



Comprehensive techno-economic and environmental assessment for 2,3-butanediol production from bread waste

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ARTICLE INFO

Keywords:

Bread waste
2,3-Butanediol
Global warming
Life cycle assessment
Pinch analysis
Techno-economic analysis

ABSTRACT

Bread waste (BW) is a common food waste in Europe and North America and has enormous potential as a biorefinery substrate for the sustainable synthesis of various platform chemicals. Our previous work made use of BW for the fermentative production of 2,3-butanediol (BDO). The present work evaluated the economic prospects and environmental consequences associated with the overall processes, handling 100 metric tons BW per day. The comprehensive process design using Aspen Plus and integrated techno-economic and environmental assessment was carried out for two different BW hydrolysis scenarios: acid and enzyme hydrolysis, followed by fermentation and extraction-based downstream BDO separation. The optimal heat exchanger network was designed using pinch analysis, which improved the energy efficiency of the processes significantly, with about 10 % savings of BDO production costs. Despite this improvement, the BDO derived from BW was exorbitant (4.2–6.9 \$/kg) compared to the market price (3.23 \$/kg) due to relatively higher capital investment for the current plant capacity. Further, the process inventory was modelled in SimaPro v9.1.0 to estimate the environmental consequences of these production processes for various impact categories, such as global warming (2.63 – 3.19 kg CO₂ eq.), marine eutrophication (3.55×10^{-4} – 4.01×10^{-4} kg N eq.), terrestrial ecotoxicity (6.44 – 7.88 kg 1,4 – DCB), etc. Sensitivity and uncertainty analyses were also conducted to establish the reliability of the results. It was found that the enzyme hydrolysis was associated with lower environmental impacts than acid hydrolysis. This comprehensive study can be used as a guideline for developing sustainable BW-based biorefinery in the future.

1. Introduction

Food waste is a major concern across the globe due to huge economic

losses and detrimental environmental consequences. The proper strategy for managing food waste is thus vital to mitigate socio-economic challenges. The starchy food waste comprises a high concentration of

Abbreviations: BDO, 2,3-butanediol; BW, bread waste; DALY, disability-adjusted life years; DCB, dichlorobenzene; FRS, fossil resource scarcity; FE, freshwater eutrophication; FET, freshwater ecotoxicity; FU, functional unit; GHG, greenhouse gas; GW, global warming; HTC, human toxicity: carcinogenic; HTnc, human toxicity: non-carcinogenic; IR, ionizing radiation; IRR, internal rate of return; LU, land use; LCA, life cycle assessment; LCI, life cycle inventory; LCIA, life cycle impact assessment; ME, marine eutrophication; MET, marine ecotoxicity; MRS, mineral resource scarcity; MT, metric tons; SOD, stratospheric ozone depletion; FPM, fine particulate matter formation; TA, terrestrial acidification; TET, terrestrial ecotoxicity; WC, water consumption.

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<https://doi.org/10.1016/j.cej.2024.157003>

Received 6 August 2024; Received in revised form 25 September 2024; Accepted 20 October 2024

Available online 22 October 2024

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clean fermentable sugars, which can be extracted easily at an affordable cost [1]. These food wastes are thus promising biorefinery feedstocks for the fermentative production of chemicals, aligning with global carbon emission commitments. Bread is a staple food of a large global population residing in Europe and North America. According to global market analysis, Europe dominates the bread market with a share of ~ 54 %, whereas the US, Asia Pacific, Middle East, and African countries account for 28.6 %, 10.9 %, and 6.9 % of bread consumption, respectively [2]. The wastage of bread is inevitable owing to the short expiry date and the preference of customers to buy fresh bread. The annual global production of bread is > 100 million tons, and it is estimated that more than 10 % of bread produced annually around the globe is wasted [3]. The economic consequences can be better gauged from the Netherlands scenario, where bread waste (BW) accounts for a loss of more than 400 million euros [4]. In terms of the environmental consequences, countries such as the UK generate about 292,000 metric tons (MT) BW per year, which can potentially contribute to 584,000 MT of CO₂ equivalent of greenhouse gas (GHG) emissions, if not properly utilized and disposed of in landfills [5].

BW is a starchy material with 50–70 % carbohydrate content and is a good source of high-quality fermentable sugars. The consistent composition is another attractive attribute of BW for the clean source of sugars. Therefore, it has the potential to serve as an excellent substrate for manufacturing various bioproducts with immense commercial potential [6,7]. The use of BW not only offers sustainable production of chemical building blocks but also cuts down carbon emissions substantially through better use and replacing fossil-based production. Currently, most of the food waste, including BW, in developed countries is treated through anaerobic digestion (AD) to produce biomethane. However, biomethane underscores the immense market potential of BW. Further, the beneficial environmental credits associated with bioconversion through AD are observed to be low [8]. Therefore, a better bioconversion technology is required to utilize this widely available organic substrate with immense potential.

Fermentation technology involves the bioconversion of organic-rich substrates to various value-added bioproducts, such as ethanol, succinic acid, lactic acid, etc. The perusal of the literature shows that BW has been transformed into a range of products via fermentation, and one good example is 2,3-butanediol (BDO) [2]. BDO is a C₄ diol with huge industrial potential and multiple applications in the food, cosmetics, and pharmaceutical industries [9,10]. Besides, it is a precursor in producing other derivatives, such as methyl ethyl ketone, 1,3-butadiene, etc. The forecast data anticipates the BDO production growth at a compound annual growth rate of 3 % from 2019 to 2027 in the automobile, textile, and construction sectors [11,12]. The global BDO market demand is projected at \$220 million by 2027. Various studies have reported BDO production using *Enterobacter* sp., *Bacillus* sp., *Klebsiella* sp., *Saccharomyces* sp., *Paenibacillaceae* sp., and *Enterococcus* sp. [9,12,13]. However, most commercial biorefineries around the world utilize edible food sources for production of biofuels and chemicals, such as sugar, corn, oils, etc., which may give rise to the food vs fuel debate in the present world scenario. In this context, utilization of inevitable food waste, such as BW, a clean source of high quality and easily extractable fermentable sugars, can mitigate the competition with edible feedstocks. Besides, the cost of feedstock procurement for BDO production will be significantly reduced as BW is a common food waste around the world. Recently, high level BDO production has been achieved using fermentable sugars obtained from acid and enzyme hydrolysis of BW by *Enterobacter ludwigii* [14]. Their work exhibited promising results in terms of BDO production parameters (titer > 130 g/L and yield > 0.40 g/g). The work clearly indicates that the bioconversion of BW to BDO has the potential to be upscaled for commercial production.

Understanding the economics and environmental consequences is essential for informed decision-making prior to pilot-scale testing and commercialization of BW valorisation into BDO. In the present work, an integrated techno-economic and environmental assessment was carried

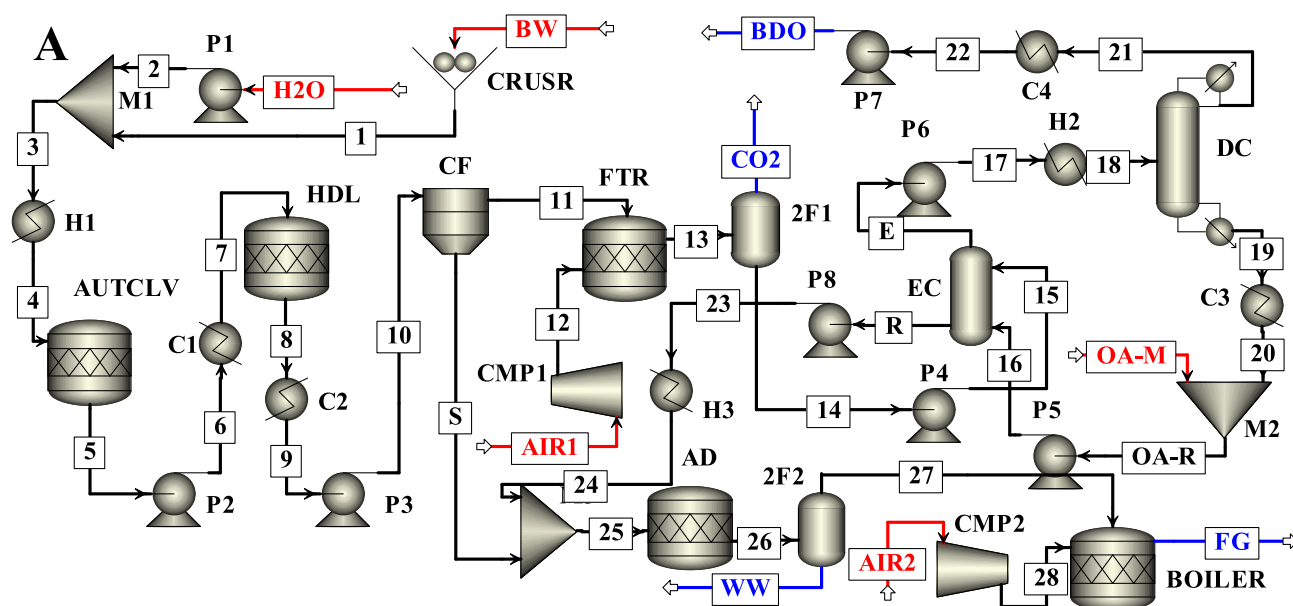
out for BDO production from BW. The fermentable sugars can be released from BW via hydrolysis of starch aided by either acid or enzyme. The present work developed two processes employing acid and enzyme hydrolysis of BW before BDO fermentation of sugars to compare their economic and environmental performance. However, a detailed process design using current state-of-the-art experimental data is essential for reliable estimates of their economic performance. The present work developed the comprehensive end-to-end processes using validated thermodynamic models available in Aspen Plus software for accurate estimation of energy consumption and sizing of the process equipment. Heat consumption is one of the key operating costs in the manufacturing of chemicals. Lowering thermal energy consumption is thus of utmost importance to enhance profitability and reduce associated environmental consequences. The pinch technology enables efficient mapping of hot and cold streams for maximum heat energy exchange within the process, reducing external thermal energy consumption. The process integration was thus carried out using pinch technology. The process economics was then evaluated using material and energy balance data obtained from these integrated processes. The economic analysis included the estimation of capital investment, production costs, major cost-contributing factors, and minimum BDO selling price.

