-5 sugar stream is sent to a Wastewater Treatment plant (WWTP) for biogas production, which is subsequently used by CHP for additional heat and electricity cogeneration (**Figure 4.1 C**).

4.3.2 Process description

Mild acid-impregnated milled corn stover is subjected to a steam explosion weak-acid pretreatment process [23] followed by detoxification. At the end of this stage, corn stover is fractionated into cellulose, lignin, and C-5 sugars. Cellulose is hydrolyzed to C-6 monomers in the enzymatic saccharification stage. *Actinobacillus succinogenes* strain, which is considered an efficient microorganism to convert both C-6 and C-5 sugars into BioSA, is utilized in the fermentation stage [24]. For the recovery of BioSA from the fermentation broth, reactive extraction [25] followed by crystallization [26], and drying are employed. In scenario 2, C-5 sugars are converted to furfural in a bi-phasic reactor, followed by distillation for product purification [27].

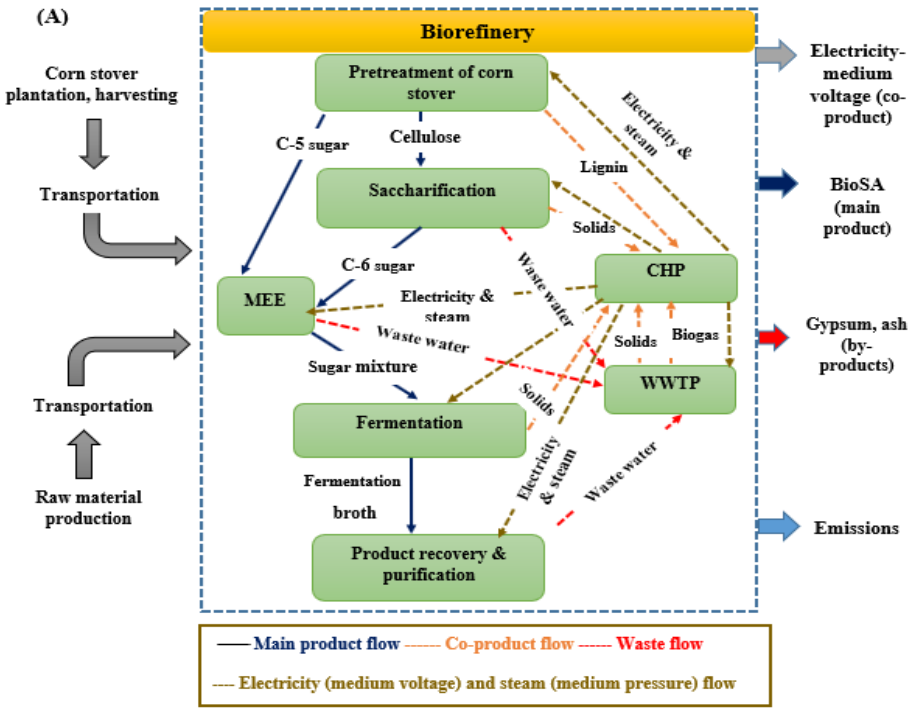
4.3.3 Life cycle assessment

The standard LCA method was followed in this work [28]. This method consists of four main steps starting from the goal and scope of study followed by Life Cycle Inventory (LCI) analysis, Life Cycle Impact Assessment (LCIA), and finally interpretation.

4.3.4 The goal, scope, boundary, and functional unit

The goal of this analysis is to calculate the environmental impacts associated with BioSA production based on eighteen midpoint impact categories and three endpoint categories. The province of Ontario, Canada, was considered as the geographical region for this study. A cradle-to-gate analysis (which does not consider the end-of-life stage) was carried out considering the following stages: feedstock production (corn stover harvesting and baling), transportation from

fields to the factory gate and biorefining (**Figure 4.2**). The fabrication (i.e., biorefining) stage is composed of different biorefining steps as discussed for each scenario. 1 kg succinic acid product is defined as the functional unit. As furfural and electricity are co-products, energy use and emissions were allocated among the main product and co-products. The system expansion approach is chosen considering corn stover as an agricultural coproduct and biorefining co-products as replacements for products currently in the market. Ecoinvent 38 apos 3011 was chosen as inventory data source. Emissions savings in fabrication stages are credited to the process [29].



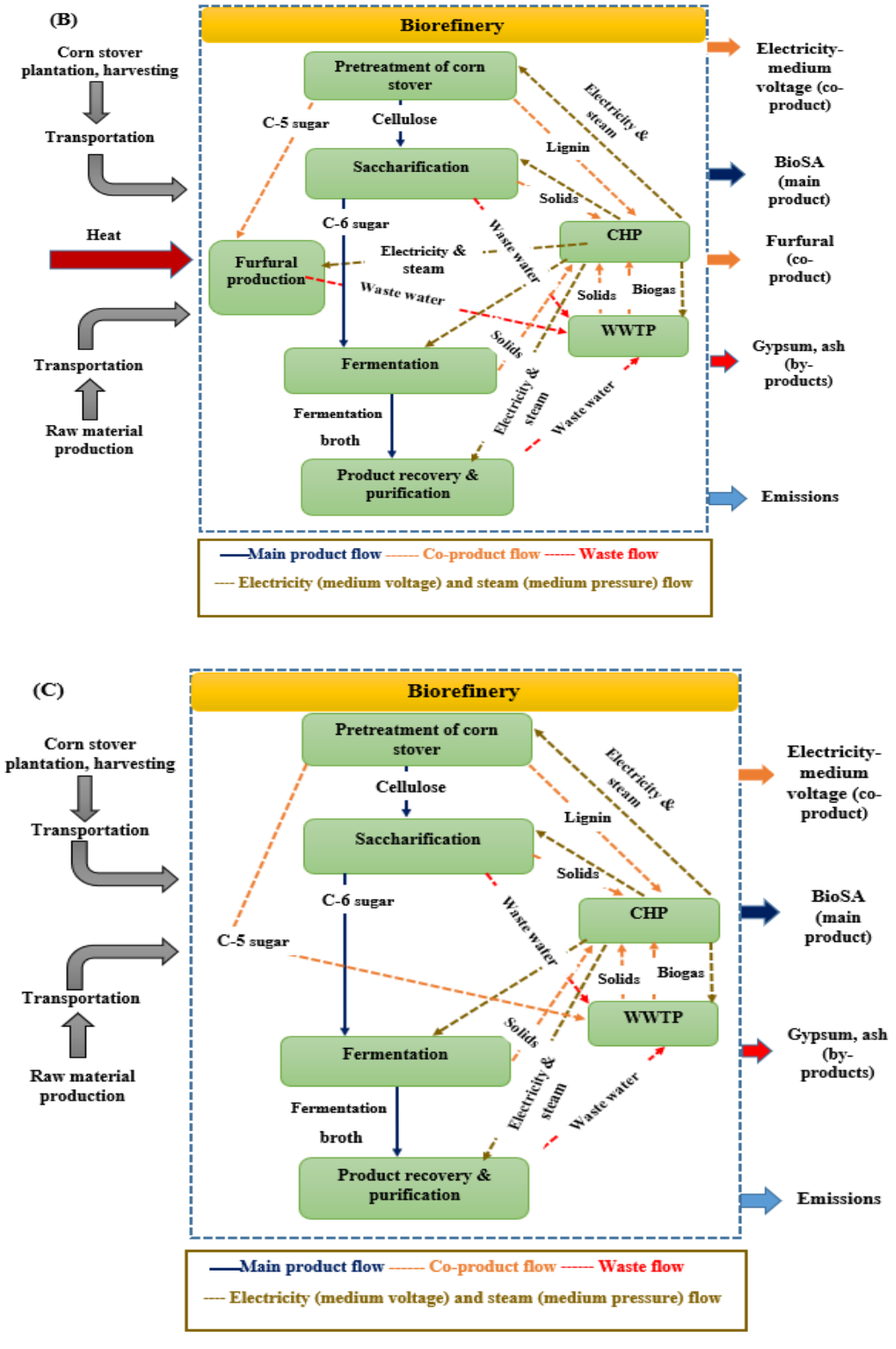


Figure 4. 2 System boundaries for life cycle assessment with BioSA as the main product and three Scenarios

(A): Scenario 1 with electricity from lignin as a co-product (B), Scenario 2 with furfural and electricity from lignin as co-products and (C), Scenario 3 with electricity from lignin and hemicellulose via a Waste Water Treatment Plant (WWTP) as a co-product

4.3.5 Process inventories and LCIA

The process inventory data for scenarios 1, 2, and 3 are based on results obtained by process simulation [22] and a standard discounted cash flow analysis for total production costs calculations using fixed selling prices for the coproducts. The plant operates 8410 hours annually. Scenarios 1 and 3 are energy self-sufficient in both heat and electricity, whereas, for scenario 2, heat/steam requirements are partially fulfilled by onsite CHP and purchased from external providers. The inventory data for the three scenarios are provided in **Table 4.2.** Ecoinvent (v3.8) database was used for LCA and fossil-based route inventory calculations. For the fossil-based SA production process, maleic anhydride derived by the oxidation of 1,4-butanediol was used as starting raw material. In a two-step process, SA is produced by hydrogenation followed by hydration of maleic anhydride [9]. Data for Canada are used when available. Alternatively, inventory data for the rest of the world (ROW) is considered for the analysis. Open LCA (version 1.10.3) is used to develop the LCA model. ReCiPe 2016 midpoint (H) and ReCiPe 2016 endpoint (H) [30] were used as an impact assessment method for this analysis. ReCiPe endpoint results target the safeguard of human health, ecosystems, and resources into three damage categories which are human wellbeing in Disability-Adjusted Life Years (DALY), biodiversity in lost species *yr and resource productivity in USD 2013 [31]. These results are further converted into monetary units by performing monetization.

Table 4. 2 Biorefinery process inventory data for all three scenarios for 1kg BioSA as a functional unit

***Note:** Inventories for the fossil-based succinic acid and corn stover at the conversion plant are adapted from the Ecoinvent database.

Main bioprocess inventories data					
	Process inventories	**Unit**	**Scenario 1**	**Scenario 2**	**Scenario 3**
Input	Corn stover at conversion plant	kg	3.03×10^{0}	4.45×10^{0}	4.45×10^{0}
	Ammonia, anhydrous, liquid	kg	1.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}
	Enzymes	kg	2.00×10^{-2}	3.00×10^{-2}	3.00×10^{-2}
	1-octanol	kg	5.00×10^{-2}	5.00×10^{-2}	5.00×10^{-2}
	Lime, hydrated, packed	kg	1.30×10^{-1}	1.90×10^{-1}	1.90×10^{-1}
	Maize starch	kg	3.9×10^{-3}	2.9×10^{-3}	2.9×10^{-3}
	Sodium bicarbonate	kg	2.10×10^{-3}	1.5×10^{-3}	1.5×10^{-3}
	Sodium hydroxide	kg	1.10×10^{-1}	1.60×10^{-1}	1.60×10^{-1}
	Sulfuric acid	kg	4.10×10^{-1}	6.00×10^{-1}	6.00×10^{-1}
	Process water	kg	3.05×10^{0}	2.97×10^{0}	2.97×10^{0}
	Tap water for washing application	kg	1.52×10^{1}	2.24×10^{1}	2.24×10^{1}
	Trimethylamine	kg	4.00×10^{-2}	3.00×10^{-2}	3.00×10^{-2}
	Cooling water	kg	1.00×10^{0}	3.07×10^{0}	1.40×10^{0}

	Steam (medium pressure)	kg		1.00×10^{1}	
	Tetrahydrofuran (THF)	kg		0.10×10^{0}	
Output	BioSA	kg	1.00×10^{0}	1.00×10^{0}	1.00×10^{0}
	Furfural	kg		3.9×10^{-1}	
	Ash	kg	1.4×10^{-1}	2.0×10^{-1}	2.0×10^{-1}
	Electricity (coal-based medium voltage)	kWh	1.8×10^{-1}	1.2×10^{-1}	3.0×10^{-1}
	Gypsum	kg	0.34×10^{0}	0.50×10^{0}	0.50×10^{0}

Corn stover at conversion plant inventories data (farming and transportation up to conversion facility gate)

***Note**: For corn stover inventory data Ecoinvent 38 apos 3011 model is used.

Input	Urea	kg	2.41×10^{-3}
	[Thio]carbamate-compound	kg	3.83×10^{-8}
	Ammonia, anhydrous, liquid	kg	1.00×10^{-4}
	Ammonium nitrite	kg	1.46×10^{-3}
	Ammonium sulfate	kg	7.15×10^{-5}
	Atrazine	kg	1.49×10^{-5}
	Pendimethalin	kg	1.40×10^{-6}
	Pesticide, unspecified	kg	2.09×10^{-6}
	Benzoic-compound	kg	2.50×10^{-6}

Carbon dioxide, in air	kg	6.10×10^{-1}
Chopping	ha	2.75×10^{-5}
Dimethenamide	kg	1.73×10^{-6}
Fodder loading, by self-loading trailer	m3	2.29×10^{-3}
Glyphosate	kg	1.76×10^{-5}
Inorganic nitrogen fertilizer, as N	kg	6.30×10^{-4}
Inorganic phosphorus fertilizer, as P2O5	kg	5.00×10^{-3}
Lime	kg	5.07×10^{-3}
Liquid manure spreading, by vacuum tanker	m3	3.90×10^{-4}
Seed, for sowing	kg	8.80×10^{-4}
Manure, liquid, cattle	kg	1.72×10^{-1}
Manure, solid, cattle	kg	5.10×10^{-2}
Metolachlor	kg	1.19×10^{-5}
Packaging, for fertilizers	kg	1.60×10^{-2}
Packaging, for pesticides	kg	1.04×10^{-4}
Poultry manure, fresh	kg	1.56×10^{-2}

	Pyrethroid-compound	kg	1.54×10^{-8}
	Solid manure loading and spreading, by hydraulic loader and spreader	kg	6.66×10^{-2}
	Sowing	ha	2.76×10^{-5}
	Tillage, ploughing	ha	2.78×10^{-5}
	Tillage, rotary cultivator	ha	4.00×10^{-5}
	Transportation	t*km	7.74×10^{-1}
Output	Corn stover at conversion plant	kg	1.0×10^{0}
	Emissions (air, water, soil)	kg	1.06×10^{-2}

4.3.6 Monetary Valuation of Impact Assessment

The monetary valuation of endpoint impacts was carried out with the budget constraint approach [32], which does not rely on revealed or stated preferences but considers the accounting balance principle to infer the Willingness To Pay (WTP) through the possible income at complete well-being condition of an individual. Other approaches like EPS, LIME, ReCiPe-CML, and NewEXT relied on European data or information. In contrast, the budget constraint approach is developed based on the available economic information of North America, which is the geographical scope of this study [31]. Weidema [32] established that DALY equals to Quality-Adjusted Life Years (QALY) and one lost species*yr is equal to 6800 Biodiversity-Adjusted Hector Year (BAHY) for biodiversity or ecosystem quality by considering the average terrestrial species density of 68

million m^2/species. To evaluate the monetary value of QALY and BAHY in this work, the method suggested by Kaenchan and Gheewala [33] was applied. QALY was determined in the form of potential annual economic production (PEP) per capita, which represents the maximum amount that an individual would be willing to pay to live one year at full well-being.

$$per\ capita\ \text{PEP} = (per\ capita\ \text{GDP} + per\ capita\ \text{GHP}) \times \text{LEP factor} \quad (1)$$

Where *per capita* GDP, GHP, and LEP represent the gross domestic product, gross household production, and lacking economic production factor (2.08) for Canada respectively.

The value of *per capita* GHP is calculated with the method suggested by Ironmonger [34] in which GHP is derived from the product of potential hours spent by Canadian citizens per household production and the average hourly base wage rate in Canada. For this assessment, 2021 was selected as a reference year. 33.6 USD and 1,644 hours were taken as Canadian annual *per capita* wage and hours spent per household production [35], respectively. The resulting *per capita* GHP was 55,342 USD. In addition, the *per capita* GDP for Canada and LEP [33] were 43,258 USD [36] and 2.08, respectively. Based on the above parameters, Canada's calculated value of *per capita* PEP is 205,089 USD, coinciding with the QALY value. Koneczny and Pennington [37] suggested that ecosystem impacts can be expressed in terms of human well-being. They suggested that, by considering 7.14 as the global species area to global human population ratio and 8.13 as the global ecosystem to human well-being ratio, 1 QALY is equivalent to 58 BAHY (i.e., 7.14 x 8.13). Therefore, one BAHY is equivalent to 3,536 USD. These values were used for the monetization of endpoint impacts. The detailed calculations to translate QALY and BAHY to USD can be found in **Table 4.3**.

Table 4. 3 Calculation details for the QALY and BAHY to USD

Monetary valuation terminology	Considered/calculated value
Currency (USD)	USD
Reference year	2021
Geography	Canada
Hourly wage (USD)	33.66 [35]
Total hours worked in a year by individual	1644 [35]
GHP per capita (USD) (Hours worked in a year) x (Hourly wage)	55342
GDP per capita in 2021 (USD)	43258.3 [36]
GEP (USD) (GHP +GDP)	98600.3
Lacking economic production (LEP) factor[4]	2.08
Potential economic production per capita (GEP X LEP)	205088.62
1 QUALY	**205088.62 USD**
1 lost species *yr.	6800 BAHY [33]
1 QALY	58 BAHY [37]
1 BAHY (205088.62 / 58)	**3536.01 USD**

4.4 Results and discussion

This section first presents the analysis of the midpoint and endpoint impact assessment results, detailing the contributions of the different inventory stages and biorefining steps. Monetization of the endpoint categories is then introduced showing how this approach contributes to the analysis of endpoint impacts. Techno-economic results from a previous study are included in the discussion

to elaborate on the advantages of using monetization to enrich the LCA analysis. In addition, a sensitivity analysis of monetized endpoint categories is also presented.

4.4.1 Impact assessment results for midpoint impact categories

The results of all eighteen impact categories of ReCiPe 2016 (H) are presented in **Table 4.4** for the three scenarios and the fossil-based route. The scenarios with the minimum value in each category are marked in green. The highest is marked in red. The worst alternative is scenario 2 with sixteen categories scoring the highest values. Among them, fine particulate matter formation, water consumption and freshwater eutrophication were an order of magnitude higher than those in scenario 1. The fossil-resource route scored minimum values in ten categories, including stratospheric ozone depletion, human non-carcinogenic toxicity, freshwater ecotoxicity, water consumption and mineral resource scarcity. However, as expected, this route obtained the highest values for global warming and fossil resource scarcity. Scenario 1 scored minimum values in eight categories, including global warming, fossil resource scarcity and freshwater eutrophication. Interestingly, fine particulate matter formation, global warming and freshwater eutrophication are of the same magnitude in scenario 1 and the fossil-resource route. Values of fossil resource scarcity, ionizing radiation, human carcinogenic toxicity and ozone formation human health were one order of magnitude lower in scenario 1 than in the fossil-based route. However, freshwater ecotoxicity, mineral resource scarcity, and terrestrial ecotoxicity are one order of magnitude larger in scenario 1 than in the fossil-based route. Moreover, in scenario 1 marine eutrophication, and land use are two orders of magnitude higher than the fossil option. Based on the midpoint category results, identifying a scenario with a clear advantage over the others becomes difficult. Further analysis including other criteria is required.

As mentioned in the Introduction, **Table 4.1** presents similar works calculating the global warming potential of BioSA production. Shaji et al. [17] carried out a cradle-to-gate LCA of BioSA production from sugarcane bagasse for midpoint impact categories using a similar methodological approach as this work, considering sugarcane bagasse as an agricultural residue in the agronomical stage and as feedstock in the fabrication (i.e., biorefining) stage. The calculated value was 1.39 kg CO_2 eq/kg BioSA, which is similar to the result of scenario 1. Mousa et al. [15] calculated 0.87 kg CO_2 eq as the global warming potential for 1 kg BioSA by using dextrose derived from sorghum grain. This value is lower than the calculated value in this work. This may be because no pretreatment stage is required unlike the lignocellulosic residues considered as a feedstock in this work. Gadkari et al. [10] calculated 1.30 kg CO_2 eq emissions per kg BioSA considering bread waste as feedstock for BioSA small-scale production.

