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Sustainability Index Accounting Food and Carbon Benefits on Circular 2,3-Butanediol Biorefinery with Oil Palm Empty Fruit Bunches

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ABSTRACT

Progressive replacement of petroleum chemicals with biomass derived products is an essential research goal toward sustainability. However, the progress of the development of new generation biorefinery has been affected by many factors, *i.e.*, prices of crude oil, food, and carbon. To quantify the environmental and social impacts of the technologies, this study constructed a sustainability index for calculating two new bio-butanediol production processes with oil palm empty fruit bunches as example feedstock. The performance of organosolv pretreatment using butanediol was compared with the whole slurry conversion process using sulfite pretreated biomass, over the petroleum refinery and first generation biorefinery with food crop feedstock. The organosolv biorefinery process successfully converted the biomass into 77.3 ± 1.63 g/L of bio-butanediol (0.45 g/g yield), which is slightly higher (5.5%) than that of the sulfite-based process. The integration of biorefinery techniques, with oil palm farming shall result in 6.8 kg-CO_2 and 0.5 kg-food benefits per kg butanediol produced, yielding a sustainability index of 7.30. The food index for first generation biorefinery is -1.04 kg food per kg butanediol produced. Using empty fruit bunches for butanediol production could save 1.54 kg food crop consumption, which turns the "food vs. fuel competition" into a "food plus fuel nexus".

Keywords: Sustainability index, butanediol, staged-organosolv-pretreatment, oil palm empty fruit bunches, energy and carbon footprint.

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1. INTRODUCTION

Global warming and depletion of fossil fuel resources have urged our research to enhance the utilization of renewable resources for biochemical production. Green bio-based technologies (e.g., fermentation) have also created growing opportunities to support agricultural industries [1]. The bio-based chemicals market is forecast to reach USD 128 billion and is with an annual growth rate of 10.27% until 2026, among which butanediol (BDO) is an important organosolv with high market demand (USD 14.5 billion) [2]. The conventional BDO produced from petroleum refinery (petro-BDO) is in the form of 1,4-BDO monomer, while bio-BDO is either 2,3-BDO or 1,4-BDO depending on the strains involved in the bioconversion process. According to National Institute of Standards and Technology (NIST, USA), the physical and thermochemical properties of both the compounds are nearly the same, *i.e.,* ideal gas heat capacity 173.7 J/mol-K for both chemicals; 200.1 and 212.4 J/mol-K liquid heat capacities; and -2495 and -2461 kJ/mol heating values for 1,4-BDO and 2,3-BDO, respectively. Both of the isomeric forms are widely used in polymer, plastic, and synthetic fibres production and have been considered as alternatives in many literatures [3–7]. At present, 1,4-BDO has higher market share than 2,3-BDO due to different production costs. Owing to its fossil nature, however, BDO market has witnessed a global shift towards the production of bio-BDO. Among all four BDO isomers (1,4-, 2,3-, 1,3-, 1,2-), 2,3-BDO is the only naturally occurring BDO, produced by bacteria during their fermentative metabolic pathway [8]. Recent studies on bio-BDO demonstrated its promising green production over petro-BDO production and considered as a low carbon economy future [9–11]. The commercial production of bio-BDO has been gaining much attention to fulfil the BDO needs in the potential market segments, mainly 1,3 butadiene and methyl ethyl ketone production [6]. The commercialized process for bio-BDO production applies the first generation feedstock (e.g., cane sugar) and

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engineered strain for direct 1,4-BDO production via fermentation [7,12], but the transition of petro-BDO to bio-BDO has involved specific challenges and bottlenecks in its economic and technological developments. The integrated platform including metabolic and process engineering, microbial strain construction, and high-throughput screening have posed critical concerns on production costs, process sustainability, and the well-known "food versus fuel" competition [1,12,13]. Hence, another paradigm for bio-BDO production is introduced to synthesize biochemicals from lignocellulosic biomass (the second-generation feedstock) [14].

Palm oil is the most cultivated crop in tropical countries, contributing 88% (67.3 million metric tons) of global oil production (76.4 million metric tons) (USDA, 2021). Almost 1.1 metric tons of empty fruit bunches (EFB) are produced as a side stream per ton of oil produced [15], estimated to reach 84 million metric tons EFB generation annually. The enormous palm oil plantations are linked closely with environmental and social concerns, due to deforestation and biodiversity loss, which have become emerging issues for sustainable development [16]. While balancing developing economies and global warming are equally important, a tentative solution has been proposed by 'The Roundtable of Sustainable Palm Oil (RSPO)' to ensure the sustainable production of oil palm products on dedicated land without any increase in deforestation [17]. To this end, EFB biorefinery serves as a sustainable alternative to the oil palm industry and waste management [18,19]. EFB contains a high fraction of cellulosic (24-65%) and hemicellulosic (21-34%) sugars [15] which can serve as excellent substrates for bioconversion to BDO. In our previous studies, a novel staged- organosolv pretreatment was employed for recovering 'whole biomass sugars' from EFB biomass and resulted in high cellulose recovery for the biorefinery process and reactive lignin extraction with a high net energy gain for biofuel production [19,20].

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Considering the sustainability of modern biorefinery studies, techno-economic and socio-environmental aspects have been conducted for assessing the potential of utilizing lignocellulosic (non-food) biomass over food crops [20,21]. Most of the cited literature studied the qualitative assessment in terms of energy security, supply chain, land use, climate change, and food security [15,22,23]. However, the quantitative sustainability analysis although important to the development of the technology, has never been developed. Herein, for the first time, we report the quantifiable extent of a sustainable biorefinery in relation to food vs. fuel impacts and global warming potential by utilizing the non-food part of crops for biochemicals production.