The life cycle assessment (LCA) of chemical manufacturing processes is based on the overall and unit-wise energy consumption and material inflow and outflow. In the absence of real plant data, the material and energy balance data stemming from the comprehensive process design formed the basis of the LCA for fermentative BDO manufacturing from BW in the present study. The comprehensive LCA incorporated the sensitivity and uncertainty analysis to identify the potential hotspots for environmental impacts. Previous studies have reported environmental impacts for BDO production from white birch [15], wood [16], oil palm empty fruit bunches [17], succinic acid [18], wheat straw [19], BSG [20], etc. Similarly, techno-economic analyses have also been conducted for BDO production from fermentable sugars derived from sugarcane [21–24], banana waste [25], wood [26], switchgrass [21], white birch [15], glucose [9], and BSG [8]. However, the process flow, energy and electricity considerations, and transportation distance assumptions are different in addition to the difference in substrate. To the best of our knowledge, this is the first study on integrated techno-economic and environmental assessment of BW based BDO production. To address the relevance of energy savings for BDO production cost, a comparison was made between process integration with and without pinch technology. The results of the study are expected to aid stakeholders and policy-makers in predicting the commercial as well as environmental prospects of BW-based biorefinery.

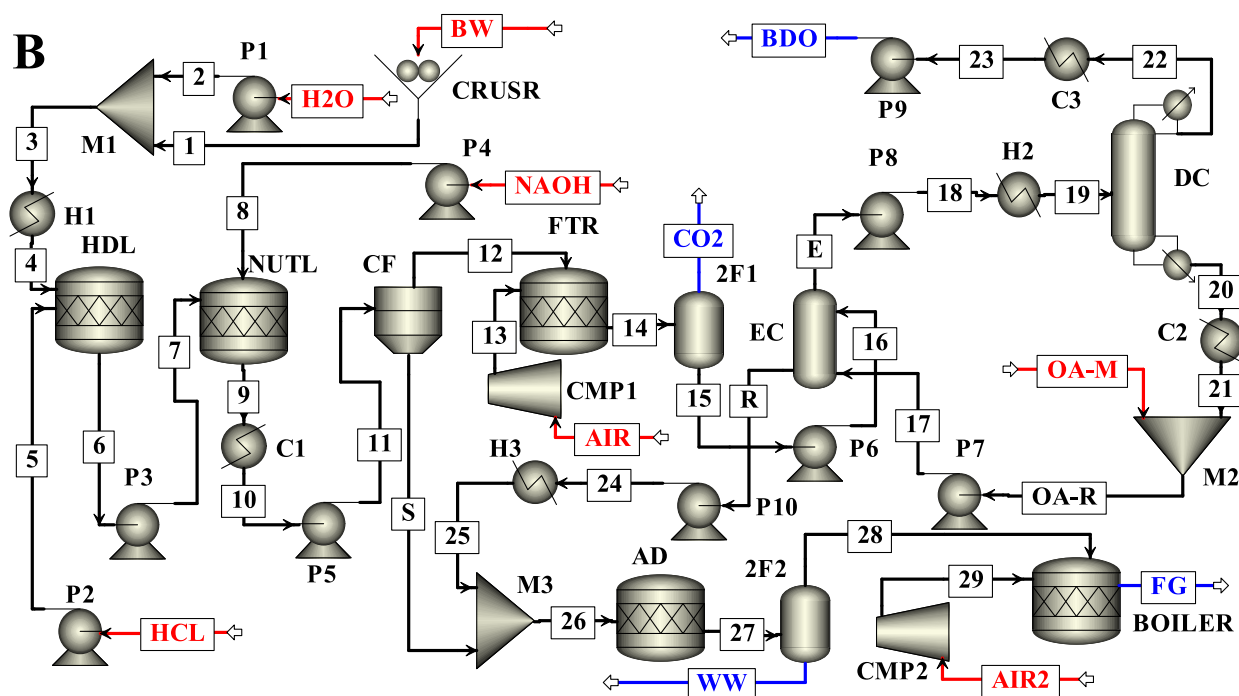
2. Methodology

2.1. Fermentative production of BDO from BW

BW feedstock employed in this work comprised 40.6 % water, with 46 % starch, 2.5 % fiber, 7.9 % protein, 2 % saturated fats, and 1 % salt [7]. The process was designed for converting 100 MT of BW into BDO. The process started with the shredding of BW, followed by enzymatic/acid hydrolysis to release the fermentable sugar from starch (Fig. 1). The saccharification of starch was carried out using 20 % BW loading, where 95 % and 90 % of starch were converted into glucose during enzymatic and acid hydrolysis, respectively. The enzyme hydrolysis was carried out at 45 °C with 48 h hydrolysis period (Fig. 1a). The acid hydrolysis of BW was carried out at 121 °C for 15 min using 2 % (v/v) hydrochloric acid (30 %), and the resulting acid solution was subsequently neutralized by 5 N NaOH (Fig. 1b). The glucose concentration obtained after enzymatic and acid saccharification was around 111 g/L and 99 g/L, respectively. The reduced glucose concentration in acid hydrolysis was due to the lower starch saccharification, extra water coming with HCl and NaOH streams, and the formation of water during acid neutralization. The



CRUSR-Crusher, AUTCLV-Sterilizer, HDL-Hydrolysis reactor, CF-Centrifuge, FTR-Fermenter, 2F-Two-phase flash
EC-Extraction column, DC-Distillation column, AD-Anaerobic digestion, CMP-compressor, C-Cooler, H-Heater, P-Pump, M-Mixer



CRUSR-Crusher, HDL-Hydrolysis reactor, NUTL-Neutralizer, CF-Centrifuge, FTR-Fermenter, 2F-Two-phase flash, C-Cooler,
EC-Extraction column, DC-Distillation column, AD-Anaerobic digestion, CMP-Compressor, H-Heater, P-Pump, M-Mixer

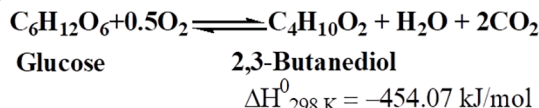
Fig. 1. Process flow diagram for BDO production using (A) enzyme and (B) acid hydrolysis of BW.

fermentable glucose was then converted to BDO by aerobic fermentation using air (Reaction 1). The fermentation was carried out at 30 °C for a three-day fermentation period, in which 95 % of fermentable glucose was converted to BDO. The BDO concentration in the fermentation broth was around 52 g/L and 46.5 g/L using glucose-rich BW hydrolysate from enzymatic and acid saccharification, respectively.

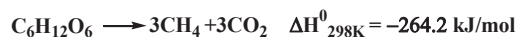
However, BDO is a fermentation product with a high-boiling point (177 °C), and further, the fermentation broth contains high-boiling soluble organics, such as unconverted glucose, salts, protein, byproducts, etc., and inorganic nutrients added to the fermenter. Therefore, we

employed solvent extraction to recover BDO from the fermentation broth [27,28]. The liquid-liquid extraction of BDO can be carried out using ethyl/butyl acetate, butanol, 2-ethyl-1-hexanol, and oleyl alcohol as a solvent. However, the oleyl alcohol offers a high BDO distribution coefficient (2.66 – 6.52), high BDO selectivity (7.24 – 421.9), and low water solubility [28]. Oleyl alcohol was thus chosen as an extractant for this work. The BDO extraction was carried out at room temperature using a solvent/feed mass ratio of 3.0, with around 99 % recovery of BDO into the extracted phase. The extraction column has ten stages, feeding fermentation broth and oleyl alcohol from the top and bottom of

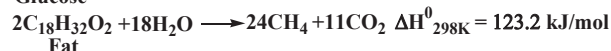
the extractor, respectively. The BDO from the extract was later separated from the oleyl alcohol by fractional distillation. The overall glucose yield was 0.49 and 0.465 kg per kg of BW for enzymatic and acid saccharification, with the yield of 0.226 and 0.214 kg BDO per kg of BW, respectively. The theoretical BDO yield is 0.50 kg/ kg glucose (Reaction 1).



Reaction 1. Reaction chemistry for aerobic fermentation of glucose to BDO.



Glucose



Fat



Protein

Reaction 2. Reaction stoichiometry for anaerobic digestion.

The oleyl alcohol is a high boiling liquid (around 329 °C). The separation of BDO from oleyl alcohol by atmospheric pressure distillation column thus involves high reboiler temperature, which needs to be fuelled by expensive fired heat. The excessive reboiler temperature may also lead to thermal degradation of BDO [28]. Therefore, the distillation column was designed under vacuum at 25 mm of Hg to keep the reboiler temperature below 250 °C to meet reboiler heating duty by high-

pressure steam. However, the distillation column involved excessive heating duty due to an enormous flow rate of oleyl alcohol. Therefore, reducing reboiler duty is of utmost importance to minimize operating expenses. The distillation column feed was thus preheated to 150 °C at atmospheric pressure to reduce reboiler duty. Further, the entire pre-heating duty can be obtained from the distillation column bottom product, thereby improving the thermal efficiency of the overall process. The oleyl alcohol loss was insignificant in the extractive distillation separation owing to its low water solubility. The distillation column had ten stages, with the fifth tray as the feed stage, and required a nominal reflux ratio of 2.0 to obtain more than 99.5 % BDO recovery. The distillation column was designed considering the sieve tray with a tray spacing of 0.61 m. The column diameter was 2.16 m and 2.26 m for enzyme and acid hydrolysis, respectively. The oleyl alcohol stream recovered from the distillation column was cooled to room temperature and recycled to the extractor after adding a small amount of makeup. The unconverted starch from the saccharification reactor and water-soluble organics (glucose, protein, and fat) present in the raffinate phase from the extractor were digested via AD at 41 °C for 16 days to generate biogas (Reaction 2). The biogas was utilized to generate high-pressure steam. The overall material balance for both processes is represented by the block diagrams (Fig. 2).