Table 4. 4 Midpoint environmental impacts

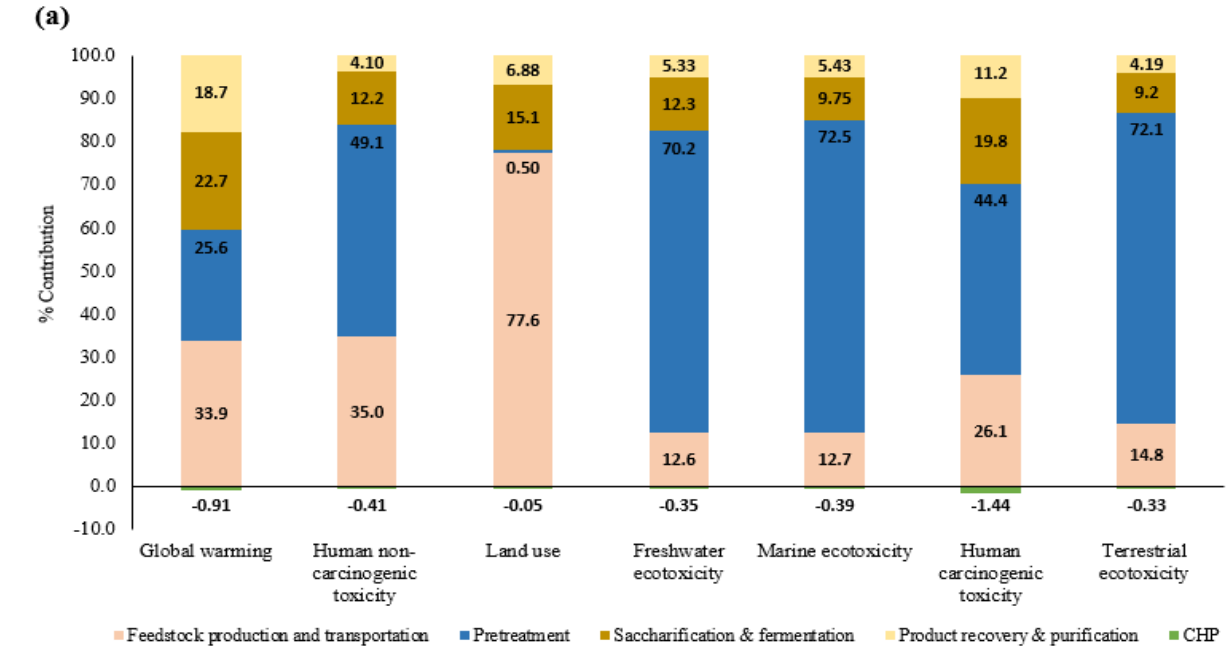
***Note:** Green and red boxes indicate the minimum and maximum values

Impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Fine particulate matter formation	kg PM 2.5 eq	3.29×10^{-3}	1.00×10^{-2}	4.59×10^{-3}	4.05×10^{-3}
Global warming	kg CO_2 eq	1.33×10^{0}	2.82×10^{0}	1.78×10^{0}	3.23×10^{0}
Stratospheric ozone depletion	kg CFC11 eq	7.59×10^{-6}	1.29×10^{-5}	1.10×10^{-5}	1.10×10^{-6}

Impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Fossil resource scarcity	kg oil eq	3.4×10^{-1}	7.9×10^{-1}	4.4×10^{-1}	1.46×10^{0}
Human non-carcinogenic toxicity	kg 1,4-DCB	3.94×10^{0}	6.96×10^{0}	5.70×10^{0}	1.80×10^{0}
Marine eutrophication	kg N eq	1.71×10^{-3}	2.53×10^{-3}	2.42×10^{-3}	4.88×10^{-5}
Ozone formation, terrestrial ecosystems	kg No_x eq	4.43×10^{-3}	8.60×10^{-3}	6.16×10^{-3}	5.74×10^{-3}
Freshwater ecotoxicity	kg 1,4-DCB	1.4×10^{-1}	2.6×10^{-1}	2.1×10^{-1}	9.00×10^{-2}
Land use	m^2a crop eq	1.01×10^{0}	1.58×10^{0}	1.47×10^{0}	2.00×10^{-2}
Water consumption	m^3	6.41×10^{-2}	3.70×10^{-1}	8.00×10^{-2}	2.00×10^{-2}
Marine ecotoxicity	kg 1,4-DCB	1.80×10^{-1}	3.30×10^{-1}	2.60×10^{-1}	1.10×10^{-1}
Mineral resource scarcity	kg Cu eq	1.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	6.25×10^{-3}
Ionizing radiation	kBq Co-60 eq	-3.00×10^{-2}	2.00×10^{-1}	-7.00×10^{-2}	1.70×10^{-1}
Freshwater eutrophication	kg P eq	6.00×10^{-4}	1.20×10^{-3}	8.60×10^{-4}	6.40×10^{-4}

Impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Terrestrial ecotoxicity	kg 1,4-DCB	1.58×10^{1}	2.72×10^{1}	2.28×10^{1}	7.98×10^{0}
Human carcinogenic toxicity	kg 1,4-DCB	8.00×10^{-2}	1.7×10^{-1}	1.00×10^{-1}	1.10×10^{-1}
Ozone formation, human health	kg NO_x eq	4.33×10^{-3}	1.00×10^{-2}	6.03×10^{-3}	1.00×10^{-2}
Terrestrial acidification	kg SO_2 eq	1.00×10^{-2}	2.00×10^{-2}	1.39×10^{-2}	1.00×10^{-2}

Figure 4.3 presents the percentage contribution of the inventory stages of each scenario to the seven impact categories with the highest values (detailed contribution data for all 18 impact categories shown in **Table 4.5**). The contribution of each biorefining step is shown to pinpoint those biorefining steps that must be improved to reduce their environmental impact.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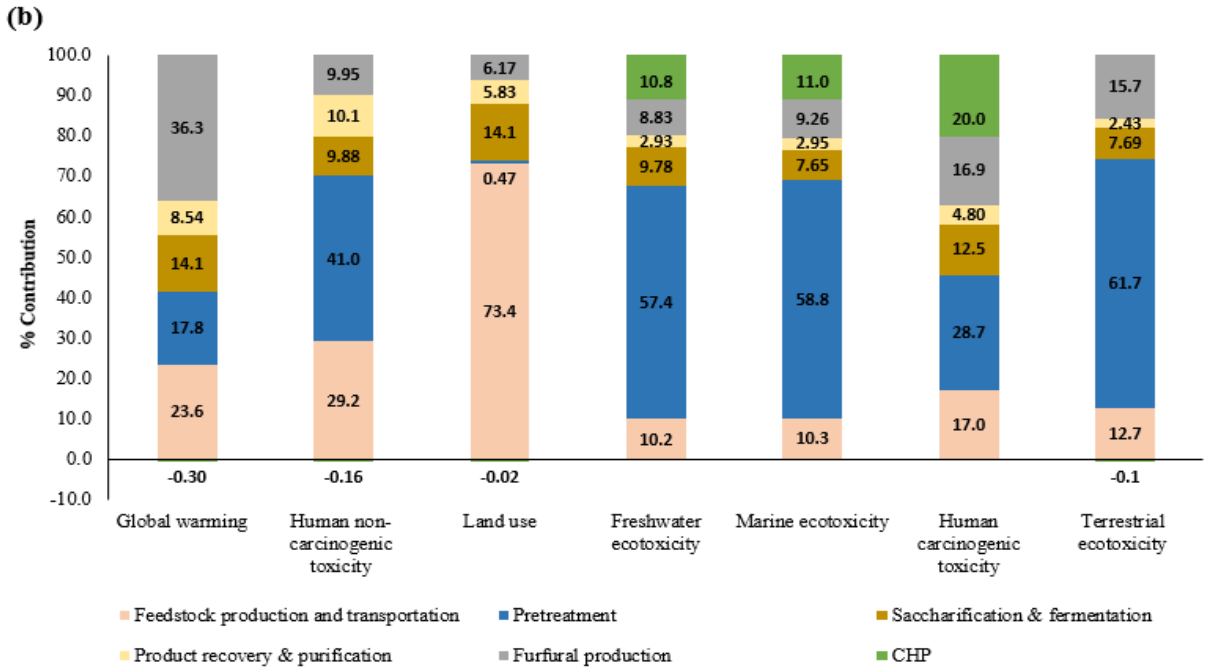
9.2
72.1
14.8
-0.33
Global warming
Human non-carcinogenic toxicity
Land use
Freshwater ecotoxicity
Marine ecotoxicity
Human carcinogenic toxicity
Terrestrial ecotoxicity
Feedstock production and transportation
Pretreatment
Saccharification & fermentation
Product recovery & purification
CHP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14.1
17.8
23.6
-0.30
9.95
10.1
9.88
41.0
29.2
-0.16
6.17
5.83
14.1
0.47
73.4
-0.02
10.8
8.83
2.93
9.78
57.4
10.2
11.0
9.26
2.95
7.65
58.8
10.3
20.0
16.9
4.80
12.5
28.7
17.0
15.7
2.43
7.69
61.7
12.7
-0.1
Global warming
Human non-carcinogenic toxicity
Land use
Freshwater ecotoxicity
Marine ecotoxicity
Human carcinogenic toxicity
Terrestrial ecotoxicity
Feedstock production and transportation
Pretreatment
Saccharification & fermentation
Product recovery & purification
Furfural production
CHP

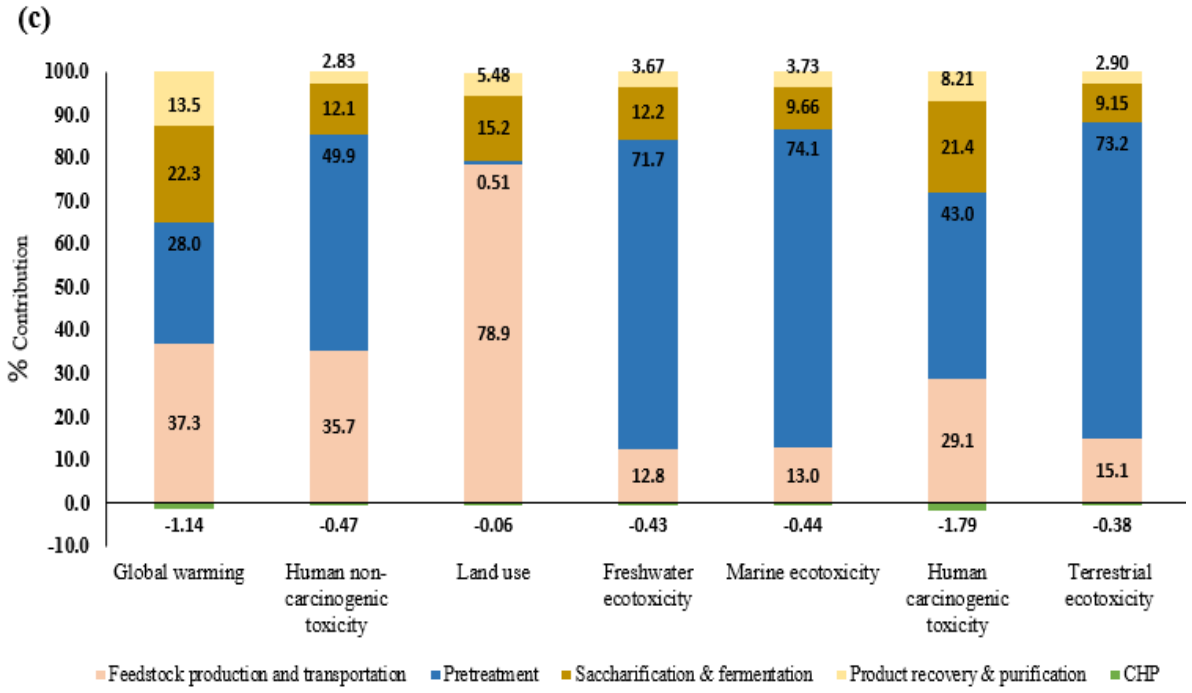


Figure 4. 3 Agronomic, transportation, and process stage-wise % contribution in environmental impacts of the three BioSA production ;a) scenario 1; b) scenario 2; and c) scenario 3.

In global warming, the feedstock production and transportation stages and the pretreatment step of the fabrication stages contribute 33.9% and 25.6% for scenario 1. In this inorganic phosphorus and ammonium nitrite-based fertilizers were identified as the main contributors whereas as in scenario 2, furfural production contributed almost 36.3 % due to the use of tetrahydrofuran (THF) as feedstock in the biorefining stage.

Table 4. 5 Biorefinery stage-wise contribution in midpoint impact categories in their specific unit

	Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Scenario 1	Fine particulate matter formation (kg PM2.5 eq)	6.50×10^{-4}	1.75×10^{-3}	5.79×10^{-4}	3.10×10^{-4}		-1.19×10^{-5}
	Global warming (kg CO_2 eq)	4.51×10^{-1}	3.41×10^{-1}	3.02×10^{-1}	2.48×10^{-1}		-1.21×10^{-2}
	Stratospheric ozone depletion (kg CFC11 eq)	6.09×10^{-6}	2.18×10^{-7}	9.98×10^{-7}	2.98×10^{-7}		-1.54×10^{-8}
	Fossil resource scarcity (kg oil eq)	8.29×10^{-2}	7.73×10^{-2}	6.72×10^{-2}	1.17×10^{-1}		-3.43×10^{-3}
	Human non-carcinogenic toxicity (kg 1,4-DCB)	1.38×10^{0}	1.94×10^{0}	4.80×10^{-1}	1.62×10^{-1}		-1.60×10^{-2}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Marine eutrophication (kg N eq)	1.17×10^{-3}	1.28×10^{-5}	3.27×10^{-4}	2.03×10^{-4}		-1.83×10^{-6}
Ozone formation, Terrestrial ecosystems (kg No_x eq)	2.08×10^{-3}	9.47×10^{-4}	8.56×10^{-4}	5.60×10^{-4}		-2.10×10^{-5}
Freshwater ecotoxicity kg (1,4-DCB)	1.79×10^{-2}	1.00×10^{-1}	1.75×10^{-2}	7.55×10^{-3}		-5.20×10^{-4}
Land use (m^2a crop eq)	7.86×10^{-1}	5.03×10^{-3}	1.53×10^{-1}	6.97×10^{-2}		-5.00×10^{-4}
Water consumption (m^3)	2.78×10^{-3}	2.81×10^{-2}	2.69×10^{-2}	8.38×10^{-3}		-5.22×10^{-3}
Marine ecotoxicity (kg 1,4-DCB)	2.29×10^{-2}	1.31×10^{-1}	1.76×10^{-2}	9.77×10^{-3}		-6.80×10^{-4}
Mineral resource scarcity (kg Cu eq)	2.96×10^{-3}	6.48×10^{-3}	1.13×10^{-3}	5.80×10^{-4}		-1.30×10^{-4}

	Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
	Ionizing radiation (kBq Co-60 eq)	9.05×10^{-3}	2.16×10^{-2}	2.76×10^{-2}	4.95×10^{-3}		-9.65×10^{-2}
	Freshwater eutrophication (kg P eq)	2.30×10^{-4}	1.92×10^{-4}	1.46×10^{-4}	4.30×10^{-5}		-1.32×10^{-6}
	Terrestrial ecotoxicity (kg 1,4-DCB)	2.34×10^{0}	1.14×10^{1}	1.45×10^{0}	6.61×10^{-1}		-5.21×10^{-2}
	Human carcinogenic toxicity (kg 1,4-DCB)	1.99×10^{-2}	3.38×10^{-2}	1.51×10^{-2}	8.54×10^{-3}		-1.07×10^{-3}
	Ozone formation, Human health (kg No_x eq)	2.05×10^{-3}	9.36×10^{-4}	8.45×10^{-4}	5.20×10^{-4}		-2.05×10^{-5}
	Terrestrial acidification (kg SO_2 eq)	1.70×10^{-3}	5.19×10^{-3}	2.12×10^{-3}	8.80×10^{-4}		-2.74×10^{-5}
Scenario 2	Fine particulate matter formation	9.60×10^{-4}	2.56×10^{-3}	7.56×10^{-4}	3.22×10^{-4}	1.07×10^{-3}	5.82×10^{-4}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
(kg PM2.5 eq)						
Global warming (kg CO_2 eq)	6.64×10^{-1}	5.02×10^{-1}	3.97×10^{-1}	2.40×10^{-1}	6.36×10^{-1}	3.78×10^{-1}
Stratospheric ozone depletion (kg CFC11 eq)	8.96×10^{-6}	3.21×10^{-7}	1.45×10^{-6}	3.30×10^{-7}	2.30×10^{-7}	1.60×10^{-6}
Fossil resource scarcity (kg oil eq)	1.22×10^{-1}	1.14×10^{-1}	9.84×10^{-2}	1.08×10^{-1}	2.30×10^{-1}	1.15×10^{-1}
Human non-carcinogenic toxicity (kg 1,4-DCB)	2.03×10^{0}	2.85×10^{0}	6.87×10^{-1}	1.61×10^{-1}	5.45×10^{-1}	6.81×10^{-1}
Marine eutrophication (kg N eq)	1.72×10^{-3}	1.89×10^{-5}	4.66×10^{-4}	2.14×10^{-4}	1.60×10^{-5}	9.83×10^{-5}
Ozone formation, Terrestrial	3.06×10^{-3}	1.40×10^{-3}	1.19×10^{-3}	5.50×10^{-4}	1.50×10^{-3}	9.06×10^{-4}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
ecosystems (kg NO_x eq)						
Freshwater ecotoxicity kg (1,4-DCB)	2.63×10^{-2}	1.47×10^{-1}	2.51×10^{-2}	7.52×10^{-3}	2.27×10^{-2}	2.77×10^{-2}
Land use (m^2a crop eq)	1.16×10^{0}	7.40×10^{-3}	2.23×10^{-1}	8.04×10^{-2}	1.08×10^{-2}	9.69×10^{-2}
Water consumption (m^3)	4.09×10^{-3}	3.98×10^{-2}	3.95×10^{-2}	9.11×10^{-3}	3.42×10^{-2}	2.42×10^{-1}
Marine ecotoxicity (kg 1,4-DCB)	3.38×10^{-2}	1.93×10^{-1}	2.51×10^{-2}	9.68×10^{-3}	3.04×10^{-2}	3.62×10^{-2}
Mineral resource scarcity (kg Cu eq)	4.36×10^{-3}	9.52×10^{-3}	1.65×10^{-3}	5.60×10^{-4}	1.56×10^{-3}	2.50×10^{-3}
Ionizing radiation (kBq Co-60 eq)	1.33×10^{-2}	8.72×10^{-3}	6.37×10^{-2}	4.80×10^{-3}	4.92×10^{-2}	6.32×10^{-2}
Freshwater eutrophication (kg P eq)	3.40×10^{-4}	2.76×10^{-4}	2.08×10^{-4}	4.17×10^{-5}	2.10×10^{-4}	1.29×10^{-4}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Terrestrial ecotoxicity (kg 1,4-DCB)	3.45×10^{0}	1.70×10^{1}	1.98×10^{0}	5.29×10^{-1}	2.25×10^{0}	1.97×10^{0}
Human carcinogenic toxicity (kg 1,4-DCB)	2.93×10^{-2}	4.94×10^{-2}	2.16×10^{-2}	8.26×10^{-3}	2.91×10^{-2}	3.44×10^{-2}
Ozone formation, Human health (kg NOx eq)	3.02×10^{-3}	1.38×10^{-3}	1.17×10^{-3}	5.10×10^{-4}	1.44×10^{-3}	8.76×10^{-4}
Terrestrial acidification (kg SO_2 eq)	2.50×10^{-3}	7.65×10^{-3}	2.94×10^{-3}	8.90×10^{-4}	2.32×10^{-3}	1.76×10^{-3}
Fine particulate matter formation (kg PM2.5 eq)	9.60×10^{-4}	2.55×10^{-3}	7.56×10^{-4}	3.22×10^{-4}		-2.00×10^{-5}
Global warming (kg CO_2 eq)	6.64×10^{-1}	4.99×10^{-1}	3.97×10^{-1}	2.40×10^{-1}		-2.04×10^{-2}

	Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Scenario 3	Stratospheric ozone depletion (kg CFC11 eq)	8.96×10^{-6}	3.23×10^{-7}	1.45×10^{-6}	3.30×10^{-7}		-2.58×10^{-8}
	Fossil resource scarcity (kg oil eq)	1.22×10^{-1}	1.13×10^{-1}	9.84×10^{-2}	1.08×10^{-1}		-5.77×10^{-3}
	Human non-carcinogenic toxicity (kg 1,4-DCB)	2.03×10^{0}	2.84×10^{0}	6.87×10^{-1}	1.61×10^{-1}		-2.68×10^{-2}
	Marine eutrophication (kg N eq)	1.72×10^{-3}	1.90×10^{-5}	4.66×10^{-4}	2.14×10^{-4}		-3.07×10^{-6}
	Ozone formation, Terrestrial ecosystems (kg NO_x eq)	3.06×10^{-3}	1.39×10^{-3}	1.19×10^{-3}	5.50×10^{-4}		-3.52×10^{-5}
	Freshwater ecotoxicity kg (1,4-DCB)	2.63×10^{-2}	1.47×10^{-1}	2.51×10^{-2}	7.52×10^{-3}		-8.80×10^{-4}
	Land use	1.16×10^{0}	7.45×10^{-3}	2.23×10^{-1}	8.04×10^{-2}		-8.40×10^{-4}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
(m^2a crop eq)						
Water consumption (m^3)	4.09×10^{-3}	3.97×10^{-2}	3.95×10^{-2}	9.11×10^{-3}		-8.77×10^{-3}
Marine ecotoxicity (kg 1,4-DCB)	3.38×10^{-2}	1.92×10^{-1}	2.51×10^{-2}	9.68×10^{-3}		-1.14×10^{-3}
Mineral resource scarcity (kg Cu eq)	4.36×10^{-3}	9.44×10^{-3}	1.65×10^{-3}	5.60×10^{-4}		-2.30×10^{-4}
Ionizing radiation (kBq Co-60 eq)	1.33×10^{-2}	3.17×10^{-2}	4.06×10^{-2}	4.80×10^{-3}		-1.62×10^{-1}
Freshwater eutrophication (kg P eq)	3.40×10^{-4}	2.75×10^{-4}	2.08×10^{-4}	4.17×10^{-5}		-2.22×10^{-6}
Terrestrial ecotoxicity (kg 1,4-DCB)	3.45×10^{0}	1.67×10^{1}	2.09×10^{0}	6.61×10^{-1}		-8.75×10^{-2}
Human carcinogenic toxicity	2.93×10^{-2}	4.33×10^{-2}	2.16×10^{-2}	8.26×10^{-3}		-1.80×10^{-3}

Impact category	Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
(kg 1,4-DCB)						
Ozone formation, Human health (kg NO_x eq)	3.02×10^{-3}	1.37×10^{-3}	1.17×10^{-3}	5.10×10^{-4}		-3.44×10^{-5}
Terrestrial acidification (kg SO_2 eq)	2.50×10^{-3}	7.64×10^{-3}	2.94×10^{-3}	8.90×10^{-4}		-4.60×10^{-5}

In all scenarios, the pretreatment section exhibits the largest contribution to human non-carcinogenic toxicity because of the sulfuric acid used in the detoxification process. For the Land use category, feedstock production and transportation are the highest contributors for all three scenarios. CHP shows a negative contribution for all three scenarios due to inhouse electricity production from lignin and biogas which replaces the conventional fossil-based medium voltage electricity. However, CHP in scenario 2 contributes, due to its higher energy requirements for furfural synthesis, to freshwater ecotoxicity, marine ecotoxicity, and human carcinogenic toxicity categories. Thus, higher temperature and pressure requirements for furfural synthesis are identified as an important hurdle for environmental sustainability. Therefore, alternative synthesis routes for furfural production under lower temperature and pressure conditions must be developed to overcome this hurdle. In addition, due to the large consumption of process water and chemicals such as sodium hydroxide, sulfuric acid, and calcium carbonate in the pretreatment stage, the contribution of this section to freshwater ecotoxicity, marine ecotoxicity, and terrestrial ecotoxicity are highest for all three scenarios.