This study aimed to examine the sustainable feasibility of EFB-to-2,3-BDO biorefinery. Organosolv-pretreatment was investigated to completely valorize the oil palm EFB for 2,3-BDO fermentation via staged- separate hydrolysis and fermentation (staged-SHF) processes. For sustainability evaluation of the proposed BDO biorefinery, numerical analysis of the energy and carbon footprint were conducted and compared with other BDO production processes (fossil-, commercial, and bio-based) using experimental data and literature sources on energy consumption and greenhouse gas (GHG) emissions of all intermediate processes. A sustainability index was developed to calculate the food (F.I.) and carbon (C.I.) indexes of BDO refinery. Throughout the proposed equations, the sustainability metrics of the biowaste studies can be analyzed, which may help in determining the magnitude of green production of biofuels and value-added chemicals in next generation biorefinery.

2. MATERIALS AND METHODS

This section contains the study design and scenario description for the petro- and bio-based BDO production. For bio-BDO production, an organosolv pretreatment method was performed,

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subsequent to 2,3-BDO fermentation. The comparative mass balance, energy consumption, carbon footprint, and sustainability index were also calculated to evaluate the sustainability of BDO production cycles.

2.1. Study design and scenario description

The process flow diagram for the BDO production via petroleum, commercial and bio-based processes is shown in **Fig. 1**. The study design included four major scenarios (Sc. I, II, III, and IV), starting from raw material consumption to intermediate products to the final product. Sc. I focuses on fossil-based 1,4-BDO production via a commercial Davy process [21]. This comprises a three-step reaction consisting of (1) butane oxidation to maleic anhydride (MAH), which undergoes (2) double-stage esterification by reacting with methanol and forms dimethyl maleate (DMM). Finally (3) hydrogenation of DMM results in 1,4-BDO production (**Fig. 1**). The whole butane/maleic anhydride process operates at high temperature (225 – 450 ^{o}C) in the presence of different catalysts *i.e.,* V_2O_5 for the butane oxidation and Cu-Cr for the hydrogenation reaction. Sc. II demonstrates the direct fermentation process for 2,3-BDO bioproduction via first generation feedstock (glucose) under aerobic conditions. The maximum 2,3-BDO yield can be obtained as 0.5 g/g using monosaccharide sugars as the sole source of energy and carbon [22]. Sc. III and IV explain the bioproduction of 2,3-BDO from second generation feedstock. In Sc. III, sulfite-pretreated (SPORL; sulfite pretreatment to overcome the recalcitrance of lignin) EFB was used for converting whole biomass sugars into 2,3-BDO. In Sc. IV, a two-stage organosolv pretreatment strategy (B40DA20; BDO followed by dilute acid pretreatment) was employed for 2,3-BDO production. The experimental data for Sc. III were obtained from our previous study [23], while

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the experiments for Sc. IV were performed during this study and are detailed in Sections 2.2 to 2.6.

[Please insert Fig.1 here]

Fig. 1. Scenario description and system boundaries of BDO production from **(I)** petrochemical; **(II)** first-generation sugars (food crops); and second-generation biomass (oil palm EFB) sugars under **(III)** sulfite-pretreated; and **(IV)** staged organosolv-pretreated biomass.

2.2. Materials and chemicals

Palm oil EFB was collected from palm oil farms in Thailand. The enzyme cellulase (Cellic® CTec2) was gifted by Novozyme China. The bacterial strain *Klebsiella pneumoniae* PM2 (MT422266) was used, which was previously isolated in our lab and reported for 2,3-BDO production from glucose, xylose and EFB biomass [23]. The chemicals and reagents used in this study were procured from Sigma Aldrich (USA) and of ACS grade.

2.3. Two-stage organosolv pretreatment of EFB (Sc. IV)

A modified two-stage organosolv pretreatment was performed using a customized rotating digester (China) according to our previous study [20]. In the first stage, 1,4-BDO (65% wt.) was used to fractionate lignin from 1 kg of EFB (1:4 solid/liquid ratio) at 170°C for 40 min. After BDO pretreatment, the reactor was allowed to cool to 50°C and then the pretreated substrate was filtered to separate the solid and spent liquid. The solid part was subjected to a second round of pretreatment with dilute acid (15 mM H_2SO_4) at a solid/liquid ratio of 1:3 for another 20 min.

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under a similar reaction temperature. After cooling, the whole slurry was milled and separated into solid and liquid portions. The aliquots (2 mL) of the pretreated substrate and spent liquors (after each stage) were drawn for determining the chemical composition according to the NREL method [24]. The B40DA20 – (BDO; 40 min., followed by dilute acid; 20 min.) pretreated washed solids and spent liquor were stored at 4°C for further use in enzymatic saccharification and fermentation experiments.

2.4. Enzymatic Hydrolysis

The pretreatment efficiency of B40DA20 pretreated substrate was evaluated via enzymatic hydrolysis. In a 500 mL flask, 2% (w/v) washed solids, 50 mM acetate buffer, and 7.5 FPU/g-cellulose enzyme were added and incubated at 50 °C, 150 rpm for 72 hours. Samples were subsequently collected after 6, 12, 24, 48 and 72 h in order to analyze the released sugar in the mixture. The substrate enzyme digestibility (S.E.D) was calculated as the concentrations of released glucose over the maximal glucose that can be produced from completely digested substrate.