2.2. Process integration by pinch analysis

The integrated processes were developed using pinch methodology, considering 10 °C as the minimum temperature difference between hot

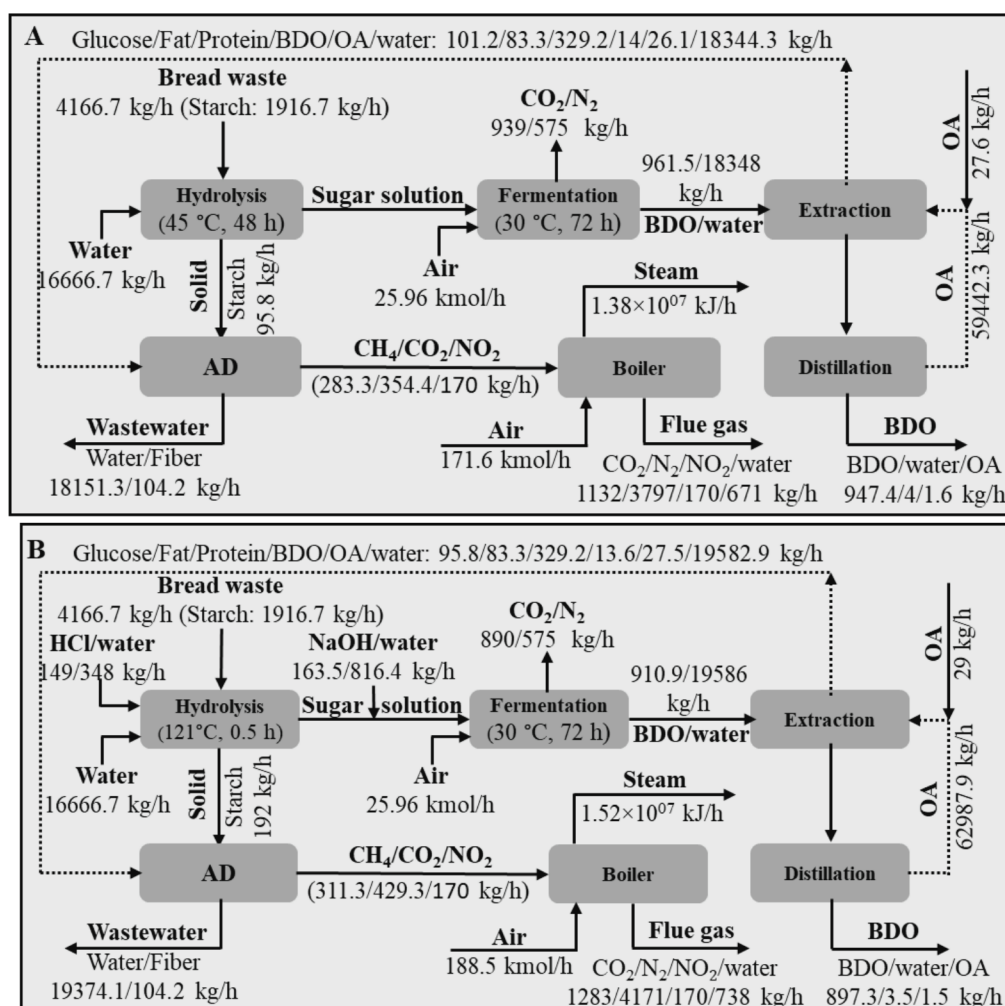


Fig. 2. The block diagram of material balance for (A) enzyme and (B) acid hydrolysis of BW.

and cold streams. The temperature vs enthalpy diagrams showed 240.1 °C as the shifted pinch point temperature for both processes (Fig. 3). The maximum process heat recovery potential was 2.64×10^7 and 2.72×10^7 kJ/h below the pinch point for enzymatic and acid hydrolysis, respectively, without any scope of process heat exchange above pinch. The minimum cooling duties were 2.03×10^7 and 2.20×10^7 kJ/h for enzymatic and acid hydrolysis, respectively (Table 1). The higher cooling duty in acid hydrolysis was due to heat generation during acid neutralization. The minimum heating duty involved in these two processes were 1.72×10^7 and 1.80×10^7 kJ/h, respectively. A slightly higher heating duty in acid hydrolysis was due to a larger oleyl alcohol flow rate in extraction with higher reboiler duty. However, the biogas generation was more in acid hydrolysis due to lower carbohydrate conversion in the hydrolysis step, resulting in more amount of carbohydrates available for AD. As a result, the heat energy generated in the reboiler was much more for acid hydrolysis. The net heating duty for acid hydrolysis was thus slightly lower than enzymatic hydrolysis. These pinch results were used in designing integrated processes for maximum process heat exchange, as shown by grid diagrams (Fig. 4). For enzymatic hydrolysis, the heat duty of H1 was partially acquired from C1, with the balance being sourced from C3. The heat duty of C3 was exploited to heat H2, H1, H3, and AD sequentially. The balanced cooling duty of C3 and remaining hot streams was obtained by cooling water. For acid hydrolysis, the heat duty of H1 and H2 was obtained from C1 and C2, respectively. The balanced heat duty of C2 was used to heat H3 and AD. The remaining heat duty of C1, C2, and all other hot streams was obtained from cooling water. The reboiler was above the pinch point for both processes and heated by high-pressure steam. The integrated processes are shown in Fig. 5.

2.3. Life cycle assessment

LCA is a useful tool based on the guidelines of ISO 14040 and 14044 to carry out environmental assessment and compare different process pathways and/or products [29,30]. It comprises four key stages: the goal and scope definition, life cycle inventory, life cycle impact assessment, and interpretation.

2.3.1. Goal and scope

This attributional LCA compared two different scenarios for the production of BDO from BW, i.e., enzyme and acid hydrolysis, and the associated environmental footprint were evaluated. The study considered a cradle-to-gate system boundary, which includes all processes starting from the transportation of BW to the biorefinery till the downstream purification of BDO in addition to wastewater treatment and sludge application to land. Since the goal was focused on the environmental assessment of BDO production, 1 kg of BDO manufacturing was selected as the functional unit for LCA. The geographical area under

Table 1

Chemicals and utility consumptions or production.

	Enzyme hydrolysis	Acid hydrolysis
BDO, MT/annum	8348.2	7904.1
Minimum cooling duty, kJ/h	2.03×10^7	2.20×10^7
Cooling water, MT/annum	8.82×10^6	9.56×10^6
Minimum heating duty, kJ/h	1.72×10^7	1.80×10^7
Generation in boiler, kJ/h	1.38×10^7	1.52×10^7
Net heating duty, kJ/h	3.37×10^6	2.84×10^6
HP steam, MT/annum	1.44×10^4	1.22×10^4
Process water, MT/annum	1.46×10^5	1.46×10^5
30 % HCl, MT/annum	—	4350.8
NaOH, MT/annum	—	3045.56
Electricity, kW-h/annum	1.55×10^6	1.66×10^6

consideration for the study was United Kingdom, and the environmental simulations were performed using SimaPro v9.1.0.

The BW was pulverized using a crusher, followed by saccharification using two different process configurations: enzyme hydrolysis and acid hydrolysis. The hydrolysate generated during hydrolysis was fermented to BDO, and the subsequent fermentation broth was subjected to solvent extraction using oleyl alcohol, followed by fractional distillation, resulting in BDO production. The solid residues from the hydrolysis and the raffinate from solvent extraction were both digested via AD to generate biogas. This biogas was combusted in a boiler to generate high-pressure steam along with flue gases. Moreover, the BDO production processes considered in this LCA incorporated pinch analysis, which includes in-process heat exchange, as shown in the process diagram (Fig. 6). The final wastes generated from the system were wastewater and sludge from the AD plant along with gaseous emissions from the fermenter and boiler.

2.3.2. Life cycle inventory (LCI)

This study is based on a biorefinery that converts 100 MT of BW into BDO per day. The inventories for the above plant capacity were extracted from process simulations in Aspen Plus v12 software and normalized per kg of BDO production (Table 1). The processes were further integrated using pinch technology to improve thermal efficiency and heat energy savings. However, the nutrient content of the sludge was based on Canote et al. [31], and the emissions associated with land application of sludge as fertilizer were derived from Adghim et al. [32]. A distance of 500 km was presumed for the transportation of BW and chemicals to the biorefinery as well as land application of sludge. In addition, the land application of sludge was assumed to be carried out using a hydraulic spreader and loader. The background data of most of the LCI were adopted from the Ecoinvent database, where a cut-off approach was selected (Table S1). The cut-off approach is the most common approach for a product-based system, where the environmental impacts are associated only with the product that generates them,

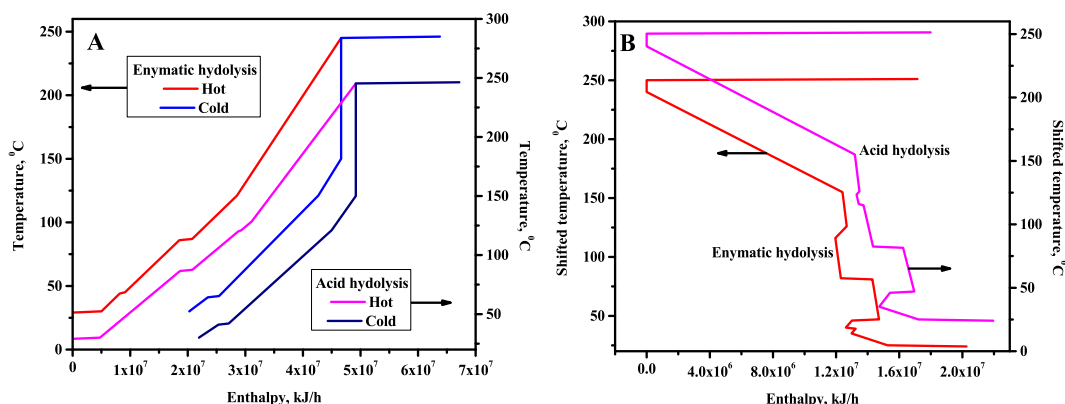


Fig. 3. (A) Composite and (B) grand composite diagrams for fermentative production of BDO from 100 MT BW per day.