Midpoint impact category results were normalized per person per year by using specific normalization factors for the ReCiPe 2016 midpoint (H) [30]. The categories with the largest normalization values are shown in **Figure 4.4**. These are freshwater ecotoxicity, human noncarcinogenic toxicity, marine ecotoxicity, terrestrial ecotoxicity, and human carcinogenic toxicity for all three scenarios and the fossil-based route. The rest of the impact categories resulted in normalized values lower than 0.01. Scenario 2 ranked as the worst option, whilst the fossil-based route ranked the best, followed by scenario 1.

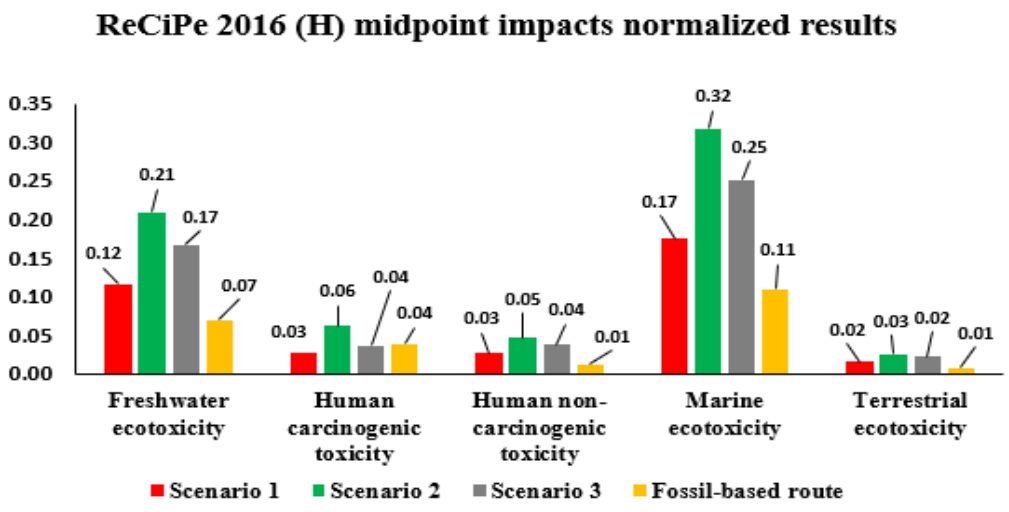


Figure 4. 4 Normalized midpoint impact assessment results for all three scenarios and fossil-based route

4.4.2 Impact assessment results at endpoint impact categories

Table 4.6 shows the endpoint impact assessment results in three damage categories (ecosystem, human health, and resources). Again, the lowest and highest values are marked in green and red boxes, respectively. The fossil-based route is the least damaging to the ecosystem scoring the lowest values in eight categories out of twelve except for global warming categories which scored the highest values. Scenario 1 followed the fossil-resource route, scoring the lowest values in four categories and with a total of 1.70 x 10^{-8} lost species*yr being 30.0 % higher than the value of the fossil-resource route.

Table 4. 6 Endpoint environmental impacts. Green and red boxes indicate the minimum and maximum values

***Note:** Green and red boxes indicate the minimum and maximum values

Endpoint impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Global warming, freshwater ecosystems	lost species *yr	1.02×10^{-13}	2.16×10^{-13}	1.36×10^{-13}	2.47×10^{-13}
Freshwater ecotoxicity	lost species *yr	9.86×10^{-11}	1.78×10^{-10}	1.42×10^{-10}	5.90×10^{-11}
Freshwater eutrophication	lost species *yr	4.04×10^{-10}	8.04×10^{-10}	5.75×10^{-10}	4.26×10^{-10}
Terrestrial ecotoxicity	lost species *yr	1.80×10^{-10}	3.10×10^{-10}	2.60×10^{-10}	9.10×10^{-11}
Ozone formation, terrestrial ecosystems	lost species *yr	5.71×10^{-10}	1.11×10^{-9}	7.94×10^{-10}	7.41×10^{-10}
Land use	lost species *yr	9.00×10^{-9}	1.40×10^{-8}	1.30×10^{-8}	2.12×10^{-10}

Endpoint impact category	**Units**	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Fossil resource route**
Global warming, terrestrial ecosystems	lost species *yr	3.73×10^{-9}	7.91×10^{-9}	4.98×10^{-9}	9.06×10^{-9}
Marine eutrophication	lost species *yr	2.90×10^{-12}	4.31×10^{-12}	4.10×10^{-12}	8.30×10^{-14}
Water consumption, aquatic ecosystems	lost species *yr	3.87×10^{-14}	2.27×10^{-13}	5.13×10^{-14}	1.27×10^{-14}
Marine ecotoxicity	lost species *yr	1.90×10^{-11}	3.45×10^{-11}	2.73×10^{-11}	1.19×10^{-11}
Terrestrial acidification	lost species *yr	2.09×10^{-9}	3.83×10^{-9}	2.95×10^{-9}	1.92×10^{-9}
Water consumption, terrestrial ecosystem	lost species *yr	8.65×10^{-10}	5.07×10^{-9}	1.15×10^{-9}	2.84×10^{-10}
Sum (ecosystem)	**lost species *yr**	**1.70×10^{-8}**	**3.32×10^{-8}**	**2.39×10^{-8}**	**1.28×10^{-8}**

Endpoint impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Human carcinogenic toxicity	DALY	2.53×10^{-7}	5.74×10^{-7}	3.34×10^{-7}	3.62×10^{-7}
Stratospheric ozone depletion	DALY	4.03×10^{-9}	6.85×10^{-9}	5.86×10^{-9}	4.11×10^{-7}
Ionizing radiation	DALY	-2.82×10^{-10}	2.28×10^{-9}	-6.07×10^{-10}	5.83×10^{-10}
Human non-carcinogenic toxicity	DALY	8.99×10^{-7}	1.59×10^{-6}	1.30×10^{-6}	1.45×10^{-9}
Ozone formation, human health	DALY	3.94×10^{-9}	7.65×10^{-9}	5.49×10^{-9}	4.99×10^{-9}
Fine particulate matter formation	DALY	2.07×10^{-6}	3.94×10^{-6}	2.88×10^{-6}	2.54×10^{-6}
Water consumption, human health	DALY	1.42×10^{-7}	8.34×10^{-7}	1.89×10^{-7}	4.67×10^{-8}
Global warming, human health	DALY	1.24×10^{-6}	2.62×10^{-6}	1.65×10^{-6}	3.00×10^{-6}
Sum (human health)	**DALY**	**4.61×10^{-6}**	**9.58×10^{-6}**	**6.37×10^{-6}**	**6.37×10^{-6}**

Endpoint impact category	Units	Scenario 1	Scenario 2	Scenario 3	Fossil resource route
Mineral resource scarcity	USD2013	2.55×10^{-3}	4.68×10^{-3}	3.65×10^{-3}	1.44×10^{-3}
Fossil resource scarcity	USD2013	1.10×10^{-1}	2.51×10^{-1}	1.42×10^{-1}	5.66×10^{-1}
Sum (resources)	**USD2013**	**1.13×10^{-1}**	**2.55×10^{-1}**	**1.46×10^{-1}**	**5.67×10^{-1}**

Scenario 2 resulted in the most damaging to the ecosystem with the highest values in ten categories and in the total amount with 3.32×10^{-8} lost species*yr, 2.6-fold the value of the fossil-resource route. However, scenario 1 ranked above all other scenarios and the fossil-based route for the human health endpoint, with the lowest values in 5 out of eight categories and a total value of 4.61×10^{-6} DALY less than half of the worst value of 9.58×10^{-6} DALY of scenario 2. Individual process stage-wise contributions in endpoint impact categories are provided in **Table 4.7**. Regarding the resource endpoint category, the fossil-based route scored the highest value with total damage of 5.67×10^{-1} USD 2013, fivefold higher than the scenario 1, which was the option with the lowest impact (1.13×10^{-1} USD 2013). For all scenarios, the contribution of feedstock production and transportation categories is considerable, in some cases above 50.0 %. Together with the pretreatment step make around 50.0 % of the contributions in most cases. The exception is scenario 2 due to the production of furfural with contributions between 9.65 and 25.8 % to all categories and CHP stage with contributions around 17.0 %

Table 4. 7 Biorefinery stage-wise contribution in endpoint impact categories in their specific unit

		Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Scenario 1	Ecosystem (lost species *yr)	9.11×10^{-9}	2.94×10^{-9}	3.18×10^{-9}	1.73×10^{-9}		-1.19×10^{-10}
	Human Health (DALY)	1.22×10^{-6}	2.03×10^{-6}	8.67×10^{-7}	5.15×10^{-7}		-3.84×10^{-8}
	Resources (USD 2013)	3.12×10^{-2}	2.38×10^{-2}	1.80×10^{-2}	4.10×10^{-2}		-1.21×10^{-3}
Scenario 2	Ecosystem (lost species *yr)	1.34×10^{-8}	4.31×10^{-9}	4.57×10^{-9}	1.81×10^{-9}	3.21×10^{-9}	5.89×10^{-9}
	Human Health (DALY)	1.80×10^{-6}	2.99×10^{-6}	1.16×10^{-6}	5.08×10^{-7}	1.56×10^{-6}	1.55×10^{-6}
	Resources (USD 2013)	4.60×10^{-2}	3.50×10^{-2}	2.89×10^{-2}	3.81×10^{-2}	6.58×10^{-2}	4.16×10^{-2}

		Feedstock production and transportation	Pretreatment	Saccharification and fermentation	Product recovery and purification	Furfural production	CHP
Scenario 3	Ecosystem (lost species *yr)	1.34×10^{-8}	4.30×10^{-9}	4.58×10^{-9}	1.81×10^{-9}		-2.00×10^{-10}
	Human Health (DALY)	1.80×10^{-6}	2.96×10^{-6}	1.16×10^{-6}	5.08×10^{-7}		-6.45×10^{-8}
	Resources (USD 2013)	4.60×10^{-2}	3.49×10^{-2}	2.89×10^{-2}	3.81×10^{-2}		-2.03×10^{-3}

The contribution of inventory stages and biorefining steps to endpoint impacts is shown in **Figure 4.5.**

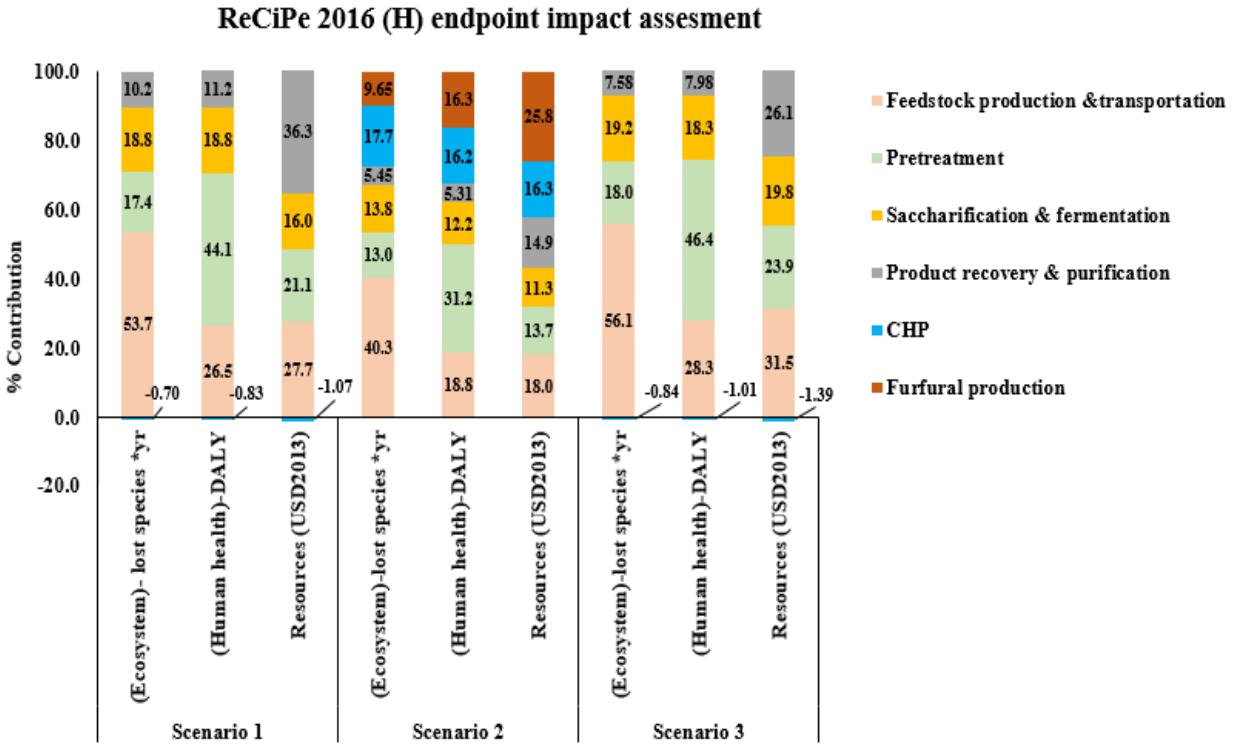


Figure 4. 5 Process area-wise percentage contribution in endpoint environmental impacts

4.4.3 Monetary valuation results

The monetization of the endpoint impacts, i.e., ecosystem, human health, and resources from **Table 4.6** are shown in **Table 4.8.** The 2013 USD of resources was updated to 2021 USD value taking into consideration an inflation rate of 11.1% [38]. Highest and lowest values are marked in red and green boxes, respectively. Note that once the impacts have been monetized, the fossil-based route scores the lowest impact in the ecosystem damage. However, the highest value in resource damage is associated with this alternative. The lowest impact on human health and

resources damages is scored by scenario 1. **Figure 4.6** compares calculated environmental costs with the minimum selling price, adapted from a recent study [22].

Table 4. 8 Monetary valuation of endpoint impacts

*** Note:** Green and red boxes indicate the minimum and maximum values

	Sum (ecosystem) in BAHY [a]	**Sum (human health) in QALY** [b]	**Sum (resources) in USD2013**	**Ecosystem (USD/kg BioSA)** [c]	**Human health (USD/kg BioSA)** [d]	**Resources (USD 2021/kg BioSA)** [e]	**Total environmental cost (USD/kg BioSA)** [f]
Scenario 1	1.15×10^{-4}	4.61×10^{-6}	1.13×10^{-1}	0.41	0.94	0.13	1.48
Scenario 2	2.26×10^{-4}	9.58×10^{-6}	2.55×10^{-1}	0.80	1.96	0.28	3.05
Scenario 3	1.63×10^{-4}	6.37×10^{-6}	1.46×10^{-1}	0.57	1.31	0.16	2.04
Fossil-based route	8.70×10^{-5}	6.37×10^{-6}	5.67×10^{-1}	0.31	1.31	0.63	2.24

[a] lost species *yr. converted to BAHY by applying a conversion factor (1 lost species *yr. = 6800 BAHY). [b] QALY is identical to DALY. [C] BAHY to USD conversion is done by applying the conversion factor (1 BAHY = 3536.01 USD). [d] QALY converted to USD by applying the conversion factor (1 QALY = 205088.62 USD). [e] adjusted by inflation rate from 2013 to 2021. [f] sum of the ecosystem (USD), human health (USD), and resources (USD 2021).

The lowest environmental cost is associated with scenario 1 (1.48 USD/kg BioSA), followed by scenario 3, the fossil-based route, and finally, scenario 2. Therefore, scenario 1, is the option with the lowest environmental impact cost and Minimum Selling Price (MSP), followed by the fossil-based route, and scenario 3. The monetized environmental impact of scenario 1 is 0.76 USD/kg BioSA lower than the corresponding value of the fossil-based route. However, monetized values of endpoint environmental impacts of scenario 2 and scenario 3, indicate that BioSA production from renewable feedstock may be more expensive than the fossil counterpart. The selection of appropriate co-product is also a vital part that can influence environmental sustainability. Environment costs can be added fully or partially (some % of the environmental cost) to product prices or, in this case, MSP, however, this thing solely depends on the country's climate change prevention and climate change tax policies.

The Social Cost of Carbon (SSC) is another approach used to estimate the monetary value of process-associated greenhouse gas emissions. For example, the Canadian government imposed an SCC of 50 Canadian dollars per tonne of carbon emissions in 2022 and is planning to increase it further in the upcoming years [39]. The US Environmental Protection Agency (EPA) estimated 190 USD per tonne of carbon emission as SCC in 2020. The imposed value of SCC by the US government was 42 USD per tonne of carbon emission in 2020, and a further increment of up to 46 USD per tonne of carbon emission is expected by 2025 [40].

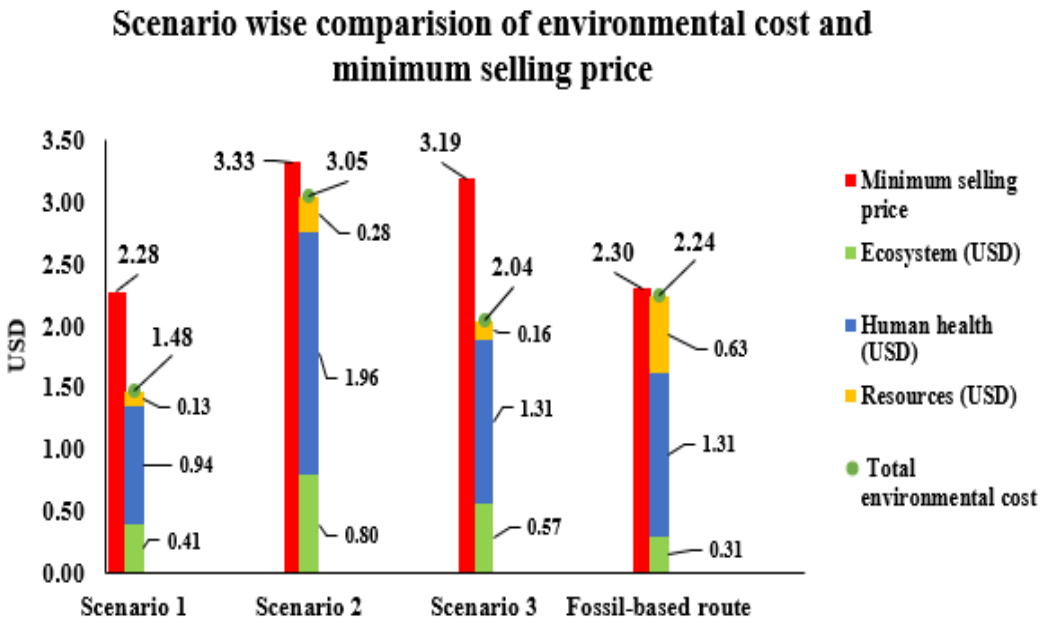


Figure 4. 6 Scenario-wise comparison of environmental cost vs. minimum selling price (real market price)

4.4.4 Sensitivity analysis of monetary valuation results

To address the uncertainty of the most important contributors to the LCA calculations and monetary valuations, a sensitivity analysis of the environmental cost was carried out. The analysis was divided into two parts. The first part considered the sensitivity to endpoint impacts: damage to resources, damage to human health, and damage to the ecosystem. The second part focused on the sensitivity to GEP, GHP and GDP employed in the monetization of the endpoint impacts. The variation range of each contributor was -50 % to +50 %, of its nominal value representing the best/worst situation, while the other contributors were kept constant. Results are shown in **Figure 4.7**. Considering sensitivity to endpoint impacts, the environmental cost of scenario 1 exhibits the largest sensitivity to damage to human health. If human health cost is increased by 50%, the environmental cost increases by 31.8 % (1.48 to 1.95 USD/kg BioSA).