2.5. 2,3-BDO Fermentation

A staged fed-batch SHF (separate hydrolysis and fermentation) was conducted for enhancing the 2,3-BDO yield under different scenarios. For Sc. II, glucose was directly added for direct fermentation. For Sc. III, fed-batch fermentation data were taken from our previous work with 87% of the maximum theoretical yield [23]. For Sc. IV, sugars were first obtained from B40DA20 pretreated EFB via enzymatic hydrolysis using 15 FPU/g Ctec2 enzyme, sodium acetate buffer (4.8 pH) with substrate (10% solid loading) and incubated at 50°C and 200 rpm for 72 h. A 10%

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(v/v) *K. pneumoniae* PM2 inoculum was seeded with 1% yeast extract and peptone into all sets of fermentations. The operational parameters were temperature 30 °C, initial pH 7, and agitation speed of 150 rpm.

For Sc. II, 100 g/L of initial pure glucose was added to start the fermentation. Then, subsequent feedings of glucose (60-70 g/L) were added when the glucose concentration was <15 g/L in the medium. For Sc. IV, a staged-SHF (fed-batch) approach was used for whole sugar fermentation according to the protocol described in Rehman et al. [23]. Briefly, the xylose obtained from the spent liquor) was fed into the SHF system at the concentration of 80 g/L as the only carbon source. Once the xylose was almost consumed, glucose solution (60-70 g/L) from hydrolyzed substrate was sequentially added for complete utilization of biomass sugars. The total sugar concentrations were maintained in all the SHF setups to reflect the exact picture of fermentation efficiency. All the experiments were run for 144 h in a duplicate manner, and samples were periodically drawn for determining the sugar consumption, 2,3-BDO, and by-product production.

2.6. Product analysis via mass balance and carbon conversion efficiency (CCE)

High performance liquid chromatography with a refractive index detector (RID; Waters, USA) was used for determining the sugar and metabolite concentrations. 2,3-BDO and organic acids were determined via Aminex HPX-87H column (Bio-Rad, USA) using 0.005 M H_2SO_4 as a mobile phase. Monomeric sugars (glucose and xylose) were analyzed via a CHO-782 Transgenomic column. The flow rate was 0.6 mL/min. at 65 °C operating temperature. A comparative mass balance was calculated on the basis of HPLC analysis of sugars produced/consumed and the BDO products obtained. The carbon conversion efficiency (CCE, %) was calculated by taking the ratio

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of carbon content in the products over it in the feedstock. All the experimental values presented in the data plots are mean ± standard deviation of duplicate tests performed during the study.

2.7. Fossil Energy Consumption (FEC) analysis

The total FEC was assessed by determining the related energy footprints of all the intermediate processes. For fossil-based 1,4-BDO production (Sc. I), input energies of butane oxidation, trans-esterification, and hydrogenation units were calculated according to the commercial Davy process, described in [13,21]. For bio-based 2,3-BDO from commercial sugars (Sc. II) and biomass sugars (Sc. III & IV), the consumption energy was the summation of energy inputs by pretreatment, milling, and/or product separation. The energy of pretreatment process was based on the change in enthalpy of each component of the system [25], and computed as follows:

$$E_H = \frac{1}{\eta}\left[\int_{T_0}^{T_t}\left(\sum_{i=1}^{n} m_i^{T_j}\cdot Cp_i^{T_j}\right)dT + \sum_{i=1}^{n} m_i^{T_k}\cdot L_i^{T_k}\right] \qquad \textit{(Eq. 1)}$$

where E_H is the total FEC during chemical/biological conversion (kJ); η is efficiency of the heat transfer; T_0 is the initial heating temperature (°C); T_t is the desired temperature (°C); m is total mass of the selected reagent (kg); C_p is heat capacity of the selected reagent (kJ/kg/°C); L is latent heat of the selected reagent (kJ/kg); Tj is specific temperature of the selected heating temperature (°C); Tk is boiling point of the selected reagent (°C); i is type of reagent in the mixture; and n is the total number of the reagents. All the energy consumption calculations were assumed as complete heat transfer without any heat loss due to radiation. The interaction among components was neglected to the heat capacity and latent heat as their mass ratios are very small in comparison

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to the water content of the system. The milling energy consumption was taken from [26]. Other variables such as solid to liquid ratio (S/L) and pretreatment temperature were also considered in the calculations. The distillation energy was determined based on the energy requirements of the conventional column distillation process with necessary solvent volume for high-purity product as a side stream along with a high volume of water and other by-products [27,28].

2.8. Carbon footprint analysis

Process-based carbon footprint analysis was performed to determine the environmental impact (GHG emissions) of the fossil-based and bio-based butanediol production. The functional unit was considered as 1 kg of bio/fossil- based BDO. The system boundary was defined as a 'cradle-to-gate' approach and included the quantification of all raw materials and related product (1,4-BDO/2,3-BDO) as carbon dioxide equivalents ($kgCO_2$-e/ kg-BDO). The key energy consumption shares of electricity and natural gas for fossil-based and bio-based BDO production were taken from [29]. The carbon conversion was calculated based upon the data sources available in the literature for 1,4-BDO production [13,21,29] and the experimental data and yields obtained during this study and Rehman et al.[23] for 2,3-BDO production. The GHG emissions were calculated as:

$$E = \sum_{i=1}^{n} A_i \cdot EF_i \cdot GWP_i \qquad \textit{(Eq. 2)}$$

where E is the total emissions as CO_2 equivalent (kg CO_2-e/kg of BDO produced); i is the specific GHG source; A_i is the activity of GHG i; EF_i is the emission factor of GHG i; and GWP_i is the Global Warming Potential; and n is the total type of GHG emission activities in concern.