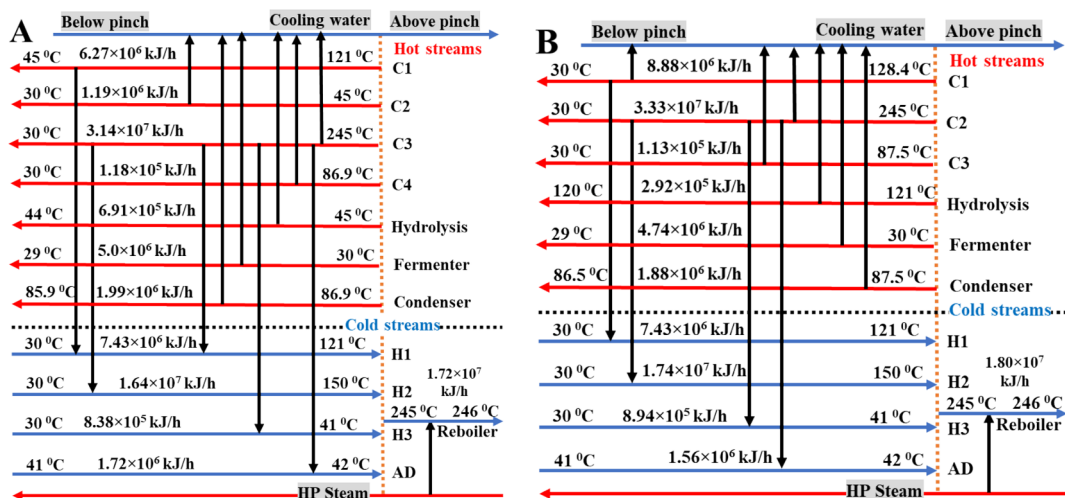


Fig. 4. Grid diagram for fermentative BDO manufacturing from 100 MT BW per day. (A) Enzyme hydrolysis. (B) Acid hydrolysis.

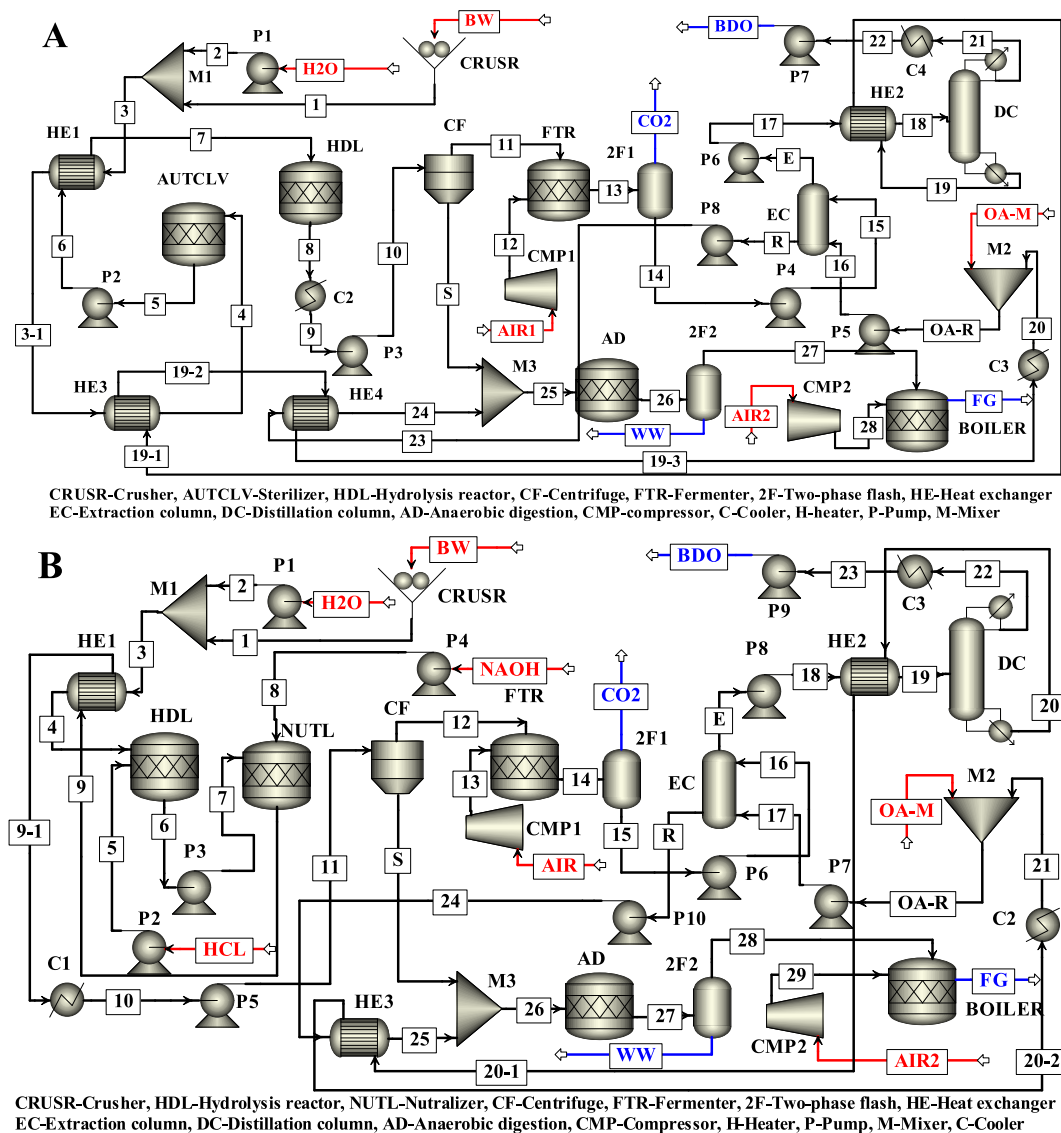


Fig. 5. Integrated process flowsheet for fermentative production of BDO from 100 MT BW per day. (A) Enzyme hydrolysis. (B) Acid hydrolysis.

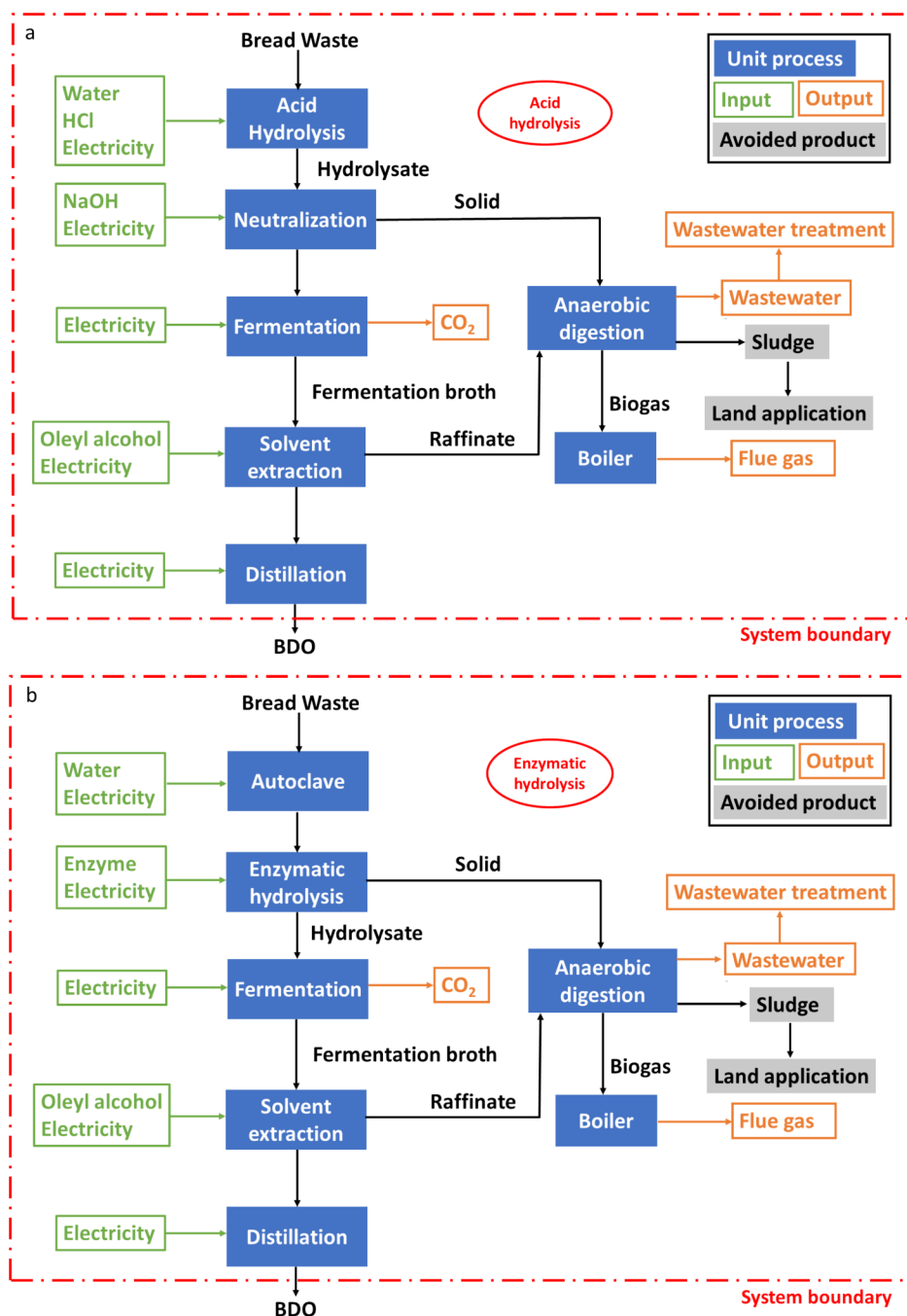


Fig. 6. System boundary for BDO production from BW using (a) acid hydrolysis and (b) enzyme hydrolysis.

irrespective of any potential future use. Therefore, it reduces the uncertainties linked with future recycling and reuse.