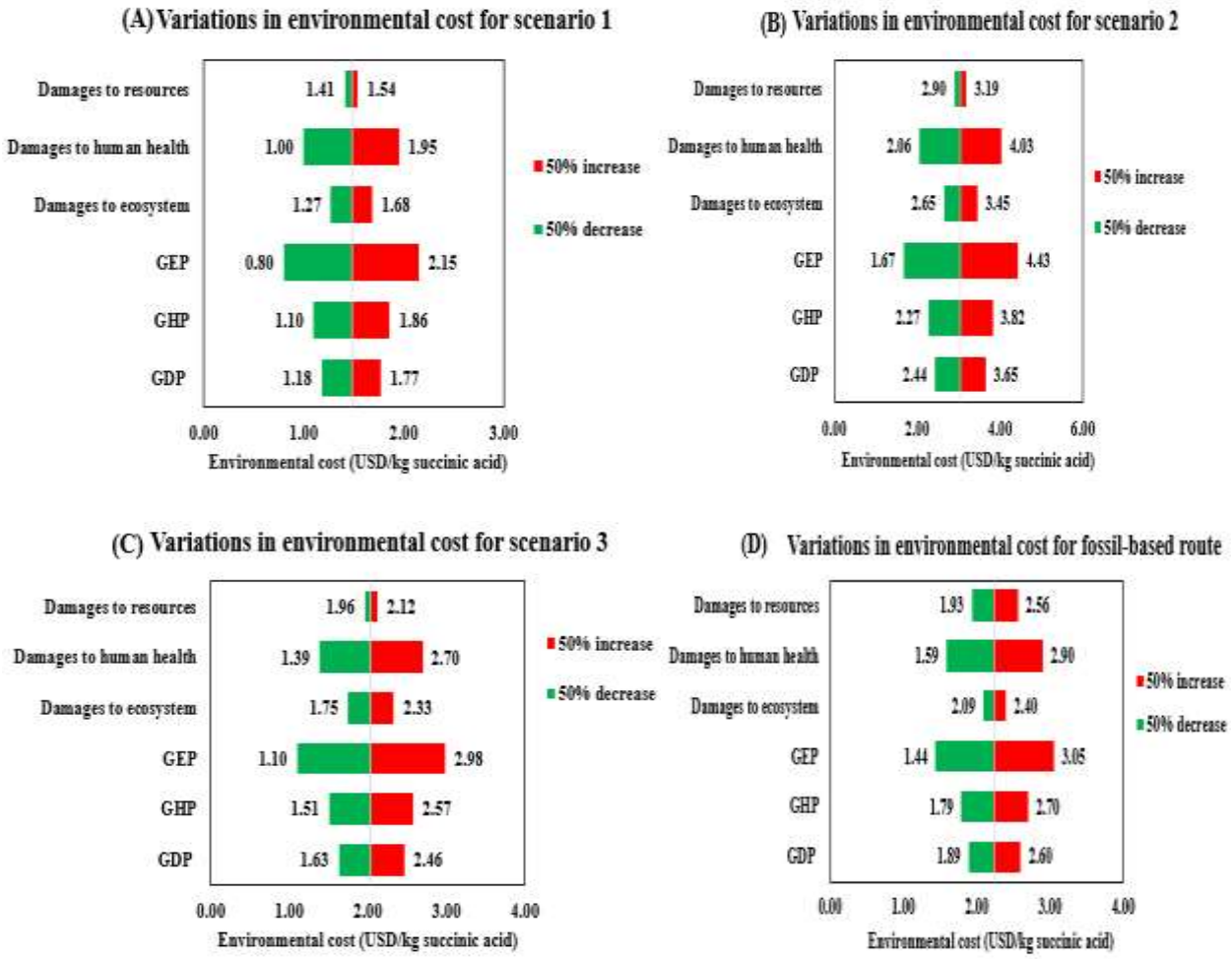


Figure 4. 7 Sensitivity analysis for environmental cost with respect to various parameters

Similarly, for the fossil route 50% reduction in damages to resources and ecosystems cause a reduction in the environmental cost of 13.8% (2.24 to 1.93 USD/kg BioSA) and 6.7 % (2.24 to 2.09 USD/kg BioSA), respectively. For scenario 3, a 50% increase and 50% reduction in human health resulted in an increment and reduction of 0.66 and 0.65 USD/kg BioSA in environmental cost, respectively. Similarly, for scenario 2, human health is the most influencing variable in environmental cost, and damage to resources is influenced the least. Regarding impacts monetization, the environmental cost is most sensitive to the GEP for all scenarios, including the

fossil-based route. A 50% reduction in GEP resulted in a significant reduction in environmental cost by 45.9%, 45.2%, 46.1%, and 35.7% for scenarios 1, 2, 3, and the fossil-based route, respectively. Furthermore, a 50 % increment in GHP caused a 25.7 %, 25.2%, 26.0%, and 20.5 % increment in environmental cost for scenarios 1, 2, 3, and the fossil-based route, respectively. Environmental costs for all scenarios are least influenced by GDP from all three variables (GEP, GHP, and GDP) considered during monetization. A 50 % increase in GDP value caused a 19.6 %, 19.7 %, 20.6 % and 16.1 % increment in environmental cost for scenarios 1, 2, 3 and fossil-based route, respectively.

4.5 Conclusion

The analysis of midpoint and endpoint categories indicates that scenario 1 and the fossil-based route scored the lowest values in these impact categories. However, identifying a scenario with a clear advantage is not straightforward. Monetary valuation contributes to this analysis with quantitative data calculated based on a unified basis. Therefore, scenario 1 (using C-6 and C-5 sugars for succinic acid and lignin for energy generation) could be considered the best option based on the environmental cost, followed by the fossil-based route. Damage to human health was identified as the leading environmental cost contributor for the studied options. From a methodology viewpoint, monetary valuation could be employed together with process economics and social policy tools such as cost-benefit analysis (CBA) and social cost of carbon (SCC) for decision-making.

4.6 References

[1] A. Ghayur, T.V. Verheyen, E. Meuleman, Techno-economic analysis of a succinic acid biorefinery coproducing acetic acid and dimethyl ether, J Clean Prod. 230 (2019) 1165–1175. https://doi.org/10.1016/j.jclepro.2019.05.180.

[2] M. Nieder-Heitmann, K. Haigh, J.F. Görgens, Process design and economic evaluation of integrated, multi-product biorefineries for the co-production of bio-energy, succinic acid, and polyhydroxybutyrate (PHB) from sugarcane bagasse and trash lignocelluloses, Biofuels, Bioproducts and Biorefining. 13 (2019) 599–617. https://doi.org/10.1002/bbb.1972.

[3] T. Werpy, G. Petersen, Top Value-Added Chemicals from Biomass Volume I, Us Nrel. (2004) Medium: ED; Size: 76 pp. pages. https://doi.org/10.2172/15008859.

[4] M. Alexandri, R. Schneider, H. Papapostolou, D. Ladakis, A. Koutinas, J. Venus, Restructuring the Conventional Sugar Beet Industry into a Novel Biorefinery: Fractionation and Bioconversion of Sugar Beet Pulp into Succinic Acid and Value-Added Coproducts, ACS Sustain Chem Eng. 7 (2019) 6569–6579. https://doi.org/10.1021/acssuschemeng.8b04874.

[5] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic acid: Technology development and commercialization, Fermentation. 3 (2017). https://doi.org/10.3390/fermentation3020026.

[6] R. Dickson, E. Mancini, N. Garg, J.M. Woodley, K. v. Gernaey, M. Pinelo, J. Liu, S.S. Mansouri, Sustainable bio-succinic acid production: superstructure optimization, techno-economic, and lifecycle assessment, Energy Environ Sci. 14 (2021) 3542–3558. https://doi.org/10.1039/d0ee03545a.

[7] X. Li, E. Mupondwa, Empirical analysis of large-scale bio-succinic acid commercialization from a technoeconomic and innovation value chain perspective: BioAmber biorefinery case study in Canada, Renewable and Sustainable Energy Reviews. 137 (2021). https://doi.org/10.1016/j.rser.2020.110587.

[8] N. Mahendrasinh Kosamia, M. Samavi, K. Piok, S. Kumar Rakshit, Perspectives for scale up of biorefineries using biochemical conversion pathways: Technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022). https://doi.org/10.1016/j.fuel.2022.124532.

[9] B. Cok, I. Tsiropoulos, A.L. Roes, M.K. Patel, Succinic acid production derived from carbohydrates: An energy and greenhouse gas assessment of a platform chemical toward a bio-based economy, Biofuels, Bioproducts and Biorefining. 8 (2014) 16–29. https://doi.org/10.1002/bbb.1427.

[10] S. Gadkari, D. Kumar, Z. hao Qin, C.S. Ki Lin, V. Kumar, Life cycle analysis of fermentative production of succinic acid from bread waste, Waste Management. 126 (2021) 861–871. https://doi.org/10.1016/j.wasman.2021.04.013.

[11] A. Foulet, T. Bouchez, E. Desmond-Le Quéméner, L. Giard, L. Renvoisé, L. Aissani, Eco-design of microbial electrochemical technologies for the production of waste-based succinic acid thanks to a life cycle assessment, J Clean Prod. 225 (2019) 1155–1168. https://doi.org/10.1016/j.jclepro.2019.03.231.

[12] P.F. Albizzati, D. Tonini, T.F. Astrup, High-value products from food waste: An environmental and socio-economic assessment, Science of the Total Environment. 755 (2021). https://doi.org/10.1016/j.scitotenv.2020.142466.

[13] S. González-García, L. Argiz, P. Míguez, B. Gullón, Exploring the production of bio-succinic acid from apple pomace using an environmental approach, Chemical Engineering Journal. 350 (2018) 982–991. https://doi.org/10.1016/j.cej.2018.06.052.

[14] B. Brunklaus, E. Rex, E. Carlsson, J. Berlin, The future of Swedish food waste: An environmental assessment of existing and prospective valorization techniques, J Clean Prod. 202 (2018) 1–10. https://doi.org/10.1016/j.jclepro.2018.07.240.

[15] H.I. Moussa, A. Elkamel, S.B. Young, Assessing energy performance of bio-based succinic acid production using LCA, J Clean Prod. 139 (2016) 761–769. https://doi.org/10.1016/j.jclepro.2016.08.104.

[16] Jo Dewulf, S. de Meester, R.A. F Alvarenga, M. Smidt, J. den Hollander, H. Bosch, Y. Xiang, M. van der Graaf, A. Lambin, J.-P. Duda, Sustainability Assessment of Renewables-Based Products: Methods and Case Studies, First Edition. Edited Life Cycle Assessment of Biobased and Fossil-Based Succinic Acid of Succinic Acid 20.1.1 Succinic Acid, A Key Biobased Building Block, n.d.

[17] A. Shaji, Y. Shastri, V. Kumar, V. v. Ranade, N. Hindle, Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse, ACS Sustain Chem Eng. 9 (2021) 12738–12746. https://doi.org/10.1021/acssuschemeng.1c02483.

[18] M. Nieder-Heitmann, K.F. Haigh, J.F. Görgens, Life cycle assessment and multi-criteria analysis of sugarcane biorefinery scenarios: Finding a sustainable solution for the South African sugar industry, J Clean Prod. 239 (2019). https://doi.org/10.1016/j.jclepro.2019.118039.

[19] Ó. Ögmundarson, S. Sukumara, M.J. Herrgård, P. Fantke, Combining Environmental and Economic Performance for Bioprocess Optimization, Trends Biotechnol. 38 (2020) 1203–1214. https://doi.org/10.1016/j.tibtech.2020.04.011.

[20] M. Pizzol, B. Weidema, M. Brandão, P. Osset, Monetary valuation in life cycle assessment: a review, J Clean Prod. 86 (2015) 170–179.

[21] Y. Dong, M. Hauschild, H. Sørup, R. Rousselet, P. Fantke, Evaluating the monetary values of greenhouse gases emissions in life cycle impact assessment, J Clean Prod. 209 (2019) 538–549.

[22] N.M. Kosamia, A. Sanchez, S.K. Rakshit, Scenario-based techno-economics and heat integration feasibility assessment of integrated multiproduct biorefineries with biosuccinic acid as the main product and various byproduct options, Biomass Convers Biorefin. (2022). https://doi.org/10.1007/s13399-022-02945-9.

[23] F. Zimbardi, E. Viola, F. Nanna, E. Larocca, M. Cardinale, D. Barisano, Acid impregnation and steam explosion of corn stover in batch processes, Ind Crops Prod. 26 (2007) 195–206. https://doi.org/10.1016/j.indcrop.2007.03.005.

[24] M.W. Guettler, M.K. Jain, United States Patent.

[25] T. Kurzrock, S. Schallinger, D. Weuster-Botz, Integrated separation process for isolation and purification of biosuccinic acid, Biotechnol Prog. 27 (2011) 1623–1628. https://doi.org/10.1002/btpr.673.

[26] B.P. Hogle, D. Shekhawat, K. Nagarajan, J.E. Jackson, D.J. Miller, Formation and recovery of itaconic acid from aqueous solutions of citraconic acid and succinic acid, Ind Eng Chem Res. 41 (2002) 2069–2073. https://doi.org/10.1021/ie010691n.

[27] R. Xing, W. Qi, G.W. Huber, Production of furfural and carboxylic acids from waste aqueous hemicellulose solutions from the pulp and paper and cellulosic ethanol industries, Energy Environ Sci. 4 (2011) 2193–2205. https://doi.org/10.1039/c1ee01022k.

[28] I.S. Arvanitoyannis, ISO 14040: life cycle assessment (LCA)–principles and guidelines, Waste Management for the Food Industries. (2008) 97–132.

[29] B.G. Hermann, K. Blok, M.K. Patel, Producing bio-based bulk chemicals using industrial biotechnology saves energy and combats climate change, Environ Sci Technol. 41 (2007) 7915–7921. https://doi.org/10.1021/es062559q.

[30] M.A.J. Huijbregts, ReCiPe 2016 A harmonized life cycle impact assessment method at midpoint and endpoint level Report I: Characterization, (n.d.).

[31] M. Goedkoop, R. Heijungs, M. Huijbregts, A. de Schryver, J. Struijs, R. van Zelm, ReCiPe 2008, A Life Cycle Impact Assessment Method Which Comprises Harmonised Category Indicators at the Midpoint and the Endpoint Level. 1 (2009) 1–126.

[32] B.P. Weidema, Comparing Three Life Cycle Impact Assessment Methods from an Endpoint Perspective, J Ind Ecol. 19 (2015) 20–26. https://doi.org/10.1111/jiec.12162.

[33] P. Kaenchan, S.H. Gheewala, Budget constraint and the valuation of environmental impacts in Thailand, International Journal of Life Cycle Assessment. 22 (2017) 1678–1691. https://doi.org/10.1007/s11367-016-1210-x.

[34] D. Ironmonger, Household Production and the Household Economy * By Duncan Ironmonger Households Research Unit, ResearchGate. (2001).

[35] OECD Data Canada, https://data.oecd.org/canada.htm (accessed July 31, 2022).

[36] GDP per capita. https://data.worldbank.org/indicator/ny.gdp.pcap.cd?locations=ca (accessed July 31, 2022).

[37] K. Koneczny, V. Dragusanu, R. Bersani, D.W. Pennington, Environmental Assessment of Municipal Waste Management Scenarios: Part I—Data Collection and Preliminary Assessments for Life Cycle Thinking Pilot Studies, JRC Scientific and Technical Reports. (2007).

[38] U.S.Inflation Calculator, (n.d.). https://www.usinflationcalculator.com/.

[39] F.L. Stewart, S. Carrière, The Greenhouse Gas Pollution Pricing Act and The Interaction of Federal and Provincial Enforcement Efforts, SSRN Electron. J. (2019).

[40] U.S. Government, Technical Update of the Social Cost of Carbon for Regulatory Impact Analysis Under Executive Order 12866 - Interagency Working Group on Social Cost of Carbon, Interagency Working Group on Social Cost of Carbon, United States Government. (2013) 1–21. https://doi.org/https://obamawhitehouse.archives.gov/sites/default/files/omb/inforeg/social_cost_of_carbon_for_ria_2013_update.pdf.

CHAPTER 5

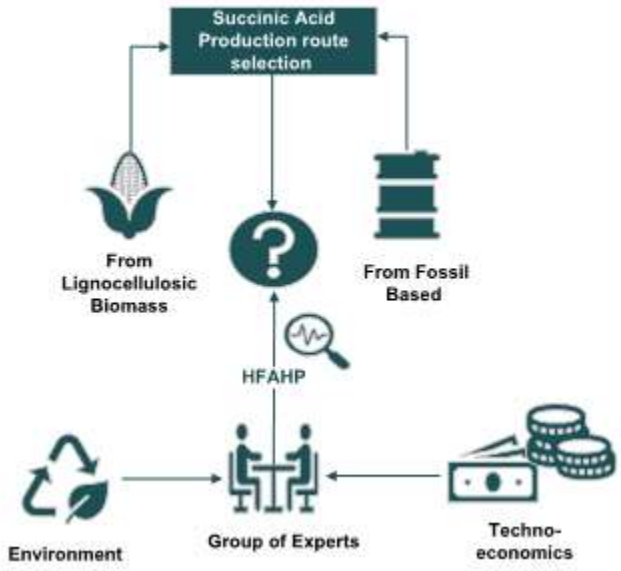
OBJECTIVE 3*

Multi-Criteria Decision Analysis of Succinic Acid Production Using Hesitant Fuzzy Analytical Hierarchy Process

* This paper from the work reported in this chapter is under preparation for submission in the **Journal of Cleaner Production** by **Elsevier**

5 Multi-criteria decision analysis of succinic acid production using hesitant fuzzy analytical hierarchy process

5.1 Abstract



For the selection of an preferred large-scale Succinic Acid (SA) production process issues related to technology, economy, and environment must be considered by decision-makers. Numerous reports were found in literature that make decisions based on either Techno-Economic Analysis (TEA) or Life Cycle Assessment (LCA). However, such decisions should be made using a comprehensive decision-making analysis method that considers both TEA and LCA, along with the involvement and inputs of experts in the relevant area. The present work performs a holistic Multi-Criteria Decision Analysis (MCDA) using the Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) for selecting the best SA production route from four studied alternatives (AL-1, AL-2, AL-3, AL-4). AL-1 utilizes both C-6 and C-5 sugar of corn stover for SA and lignin for electricity production. AL-2 produced SA, furfural, and electricity from C-6, C-5, and lignin respectively.

AL-3 considered SA production from C-6 sugar and biogas from C-5 sugar. Biogas which is subsequently used for electricity production along with lignin in a CHP. AL-4 considered SA production using a conventional fossil-based route. The hierarchical decision model consisting two main criteria, techno-economics and environment, and seven sub-criteria was developed. Fuzzy Set Theory (FST) involves expert's judgments that are used for the evaluation process. Based on these inputs the results indicate a slightly higher weightage of techno-economic criteria (55.0 %) than environmental criteria (45.0 %). AL-1 was found to be the preferred alternative for SA production with 35.0 % weightage, followed by AL-3 (24.0 %), AL-2 (22.0 %), and AL-4 (19.0 %). The sensitivity analysis results demonstrate that AL-1 remains the most preferred alternative throughout variation in the range of 0.10 to 1.00 of the main criteria weightage, whereas the remaining three alternatives were found sensitive to the variations.