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2.9.Sustainability index

A sustainability index was measured against the food and carbon indexes of all the four scenarios to determine their social and environmental impacts. The food index (F.I.) was determined to ensure the food security through utilization of first-generation sugars for biochemical production and calculated as follows:

$$F.I. = \frac{F_B - F_F}{F_B \cdot f_S \cdot Y_p \cdot Y_h \cdot Y_{SHF}^S} \cdot \frac{1}{Y_{SHF}^F} \qquad \textit{(Eq. 3)}$$

where F_B is the fraction of biomass from the crop; F_F is the fraction of food produced from the crop; Y_{SHF}^F is the fermentation yield on the hydrolysed food; f_S is the fraction of sugar in the biomass; Y_P is the pretreatment yield; Y_h is the sugar yield obtained after enzymatic hydrolysis of the pretreated biomass; and Y_{SHF}^S is the fermentation yield on the hydrolysed biomass substrate.

The carbon index (C.I.) was used as a measure of GHG emissions (CO_2-e) for determining the GHG impact of various BDO production from their related processes, and it was calculated as:

$$C.I. = \frac{\text{Net Carbon}}{\text{BDO producted}} = \frac{C_B - E}{Y_P^{BDO} + Y_B^{BDO}} \qquad \textit{(Eq.4)}$$

where C_B is carbon content in biomass that has been converted into final products (i.e., 2,3-BDO and lignin); Y_P^{BDO} is the yield of BDO produced from petro-chemical; and Y_B^{BDO} is the yield of BDO produced from biomass.

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The three separate fermentation yields were taken for the bio- BDO production from the first- and second-generation feedstock, whereas the yields for the commercial Davy process were accounted for 32-45% of the petro-BDO production from the butane/maleic anhydride process [30]. Overall, the sustainability index was calculated through the summation of food (F.I.) and carbon indexes (C.I.) to obtain the sustainable number of producing biofuels and biochemicals.

3. Results and discussion

To assess the prospective advantages of the 2,3-BDO biorefinery from oil palm EFB, the following sections present the methodological comparison of the scenarios relative to their experimental findings and key data outputs. The chemical composition of the two-stage-organosolv-pretreated (B40DA20) EFB was determined to check the pretreatment efficiency and subsequent enzymatic hydrolysis for 2,3-BDO production. The critical assessment was presented by comparing the B40DA20- BDO biorefinery with that of sulfite- BDO biorefinery, commercial, and fossil-based BDO production. The mass balance, overall fossil energy requirement, GHG emission, food, and carbon benefits of all four scenarios are also provided for a detailed sustainability picture of the BDO production processes to be presented.

3.1. Effect of two-stage organosolv pretreatment (Sc. IV)

The chemical compositions of the raw and B40DA20-pretreated EFB biomass in comparison with the sulfite-pretreated EFB are shown in **Fig.2**. The extractive-free raw EFB cell wall was composed of 36.09% cellulose, 25.85% hemicellulose, and 23.39% lignin. After the first stage (B40) of the organosolv pretreatment, cellulose recovery was negligible, while 22.5% of

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hemicellulose and 15% of lignin were solubilized in the solvent. Thereafter, dilute acid (DA20) pretreatment in the second stage enhanced the cell wall fractionation. Around 89% of the cellulose was recovered in the pretreated solids. High removal of hemicellulose and lignin structure (77.6% and 61.4%, respectively) was observed in this stage as the result of optimal acid charge (15 mM), which impeded lignin condensation [10]. In our previous study on one stage acid-catalyzed organosolv pretreatment, the formation of condensed lignin was observed which reduced the substrate digestibility, whereas in two-stage (B40DA20) pretreatment, the condensation effects were minimized due to lower lignin acidolysis and preservation of lignin carbocation by the solvent [19]. This might be the reason for the high digestibility of the substrate (discussed in Section 3.2).

[Please insert Fig.2 here]

Fig. 2. Chemical composition analysis of **(a)** the raw and staged pretreated (B40DA20) EFB (Sc. IV). For comparison, Sc. III was also described as sulfite- pretreated EFB; and **(b)** Substrate enzyme digestibility (S.E.D) of the respective pretreated substrates.

In contrast, the sulfite-pretreatment removed 72% of hemicellulose and 52% of lignin [23]. Studies suggest that partial delignification resulted in lignosulfonate formation which might serve as a surfactant and facilitate substrate digestion [25,31]. Therefore, sulfite pretreatment was selected as a fair comparison to staged-organosolv pretreatment. The increased cellulose and hemicellulose yield along with the high-quality lignin fractionation/ lignosulfonate formation may offer the dual benefits of the pretreatment process in the circular biorefinery.