2.3.3. Life cycle impact assessment (LCIA)

The various unit operations leading to the production of BDO from BW were categorized under four phases, i.e., pretreatment, fermentation, distillation, and ancillary processes. The pretreatment includes all activities prior to the fermentation phase, and the distillation represents both solvent extraction and downstream separation of BDO by distillation, while the ancillary processes were associated with the AD plant and boiler. ReCiPe 2016 was chosen as the LCIA method as it is commonly used to evaluate the mid-point impacts related to global warming (GW), terrestrial acidification (TA), freshwater eutrophication (FE), carcinogenic human toxicity (HTC), non-carcinogenic human toxicity (HnTC),

terrestrial ecotoxicity (TET), freshwater ecotoxicity (FET), marine ecotoxicity (MET), land use (LU) and ionizing radiation (IR) [33]. The land application of sludge was based on the avoided burden approach, where the sludge substituted the need for chemical fertilizers based on the corresponding nutrient content.

2.3.4. Sensitivity and uncertainty analysis

The total environmental impacts and various phase contributions can fluctuate substantially with the variation in input–output parameters. These aspects can be electricity mix, transportation distance, product yield, BDO titer, etc. Environmental consequences such as IR, LU, HTC, HnTC, FET, as well as the production cost for BDO were found to reduce with increase in BDO titer [8,20]. Hence, the implication of such alternate scenarios is evaluated by conducting a sensitivity analysis

[34]. In this LCA study, the distance for transporting raw materials or products was varied, and the corresponding changes in the various impact categories were observed. Uncertainty analysis was performed via 10,000 Monte Carlo simulations and 95 % confidence interval to judge the accuracy and reliability of the obtained results [35].

3. Results and discussion

3.1. Capital investment

The capital investment was estimated following the six-tenth rule using the Chemical Engineering Plant Cost Index of 813 for 2022. The same cost index was also used to calculate retail price of chemicals (Table 2). The equipment cost for hydrolysis and fermentation was calculated considering the number of 500 or 250 cum reactors, with 75 % of the volume as usable for reaction. The nine 500 cum fermenters were considered for both processes, with three 500 cum reactor for enzymatic hydrolysis and one 250 cum reactor for acid hydrolysis. The fermenters and AD reactors were thus the major capital-intensive equipment, contributing 41–45 % and 26–30 % of the total capital expenditure due to prolonged residence time (Table 3 and Fig. S1). These results demonstrated that AD had significant impacts on process economics despite being vital for waste management. On the other hand, the hydrolysis reactors contributed around 14 % and 3 % of the total capital investment for the enzyme and acid hydrolysis, respectively. The distillation and extraction columns were other major process equipment involved in complex downstream BDO separation, contributing 4–5 % of the total capital expenditure. The storage tank cost was calculated considering twenty-five and twelve-day stocks of product and chemicals, respectively, and it contributed around 3–4 % of total capital investment. The total capital expenditure in enzyme hydrolysis was slightly more than in acid hydrolysis due to the excessive costs involved in enzyme hydrolysis reactors with prolonged residence time (Table 3).

3.2. Operating costs and cost-contributing factors

The operating cost was calculated using the costs of utility/electrical energy and chemicals acquired from different sources (Table 2). The economic analysis considered borrowing the entire capital investment with a 5.5 % annual interest rate. The depreciation cost of the equipment was calculated using the straight-line method, with 20 % of the original equipment cost being the end-of-life value. The BW was the major cost-contributing operating costs, with 56–62 % of the share of the total cost of raw material and energy (Fig. S1). The enzyme cost (22 %) was significantly higher in enzyme hydrolysis compared to the corresponding chemical costs in acid hydrolysis (15 %). The nutrients (9 %) and heat energy (10 %) were other prominent operating costs. The total operating cost in enzyme hydrolysis was slightly higher than in acid hydrolysis (Table 3). It was due to the high price of enzymes and higher direct and indirect costs stemming from excessive capital investment. Although the BDO production cost was higher in enzyme hydrolysis than in acid hydrolysis, the difference was practically negligible. However,

Table 2
Retail price of chemicals and utilities.^a

Bread waste (BW)	100 \$/MT [36]
NaOH	0.172 \$/kg [37]
30 % HCl	0.15 \$/kg
Cooling water	0.032 \$/1000 L
Electricity	0.0775 \$/kW-h
Enzymes	3.21 \$/kg [36]
Inoculum	0.007 \$/kg [36]
Nutrients	0.248 \$/kg [36]
Steam@100 psi	0.018 \$/kg
Steam@400 psi	0.027 \$/kg

^a Based on Chemical Engineering Plant Cost Index of 813.0 for 2022.

Table 3

Capital expenditure and BDO manufacturing costs in million US\$.

	EH	AH		EH	AH
Crusher	0.22	0.22	Production costs		
Sterilizer	0.5	–	Direct cost	9.8	9.18
Hydrolysis	2.21	0.5	Bread waste	3.65	3.65
Fermenters	6.62	6.62	Chemicals	1.39	0.9
Anaerobic digester	4.21	4.42	Inoculum & nutrients	0.65	0.61
Neutralization	–	0.5	Utilities	0.67	0.63
Columns	0.69	0.69	Electricity	0.12	0.13
Centrifuge	0.02	0.03	Indirect costs	5.79	5.34
Boiler	0.3	0.31	General & admin expenses	0.78	0.73
Heat exchangers	0.17	0.18	Total operating cost	22.86	21.18
Pumps and compressors	0.63	0.68	Production cost, \$/kg	2.74	2.68
Storage tanks	0.45	0.63	Without pinch analysis		
Total equipment cost	16.02	14.78	Additional utility costs	2.4	2.48
Fixed capital cost (a)	85.06	78.46	Production cost, \$/kg	3.03	2.99
Working capital (b)	4.25	3.92			
Capital expenditure (a + b)	89.31	82.38			

EH: Enzyme hydrolysis, AH: Acid hydrolysis.

the BDO manufacturing cost from BW was higher than that of the petrochemical route. Currently, the commercial BDO selling price is reported to be around \$3.23 per kg [8]. The high BDO manufacturing costs stemmed from a smaller plant capacity than the economics of scale and low carbon conservation. In the present fermentation route, only two-thirds of the carbon in sugar was retained with the BDO, and the remaining one-third of the carbon was lost as CO₂ (Reaction 1). As a result, relatively less quantity of BDO was produced with high unitary production costs. It might be noted that pinch analysis diminished around 10 % of production costs; however, it was not sufficient to make BDO economical.

The indirect costs (taxes, insurance, interest, and depreciation) stemming from capital investment contributed about 25 % of the total operating cost (Fig. 7a). Besides, the share of direct costs (operating labour, maintenance, operating charges, and plant overhead charges) was around 43 % of the operating costs. These operating costs are related to the capital investment, implying relatively huge capital expenditure for the current production scale. The result further implies that capital expenditure can be reduced by taking advantage of economies of scale. However, the feedstock, BW, contributed only about 16–17 % of the manufacturing cost.

3.3. Minimum BDO selling price

The profitability analysis was carried out assuming twenty years as the life of the equipment and 34 % income tax. The analysis also considered the cost escalation of 3.5 % for chemicals and feedstock, 3 % for utilities and operating labour, and 5 % for products. The minimum BDO selling price was estimated for 7.5–15 % internal rate of return and 5–10 years payback time. However, the minimum BDO selling prices were exorbitant, \$4.3–6.9 per kg for enzyme hydrolysis and \$4.2–6.8 per kg for acid hydrolysis, depending on the payback period and internal rate of return (Fig. 7b). The economic analysis results were further compared with the literature (Table 4). These data show that BDO is economically viable from various biomass feedstock with large biomass processing capacities. However, bio-based BDO is more expensive than the current market price for lower plant capacities. We should either take advantage of the economics of scale to make BDO viable or future research should be focused on increasing the current benchmark BDO titer and productivity to make decentralized technology feasible.

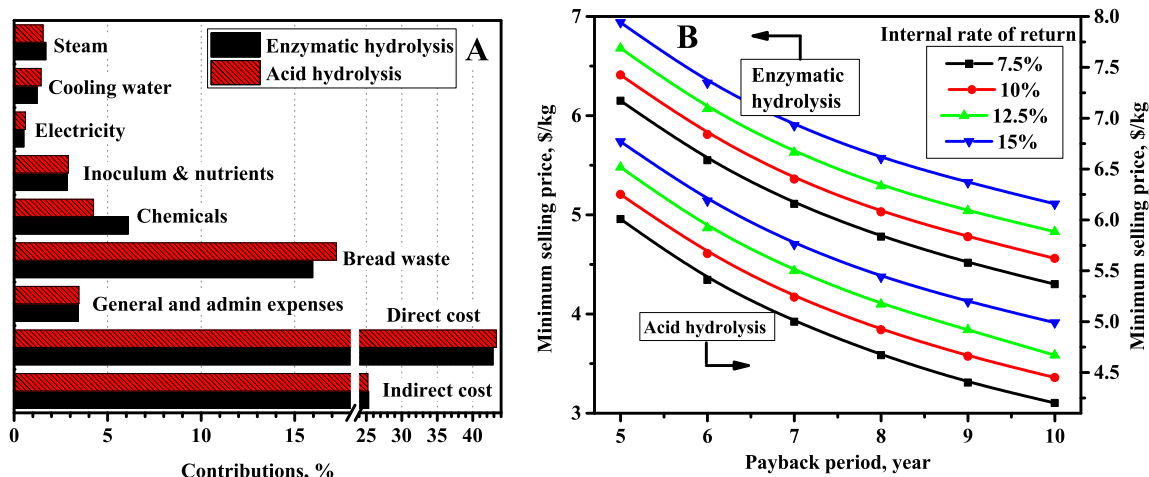


Fig. 7. (A) Cost-controlling operating cost factors on the BDO production cost. (B) Profitability analysis for minimum BDO selling price.