Keywords: Hesitant Fuzzy AHP, Succinic acid, Multi-criteria decision analysis, Sustainability assessment, Biochemicals.

5.2 Introduction

In the recent decade, for the reduction of mankind's environmental footprint and to reduce dependency on crude oil, special attention has been given to biochemical production using lignocellulosic biomass as feedstock [1]. The production of chemicals using carbon-negative green technology from renewable resources needs to take into consideration technical, economic, and environmental aspects [2]. Succinic acid (SA) is a platform chemical which has applications in the food, pharmaceutical, detergents, cosmetic, and pigment industries. The worldwide market demand for SA is steadily increasing, with a compound annual growth rate (CAGR) of 27.4 % [3]. The Department of Energy (DoE) in the USA identified SA as one of the compounds of strategic interest among 12 platform chemicals that can be produced from renewable feedstock [4]. SA

production from renewable starch based feedstock using mature carbon-negative technologies has drawn attention for commercial manufacture due to its competitiveness to the conventional fossil-based SA production route in the last decade. However, by the end of the decade, with large fluctuation of fossil resources prices many of these commercial-scale units either closed or changed their corporate goals [5]. Various studies have been performed to assess SA production's economic and environmental sustainability. For instance, Ghayur et al. [6] employed techno-economic analysis (TEA) to evaluate capital expenditure (CAPEX), operating expenditure (OPEX), and Minimum Selling Price (MSP) for coproduction of SA, acetic acid, and dimethyl ether from pulp logs as a feedstock. Similarly, Kosamia et al. [7] also performed TEA comparison for a multiproduct biorefinery coproducing SA, furfural, and electricity from corn stover following three different production scenarios. In order to evaluate the energy performance of SA production from sorghum, Moussa et al. [8] performed a cradle-to-gate LCA. Based on TEA and LCA, Ioannidou et al. [9] estimated values of 1.23 - 2.76 USD/kg SA and 1.47 kg CO_2 eq per dry waste as MSP and GHG emissions for SA production from winery waste. Similarly, Shaji et al. [10] studied TEA and LCA for SA production from sugarcane bagasse and calculated the MSP and greenhouse gas (GHG) emission of 2.37 USD/kg SA and 1.39 kg of CO_2 eq/ kg SA respectively. Dickson et al. [11] also assessed SA production economic and environmental criteria using multiple feedstocks, including glucose, corn stover, glycerol, and seaweed. They recommended the application of Multi-Criteria Decision Analysis (MCDA) for SA production option selection by considering economic and environmental aspects as a decision-making criteria. Nieder-Heitmann et al. [12] performed MCDA for assessing coproduction schemes, including SA, itaconic acid, polyhydroxy butyrate, together with electricity cogeneration. In this investigation, techno-economic and environmental sustainability parameters were normalized and used a MCDA. They

recommended the involvement of local experts and relevant stakeholders to standardize the decision-making process.

The main goal of this study is to facilitate researchers, policymakers, and market customers with a decision-making tool for selecting a preferred SA production alternative. This study evaluated SA production performance using the Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) as a MCDA tool based on two main criteria and seven sub-criteria among four available SA production alternatives. Three biochemical based biorefineries using corn stover as feedstock and a fossil resource-based alternative were compared. The analysis includes the involvement of experts in decision-making. This paper reports a novel approach using HFAHP as MCDA tool for decision-making of SA production alternative selection from a techno-economic and environmental perspective.

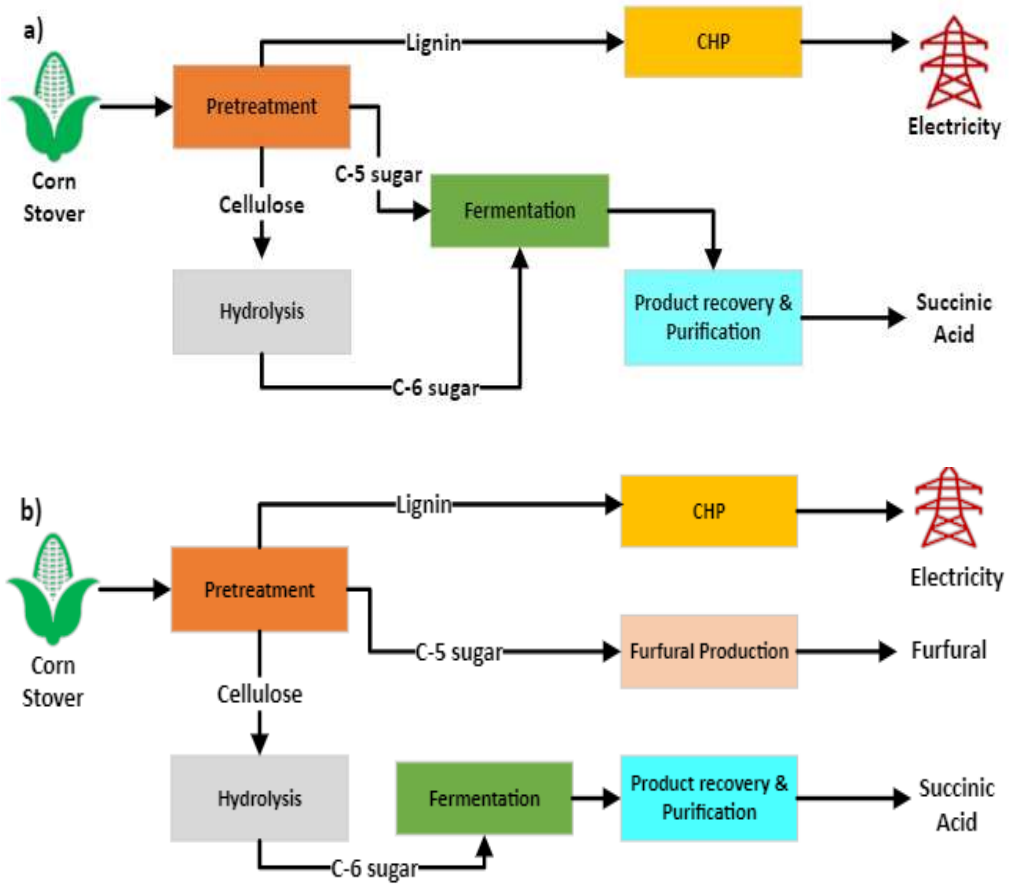
5.3 Succinic acid production alternatives considered in this work

In this paper four SA production alternatives studied are classified based on their design and starting material**.** It should be noted that three alternatives (AL-1, AL-2, AL-3) utilize corn stover as a starting feedstock and the fourth alternative (AL-4) uses crude oil-derived maleic anhydride as a starting feedstock.

5.3.1 Succinic acid production from corn stover

The biorefinery that produces SA from corn stover comprises six stages: pretreatment, hydrolysis, fermentation, product recovery and purification, Combined Heat and Power generation (CHP) unit and a Wastewater Treatment Plant (WWTP). In our previous article [7], mass-energy balance, process economy, and profitability were assessed for such a biorefinery. Three different alternative scenarios for the main product (SA) production were compared. C-6 sugars were used for SA production in all three alternatives. C-5 sugars were used for SA, furfural and biogas production

in AL-1 to three respectively. Lignin was used for electricity production in all three scenarios. Furfural in predicted to have a future market value of 896 million USD between 2020 to 2027 and is used as a primary solvent in oil refineries [13]. It was thus chosen as a co-product in AL-2. The biogas produced in a WWTP plant in AL-3 was used to produce electricity along with electricity in a CHP in AL-3. A detailed biorefinery description for AL-1, AL-2, and AL-3 can be found in **Figure 5.1**.



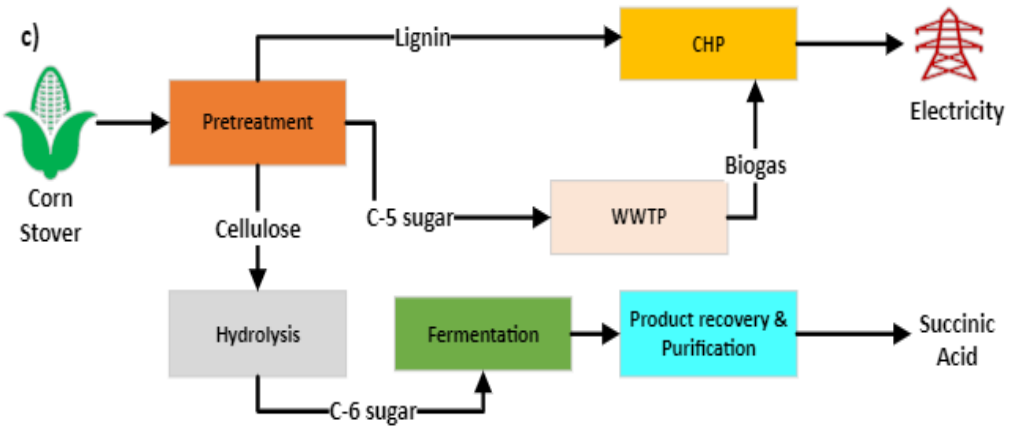


Figure 5. 1 Succinic acid and co-products production from corn stover (a) Alternative 1 (b) Alternative 2 (c) Alternative 3

Alternative 2 (AL-2) Succinic acid, furfural and electricity from corn stover: C-6 and C-5 sugar derived after the pretreatment and hydrolysis stage from cellulose and hemicellulose were utilized by *A. succinogenes* assisted fermentation stage for SA production. CHP uses the third component lignin of corn stover to produce electricity to power the biorefinery operation and sell it to district heating.

Alternative 3 (AL-3) Succinic acid, biogas and electricity from corn stover: In this alternative, after the pretreatment stage, C-5 sugar derived from hemicellulose is diverted for furfural production, and C-6 sugar, after hydrolysis, is diverted to SA production in the fermentation stage by using *A. succinogenes*. As in alternative 1, lignin is used for heat and electricity production in the CHP stage. Furfural, as a coproduct, contributes to the Minimum Selling Price (MSP) improvement of the main product SA.

Alternative 4 (AL-4)- Succinic acid production from crude oil-based maleic anhydride: SA and electricity are coproduced in this alternative. C-6 sugar from cellulose is used for SA

production, and lignin is used in the CHP stage for electricity production. The C-5 sugar stream is diverted to WWTP for biogas generation, which is later used in the CHP for additional electricity production.

5.3.2 Alternative 4 (AL-4)- Succinic acid production from crude oil-based maleic anhydride

The process for SA production from fossil route uses maleic anhydride in a liquid phase as a raw material. The two-step process starts with the hydrogenation of maleic anhydride to succinic anhydride and is followed by hydration into the final product SA [14]. Hydrogenation of maleic anhydride takes place at 120 to 180 ˚C and 0.5 to 4.0 MPa in the presence of Ni or Pd as a catalyst, and hydration is performed by dissolving succinic anhydride into hot water [15].

5.4 Multicriteria decision-making for biochemicals production from renewable resources

MCDA is a methodology used in operational research that helps in decision-making and evaluation of problems with conflicting criteria and uncertainties. It is used to solve complex decision-making problems with little or poor available data [16–19]. This technique identifies the most preferred or suitable alternative by giving them rankings based on final weightage after sorting out the various available alternatives. MCDA methods such as Multi Attributional Utility Theory (MAUT), Analytical Hierarchy Process (AHP), Analytical Network Process (ANP), Elimination and Choice Translating Reality (ELECTRE), Preference Ranking Organization Method for Enrichment of Evaluations (PROMETHEE), Dominance based Rough Set Approach (DRSA) and Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) have been suggested for making a decision based on mixed data from the different sustainability aspects such as techno-economics, environment and social aspects [5]. However, the conventional MCDA methods are inadequate to handle uncertainty in crisp numeric weights. Thus, a MCDA method with linguistic weights such as Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) was used in this study.

5.5 Methodology

In this section, the methodology adopted for HFAHP is explained in detail. The section is framed in three parts. In the first part hesitant fuzzy sets and hesitant fuzzy linguistic terms are discussed. This is followed by detailed steps of HFAHP, and finally the proposed model for the preferred SA production route selection is discussed.

5.5.1 Hesitant fuzzy sets and hesitant fuzzy linguistic terms

For handling MCDA problems, the Analytical Hierarchy Process (AHP) developed by Saaty [20] is widely employed. The problem is initially structured in a hierarchy that starts with the overall goal of the exercise, followed by criteria, sub-criteria, and alternatives at successive levels. At each level, pairwise comparisons are performed, and experts independently provide their preferences by using a discrete scale starting from zero to nine. However, this basic method faced criticism because of its inability to address imprecision in an expert's opinion. The reason for this is that in real-life decision-making problems, the experts are usually unable to explicitly provide their preferences due to the complicated nature of the comparison process. Thus, they are more confident to provide a preference interval (range) rather than a fixed value one. There is no provision in AHP to give a preference interval or fractional value between two discrete values. In order, to overcome this imprecision of AHP, Hesitant Fuzzy Sets (HFS) were introduced by Torra and Narukawa [21]. In the latter method, preferences can also be provided by a fuzzy expression in an interval. In this, the expert can provide fractional inputs instead of a fixed integer value preference used in AHP [22]. Hesitant Fuzzy Linguistic Terms (HFLTS) were developed by Rodriguez et al. [23] to help experts to give their hesitant preference in the form of linguistic terms, like Absolutely High Importance (AHI) for 10, Very Low Importance (VLI) for 1. In HFAHP, expert's preferences are given using the interval-based linguistic scale shown in **Table 5.1**. In

addition, in a real-world problem were more than two experts are involved in a decision-making process, Ordered Weighted Averaging (OWA) can be employed for aggregating the expert's evaluations [24]. These methods were used in this study to determine the best route to produce SA.

Table 5. 1 Linguistic scales for the Hesitant Fuzzy Analytical Hierarchy Process (HFAHP) [20]

Rank	Linguistic term	Triangular fuzzy number
10	Absolutely High Importance (AHI)	(7,9,9)
9	Very High Importance (VHI)	(5,7,9)
8	Essentially High Importance (ESHI)	(3,5,7)
7	Weakly High Importance (WHI)	(1,3,5)
6	Equally High Importance (EHI)	(1,1,3)
5	Exactly Equal (EE)	(1,1,1)
4	Equally Low Importance (ELI)	(0.33,1,1)
3	Weakly Low Importance (WLI)	(0.2,0.33,1)

2	Essentially Low Importance (ESLI)	(0.14,0.2,0.33)
1	Very Low Importance (VLI)	(0.11,0.14,0.2)
0	Absolutely Low Importance (ALI)	(0.11,0.11,0.14)

5.5.2 Main criteria and sub-criteria description

Criteria for the sustainability assessment of biochemical production primarily include economic, environmental, technological, and social aspects. However, some criteria may belong to more than one aspect and can overlap between two aspects, say techno-economic and socio-economic, etc. Considering the actual situation of SA production, two main criteria, techno-economic (CT-1) and environmental (CT-2), were chosen for this analysis. It was difficult to get feedback on the social aspect of SA production and was thus not considered in this analysis.

5.5.2.1 Techno-economic (CT-1) and its sub-criteria

The techno-economic criteria describe the technical and economic aspects of SA production. Technical performance was addressed based on process maturity, energy efficiency, and waste generation [25]. For process economics, profitability is an essential indicator. The targeted questions are whether the production of SA is economically feasible and whether it can make a profit or not. Net Present Value (NPV), Minimum Selling Price (MSP), and Return on Investment (ROI) are indicators that reflect economic performance efficiently [26]. In this analysis, to address process economy the sub-criteria selected included MSP (ST-1), waste generation (ST-2), raw material input (ST-3), and energy requirement (ST-4). MSP (ST-1) was calculated using standard

Discount Cash Flow Analysis (DCFA), which considered costs associated with the land, site establishment, construction, equipment purchases to installation, utility requirements, and salaries [27]. Raw material input (ST-3) represents the requirement of all feed associated with the SA production process. During the process, byproducts such as gypsum are also generated that demand treatment before disposal into landfills or incineration. This was addressed by choosing waste as a sub-criteria. Energy requirement (SE-4) calculates the amount of energy used for SA production by each alternative. These sub-criteria are necessary to address the techno-economic aspect, as it relies solely on process operating conditions which affect both the process economy and technical maturity.

5.5.2.2 Environment (CT-2) and its sub-criteria

The environmental performance of SA production is addressed by considering the pollution and resource consumption associated with the SA production process. These can be estimated by performing the Life Cycle Analysis (LCA) of SA production. In this analysis, damage-oriented (endpoint) impacts on three Areas of Protection (AOPs) of the environment, humans, ecosystem, and resources, are addressed by selecting sub-criteria such as damages to human health (SE-1), damage to the ecosystem (SE-2), and damage to resources (SE-3). Damage to human health (SE-1) covers the various impacts (total of eight impacts), including, Human carcinogenic toxicity, Stratospheric ozone depletion, Ionizing radiation, Human non-carcinogenic toxicity, Ozone formation-human health, Fine particulate matter formation, Water consumption-human health, Global warming-human health, and its end damaging results on human beings. Damage to the ecosystem (SE-2) covers a total of 12 impacts, including, i.e., Global warming-freshwater ecosystems, Freshwater ecotoxicity, Freshwater eutrophication, Terrestrial ecotoxicity, Ozone formation-terrestrial ecosystems, Land use, Global warming-terrestrial ecosystems, Marine

eutrophication, Water consumption-aquatic ecosystems, Marine ecotoxicity, Terrestrial acidification and Water consumption- terrestrial ecosystem damage to resources (SE-3). The impacts on mineral and fossil resources scarcity are considered in this analysis based on work reported by Goedkoop et al [28].

5.5.3 Hesitant fuzzy analytical hierarchy process

In section 5.5, the advantages of HFAHP over AHP, to determine the weight of criteria and sub-criteria was discussed. The detailed steps for evaluating the model's criteria, sub-criteria, and alternative weightage derived from three expert preference inputs are summarized below. These steps had to be appropriately modified from the method suggested by Öztaysi et al. [24] for the SA production process.

Step 1. The hierarchical model with two main criteria, seven sub-criteria, and four alternatives was constructed for to get three expert's preferences **(as shown in Figure 5.2)**.

Step 2. Experts assessed the main criteria and sub-criteria using the linguistic fuzzy set presented in **Table 5.1.** The experts were allowed to express their preference as an interval if they wanted. However, as a rule for utilizing the OWA operator, the maximum allowable difference between the Ranks was set as two. For example, a preference by an expert between EHI and WHI is acceptable as the difference between the ranks is 1 (which is less than 2). But if a preference is between ELI and VHI it would not be acceptable as the difference is greater than 2.