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3.2. Enzymatic hydrolysis

To further evaluate the staged-pretreatment efficiency, the substrate enzyme digestibility (S.E.D) is presented in **Fig. 2 (b)**. By using B40DA20- pretreated EFB, almost 85% of the cellulose was converted into monomeric sugars within the first 24 hours of the reaction. The cellulose conversion reached 88% after 72 h. Similarly, 98.6% of S.E.D. (72h) was measured by sulfite-pretreated EFB [23]. These results revealed that cellulose accessibility was quite high due to the high hemicellulose removal and delignification. The higher S.E.D also reflected the low affinity of lignin adsorption (due to reactive lignin/ lignosulfonation) at the active sites of enzymes, leading to improved lignocellulosic saccharification [19,32].

3.3. 2,3-BDO production via staged fed-batch SHF

2,3-BDO bioproduction was quantified under different scenarios (II, III, and IV) using *K. pneumoniae* PM2, isolated in our previous study [23]. Sc. II depicted the utilization of pure glucose via fed-batch SHF. The fermentation profile for Sc. III by staged-fed batch SHF using sulfite-pretreated EFB was taken from [23]. Sc. IV showed the 2,3-BDO production from B40DA20-pretreated EFB via staged fed-batch SHF. The results in **Fig. 3a** show that the cells rapidly consumed ~60% of glucose in the first 24 h of cultivation, yielding 30 ± 0.32 g/L of 2,3-BDO concentration at the rate of 1.25 g/L/h. After glucose feedings, the production rate was steadily increased to 1.7 ± 0.29 g/L/h and 85.9 ± 1.05 g/L 2,3-BDO titer was achieved after 86 h with 0.48 g/g yield. Afterwards, the glucose consumption as well as 2,3-BDO productivity decreased along with the declining growth rate of strain PM2. Consequently, other by-products, mainly acetoin, drastically increased and reached 18 ± 0.51 g/L by the end of fermentation.

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In the case of EFB biomass for Sc. III and IV, staged SHF (fed-batch) was performed. As a sole carbon source, xylose from spent liquor (80 g/L) was added into the system. As *K. pneumoniae* PM2 is a xylose-consuming strain, it quickly assimilated the pentose sugar at the rate of 0.83 ± 0.63 g/L/h and 2,3-BDO production reached >33 g/L from sulfite- and B40DA20- pretreatment liquor, respectively **(Fig. 3b**). At the second stage, EFB hydrolyzed glucose was added to the system for the purpose of whole sugar fermentation. The maximum 2,3-BDO produced from these processes were 75.03 ± 1.32 [23] and 77.29 ± 1.63 g/L with an overall yield of 86% and 91% of the maximum theoretical value for Sc. III and IV, respectively. Because 2,3-BDO production depends on cell growth factor, higher concentrations are observed in the late stationary period of cell growth [33]. The sugar consumption was reduced toa steady rate of 0.6 g/L and other by-products (*i.e.*, acetoin and organic acids) had slightly increased by the end of cultivation, indicating the diversion of metabolic route towards mixed-acid fermentation [34]. By comparing III and IV results, an increment of 5.5 % yield from B40DA20 substrate was observed which might be due to the high solubilization of xylose in the spent liquor. Studies on sulfite pretreatment reported that the liquor contains many fermentation inhibitors such as acetic acid, HMF and furfural, which might delay the xylose consumption, thereby reducing the fermentation efficiency [25,35], whereas organosolv pretreatment was found to be more promising due to less inhibitor formation and enhanced overall fermentation yield and productivity [36,37].

[Please insert Fig.3 here]

Fig. 3. Fed-batch SHF profile for **(a)** Sc. II using pure glucose as the sole substrate; and staged-fed batch SHF profile for **(b)** Sc. IV using staged organosolv-pretreated oil palm EFB. The data

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plots are the average of independent sets of experiment with ±S.D. as the error bars (Note: data used in Sc. III using sulfite-pretreated substrate has been reported elsewhere [23]).

Results obtained from both scenarios (Sc. III and IV) revealed that utilization of EFB sugars can be a suitable alternative for 2,3-BDO bioproduction as compared with the direct fermentation using glucose. This in turn also favors resource recovery and somewhat ends the food-feed-fuel debate by managing the utilization of biomass in an economical and sustainable way [1,12,13].

3.4. Mass balance of the bio-BDO production processes

The mass balance of the first-generation and second-generation 2,3-BDO biorefinery was calculated for determining the total production capacity of the different scenarios for 2,3-BDO production and other products (**Fig. 4**). The process flow for Sc. II was based on the total glucose added to the system and the products obtained via direct fermentation. The process yield was 96% with the highest CCE value of 64%. The CO_2 produced during the process was equivalent to the amount of 2,3-BDO produced (**Fig. 4a**). For Sc. III and IV, the calculations were dependent on the sugars obtained after EFB pretreatment. Since the hemicellulose dissolution in Sc. IV was superior to Sc. III, it reflected more carbon conversion from xylose to 2,3-BDO. The 2,3-BDO yield and CCE were 86% & 91%, and 57.3% & 60% for Sc. III and IV, respectively **(Fig. 4b and c)**. The calculated 2,3-BDO productions in terms of mass balance were 430, 175.5, and 247 g from 1 kg of pure sugars, sulfite-pretreated, and organosolv-pretreated EFB biomass substrate, respectively. Among by-products, CO_2 was the major contributor to capture carbon content from the substrate, which was followed by acetoin (2,3-BDO precursor) and other organic acid production during mixed-acid fermentation.

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[Please insert Fig.4 here]

Fig. 4. Mass balance of the 2,3-BDO fermentation from **(a)** Sc. II, **(b)** Sc. III, and **(c)** Sc. IV. The values in brackets are counted as 'grams' of the substrates and corresponding products.