Table 4

Comparison of BDO production cost and minimum selling price with the literature reports.

Feedstock	Plant capacity	Production cost, \$/kg	Minimum selling price, \$/kg	Major cost factors	Ref.
Brewers' spent grain (BSG)	100 MT/day	1.894	2.7 (8.5 % IRR and 09 years payback period)	Feedstock: 18 %, Direct cost: 47 %	[8]
	2000 MT/day	1.199	1.53 (8.5 % IRR and 09 years payback period)	Feedstock: 40 %, Direct cost: 27 %	
White birch	2,000 MT (dry)/day	—	1.292 (8 % IRR and 10 years payback period)	—	[15]
Sugarcane bagasse (SCB)	96 MT/day	2.28 (only xylose), 1.21 (both C5 and C6 sugars)	3.99 (only xylose), 1.86 (both C5 and C6 sugars)	—	[21]
Sugarcane	2000 MT/day	0.904	1.1 (8.5 % IRR and 10 years payback period)	Feedstock: 53 %, Direct cost: 20 %	[22]
Molasses	610 MT/day	1.18	1.91 (20 % IRR and 10 years payback period)	Feedstock: 49 %	[23]
Whole banana (WB), Banana peels (BP)	2.4 MT/day	—	21.8–28.5 (WB), 38.8–48.8 (BP) (10 % IRR)	—	[25]
Bread waste	100 MT/day	2.74 (EH), 2.68 (AH)	4.3 (EH), 4.2 (AH) (7.5 % IRR and 10 years payback period)	Feedstock: 16–17 %, Direct cost: 43 %	Present study

3.4. Sensitivity analysis

The equipment cost is vendor-specific, with wide variation across different continents. Similarly, the retail prices of BW, chemicals, and energy are sensitive to geographical location and time. Therefore, a sensitivity study was performed to evaluate the effect of $\pm 30\%$ change in the above factors on BDO manufacturing cost and minimum selling price (Fig. 8). The capital investment was the most sensitive parameter, with $\pm 19\%$ and $\pm 24\%$ change in production cost and minimum selling price, respectively, for both enzyme and acid hydrolysis. The production cost and minimum selling price per kg of BDO were reduced to merely \$2.22 and \$3.29 for enzyme hydrolysis and \$2.17 and \$3.22 for acid hydrolysis for a 30% reduction in capital investment, which was marginally lower than the current BDO retail price. However, the effect of other parameters had negligible effect, with less than $\pm 5\%$ change in the production cost and minimum selling price. These results demonstrate that the economics-of-scale benefits of centralized plants can make this biorefinery feasible.

The return on investment of these processes was further analysed using various profitability indicators, such as net present value, internal rate of return (IRR), and payback period, considering factory gate BDO selling price of \$3.5 per kg. The enzyme hydrolysis showed a net present value of \$21.92 million for a 7.5% discount factor and 20 years of plant life, with a 9.88% IRR and 16.3-year payback period. However, acid hydrolysis showed a slightly higher net present value (\$26.52 million) and IRR (10.53%) and a lower payback period (15.3 years).

3.5. Environmental assessment

3.5.1. Life cycle impact assessment of BDO production

This section provides a comparative analysis of the two BDO production scenarios based on their hydrolysis stage, i.e., acid and enzyme hydrolysis. A base scenario derived from the Ecoinvent database that considers fossil-based BDO production was also included to analyze the environmental consequences of the established technology. It is to be noted that BDO and 1,4-butanediol have different physicochemical properties. Moreover, BDO is mostly used in the food, cosmetics, and pharmaceutical industries [15], while 1,4-butanediol is a chemical intermediate for resins and plasticizers as a humectant [38,39]. Although they are different isomeric forms, 1,4-butanediol was still selected for comparison. Previous studies have also used this analogy to compare their production pathways [17,26]. The fossil-based BDO is produced at a high temperature (225–450 °C) by butane oxidation in the presence of V_2O_5 catalyst to maleic anhydride, followed by two-stage esterification of maleic anhydride with methanol to form dimethyl maleate, and then its eventual hydrogenation in the presence of Cu-Cr catalyst. The entire

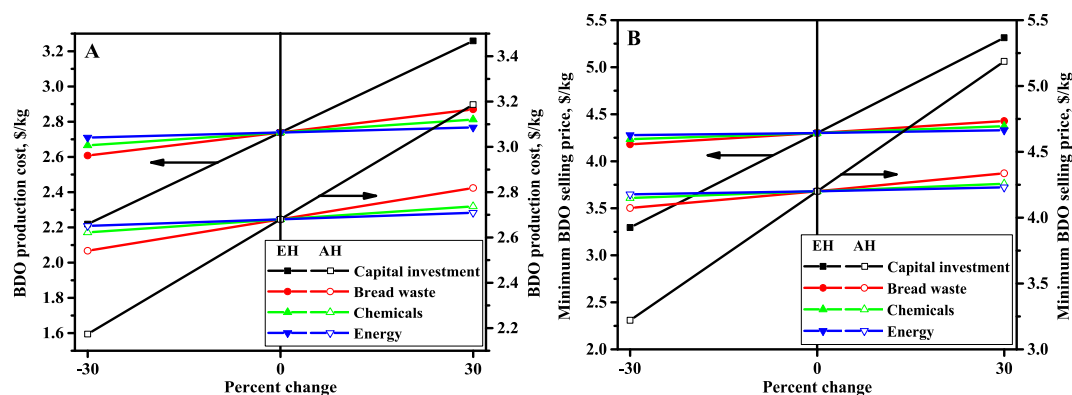


Fig. 8. Sensitivity analysis on the (A) BDO production cost and (B) minimum BDO selling price for 7.5% discount factor and ten-year payback period.

process is carried out at high temperatures.

The acid hydrolysis scenario reported higher environmental impacts than enzyme hydrolysis for all categories. While the downstream processes were the same, this difference in impacts is attributed to the difference in inventories related to BDO production stages, specifically the pretreatment stage, i.e., acid and enzyme pretreatment (Tables S2–S3). Dextrose peak enzyme was administered during hydrolysis to produce BDO in enzyme hydrolysis scenario, whereas HCl was used in the acid hydrolysis scenario, which was followed by NaOH for neutralization. Moreover, the BDO yield from enzyme pretreatment (947.4 kg/h) was higher than the acid pretreatment (897.2 kg/h). The direct emission of CO₂ from the biorefinery during the fermentation stage and ancillary process contributed to GW. In addition, the combustion of fossil fuels during transportation of various inventories, such as chemicals, BW, etc., also contributed to GW. The acid hydrolysis scenario accounted for a GW of 3.19 kg CO₂ eq., which was around 21 % higher than enzyme hydrolysis (2.64 kg CO₂ eq., Table 5). However, both these pathways accumulate lower GW as compared to fossil-derived BDO, which generates a GW of 4.46 kg CO₂ eq. Hence, in terms of GW, both the biorefineries modelled in this study based on acid and enzyme pretreatment can provide a more environmental-friendly alternative to the fossil-derived BDO. Specifically, CO₂ released from the fermenter and boiler combined together contributed around 74–81 % of the total CO₂ emission, apart from major contributions from transportation-related emissions (~11 %). CO₂ released from the fermenter can be utilized in

carbon capture and utilization (CCU) technologies for microalgae cultivation to produce biodiesel [42], biohydrogen [43], bioenergy [44], and human and animal nutrient supplements [45,46]. This could reduce the GWP of the BDO production. Electricity and oleyl alcohol consumption also contributed to GW for both processes. However, HCl and NaOH used in the case of acid pretreatment contributed around 0.13 kg CO₂ eq. each, which led to higher GW for acid hydrolysis.

Freshwater eutrophication registered significant environmental burdens of 3.22×10^{-5} kg P eq. for acid hydrolysis scenario, which was around four-fold higher than enzyme hydrolysis scenario. Wastewater generated from the ancillary processes during BDO production via acid hydrolysis accounted for around 34 % of these adverse impacts. However, the marked difference in comparison to enzyme hydrolysis was attributed to the pretreatment stage owing to the use of HCl for hydrolysis and NaOH for neutralization, which together contributed around 2.47×10^{-5} kg P eq., accounting for 40 % of the corresponding adverse impacts. However, both these inventories, acid, and alkali, were absent in the case of BDO production via enzyme hydrolysis. The hydrolysis was facilitated by enzyme, which had a comparatively lower contribution of 2.26×10^{-6} kg P eq. Hence, a lower FE of 7.63×10^{-6} kg P eq. was observed for enzyme hydrolysis with wastewater from ancillary processes, contributing around 55 % of the cumulative adverse impacts. Oleyl alcohol utilization during distillation and electricity consumption for various operations in the biorefinery was also responsible for FE, although the contributions were almost similar for both scenarios. Contrary to FE, adverse impacts associated with marine eutrophication (ME) for both processes were shared between oleyl alcohol consumption and wastewater generation. While oleyl alcohol utilization for distillation resulted in around two-thirds of the ME, the remaining one-third was mostly attributed to wastewater generated from the ancillary processes. The comparison with fossil-derived BDO showed a contrasting picture for the environmental categories of freshwater and marine eutrophication. While both process scenarios reported lower values for FE, the ME values were higher than the fossil-derived BDO (1.7×10^{-4} kg P eq., 9.26×10^{-6} kg N eq.).