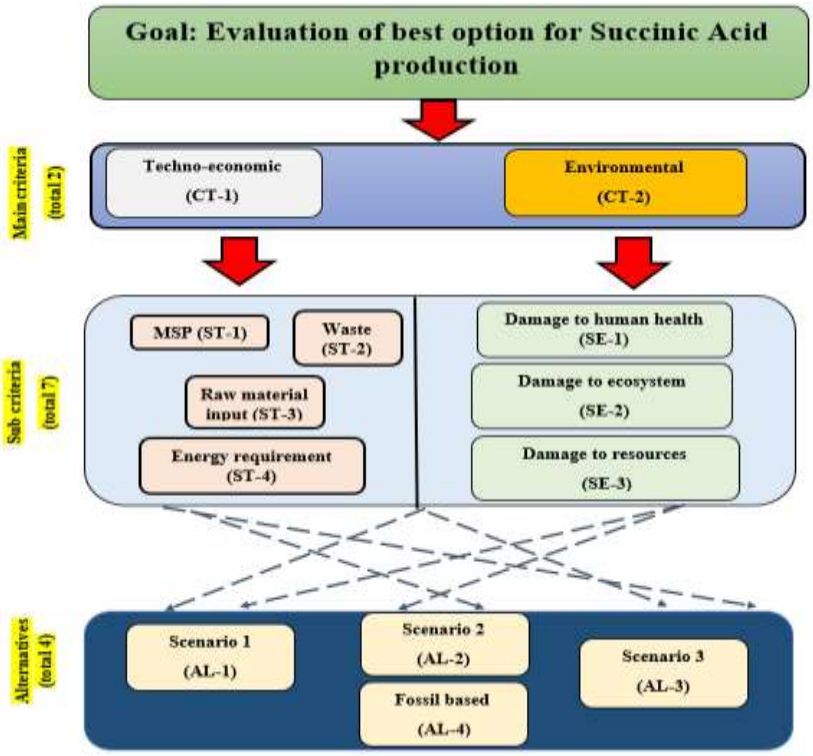


Figure 5. 2 Proposed model for SA production HFAHP

Step 3. The fuzzy envelope approach given by Liu and Rodríguez [29], was used to convert expert's preferences into trapezoidal fuzzy numbers. For the trapezoidal fuzzy interval, the lowest and highest boundary of scales are s_0 and s_g, respectively. The preferences vary between the two terms s_i and s_j. Therefore, it can be mathematically denoted as $s_0 \leq s_i \leq s_j \leq s_g$. For the evaluation of parameters (a, b, c, d) in the trapezoidal fuzzy number, Ă = (a, b, c, d), Equations **(1), (2), (3),** and **(4)** are used**.** j is the rank of highest preference, and *i* is the rank of lowest preference.

$$a = min\left\{a_L^i, a_M^i, a^{i+1}_M, \ldots\ldots a_M^j, a_R^j\right\} = a_L^i \quad (1)$$

$$d = max\left\{a_L^i, a_M^i, a^{i+1}_M, \ldots\ldots a_M^j, a_R^j\right\} = a_R^j \quad (2)$$

$$b = \begin{cases} a_{M}^{i}, if\ i+1=j \\ OWA_{W^2}\left(a_{m}^{i}, \ldots\ldots a_{m}^{\frac{i+j}{2}}\right), if\ i+j\ is\ even \\ OWA_{W^2}\left(a_{m}^{i}, \ldots\ldots a_{m}^{\frac{i+j-1}{2}}\right), if\ i+j\ is\ odd \end{cases} \quad (3)$$

$$c = \begin{cases} a_{M}^{i+1}, if\ i+1=j \\ OWA_{W^1}\left(a_{m}^{j}, a_{m}^{j-1}, \ldots\ldots a_{m}^{\frac{i+j}{2}}\right), if\ i+j\ is\ even \\ OWA_{W^1}\left(a_{m}^{j}, a_{m}^{j-1}, \ldots\ldots a_{m}^{\frac{i+j+1}{2}}\right), if\ i+j\ is\ odd \end{cases} \quad (4)$$

In addition, the OWA operator of a dimension of *n* given by Öztaysi et al. [24] is used for the fuzzy envelopes approach, which can be defined by

$$\mathrm{OWA}(a_1, a_2, \ldots\ldots, a_n) = \sum_{j=1}^{n} w_j\, b_j \quad (5)$$

Where b_j is the largest of the aggregated arguments $a_1, a_2, \ldots\ldots, a_n$ and $W = (w_1, w_2, \ldots\ldots\ldots, w_n)^T$ is the weighting vector where $w_i \in [0,1]$, i= 1,2,……n and $\sum_{i=1}^{n} w_i = 1$ The first type of weight $W^1 = (W_1^1, W_2^1, \ldots\ldots W_n^1)$ and the second type of weight $W^2 = (W_1^2, W_2^2, \ldots. W_n^2)$ defined in terms of α [30] as shown in Equations **(6)** and **(7)**.

$$W_1^1 = \alpha_2, W_2^1 = \alpha_2(1-\alpha_2), \ldots\ldots, W_n^1 = \alpha_2(1-\alpha_2)^{n-2} \quad (6)$$

$$W_1^2 == \alpha_1^{n-1}, W_2^2 = (1-\alpha_1)\alpha_1^{n-2}, \ldots\ldots, W_n^2 = (1-\alpha_1), W \quad (7)$$

Where $\alpha_1 = \frac{g-(j-i)}{(g-1)}$, $\alpha_2 = \frac{(j-i)-1}{(g-1)}$ and g is the maximum rank number (10 from **Table 5.1**).

Step 4. A collaborative pairwise comparison matrix ($\tilde{A}^k$) is formed for expert k as shown in Eq. **(8)** where $a_{ij} = (a_{ijl}, a_{ijm1}, a_{ijm2}, a_{iju})$. The reciprocal values were evaluated using Equation **(9)**.

$$\tilde{A}^k = \begin{bmatrix} 1 & \cdots & \tilde{a}_{ln} \\ \vdots & \ddots & \vdots \\ \tilde{a}_{nl} & \cdots & 1 \end{bmatrix} \quad (8)$$

$$\tilde{a}_{ji} = \left(\frac{1}{a_{iju}}, \frac{1}{a_{ijm2}}, \frac{1}{a_{ijm1}}, \frac{1}{a_{ijl}}\right) \quad (9)$$

Step 5. Before the formation of the aggregated decision matrix, the consistency of each fuzzy pairwise matrix is checked. The graded mean integration approach [31] was used to defuzzified the comparison matrices. For the trapezoidal fuzzy number $d = (l, m_1, m_{2,} u)$ the crisp number (μ_d) can be evaluated by

$$\mu_d = \frac{l+2m_1+2m_2+u}{6} \quad (10)$$

After evaluating the crisp number, the Consistency Ratio (*CR)* was calculated using Equations **(11**) and **(12)**.

$$CI = \frac{\lambda_{max-n}}{n-1} \quad (11)$$

$$CR = \frac{CI}{RI} \quad (12)$$

Where *CI* is the consistency index, λ_{max} is the largest eigenvector of the matrix, n is the number of criteria, and *RI* is the random index that differs for each n. A value of *CR* less or equal to 0.10 is acceptable [31]. If any pairwise comparison matrix is not consistent, then experts were asked to revise the preferences until the pairwise comparison matrix becomes consistent.

Step 6. Once the consistency is established in every matrix, individual matrices are aggregated into the aggregated matrix $\tilde{C}$.

$$\tilde{C} = \begin{bmatrix} 1 & \cdots & \tilde{C}_{xy} \\ \vdots & \ddots & \vdots \\ \tilde{C}_{yx} & \cdots & 1 \end{bmatrix} \quad (13)$$

Here $\tilde{C}_{ij} = \sqrt[n]{\tilde{a}_{ij}} \prod_{k=1}^{n}$, Where n is the total number of experts and k represents individual experts.

Step 7. In this step, the geometric mean ($\tilde{r}_i$) was calculated for each raw of aggregated matrix by using Equation **(14)**.

$$\tilde{r}_i = \left(\tilde{C}_{i1} \otimes \tilde{C}_{i2\ldots\ldots\ldots} \otimes \tilde{C}_{in}\right)^{1/n} \quad (14)$$

Step 8. By using Eq. **(15),** weights of main criteria, sub-criteria, and alternatives are calculated.

$$\widetilde{w}_i = \tilde{r}_i \otimes (\tilde{r}_1 \otimes \tilde{r}_{2\ldots\ldots\ldots} \otimes \tilde{r}_n)^{-1} \quad (15)$$

Step 9. The fuzzy numbers are defuzzified with the help of Equation **(16)**.

$$\mathrm{D} = \frac{C_l + 2C_{m1} + 2C_{m2} + C_u}{6} \quad (16)$$

Step 10. The defuzzified weights are normalized, and the local weights of the criteria are obtained. For the global weight of sub-criteria, local weights are multiplied by the weight of their respective main criteria.

Step 11. All the above steps are performed for each matrix and preference score (S_i) for alternative (i) calculated. The final score for each alternative can be calculated using Equation **(17)**.

$$S_i = \sum_{j=1}^{n} \forall i, w_j s_{ij} \quad (17)$$

Where w_j is the global weight of criteria j and s_{ij} is the score of alternative criteria i with respect to j. The best alternative can be evaluated by ranking the defuzzified values.

5.6 Results and discussion

Three experts with different backgrounds had scored the criteria, sub-criteria, and alternatives using pairwise comparisons at each level. Expert 1 has a work experience in the pulp and paper industry with specific expertise in biochemical process operations and their technical and economic aspect from a stakeholder point of view. Expert 2 works sustainability assessment of

biorefinery design with specific expertise in TEA and LCA. Expert 3 is works on laboratory scale design of biorefining processes.

5.6.1 Main criteria weights

All three experts evaluated two main criteria (CT-1 and CT-2), and provided individual preferences. As study has two main criteria; a 2 X 2 matrix form resulted for each expert's evaluation. The preferences provided by each expert is presented in **Table 5.2**. According to Saaty's rule [33] there is no need to check the consistency ratio if there are two or fewer criteria. Thus, for the main criteria, step 5 is skipped before the formation of a single aggerated matrix was obtained by combining three individual matrices using geometric means (as mentioned in step 6).

Table 5. 2 Fuzzy envelopes inputs for the main criteria from the three experts

		CT-1	**CT-2**
Expert-1			
	CT-1	EE	WLI
	CT-2		EE
Expert-2			
	CT-1	EE	Between ESHI and VHI
	CT-2		EE
Expert-3			
	CT-1	EE	Between ELI and EE
	CT-2		EE

After the aggregation of matrices, in order to form trapezoidal fuzzy sets in the form of a, b, c and d, the OWA operator was applied. For example, in **Table 5.2,** Expert 2 evaluation of CT-1 and CT-2, between ESHI and VHI is found (3,5,7,9). It is very important to find α_1 and α_2 using the formula given in Step 3. Here g is a top rank number 10; *i* is the rank of lowest evaluation (ESHI), equal to 8; *j* is the rank of highest evolution (VHI), equal to 9. Then,

$\alpha_1 = \frac{10-(9-8)}{(10-1)} = 1$

$\alpha_2 = \frac{(9-8)-1}{(10-1)} = 0$

As a = a_L^i and d =a_R^j; a = 3 (minimum value of ESHI shown as 3,5,7) and d = 9 (maximum value of VHI shown as 5,7,9). From Equations **(3)** and **(4)**, ,if *i+1 =j,* then b = a_M^i. In our case, *i*+1 =*j;* therefore, b = 5. In addition, if *i+1 =j;* then c = a_M^{i+1}. In our case, *i*+1 =*j;* thus, c = 7. Hence, the fuzzy envelope for CT-1 and CT-2 for expert-2 is (3,5,7,9). Similarly, the fuzzy envelope was created for the remaining evaluations (see **Table 5.3**).

Table 5. 3 Fuzzy envelopes for the main criteria evaluation for all three experts (after applying the OWA operator)

		CT-1	**CT-2**
Expert-1			
	CT-1	(1,1,1,1)	(0.2,0.33,0.33,1)
	CT-2	(1,3,3,5)	(1,1,1,1)
Expert-2			
	CT-1	(1,1,1,1)	(3,5,7,9)

	CT-2	(0.11,0.14,0.2,0.33)	(1,1,1,1)
Expert-3			
	CT-1	(1,1,1,1)	(0.33,1,1,1)
	CT-2	(1,1,1,3)	(1,1,1,1)

The geometric means are then calculated for the trapezoidal fuzzy sets. For example, CT-1 and CT-2 were evaluated as (0.58,1.19,1.33,2.1). This is as per the explanation given below.

$a_g = (0.2 * 3 * 0.33)^{1/3} = 0.58$

$b_g = (0.33 * 5 * 1)^{1/3} = 1.19$

$c_g = (0.33 * 7 * 1)^{1/3} = 1.33$

$a_g = (1 * 9 * 1)^{1/3} = 2.1$

The trapezoidal fuzzy aggregated matrix was calculated for the rest of the comparisons is own in **Table 5.4**.

Table 5. 4 Aggregated trapezoidal fuzzy sets of main criteria

	CT-1	**CT-2**
CT-1	(1,1,1,1)	(0.58,1.19,1.33,2.1)
CT-2	(0.48,0.75,0.84,1.70)	(1,1,1,1)

Once the combined aggregated matrix is established in a trapezoidal form, steps 7 and step 8 are applied to get the criteria weights in fuzzy form (see **Table 5.5)**. Furthermore, the final weights of the main criteria were obtained in crisp numbers by de-fuzzification.

Table 5. 5 Main criteria weights in the trapezoidal fuzzy form before applying steps 7 and step 8

C1	(1.58,2.19,2.33,3.1)
C2	(1.48,1.75,1.84,2.70)

This is followed by normalization of criteria weightage in fuzzy forms, as shown in **Table 5.6** and **Table 5**.**7** The same steps are applied for all sub-criteria and alternatives too for obtaining their weights.

Table 5. 6 Trapezoidal fuzzy weights of main criteria

Main criteria	**Trapezoidal fuzzy weights**
CT-1	(0.27,0.53,0.58,1.02)
CT-2	(0.25,0.42,0.46,0.89)

Table 5.7 shows that techno economics has higher weightage (55%) than the environment (45 %) as per the inputs provided by the experts for the main criterion. The experts who provided inputs for this study have indicated that at the beginning of commercialization, techno economics is

slightly more important than the environmental criteria. This weightage can be vary based on the expert's opinion that may be obtained.

Table 5. 7 Normalized crisp weights of the main criteria

Main criteria	Normalized crisp weight
CT-1	0.55
CT-2	0.45

5.6.2 Sub-criteria weights

Table 5.8 and **Table 5.9** represent the expert's evaluations for four sub-criteria of techno-economic and three sub-criteria of environment. In **Table 5.8**, the evaluated consistency ratios for expert-1, expert-2 and expert-3 are 0.06,0.07, and 0.08, respectively, which is acceptable. In addition, for **Table 5.9,** the evaluated consistency ratios for expert-1, expert-2, and expert-3 are 0.06,0.09, and 0.09.

Table 5. 8 Fuzzy envelopes for the sub-criteria (ST's) of main Criteria Techno-Economics Aspects (CT-1) as evaluated by three experts

		ST-1	ST-2	ST-3	ST-4
Expert-1					
	ST-1	EE	Between ELI and EE	ESHI	EE
	ST-2		EE	ESHI	EE

	ST-3			EE	WLI
	ST-4				EE
Expert-2					
	ST-1	EE	Between ELI and EE	Between ELI and EE	Between ELI and EE
	ST-2		EE	ELI	ELI
	ST-3			EE	Between ELI and EE
	ST-4				EE
Expert-3					
	ST-1	EE	ELI	ESHI	EE
	ST-2		EE	VHI	EHI
	ST-3			EE	WLI
	ST-4				EE

Table 5. 9 Fuzzy envelopes for the sub-criteria (ST's) of main criteria Environmental Aspects (CT-2) as evaluated by three experts

		SE-1	SE-2	SE-3
Expert-1				
	SE-1	EE	EE	EE
	SE-2		EE	ELI
	SE-3			EE
Expert-2				
	SE-1	EE	Between EE and EHI	EE
	SE-2		EE	ELI
	SE-3			EE
Expert-3				
	SE-1	EE	Between ELI and EE	EE
	SE-2		EE	Between EE and EHI
	SE-3			EE

After implementing all the steps mentioned in section 3.3, the final normalized crisp weightage of sub-criteria for CT-1 and CT-2 can be seen in **Tables 5.10** and **5.11,** respectively.

Table 5. 10 Normalized crisp weights of sub-criteria for CT-1

Sub-criteria	Normalized crisp weight
ST-1	0.28
ST-2	0.32
ST-3	0.12
ST-4	0.28

Table 5. 11 Normalized crisp weights of sub-criteria for CT-2

Sub-criteria	Normalized crisp weight
SE-1	0.33
SE-2	0.33
SE-3	0.34

Waste (ST-2) has been found to have the highest weightage, while raw material input (ST-3) has the least weightage. Our experts believe that the generation of waste hampers the improvement in the process economy the most and indirectly reflects on the selling price of SA. In addition, energy requirement has 28.0 % weightage as a sub-criteria for SA production. For the main criteria CT-

2, all three experts believe that all three sub-criteria have almost equal importance. Thus, damage to human health (SE-1), damage to the ecosystem (ST-2), and damage to resources (SE-3) have been assigned 33.0 %, 33.0 %, and 34.0 % weightage respectively.

5.6.3 Alternative weights

Similarly, the expert's evaluations for alternatives with respect to each sub-criteria (see **Table 5.12**) were converted into weights is shown in **Table 5.13**.

Table 5. 12 Fuzzy envelopes for the alternatives for all experts

		AL-1	AL-2	AL-3	AL-4
Alternatives with respect to MSP (ST-1)					
Expert-1					
	AL-1	EE	WHI	WHI	Between EE and EHI
	AL-2		EE	WHI	Between EE and EHI
	AL-3			EE	Between ELI and EE
	AL-4				EE
Expert-2					
	AL-1	EE	Between EE and EHI	ELI	EE
	AL-2		EE	ELI	Between ELI and EE
	AL-3			EE	Between EE and EHI

		AL-1	AL-2	AL-3	AL-4
	AL-4				EE
Expert-3					
	AL-1	EE	ESHI	ESHI	WHI
	AL-2		EE	ELI	ELI
	AL-3			EE	ELI
	AL-4				EE
Alternatives with respect to Waste (ST-2)					
Expert-1					
	AL-1	EE	WLI	EE	Between EE and EHI
	AL-2		EE	Between EE and EHI	Between EE and EHI
	AL-3			EE	Between ELI and EE
	AL-4				EE
Expert-2					
	AL-1	EE	Between EE and EHI	EE	Between EE and EHI
	AL-2		EE	Between ELI and EE	EHI
	AL-3			EE	Between ELI and EE
	AL-4				EE
Expert-3					

		AL-1	AL-2	AL-3	AL-4
	AL-1	EE	Between EE and EHI	ELI	Between ELI and EE
	AL-2		EE	EE	ELI
	AL-3			EE	Between ELI and EE
	AL-4				EE
Alternatives with respect to Raw material input (ST-3)					
Expert-1					
	AL-1	EE	ELI	Between EE and EHI	EE
	AL-2		EE	Between EE and EHI	Between EE and EHI
	AL-3			EE	Between ELI and EE
	AL-4				EE
Expert-2					
	AL-1	EE	WHI	EE	WLI
	AL-2		EE	ELI	VLI
	AL-3			EE	ESLI
	AL-4				EE
Expert-3					
	AL-1	EE	Between ESHI and VHI	Between EE and EHI	EE
	AL-2		EE	WLI	VLI

		AL-1	AL-2	AL-3	AL-4
	AL-3			EE	ELI
	AL-4				EE
Alternatives with respect to Energy requirement (ST-4)					
Expert-1					
	AL-1	EE	Between EE and EHI	EE	ESHI
	AL-2		EE	ELI	Between WHI and ESHI
	AL-3			EE	VHI
	AL-4				EE
Expert-2					
	AL-1	EE	EHI	EE	Between EE and EHI
	AL-2		EE	EHI	EHI
	AL-3			EE	Between EE and EHI
	AL-4				EE
Expert-3					
	AL-1	EE	WHI	EE	EE
	AL-2		EE	WLI	WLI
	AL-3			EE	ELI
	AL-4				EE
Alternatives with respect to Damage to human health (SE-1)					
Expert-1					

		AL-1	AL-2	AL-3	AL-4
	AL-1	EE	Between ELI and EE	EE	Between EE and EHI
	AL-2		EE	Between EE and EHI	Between EE and EHI
	AL-3			EE	Between EE and EHI
	AL-4				EE
Expert-2					
	AL-1	EE	WHI	ESHI	VHI
	AL-2		EE	Between EHI and WHI	WHI
	AL-3			EE	EE
	AL-4				EE
Expert-3					
	AL-1	EE	ESHI	Between EHI and WHI	WHI
	AL-2		EE	WLI	WLI
	AL-3			EE	EE
	AL-4				EE
Alternatives with respect to Damage to eco system (SE-2)					
Expert-1					
	AL-1	EE	EHI	EHI	Between ESHI and VHI

		AL-1	AL-2	AL-3	AL-4
	AL-2		EE	Between ELI and EE	Between ESHI and VHI
	AL-3			EE	Between ESHI and VHI
	AL-4				EE
Expert-2					
	AL-1	EE	Between EE and EHI	EHI	EE
	AL-2		EE	EHI	ELI
	AL-3			EE	ELI
	AL-4				EE
Expert-3					
	AL-1	EE	EHI	WHI	VHI
	AL-2		EE	Between EE and EHI	ESHI
	AL-3			EE	WHI
	AL-4				EE
Alternatives with respect to Damage to resources (SE-3)					
Expert-1					
	AL-1	EE	ELI	EHI	VHI
	AL-2		EE	Between EHI and WHI	VHI
	AL-3			EE	VHI
	AL-4				EE

		AL-1	AL-2	AL-3	AL-4
Expert-2					
	AL-1	EE	Between ELI and EE	Between EE and EHI	AHI
	AL-2		EE	Between ELI and EE	ESHI
	AL-3			EE	VHI
	AL-4				EE
Expert-3					
	AL-1	EE	WHI	Between EE and EHI	VHI
	AL-2		EE	WLI	ESHI
	AL-3			EE	VHI
	AL-4				EE

Table 5. 13 Normalized crisp weights of alternatives with respect to all sub-criteria

	ST-1	ST-2	ST-3	ST-4	SE-1	SE-2	SE-3
AL-1	0.43	0.24	0.23	0.32	0.44	0.41	0.32
AL-2	0.20	0.27	0.13	0.20	0.20	0.25	0.24
AL-3	0.19	0.23	0.21	0.31	0.19	0.21	0.29
AL-4	0.18	0.26	0.43	0.17	0.17	0.13	0.15

It can be seen that with respect to MSP (ST-1), experts gave the highest weightage of 43.0 % to AL-1, followed by AL-2, and AL-3 with a weightage of 20.0 % and 19.0 %, respectively, as shown in **Figure 5.3**. For the environmental sub-criteria (SE-1, SE-2, SE-3) alternatives AL-1 (both C-6 and C-5 for SA production and lignin for electricity) and AL-4 (fossil route) obtained the highest and least weightage respectively. However, from the raw material input (ST-3) perspective, experts suggested AL-4 is better than other alternatives. The fossil route-based SA production process is old compared to relatively new and developing bio-based routes and hence has a higher process efficiency compared to the bio routes.