Besides biomass sugars, approximately 126 g of lignosulfonate (from Sc. III) and 144 g of high-quality lignin (from Sc. IV) could be procured from the pretreatment liquor, and these are the valuable industrial chemicals [20,31]. Specifically, the lignin from B40DA20 pretreatment is considered as non-condensed and highly reactive for the production of other value-added compounds [19], hence adding benefits to the carbon flow towards the sustainability of the pretreatment process.

3.5. Fossil energy consumption (FEC)

The net FEC of the processes was determined based on the enthalpy of all system factors. As shown in **Fig. 5a**, the cumulative energy consumption (based on the final BDO yield) of solely bio-2,3-BDO production processes was lower than the petro-1,4-BDO production [21]. The highest FEC of Sc. I was calculated as 87.27 MJ/kg, in which natural gas (25.6%) and product distillation energy (58.6%) were the predominant contributors. The reduction of 41.4% was observed when first generation sugar (Sc. II) was used for bio-BDO production. While in the case of bio-BDO production from second-generation sugars (Sc. III and IV), the reduction was about 27.5% and 15.5% for FEC as compared to the petro-BDO production from fossil-derived chemicals. In Sc. IV, the energy consumed during B40DA20- EFB pretreatment was much higher

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than the sulfite-EFB pretreatment, which was obvious in the two-stage strategy followed in Sc. IV. Consumption of other inputs such as natural gas, electricity, and milling contributed about 5% to life-cycle FEC. The energy input of key materials is also tabulated in **Table S1**. The top energy consumer (58-66%) was the conventional distillation process among all the scenarios. It can be reduced by using hybrid energy-efficient distillation units for separating the BDO stream from other chemicals, present in the chemical plant/ fermentation broth [27,28]. In a study by Adom et al., two different configurations for 1,4-BDO separation were compared. They reported that moisture removal prior to product separation might have reduced >80% of the FEC consumption with the high yield product baseline [29]. The results suggested that the product yield integrated with the energy-efficient process design can affect the FEC reduction of BDO production.

[Please insert Fig.5 here]

Fig. 5. (a) Fossil energy consumption (FEC) as MJ/kg of the BDO produced; and **(b)** greenhouse gas (GHG) emissions as kgCO_2-e/kg-BDO for all four scenarios of BDO production.

3.6. Greenhouse gas (GHG) emissions

Carbon footprint analysis from bio-BDO was conducted to determine the sustainability of the processes in comparison to the fossil-derived counterpart. **Fig. 5b** revealed that GHG emissions from petro-BDO was 43.3% higher than the commercial bio-BDO production using first generation feedstock. While the lignocellulosic biorefinery products counted as carbon-neutral since the related carbon is biogenic and help in reducing GHG emissions up to 90% of the fossil-based GHG emissions [38]. The remaining 10% of life- cycle GHG emissions was contributed

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from indirect GHG emissions such as electricity, natural gas and chemicals used during biomass pretreatment (**Table S2**). Another advantage of biomass utilization for bio-BDO from Sc. IV is the 'carbon benefits' obtained from the recovery of high-quality lignin which helped in mitigating 0.335 $kgCO_2$-e/kg BDO through the production of value-added compounds as a carbon sequestration tool.

A comparative analysis of the bio-BDO production lines revealed that FEC and GHG contributions of biomass sugar feedstock were about twice compared to that of the pure sugar feedstock. This might be due to the high- yield BDO from Sc. I as compared to the biomass conversion ratios. Another major factor was the high pretreatment energy inputs and related carbon emissions, which also affect the GHG emissions from the process. Biorefineries play a positive role in energy and GHG emissions savings over conventional BDO production, as half of the energy can be recovered by utilizing the residual biomass (lignin, unconverted sugars, etc.) for generating in-house electricity and easier solvent recovery for pretreatment plants, thereby aiming for more carbon neutrality [29].

3.7. Sustainability index of the BDO production

A sustainability index was used to develop the food vs. fuel index to quantify the relationship between biorefinery and the crop industry. The food and carbon indices were calculated related to 1 kg of petro-/bio-based BDO production. **Fig. 6** shows a positive sustainability shift for changing petro-BDO (-4.2 for Sc. I) to second-generation bio-BDO (+9.6 for Sc. III; +7.3 for Sc. IV), whereas the low index value of first-generation bio-BDO (+1.6 for Sc. II) clearly demonstrated the food security burden on the first-generation biorefinery, though the process has some carbon benefits over petro-based BDO production due to the carbon sequestration during the food crop

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plantation. In addition, the fuel produced from the EFB biomass will not only provide a high-demand food (palm oil), but also high-quality lignin obtained from staged-organosolv (Sc. IV) will facilitate the additional carbon benefits for the system.

Utilization of second-generation feedstock is proposed as a sustainable approach with carbon-negative BDO biorefinery. To support, the developed equations were used to calculate the food and carbon benefit indexes for some other published studies on 2,3-BDO production from non-food biomass. **Table 1** shows that efficient valorization of agro-industrial biowaste, such as wheat straw [39], corn cob [40], soy hull [41], wood [42], and sugarcane bagasse [43] for value-added BDO production can help in sequestering carbon without compromising the food security. Nonetheless, uncertainty of the bio-BDO output is highly linked to the feedstock cultivation, material and energy prices, input of any additional heat during lignocellulosic feedstock bioconversion (pretreatment/hydrolysis), and combustion of unconverted biomass solids in a biorefinery plant, which may affect the overall 2,3-BDO recovery efficiency via fermentation [13]. As the second and third generation bioconversion technologies are gaining attention, it is imperative to consider the availability of natural resources to fulfill the ever-increasing energy needs. Therefore, a sustainability index is important to direct the sustainability issues associated with the depletion of food resources and loss of biodiversity and biosecurity [13,16]. By considering these critical impacts, integrated approaches in the bio-market dynamics may help addressing the social and sustainable needs of strengthening the life- cycle of biorefineries in terms of economic and environmental sustainability.