Transportation was the single largest contributor to the impact categories of terrestrial (93–97 %) and marine ecotoxicity (68–70 %) for both BDO production pathways. However, transportation only contributed around 14 % for both pathways in the case of FET, where the highest impact was generated owing to the use of oleyl alcohol in the range of 80–83 %. Although the attributable trend in the case of FET, MET, and TET were similar for both pathways, the scenario is different for HCT and HnCT primarily due to the contributions of HCl and NaOH in the case of acid hydrolysis. Wastewater generation was responsible for around one-third of the impacts associated with HCT for acid hydrolysis, along with contributions in the range of 16–18 % from oleyl alcohol, HCl, and NaOH. Contrary to HCT, where transportation only corresponded to around 6 % of the adverse impacts, the share increased to around 32 % for HnCT. This was followed by contributions from oleyl

Table 5

Overall environmental impacts of 1 kg BDO production for acid and enzyme hydrolysis configurations.

Impact category	Unit	Acid hydrolysis	Enzyme hydrolysis
Global warming	kg CO ₂ eq	3.19	2.63
Stratospheric ozone depletion	kg CFC11 eq	8.01×10^{-07}	3.18×10^{-07}
Ionizing radiation	kBq Co-60 eq	1.50×10^{-02}	6.90×10^{-03}
Terrestrial acidification	kg SO ₂ eq	2.30×10^{-03}	1.14×10^{-03}
Freshwater eutrophication	kg P eq	3.22×10^{-05}	7.63×10^{-06}
Marine eutrophication	kg N eq	4.01×10^{-04}	3.55×10^{-04}
Terrestrial ecotoxicity	kg 1,4-DCB	7.88	6.44
Freshwater ecotoxicity	kg 1,4-DCB	7.48×10^{-03}	6.60×10^{-03}
Marine ecotoxicity	kg 1,4-DCB	7.40×10^{-03}	6.12×10^{-03}
Human carcinogenic toxicity	kg 1,4-DCB	2.92×10^{-03}	1.62×10^{-03}
Human non-carcinogenic toxicity	kg 1,4-DCB	3.02×10^{-01}	2.18×10^{-01}
Land use	m ² a crop eq	1.86×10^{-01}	1.61×10^{-01}
Mineral resource scarcity	kg Cu eq	-1.56×10^{-03}	-1.67×10^{-03}
Fossil resource scarcity	kg oil eq	2.26×10^{-01}	1.36×10^{-01}
Water consumption	m ³	3.24×10^{-02}	1.97×10^{-02}

alcohol (~30 %) and wastewater-related emissions (~16 %). In addition, contributions from HCl and NaOH were reduced to half as compared to HCT. In the case of enzyme hydrolysis, wastewater contributed around half of the adverse impacts associated with HCT, followed by oleyl alcohol (24 %). Further, transportation and electricity were also responsible for HCT in the range of 7–10 %. The absence of acid hydrolysis and neutralization step for enzyme hydrolysis led to considerably lower HCT values than acid hydrolysis. Impacts associated with HnCT were majorly ascribed to transportation and oleyl alcohol, each contributing around 37 % of the total impacts. Additionally, around one-fifth of the HnCT impacts were ascribed to wastewater-related emissions. Fossil-derived BDO generated a higher impact for both HCT and HnCT than acid and enzyme hydrolysis.

This study also discusses the impacts generated from the utilization of resources, such as minerals, fossils, water, and land. Impacts related to water consumption for BDO production via enzyme hydrolysis were mostly concentrated in two stages, i.e., process water consumption in the pretreatment stage and oleyl alcohol consumed in the distillation stage, each accounting for nearly half of the total consumption. However, in the case of BDO production via acid hydrolysis, around 10 % was attributed to each HCl and NaOH, while the rest was distributed between process water and oleyl alcohol consumption. Consumption of fossil during transportation accounted for the highest impacts in the fossil resource category for both acid (~50 %) and enzyme (~70 %) hydrolysis in addition to oleyl alcohol (7–10 %). As observed for other impact categories, HCl and NaOH consumption also led to around 30 % of total adverse consequences in FRS. A common consumable for both processes in this FRS was electricity. The electricity in the UK is mostly derived from fossil fuels (76.42 %), apart from a combination of nuclear, renewables, hydropower and imports from France and Ireland [40]. This utilization of primarily fossil-based electricity is responsible for the adverse environmental footprint in FRS.

Ancillary processes have a significant contribution to the beneficial impacts of BDO production for both pathways. The sludge produced from the AD of fermentation solid residue has fertilizer potential owing to the nitrogen, potassium, and phosphorus content. This could be used for land application, which could replace or avoid a part of commercial fertilizer production and, in turn, reduce the environmental burdens generated from BDO production. This contributed significantly to the mineral resource category by overcoming the total adverse impacts and eventually scoring -1.56×10^{-3} kg Cu eq. and -1.67×10^{-3} kg Cu eq. for acid and enzyme hydrolysis, respectively. Similarly, the ancillary process could offset nearly all the environmental burdens for the land use category and about 77 % for FE. Moreover, adverse impacts for MET, HCT, and HnCT were reduced in the range of 5–9 % for enzyme and 5–7 % for acid hydrolysis.

The inventories generating adverse impacts can be mostly

categorized under consumables, electricity, transportation, and miscellaneous (Fig. 9). Consumables include chemical and water consumption, while miscellaneous indicates process emissions, such as gases and wastewater. In the case of BDO production via acid hydrolysis, miscellaneous was the highest contributor at 75 % to GW, although the contribution was also substantial, around one-third to FE, ME, and HCT. As previously mentioned, transportation was the dominant inventory for FRS, TET, and MET while consumables contributed the highest impact for the rest. Consumables single-handedly accounted for more than 82 % of FET, LU, MRS, and WC, while the contribution was in the range of 54–67 % for TA, FE, ME, and HCT. However, the contributions of the inventories for various impact categories were different for enzyme hydrolysis. In addition to GW, miscellaneous was also the highest contributor to FE and HCT. Similar to acid hydrolysis, transportation was again the highest contributor to TET, MET, and FRS. In the case of both TA and HnCT, the contributions were almost equally shared between consumables and transportation. However, consumables accounted for the highest contributions for the rest of the impact categories.

The end-point impacts also followed the same trend as mid-point impacts, where the BDO production via acid hydrolysis was associated with higher environmental consequences than enzyme hydrolysis. The end-point categories are derived from mid-point categories and are expressed in different units. For example, the impact categories of human health, ecosystems, and resources are expressed in terms of disability affected light years (DALY), species.yr and USD2013. The acid hydrolysis generated a human health impact of 3.62×10^{-6} DALY and ecosystems impacts of 1.16×10^{-8} species.yr, which are comparatively higher as compared to enzyme hydrolysis (3.62×10^{-6} DALY, 9.37×10^{-9} species.yr). The maximum contribution to these two end-point categories for both pathways was attributed to direct CO₂ emissions. However, impacts in the resources category were mainly attributed to transportation and the subsequent use of fossil fuels and related emissions, which led to an impact of around 0.07 and 0.05 USD2013, respectively.

3.5.2. Sensitivity and uncertainty analysis

It was clear from the contribution analysis that transportation distance has considerable influence over multiple environmental categories, such as GW, IR, ecotoxicity, HnCT, and FRS, for both production pathways. Transportation is directly associated with the emission of GHG, which not only contributes to GW but also contributes to deterioration in land, air, and water quality. In addition, the consumption of fuel leads to a reduction in fossil reserves, thus contributing to FRS. This information is of immense importance as the impacts can be significantly reduced, which could lead to a more environment-friendly product without altering the production process. Hence, a sensitivity

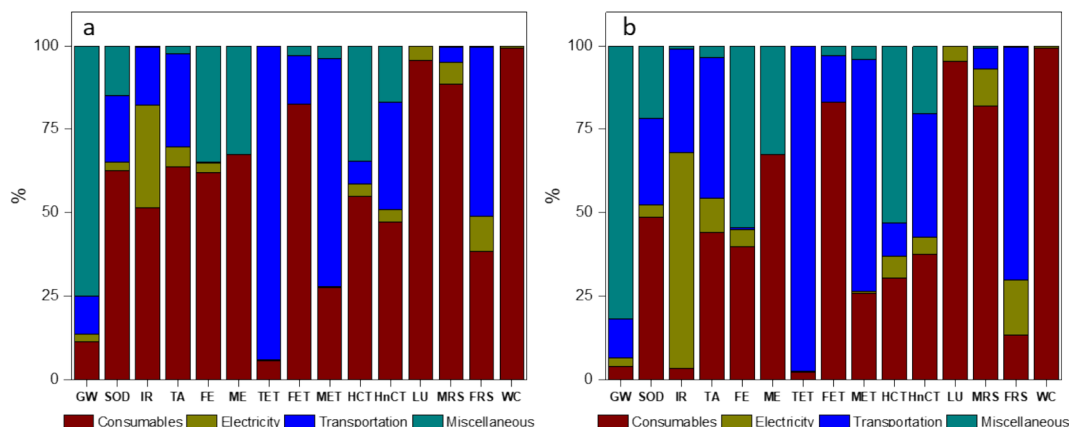


Fig. 9. Contribution of inventory to adverse environmental impacts for (a) acid hydrolysis and (b) enzyme hydrolysis.

analysis was performed for the transportation distance between the source of BW and the biorefinery producing BDO (Fig. 10). In the case of acid hydrolysis, the highest variation of impacts was noticed for TET and MET, where the values were reduced by around two-thirds and half of the original values, respectively, for a reduction in distance from 500 km to 100 km. As a consequence of this reduction in the distance by 400 km, a substantial decrease in adverse impacts was also noticed for FRS (37 %), SOD (25 %), and HnCT (32.4 %). However, the reduction in GW, FET, and IR was comparatively milder in the range of 8–12 %. In the case of enzyme hydrolysis, the consequence of this reduction in transportation distance was more pronounced than that of acid hydrolysis. The reduction in the distance between the source of BW and the biorefinery led to a decrease in TET, SOD, FRS, MET, HnCT, IR, FET, and GW by ~ 76 %, 60 %, 58 %, 57 %, 31 %, 25 %, 11 %, and 9 %, respectively. Hence, it is evident that locating the biorefinery near the source of BW could significantly reduce the adverse impacts on the environment.