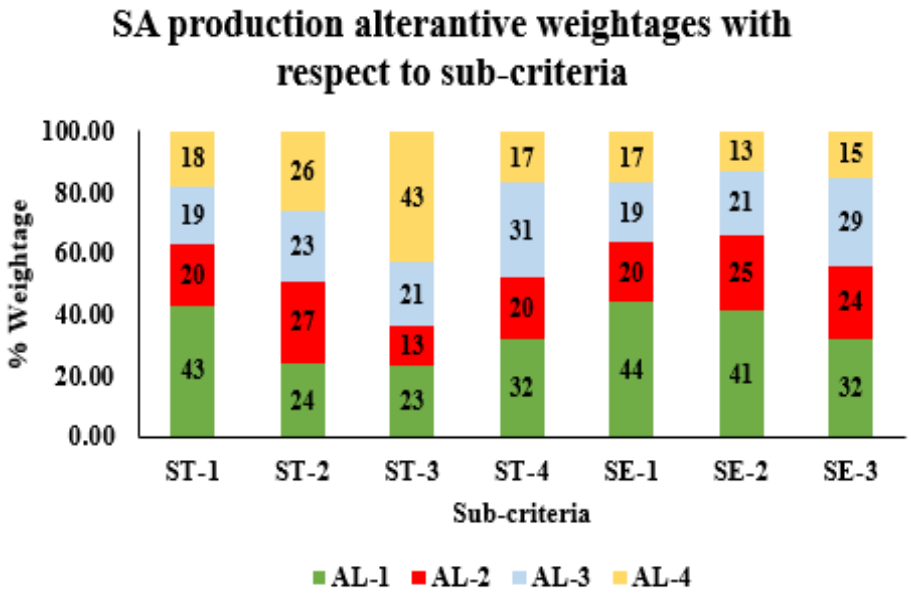


Figure 5. 3 Alternative weights for individual sub-criteria

5.6.4 SA production option selection

Once the weightage of all main criteria, sub-criteria, and alternatives were evaluated, the global weights of alternatives were calculated by multiplying the local weight of the alternative by the

local weight of the relevant sub-criteria. Finally, to obtain the final weightage of SA production alternatives, evaluated global weights of alternatives multiplied with relevant main criteria weights and summation of an individual SA production option produced the final weightage as shown in **Table 5.14**. The techno-economic criteria are the most influential, with the highest global weightage of 55.0 % for SA production. For techno economics, waste is identified as the most important sub-criteria with a 32.0 % local weightage.

Table 5. 14 Local and global weights of SA production alternatives with respect to sub-criteria

Main criteria	Global weights of main criteria	Sub-criteria	Local weight of sub-criteria	Crisp local weights of alternatives				Crisp global weights of alternatives			
				AL-1	AL-2	AL-3	AL-4	AL-1	AL-2	AL-3	AL-4
CT-1	0.55	**ST-1**	0.28	0.43	0.20	0.20	0.18	0.12	0.06	0.06	0.05
		ST-2	0.32	0.24	0.27	0.23	0.26	0.08	0.09	0.08	0.08
		ST-3	0.12	0.23	0.13	0.21	0.43	0.03	0.01	0.02	0.05
		ST-4	0.28	0.32	0.20	0.31	0.18	0.09	0.06	0.09	0.05
CT-2	0.45	**SE-1**	0.33	0.44	0.20	0.19	0.17	0.14	0.07	0.06	0.06
		SE-2	0.33	0.41	0.26	0.21	0.13	0.13	0.08	0.07	0.04
		SE-3	0.34	0.31	0.24	0.29	0.15	0.11	0.08	0.10	0.05

The final results in are visually presented in **Figure 5.4**. The results indicate that the most suitable option for SA production, alternative 1 outweighs all other alternatives with a final overall weightage of 35 %.

Experts gave the last priority to SA production from the fossil-based route (alternative 4) with a weightage of 20.0 %. Alternative 2 and 3 have were prioritized third and second place with 22.0 % and 24.0 % final weightage, respectively.

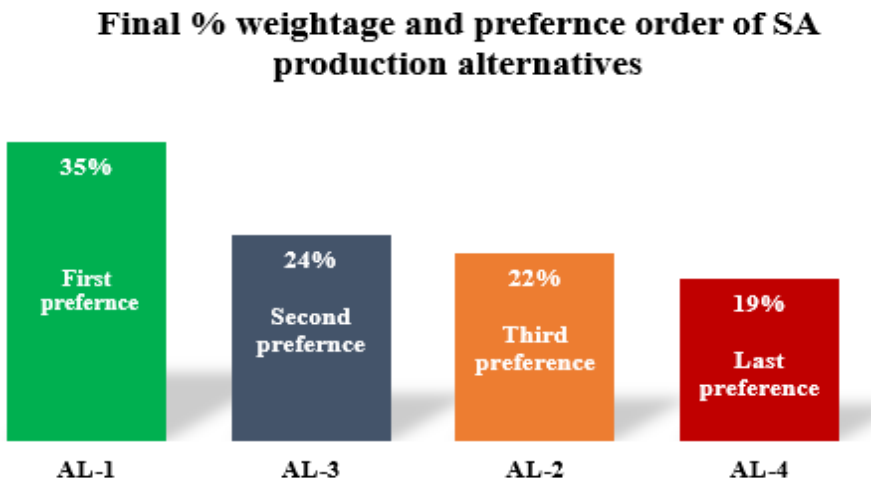


Figure 5. 4 Final weightage and preference order of alternatives for SA production

5.6.5 Sensitivity analysis

Sensitivity analysis was then performed to assess the stability of evaluated preferred alternatives for SA production against changes in criteria weights. For this, criteria weights were altered from 0 to 1 by increasing increments of 0.10 at a time. The weights of the remaining criteria were kept the same proportionally when the weight of one criteria changed. **Figure 5.5** and **Figure 5.6** demonstrate the sensitivity analysis results for two main criteria, techno-economics and environmental issues respectively. As can be seen from **Figure 5.5,** AL-1 and AL-3 remain the

best two alternatives even after the major variations in the weightage of techno-economics criteria. However, over a value 0.90, a further increment in the weightage of techno-economics makes AL-4 the better option than AL-2.

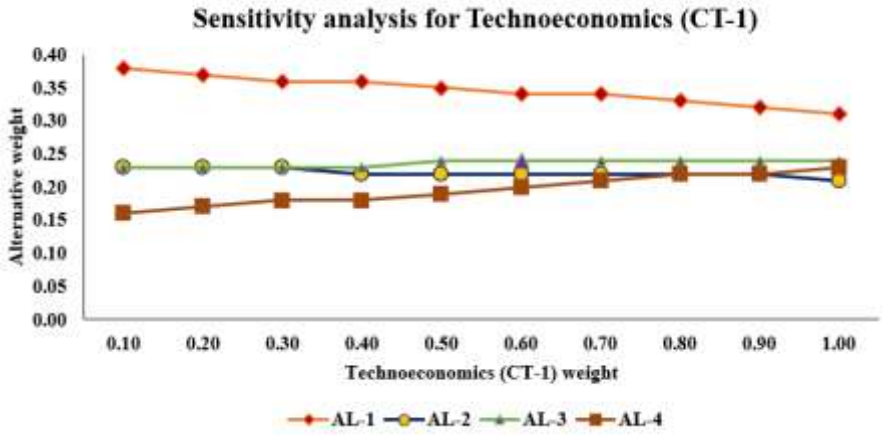


Figure 5. 5 Sensitivity analysis of techno-economic (CT-1) and its impact on the final weightage of alternatives

For environmental criteria (**Figure 5.6**), after a value of 0.60, dramatic changes were observed for the weightage of AL-2. AL-2 and AL-3 which become equally important as AL-1. It was observed that, throughout variations from 0.10 to 1.00, the fossil-based route is considered the least preferred option all the time. These results indicate that AL-1 and AL-4 are not highly sensitive to changes in the weightage. On the contrary, AL-2 and AL-3 are slightly sensitive to changes in both main criteria.

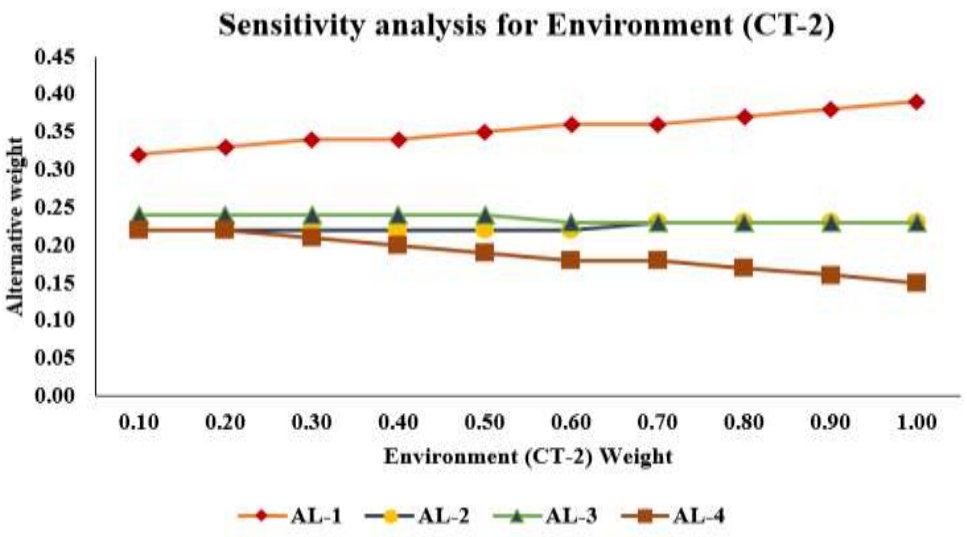


Figure 5. 6 Sensitivity analysis of environment (CT-2) and its impact on the final weightage of alternatives

5.7 Conclusion

This study applied MCDA for an evaluation of the best option for SA production by using hesitant fussy AHP. Techno-economic and environmental aspects were considered as the main two criteria in the analysis. In addition, seven sub-criteria relevant to their respective main criteria were also considered during the analysis. From the two main criteria, experts gave slightly higher preference to techno-economic (CT-1) than environmental (CT-2) criteria, with a nominal difference of 10.0 %. In the techno-economic criteria, the highest weightage is given to waste. On the other hand, the least weightage is given to raw material input. Experts assigned equal weightage to MSP and energy requirements. For the environmental criteria, all three sub-criteria have the same weightage. Considering all main criteria and sub-criteria alternative 1 was found to be the most suitable option for SA production, followed by alternative 3 and alternative 2. Alternative 4 is seen as the least suitable production alternative. The results derived from this analysis can assist decision makers take a decision as regards SA production route selection between renewable resources and

conventional fossil-based resources and alternative co-product routes. It is important to note that the obtained ranking results of SA production alternatives do not mean policymakers omit the low-ranked SA production alternatives. The obtained ranking results demonstrate the comparative significance of each SA production alternative versus other alternatives. The methodology used in this study can be used to compare methods for other products and production alternatives which make decision making a complex process.

5.8 References

[1] B.G. Hermann, K. Blok, M.K. Patel, Producing bio-based bulk chemicals using industrial biotechnology saves energy and combats climate change, Environ Sci Technol. 41 (2007) 7915–7921. https://doi.org/10.1021/es062559q.

[2] V. Masson-Delmotte, P. Zhai, H.-O. Pörtner, D. Roberts, J. Skea, P.R. Shukla, A. Pirani, W. Moufouma-Okia, C. Péan, R. Pidcock, Global warming of 1.5 C, An IPCC Special Report on the Impacts of Global Warming Of. 1 (2018).

[3] N.P. Nghiem, S. Kleff, S. Schwegmann, Succinic acid: technology development and commercialization, Fermentation. 3 (2017) 26.

[4] T. Werpy, G. Petersen, Top value-added chemicals from biomass: volume I--results of screening for potential candidates from sugars and synthesis gas, National Renewable Energy Lab., Golden, CO (US), 2004.

[5] N.M. Kosamia, M. Samavi, K. Piok, S.K. Rakshit, Perspectives for scale up of biorefineries using biochemical conversion pathways: Technology status, techno-economic, and sustainable approaches, Fuel. 324 (2022). https://doi.org/10.1016/j.fuel.2022.124532.

[6] A. Ghayur, T.V. Verheyen, E. Meuleman, Techno-economic analysis of a succinic acid biorefinery coproducing acetic acid and dimethyl ether, J Clean Prod. 230 (2019) 1165–1175. https://doi.org/10.1016/j.jclepro.2019.05.180.

[7] N.M. Kosamia, A. Sanchez, S.K. Rakshit, Scenario-based techno-economics and heat integration feasibility assessment of integrated multiproduct biorefineries with biosuccinic acid as the main product and various byproduct options, Biomass Convers Biorefin. (2022). https://doi.org/10.1007/s13399-022-02945-9.

[8] H.I. Moussa, A. Elkamel, S.B. Young, Assessing energy performance of bio-based succinic acid production using LCA, J Clean Prod. 139 (2016) 761–769. https://doi.org/10.1016/j.jclepro.2016.08.104.

[9] S.M. Ioannidou, K. Filippi, I.K. Kookos, A. Koutinas, D. Ladakis, Techno-economic evaluation and life cycle assessment of a biorefinery using winery waste streams for the production of succinic acid and value-added co-products, Bioresour Technol. 348 (2022) 126295.

[10] A. Shaji, Y. Shastri, V. Kumar, V. v. Ranade, N. Hindle, Economic and Environmental Assessment of Succinic Acid Production from Sugarcane Bagasse, ACS Sustain Chem Eng. 9 (2021) 12738–12746. https://doi.org/10.1021/acssuschemeng.1c02483.

[11] R. Dickson, E. Mancini, N. Garg, J.M. Woodley, K. v Gernaey, M. Pinelo, J. Liu, S.S. Mansouri, Sustainable bio-succinic acid production: superstructure optimization, techno-economic, and lifecycle assessment, Energy Environ Sci. 14 (2021) 3542–3558. https://doi.org/10.1039/d0ee03545a.

[12] M. Nieder-Heitmann, K.F. Haigh, J.F. Görgens, Life cycle assessment and multi-criteria analysis of sugarcane biorefinery scenarios: Finding a sustainable solution for the South African sugar industry, J Clean Prod. 239 (2019). https://doi.org/10.1016/j.jclepro.2019.118039.

[13] C. Xu, E. Paone, D. Rodríguez-Padrón, R. Luque, F. Mauriello, Recent catalytic routes for the preparation and the upgrading of biomass derived furfural and 5-hydroxymethylfurfural, Chem Soc Rev. 49 (2020) 4273–4306.

[14] C.E. Mabermann, J.I. Kroschwitz), Encyclopedia of Chemical Technology, John Wiley & Sons, New York. 1 (1991) 251.

[15] J.M. Pinazo, M.E. Domine, V. Parvulescu, F. Petru, Sustainability metrics for succinic acid production: A comparison between biomass-based and petrochemical routes, Catal Today. 239 (2015) 17–24.

[16] S. Kheybari, M. Javdanmehr, F.M. Rezaie, J. Rezaei, Corn cultivation location selection for bioethanol production: An application of BWM and extended PROMETHEE II, Energy. 228 (2021) 120593. https://doi.org/10.1016/j.energy.2021.120593.

[17] C. Emeksiz, A. Yüksel, A suitable site selection for sustainable bioenergy production facility by using hybrid multi-criteria decision making approach, case study: Turkey, Fuel. 315 (2022) 123214. https://doi.org/10.1016/j.fuel.2022.123214.

[18] A. Mostafaeipour, A. Sedaghat, M. Hedayatpour, M. Jahangiri, Location planning for production of bioethanol fuel from agricultural residues in the south of Caspian Sea, Environ Dev. 33 (2020) 100500. https://doi.org/10.1016/j.envdev.2020.100500.

[19] A. Chanthawong, S. Dhakal, Stakeholders' perceptions on challenges and opportunities for biodiesel and bioethanol policy development in Thailand, Energy Policy. 91 (2016) 189–206. https://doi.org/10.1016/j.enpol.2016.01.008.

[20] T.L. Saaty, How to make a decision: the analytic hierarchy process, Eur J Oper Res. 48 (1990) 9–26.

[21] V. Torra, Y. Narukawa, On hesitant fuzzy sets and decision, in: 2009 IEEE International Conference on Fuzzy Systems, IEEE, 2009: pp. 1378–1382.

[22] A. Beskese, C. Kahraman, Z. Irani, Quantification of flexibility in advanced manufacturing systems using fuzzy concept, Int J Prod Econ. 89 (2004) 45–56.

[23] R.M. Rodriguez, L. Martinez, F. Herrera, Hesitant fuzzy linguistic term sets for decision making, IEEE Transactions on Fuzzy Systems. 20 (2011) 109–119.

[24] B. Öztaysi, S.C. Onar, E. Boltürk, C. Kahraman, Hesitant fuzzy analytic hierarchy process, in: 2015 IEEE International Conference on Fuzzy Systems (FUZZ-IEEE), IEEE, 2015: pp. 1–7.

[25] R. Lin, Y. Man, C.K.M. Lee, P. Ji, J. Ren, Sustainability prioritization framework of biorefinery: a novel multi-criteria decision-making model under uncertainty based on an improved interval goal programming method, J Clean Prod. 251 (2020) 119729.

[26] D. Humbird, R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol: dilute-acid pretreatment and enzymatic hydrolysis of corn stover, National Renewable Energy Lab. (NREL), Golden, CO (United States), 2011.

[27] A. Sanchez, G. Magaña, L. Gutierrez, Parametric analysis of total costs and energy efficiency of 2G enzymatic ethanol production, Fuel. 113 (2013) 165–179. https://doi.org/10.1016/j.fuel.2013.05.034.

[28] M. Goedkoop, R. Heijungs, M. Huijbregts, A. de Schryver, J. Struijs, R. van Zelm, ReCiPe 2008, A Life Cycle Impact Assessment Method Which Comprises Harmonized Category Indicators at the Midpoint and the Endpoint Level. 1 (2009) 1–126.

[29] H. Liu, R.M. Rodríguez, A fuzzy envelope for hesitant fuzzy linguistic term set and its application to multicriteria decision making, Inf Sci (N Y). 258 (2014) 220–238.

[30] D. Filev, R.R. Yager, On the issue of obtaining OWA operator weights, Fuzzy Sets Syst. 94 (1998) 157–169.

[31] C.-H. Hsieh, S.-H. Chen, A model and algorithm of fuzzy product positioning, Inf Sci (N Y). 121 (1999) 61–82.

[32] F. Liu, Y. Peng, W. Zhang, W. Pedrycz, On consistency in AHP and fuzzy AHP, Journal of Systems Science and Information. 5 (2017) 128–147.

[33] T.L. Saaty, Decision making for leaders: the analytic hierarchy process for decisions in a complex world, RWS publications, 2001.

CHAPTER 6

Summary and Recommendations

6 Summary and recommendations

6.1 Summary of the thesis

Lignocellulosic biomass residues such as corn stover have considerable potential to be used as a renewable resource to produce BioSA. However, the commercialization of this biorefining process faces several challenges. In the present thesis, a sustainability assessment framework was developed and implemented to address the issues associated with the successful commercialization of BioSA production from lignocellulosic biomass in competition with conventional fossil-based SA production route.

The initial comprehensive literature review helped to identify the research gaps for the sustainable production of BioSA. At the outset, it was clear that products like ethanol which are required in high volumes but have a low price will not be competitive, if produced from lignocellulosic biomass. On the other hand, a product like succinic acid which can be used in a number of applications (middle-level bulk chemical), and hence called a platform chemical, has a higher market value and would make such biorefining processes economically feasible. Secondly, utilization of all three main components of biomass for producing products and co-products was essential for such system to be competitive economically. The environmental benefits of biorefining processes are often made by qualitative statements or by quantifying the amount of GHG emissions. **The novel contribution** of this study is that it includes the development of a sustainability framework that addresses techno-economic and environmental aspects of sustainability in a single monetary unit, making it easy to compare between different scenarios. The social aspect of sustainability is not explored in this work.