[Please insert Fig.6 here]

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Fig. 6. Sustainability index of the petro-BDO and three bio-BDO production processes as the function of food index (F.I) and carbon index (C.I.).

4. Conclusion

This study elaborated the four processes of BDO production among fossil-, commercial-, and two bio-based pathways. The staged organosolv-pretreatment was demonstrated to be an efficient strategy for oil palm biomass bioconversion, and this approach has become more sustainable through integrating the staged fed-batch fermentation product into the pretreatment process. The energy and carbon footprint analyses indicate that the integrated biorefinery process can result into a carbon benefit from -4.20 $kgCO_2$-e to 6.80 $kgCO_2$-e per kg-BDO produced, in comparison with petroleum refinery. The food vs. fuel index demonstrates that the transition from first generation biorefinery to second-generation bio-BDO may shift the sustainability index from -1.04 to +0.45. Further improvements to reduce the carbon footprint and energy consumption may be achieved by process optimization and recyclability of renewable materials. This approach may also offer a cost-effective, energy-efficient integrated biorefinery system, thereby strengthening the bio-based economy and environmental sustainability of the palm oil industry and lignocellulosic biorefinery.

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

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Nomenclature and units

2,3-BDO	2,3-Butanediol
1,4-BDO	1,4-Butanediol
EFB	Empty fruit bunches
MMT	Million metric tons
FEC	Fossil Energy consumption
GHGs	Greenhouse gases
kg CO2-e	Kilogram carbon dioxide equivalent
Staged-SHF	Staged separate hydrolysis and fermentation
SPORL	Sulfite pretreatment to overcome the recalcitrance of lignin
CCE	Carbon conversion efficiency
F.I.	Food index
C.I.	Carbon index
qCO_2	Specific CO_2 emission ($kgCO_2$-e/MJ)

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Figure Captions

Fig. 1. Scenario description and system boundaries of BDO production from **(I)** petrochemical; **(II)** first-generation sugars (food crops); and second-generation biomass (oil palm EFB) sugars under **(III)** sulfite-pretreated; and **(IV)** staged organosolv-pretreated biomass.

Fig. 2. Chemical composition analysis of **(a)** the raw and staged pretreated (B40DA20) EFB (Sc. IV). For comparison, Sc. III is also described as sulfite- pretreated EFB; and **(b)** Substrate enzyme digestibility (S.E.D) of the respective pretreated substrates.

Fig. 3. Fed-batch SHF profile for **(a)** Sc. II using pure glucose as the sole substrate; and staged-fed batch SHF profile for **(b)** Sc. IV using staged organosolv-pretreated oil palm EFB. The data plots are the average of independent sets of experiment with ±S.D. as the error bars (Note: data used in Sc. III using sulfite-pretreated substrate has been reported elsewhere [26]).

Fig. 4. The mass balance of the 2,3-BDO fermentation from Sc. II, III and IV. All the proportions are counted as 'gram' weight of the substrates and corresponding products.

Fig. 5. (a) Fossil energy consumption (FEC) as MJ/kg of the BDO produced; and **(b)** greenhouse gas (GHG) emissions as kgCO_2-e/kg-BDO for all four scenarios of BDO production.

Fig. 6. Sustainability index of the petro-BDO and three bio-BDO production processes as the function of food index (F.I.) and carbon index (C.I.).