LCA is quite data-intensive, and it is possible that some data are unaccounted for or not representative but derived based on suitable assumptions or estimations. This may eventually be reflected in the form of uncertainty about the impacts associated with the inventory data. This uncertainty in results, if not accounted for, may affect the subsequent decision-making process. Hence, uncertainty should always be addressed to establish the validity of the results and increase confidence in the corresponding outcomes of an LCA study. A Monte Carlo simulation generates repetitive random values that provide an estimation of how accurate the predicted results are (Tables S4–S5). For acid hydrolysis, CV-values lower than 12 % were observed for FRS, GW, ME, TA, and TET, which was also true for enzyme hydrolysis. Comparatively, CV values in the range of 22–50 % were observed for FET, LU, MET and SOD for acid hydrolysis. The mid-range categories were different for enzyme hydrolysis, as a CV value of 87 % was observed for LU, whereas HnCT reported a CV value of 27.5 %. However, higher CV values were reported for FE (57 %), HnCT (53 %), HCT (344 %), and IR (143 %). Similarly, in the case of enzyme hydrolysis, higher CV values were observed for FE (62.7 %), HCT (122 %), and IR (137 %).

3.5.3. Comparison with previous studies

Various studies have estimated impacts generated from BDO production with different biobased processes while considering different system boundaries or process flows and activities. A discussion is still carried out in this section to provide insight into the present study, which mostly discusses GW impacts. BDO production from white birch resulted in a GW of 0.98–1.27 kg CO₂ eq./ kg BDO [15]. Although the process flow was designed by Aspen Plus, and the authors used the

ReCiPe method for impact assessment similar to the present study, there was a deviation in the production process. The present study follows a route where BDO is generated as a single product while white birch was used for co-production of both BDO and adipic acid. Hence, mass, and economic allocations were followed for impact calculations. Moreover, the liquid–liquid extraction step using isobutyl alcohol was adopted for BDO extraction, and the transportation of materials was not considered. Similarly, another study also estimated the end point impacts of wood-based BDO production [26]. However, the assumptions for CO₂ emissions considerations for the climate change category were different than the present study. For wood-based BDO production, all the CO₂ emissions were considered biogenic and hence were not accounted in the estimation of total CO₂ eq. In contrast, the present study includes all the CO₂ emissions in the process. The present study would result in a GW of 0.49 – 0.77 kg CO₂ eq./kg BDO if biogenic emissions were excluded from the total CO₂ emissions. This could lead to a decrease in GW by 3.7 – 4.0 kg CO₂ as compared to the fossil-based BDO production, allowing a reduction of 82–89 %. This reduction is higher than that reported by other studies for biobased BDO production. The wood-based BDO recorded a reduction of 52 %, which is similar to that achieved from corn stover feedstock [41] and 43 % reduction in the case of food crops (oil palm farming integrated with biorefinery) as feedstock [17]. In comparison to the present study, where the system boundary covers all upstream and downstream production processes in addition to transportation and wastewater treatment, Rehman et al. [17] conducted an LCA considering only the key inputs which led to the eventual 6.8 kg CO₂ benefits/ kg BDO. Another study where BDO was produced while utilizing 2G succinic acid and direct sugars as substrates through the fermentative pathway generated a GW of 2.05 – 2.37 and 0.16 – 0.54 kg CO₂ eq., respectively [18]. Again, it was considered that embedded biogenic carbon is classified as negative emissions. BDO production from cardoon lignocellulosic biomass emitted 2.82 kg CO₂ eq., where a comprehensive LCA was conducted as the impacts were considered for the cultivation phase, biorefinery phase, and transportation. However, only 100 km distance (return) was considered as compared to 500 km for the transportation of BW and chemicals in the present study. Further, the fossil-derived high-pressure steam used for distillation also contributed to GW. Another LCA that reported a lower emission than fossil-derived BDO was based on BDO production from wheat straw [19]. A CO₂ eq. of 5 kg/ kg BDO originating from the combustion of solid residue in the CHP plant was considered biogenic and hence, not included in the cumulative GW calculations. In a previous study by the authors, BDO derived from brewers spent grain was modelled for LCA. The GW was reported to be around 7.25 kg CO₂ eq. owing to the CO₂ emission during fermentation [20]. The present study with BW as

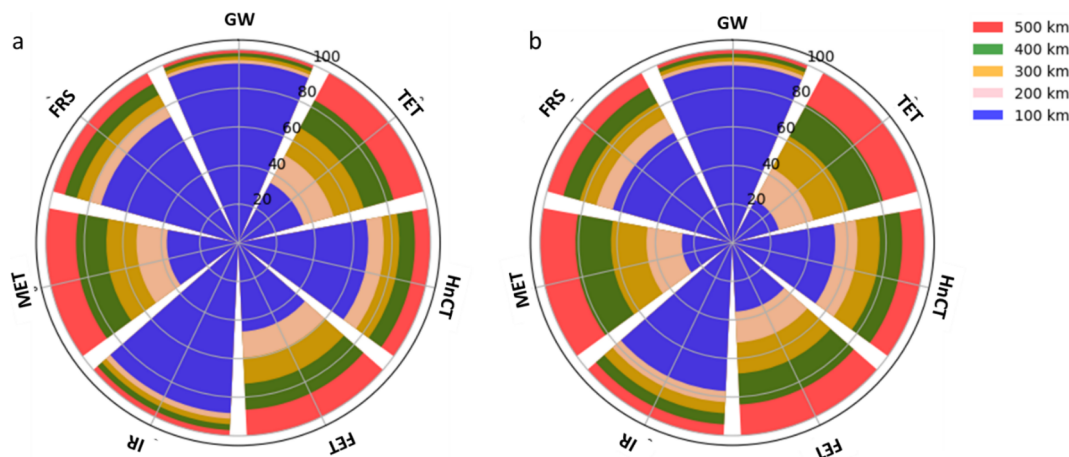


Fig. 10. Percentage variation in environmental impacts with change in transportation distance of BW to biorefinery for (a) acid hydrolysis and (b) enzyme hydrolysis.

substrate reported a considerably lower GW of more than 50 % reduction.

4. Conclusions and future perspectives

An integrated techno-economic and environmental assessment was reported in this work for sustainable BDO production by fermentation of sugars derived from the enzyme and acid hydrolysis of 100 MT of BW per day. The environmental assessment was performed based on the pinch analysis-based comprehensive process design using Aspen Plus for two different scenarios: enzyme and acid hydrolysis of BW, followed by fermentation and extraction-based downstream BDO separation. The energy efficiency of these bioprocesses was enhanced significantly using pinch analysis, with around 10 % reduction in production costs. However, the capital investment was relatively high for the proposed BW processing capacity, with excessive contributions of direct (~43 %) and indirect (~25 %) costs to the total operating costs. The BDO production cost was slightly higher for enzyme hydrolysis (2.74 \$/kg) than acid hydrolysis (2.68 \$/kg) due to the high cost of enzyme and higher capital investment for enzyme hydrolysis. The biobased BDO was more expensive than the current market price. However, the biobased BDO pathways were environmentally promising, with lower global warming impacts than fossil-based BDO production. The enzyme hydrolysis was associated with comparatively lower environmental impacts than acid hydrolysis, mostly due to the higher BDO yield and difference in inventories related to the pretreatment stage. The sensitivity analysis ascertained that a decrease in transportation distance could further reduce the overall impacts for both pathways. Improvements to the present system boundary can generate lower environmental impacts and BDO production costs. The fermentation and downstream BDO separation can be improved to increase the BDO titer and reduce energy consumption, respectively. This increase in BDO titer can subsequently lead to reduction in the production cost and environmental burdens. Further the fermentation route retains only two-thirds of the carbon of sugar in the form of BDO, with one-third of the carbon being lost as CO₂. Hence, environmental consequences can be further reduced by improving the carbon economy of fermentation via implementing CCU technologies making use of biogenic CO₂ released during fermentation. Besides, the biorefinery should be located close to the BW source to reduce transportation costs and associated environmental impacts due to fuel consumption. Finally, the scaling-up process can reduce capital expenditure and production costs.

CRedit authorship contribution statement

Bikash R Tiwari: Writing – original draft, Software, Methodology, Conceptualization. **Sunil K. Maity:** Software, Conceptualization, Data curation, Writing – original draft, Writing – review & editing. **Satinder K Brar:** Supervision, Resources. **Kit Wayne Chen:** Writing – review & editing. **Gopalakrishnan Kumar:** Writing – review & editing. **Vinod Kumar:** Writing – review & editing, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors would like to acknowledge NSERC CRD grants and James and Joanne Love Chair in Environmental Engineering for funding this research.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.cej.2024.157003>.

Data availability

No data was used for the research described in the article.

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2024-11-15

Elsevier

<https://doi.org/10.1016/j.cej.2024.157003>

Tiwari BR, Maity SK, Brar SK, et al., (2024) Comprehensive techno-economic and environmental assessment for 2,3-butanediol production from bread waste. Chemical Engineering Journal, Volume 500, November 2024, Article number 157003