The first objective was to develop a conceptual process design and techno-economic analysis of a biorefinery product BioSA as a primary product and a combination of co-products identified to have the potential for good economic returns and market. The coproducts chosen in this study included furfural and electricity were based on a detailed review of possible alternative products. Three scenarios were studied for the production of BioSA from corn stover. Initially mass and energy balance of a conceptual design was performed, followed by equipment sizing, mapping, and profitability analysis. Subsequently, heat integration and profitability were also evaluated for all three scenarios. Among the three scenarios studied, the production of BioSA using both C-6 and C-5 sugar and electricity from lignin (scenario 1) was found to be the most economically preferable with the lowest MSP value of 2.28 USD/kg BioSA and an 8-year payback period. This biorefinery scenario was also found to be self-reliant energy wise and could sustain itself for electricity and steam needs. Due to the higher energy requirement in the furfural production process, scenario 2 (in which C-6, C-5 sugars, and lignin were used for BioSA, furfural, and electricity production, respectively) was found to be economically least profitable with the highest value of MSP (3.33 USD/kg BioSA) among all studied scenarios. Scenario 3 in which C-5 sugars and lignin were used for energy production was found to be less profitable compared to scenario 1. Based on MSP values, scenario 1 and scenario 3 were found to be better than the conventional fossil resources route which has MSP of 2.30 USD/kg SA.

The second objective of this study involved a Life Cycle Assessment (LCA) of all three scenarios along with the fossil-based route of SA production. Environmental impacts were assessed at the midpoint and endpoint. Applying the budget constraint method, the evaluated environmental impacts were converted to monetary units to get the environmental cost of BioSA production for each scenario. Evaluating the environmental cost of BioSA production from corn stover and

comparing it to the fossil-based route in terms of USD is a novel idea that has not been done with biorefining processes of this type earlier. This study also showed that scenario 1 is the best option, if the decision should be made based on the environmental cost. Calculations show that the subsequent choices would be scenario 3 followed by the fossil route. The MSP values for the combined techno-economic and environmental costs derived from LCA were 3.76 and 4.54 USD for scenario 1 and fossil resource route, respectively. Sensitivity analysis of these processes showed that environmental cost for scenario 1 was most sensitive to endpoint impact category named damage to human health.

As part of the third objective, a decision-making method was used to select the best SA production route among those chosen by considering techno-economic and environment assessments as the main criteria. Experts working in fields related to biorefining of BioSA provided their weighed inputs from available choices. Seven sub-criteria and four alternatives were also considered during the application of the MCDA tool for SA production option selection. A novel hesitant fuzzy analytical hierarchy process involving inputs from real expert's opinion was used in MCDA analysis for finding the best route among the alternatives studied.

The seven sub criteria used in this study were MSP, waste generation, raw material input, energy requirement, damage to human health, damage to ecosystem, and damage to resources. Alternative 1 (SA production from C-6 and C-5 sugar and electricity production from lignin) was found as the most preferred option with a highest weightage of 35%, followed by alternative 3 (SA production from C-6 sugar, biogas generation from C-5 sugar subsequently utilized by CHP for electricity production along with lignin) with 24% given weightage and alternative 2 (SA, furfural and electricity production from C-6 sugar, C-5 sugar, and lignin, respectively) with 22% weightage.

6.2 Major conclusions and limitations

An overview of the major conclusions and limitations that can be drawn from this study are as follows:

- As the growing needs for chemicals need to be aligned with circular economy targets, it is essential to address the techno-economic, environment sustainability domains simultaneously in a single monetary unit (dollar value). A framework suggested in this study including TEA, LCA followed by monetization provides very good inputs that decision makers can use to determine holistically the sustainable production of platform chemicals like succinic acid.
- At the preliminary sustainability assessment stage, based on lab or pilot scale results, an assumption of a conceptual N^{th} plant is often made. This can result in discrepancies in the development of new biorefining processes. This issue can be overcome by involving real experts who have experience in the field. Incorporating their inputs at various stages of biochemical process development stages starting from research and development to commercial-scale production is essential. The application of MCDA analysis methods with an involvement of such experts from different relevant areas, as carried out in this study, can provide practical guidelines and make commercial-scale production of biochemicals successful.
- The data used in this study is specific to the geographical location of Canada and has to be suitably modifies for other locations.
- The process economy results calculated in this study were based on classical theoretical methods. This needs to be validated by real-time vendor quotes before commercialization.

- Discrepancies related to the choice of allocation method selected is an issue faced by LCA researchers. The environmental cost based on those results is very specific to the selected allocation approach chosen. Hence these results need to be verified carefully using alternate equivalent methods.

6.3 Recommendations for future studies

Based on this study, the recommendations that can be made for the sustainable production of BioSA and other platform chemicals from lignocellulosic biomass are as follows:

- Validate the process simulation and TEA outcomes by further experimental confirmation at the lab and pilot scales.
- Conduct detailed market research to prioritize co-products that can be produced from C-5 sugars and lignin along with the main product BioSA. Collaboration with potential industries or partners will help to identify the most suitable co-product based on market needs and future demands.
- To address the social aspect of sustainability, it is recommended to conduct a detailed social life cycle assessment in the suggested sustainability framework along with techno-economic and environmental aspects.
- Extend research on methodology taking into account country-specific environmental policies such as Social Cost of Carbon (SCC) and Cost Benefit Analysis (CBA).
- Develop a hierarchical method involving all three sustainability criteria which can be used to evaluate the production of such products in various countries and regions of the world where lignocellulosic resources are abundantly available.

Appendix A

Appendix A: Brief description of theories behind Aspen plus models and stream output data

Table A.1 Aspen models and key description of theories

Process model	Description and theory
Heater and cooler model	In present work, heating and cooling operations were simulated using heater and cooler model. The heater and cooler model of Aspen plus considers material and energy balances as well as phase thermodynamic calculations. Aspen plus uses a single unit operation model for both heating and cooling operations. The difference between heater and cooler is only given by the sign of the heat duty. The material balance equation [1] for heater and cooler model can be given by below equation $$\sum_{i,j} m_{i,in}^{j} = \sum_{i,j} m_{i,out}^{j} = m_{in} = m_{out} = m$$ Where, i represents streams, j represents components, *in* stands for input and *out* stands for output. For this model the energy balance [1] can be represented by below equation $$q = m(h_{out} - h_{in}) + q_{loss}$$ Where, m stands for total feed mass flow, q is heat duty and q_{loss} stands for the heat losses.
Pressure changing equipment (pump)	For pressure related operations Aspen plus provides a model called *Pump*. *Pump* increases the liquid pressure between its inlet (P_1) and outlet (P_2) by ΔP. Pump efficiency (n) is defined as the ratio between hydraulic power (P_w) and mechanical power (P_f). To model the reduction in pressure of a liquid stream there is a provision for *Valve* model in Aspen plus.

Stoichiometry (*RStoic*) reactor model	This model is basically used when the reaction stoichiometry and conversion or molar extent for each reaction is known. For this thesis fermentation and hydrolysis reactions were simulated using *RStoic* model. In *RStoic* as an input, all the details related to process such as reaction stoichiometry, conversion factors, molar extent, stoichiometry coefficient are mandatory. If no information on the reactions and their stoichiometry is available, but the number of individual components produced per unit of mass or unit of mole available then *RYield* model can be used. In steady-state condition, the material balance equation [1] of component *i* taking part in *n* reactions in a reactor with *j* inlet streams can be written for these models as $$\left(\sum_{j} n_{ij}\right)_{in} - \left(\sum_{k} n_{ik}\right)_{out} + \left(\sum_{n} v_{in}\xi_n\right)_{R} = 0$$ Where, n_{ij} represents the mole flow of component *i* in the *j* inlet stream, n_{ik} is the mole of component *i* the *k* outlet stream, v_{in} is the stochiometric coefficient of component *i* in the *n*th reaction and ξn is the reaction extent of the *n*th reaction. Considering the steady-state condition, the general energy balance equation of reactor can be written as $$\left(\sum_{j} n_j\ h_j\right)_{in} - \left(\sum_{k} n_k\, h_k\right)_{out} + \sum_{n} \Delta_r H_n\ \xi_n + Q + W = 0$$ Where, n_j is the mole flow of inlet stream *j,* n_k is the mole flow of outlet stream *k,* h_j is the enthalpy of inlet stream *j,* h_k is the enthalpy of outlet stream *k.* Q is the heat flow added or removed, *W* is the rate of work

	added or done by the system, H_n is the reaction enthalpy.
Separation models	In present work, reactive extraction operation in the downstream processing were simulated using this model of Aspen plus. For the separation models Aspen plus uses two approaches. Approach one uses rate equation of mass transfer using Fick's law by considering partial and overall mass transfer coefficients. For distillation, extraction, absorption operation simulation, separation models consider the second approach by using the concept of theoretical (equilibrium) stages. Several models for single contact and multiple contact are available in aspen plus. For example, for single stage liquid -vapor process *FLASH2,* for liquid-liquid separation *DECANTER* models are available. For distillation operation simulation Aspen plus uses shortcut distillation method named Fenske-Underwood-Gilliland method. There is a provision for simulating unit operations such as extractive distillation, reactive distillation, azeotropic distillation in separation models of Aspen plus.
Solid handling	With the help of solid handling models of Aspen plus unit operations such as drying, crystallization and filtration can be simulated. There is also a provision for granulation, screening, clarifiers, cyclone operations in this category of models in Aspen plus. In the present work, crystallization, drying and size reduction operations were simulated using these models of Aspen plus.

Table A.2 Pretreatment section streams simulation data

Description	Units	R-1OUT	R-2OUT	R-3OUT	Hemicellulose stream	Cellulose stream	Lignin	Gypsum	M-5OUT
Temperature	**C**	**190.00**	**50.00**	**30.00**	**30.43**	**30.34**	**30.10**	**30.00**	**30.10**
Pressure	**atm**	**11.35**	**1.00**	**1.00**	**11.84**	**1.00**	**1.00**	**1.00**	**1.00**
GLUCOSE	kg/hr	29.09	28.80	28.80	28.51	0.29	0.00	0.29	0.00
CELLULOS	kg/hr	342.58	0.09	0.09	0.00	342.49	0.00	0.09	0.00
XYLOSE	kg/hr	177.43	175.65	175.65	173.90	1.77	0.00	1.76	0.00
HEMICELL	kg/hr	39.04	0.01	0.01	0.00	39.02	0.00	0.01	0.00
LIGNIN	kg/hr	171.00	0.05	0.05	0.00	0.85	170.10	0.04	170.10
CELLULAS	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
BIOMASS	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZYMO	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
UNKNOWN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SOLSDS	kg/hr	11.00	10.89	10.89	10.78	0.11	0.00	0.11	0.00
GYPSUM	kg/hr	0.00	72.79	116.19	3.21	0.00	0.00	112.98	0.00
ACETATE	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LGNSOL	kg/hr	9.00	8.91	8.91	8.82	0.09	0.00	0.09	0.00
HMF	kg/hr	1.40	0.56	0.56	0.56	0.01	0.00	0.01	0.00
ARABINOS	kg/hr	29.66	29.36	29.36	29.07	0.30	0.00	0.29	0.00
GALACTOS	kg/hr	20.00	19.80	19.80	19.60	0.20	0.00	0.20	0.00
MANNOSE	kg/hr	16.00	15.84	15.84	15.68	0.16	0.00	0.16	0.00
ARABINAN	kg/hr	0.73	0.00	0.00	0.00	0.72	0.00	0.00	0.00
MANNAN	kg/hr	0.40	0.00	0.00	0.00	0.40	0.00	0.00	0.00
GALACTAN	kg/hr	0.50	0.00	0.00	0.00	0.50	0.00	0.00	0.00
GLUCOLIG	kg/hr	2.62	2.59	2.59	2.57	0.03	0.00	0.03	0.00
CELLOB	kg/hr	2.76	2.74	2.74	2.71	0.03	0.00	0.03	0.00
XYLOLIG	kg/hr	5.27	5.22	5.22	5.17	0.05	0.00	0.05	0.00
MANOLIG	kg/hr	0.40	0.40	0.40	0.39	0.00	0.00	0.00	0.00
GALAOLIG	kg/hr	0.50	0.49	0.49	0.49	0.00	0.00	0.00	0.00
ARABOLIG	kg/hr	0.72	0.72	0.72	0.71	0.01	0.00	0.01	0.00
ACETOLIG	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
XYLITOL	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EXTRACT	kg/hr	47.00	46.53	46.53	46.06	0.47	0.00	0.47	0.00
PROTEIN	kg/hr	31.00	30.69	30.69	30.38	0.31	0.00	0.31	0.00
CASO4	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CAH2O2	kg/hr	0.00	18.68	0.00	0.00	0.00	0.00	0.00	0.00
ASH	kg/hr	52.00	0.01	0.01	0.00	0.00	51.99	0.01	51.99
H2O	kg/hr	1054.00	1212.77	1212.77	1200.65	1368.32	39.55	12.13	3954.93
FURFURAL	kg/hr	8.73	0.24	0.24	0.23	0.00	0.00	0.00	0.00
H2SO4	kg/hr	60.00	0.00	30.28	29.98	0.42	0.08	0.30	40.00
AACID	kg/hr	29.00	0.27	0.27	0.27	0.00	0.00	0.00	0.00
NAOH	kg/hr	0.00	0.00	0.00	0.00	0.41	40.59	0.00	40.59
Mass Flows	**kg/hr**	**2141.83**	**1684.10**	**1739.10**	**1609.74**	**1756.98**	**302.30**	**129.36**	**4257.61**

Table A.3 Scenario-1 downstream process streams simulation results

Description	Units	C-1-BTM	C-2-BTM	C-3-BTM	C-3-TOP	BC-1-TOP	CRY-OUT	F-1SOLID	SA	To WWT
Temperature	**C**	**38.16**	**38.33**	**38.37**	**38.37**	**45.84**	**20.00**	**20.00**	**130.00**	**36.82**
Pressure	**atm**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**1.00**	**11.84**
GLUCOSE	kg/hr	0.00	0.00	0.00	29.28	0.00	0.00	0.00	0.00	29.28
XYLOSE	kg/hr	0.00	0.00	0.00	65.96	0.00	0.00	0.00	0.00	65.96
SOLSDS	kg/hr	0.00	0.00	0.00	10.89	0.00	0.00	0.00	0.00	10.89
LGNSOL	kg/hr	0.00	0.00	0.00	8.91	0.00	0.00	0.00	0.00	8.91
HMF	kg/hr	0.00	0.00	0.00	0.56	0.00	0.00	0.00	0.00	0.56
ARABINOS	kg/hr	0.00	0.00	0.00	23.34	0.00	0.00	0.00	0.00	23.34
GALACTOS	kg/hr	0.00	0.00	0.00	19.80	0.00	0.00	0.00	0.00	19.80
MANNOSE	kg/hr	0.00	0.00	0.00	15.84	0.00	0.00	0.00	0.00	15.84
GLUCOLIG	kg/hr	0.00	0.00	0.00	16.02	0.00	0.00	0.00	0.00	16.02
CELLOB	kg/hr	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.20
XYLOLIG	kg/hr	0.00	0.00	0.00	5.22	0.00	0.00	0.00	0.00	5.22
MANOLIG	kg/hr	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.40
GALAOLIG	kg/hr	0.00	0.00	0.00	0.49	0.00	0.00	0.00	0.00	0.49
ARABOLIG	kg/hr	0.00	0.00	0.00	0.72	0.00	0.00	0.00	0.00	0.72
EXTRACT	kg/hr	0.00	0.00	0.00	46.53	0.00	0.00	0.00	0.00	46.53
PROTEIN	kg/hr	0.00	0.00	0.00	30.69	0.00	0.00	0.00	0.00	30.69
H2O	kg/hr	21.89	0.00	0.00	2169.87	1168.84	449.05	13.47	0.00	2605.45
FURFURAL	kg/hr	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.02
H2SO4	kg/hr	0.00	0.00	0.00	30.38	0.00	0.00	0.00	0.00	30.38
CO2	kg/hr	0.00	0.00	0.00	2.10	0.00	0.00	0.00	0.00	2.10
NH3	kg/hr	0.00	0.00	0.00	122.74	0.00	0.00	0.00	0.00	122.74
AACID	kg/hr	0.00	0.00	0.00	18.84	0.00	0.00	0.00	0.00	18.84
SUCCACID	kg/hr	371.73	52.64	7.49	1.22	427.53	34.64	1.04	0.00	34.82
CSL	kg/hr	0.00	0.00	0.00	1.50	0.00	0.00	0.00	0.00	1.50
NAOH	kg/hr	0.00	0.00	0.00	0.40	0.00	0.00	0.00	0.00	0.40
1-Oct-01	kg/hr	590.85	123.54	25.74	0.26	0.00	0.00	0.00	0.00	0.26
TRI-N-01	kg/hr	89.18	17.76	3.70	0.00	0.00	0.00	0.00	0.00	0.00
TRIME-01	kg/hr	0.00	0.00	0.00	0.00	386.25	16.64	0.50	0.00	16.14
SACRSTL	kg/hr	0.00	0.00	0.00	0.00	0.00	392.87	383.16	383.16	9.71
SODIU-01	kg/hr	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.80
DIPOT-01	kg/hr	0.00	0.00	0.00	1.62	0.00	0.00	0.00	0.00	1.62
MONOSODI	kg/hr	0.00	0.00	0.00	0.77	0.00	0.00	0.00	0.00	0.77
Mass Flows	**kg/hr**	**1073.66**	**193.94**	**36.93**	**2625.35**	**1982.62**	**893.20**	**398.17**	**383.1**	**3120.37**

Table A4 Furfural production main streams simulation results

Description	Units	C-5 STRM	M-2-OUT	H-FUROUT	SEP-1-AQ	SEP-1-OR	C-1TOP	C-2BTM	C-2BTM	C-2TOP
Temperature	C	30.43	31.06	110.00	25.00	25.00	66.00	158.43	158.43	118.01
Pressure	Atm	11.84	1.00	15.00	1.00	1.00	1.00	1.00	1.00	1.00
GLUCOSE	kg/hr	28.51	28.51	28.51	28.51	0.00	0.00	0.00	0.00	0.00
CELLULOS	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
XYLOSE	kg/hr	173.90	173.90	173.90	0.00	0.00	0.00	0.00	0.00	0.00
HEMICELL	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LIGNIN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SOLSDS	kg/hr	10.78	10.78	10.78	10.78	0.00	0.00	0.00	0.00	0.00
GYPSUM	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LGNSOL	kg/hr	8.82	8.82	8.82	8.82	0.00	0.00	0.00	0.00	0.00
HMF	kg/hr	0.56	0.56	0.56	0.56	0.00	0.00	0.00	0.00	0.00
ARABINOS	kg/hr	29.07	29.07	29.07	2.91	0.00	0.00	0.00	0.00	0.00
GALACTOS	kg/hr	19.60	19.60	19.60	19.60	0.00	0.00	0.00	0.00	0.00
MANNOSE	kg/hr	15.68	15.68	15.68	15.68	0.00	0.00	0.00	0.00	0.00
ARABINAN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MANNAN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GALACTAN	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLUCOLIG	kg/hr	2.57	2.57	2.57	2.57	0.00	0.00	0.00	0.00	0.00
CELLOB	kg/hr	2.71	2.71	2.71	2.71	0.00	0.00	0.00	0.00	0.00
XYLOLIG	kg/hr	5.17	5.17	5.17	5.17	0.00	0.00	0.00	0.00	0.00
MANOLIG	kg/hr	0.39	0.39	0.39	0.39	0.00	0.00	0.00	0.00	0.00
GALAOLIG	kg/hr	0.49	0.49	0.49	0.49	0.00	0.00	0.00	0.00	0.00
ARABOLIG	kg/hr	0.71	0.71	0.71	0.71	0.00	0.00	0.00	0.00	0.00
EXTRACT	kg/hr	46.06	46.06	46.06	46.06	0.00	0.00	0.00	0.00	0.00
PROTEIN	kg/hr	30.38	30.38	30.38	30.38	0.00	0.00	0.00	0.00	0.00
ASH	kg/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2O	kg/hr	1201.85	1201.85	1201.85	1278.04	0.00	0.00	0.00	0.00	0.00
FURFURAL	kg/hr	0.28	0.28	0.28	18.31	98.88	0.00	98.88	98.88	0.00
H2SO4	kg/hr	30.14	30.14	30.14	30.14	0.00	0.00	0.00	0.00	0.00
AACID	kg/hr	2.71	2.71	2.71	1.45	8.22	1.10	1.11	1.11	6.01
NACL	kg/hr	0.00	1.32	1.32	1.32	0.00	0.00	0.00	0.00	0.00
HCL	kg/hr	0.00	2.31	2.31	2.31	0.00	0.00	0.00	0.00	0.00
THF	kg/hr	0.00	1773.75	1773.75	481.75	1292.00	1292.00	0.00	0.00	0.00
Mass Flows	**kg/hr**	**1610.39**	**3387.77**	**3387.77**	**1988.68**	**1399.10**	**1293.10**	**99.99**	**99.99**	**6.01**

References

[1] J. Haydary, Chemical process design and simulation: Aspen Plus and Aspen Hysys applications, John Wiley & Sons, 2019.

"वीर भोग्या वसुंधरा"

~ Shiv Purana