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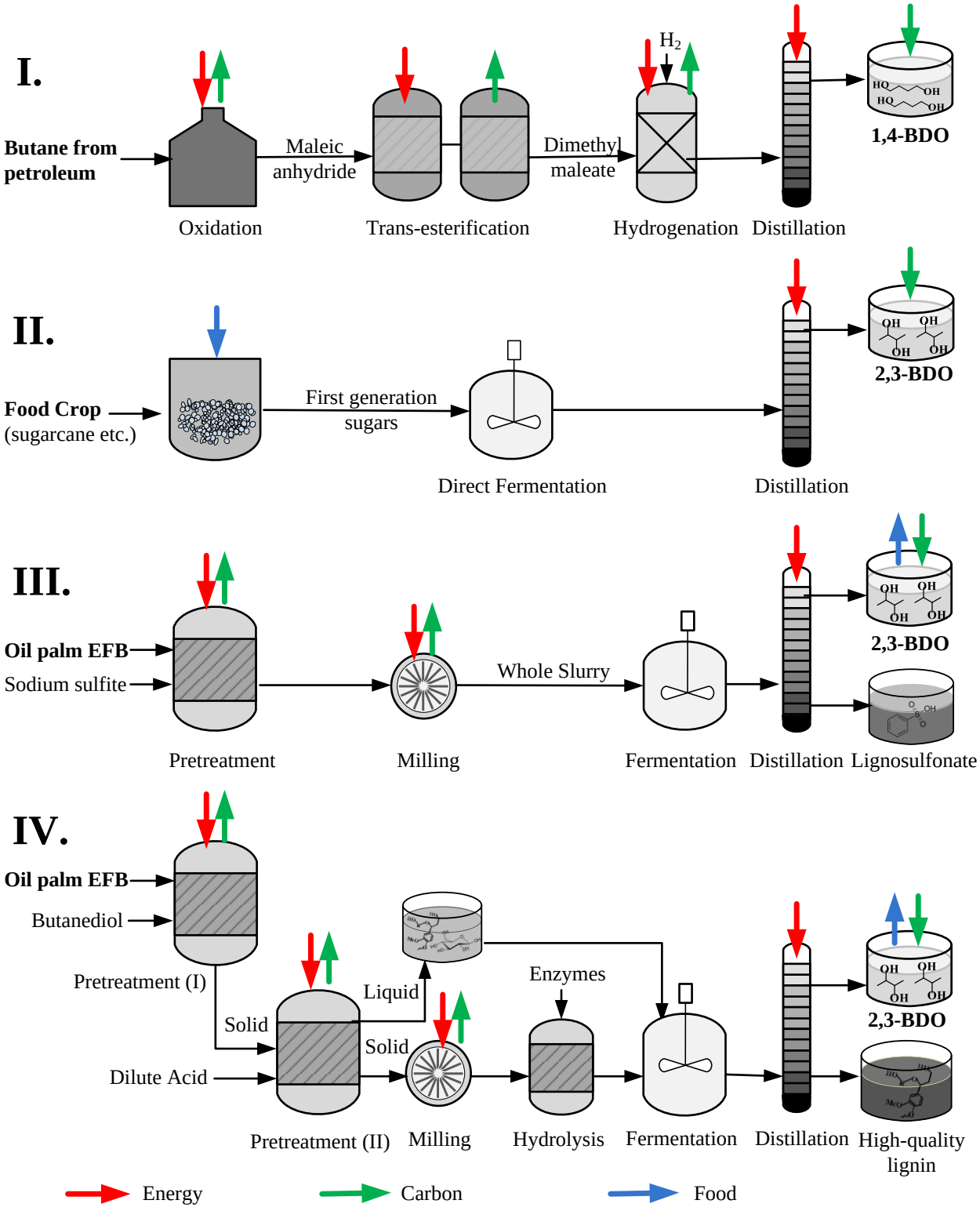

Fig. 1

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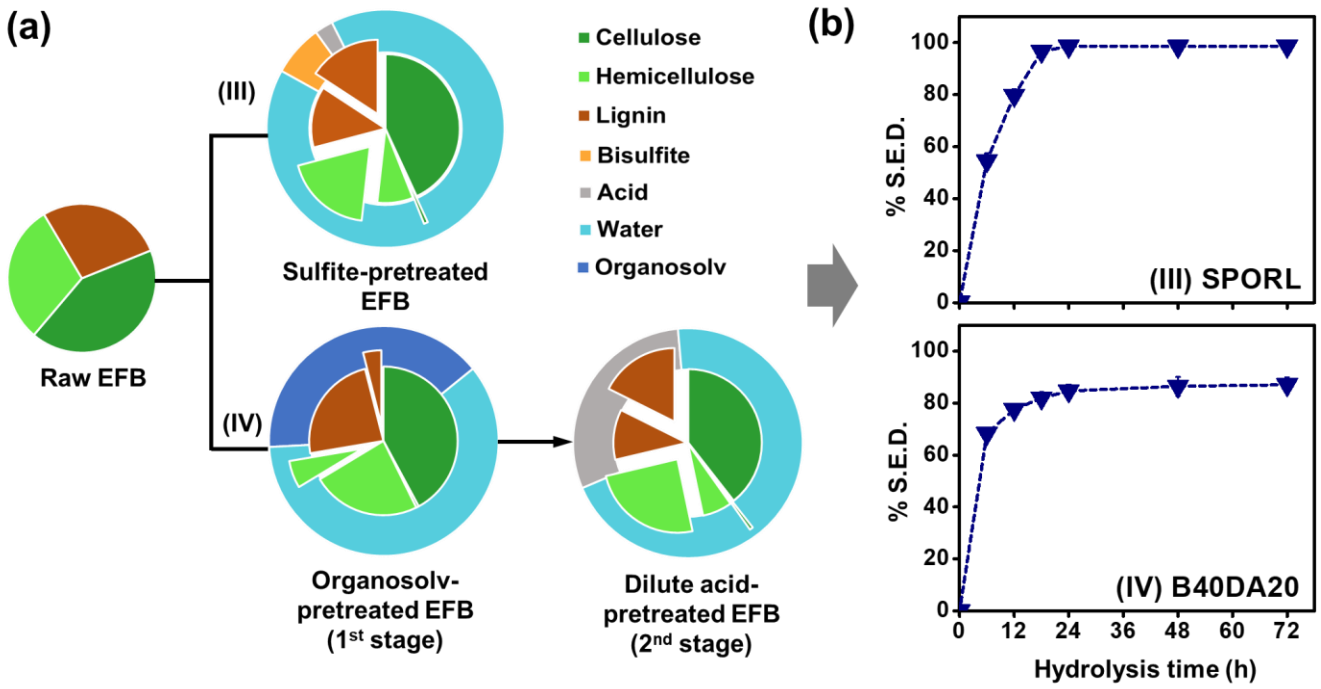

Fig. 2

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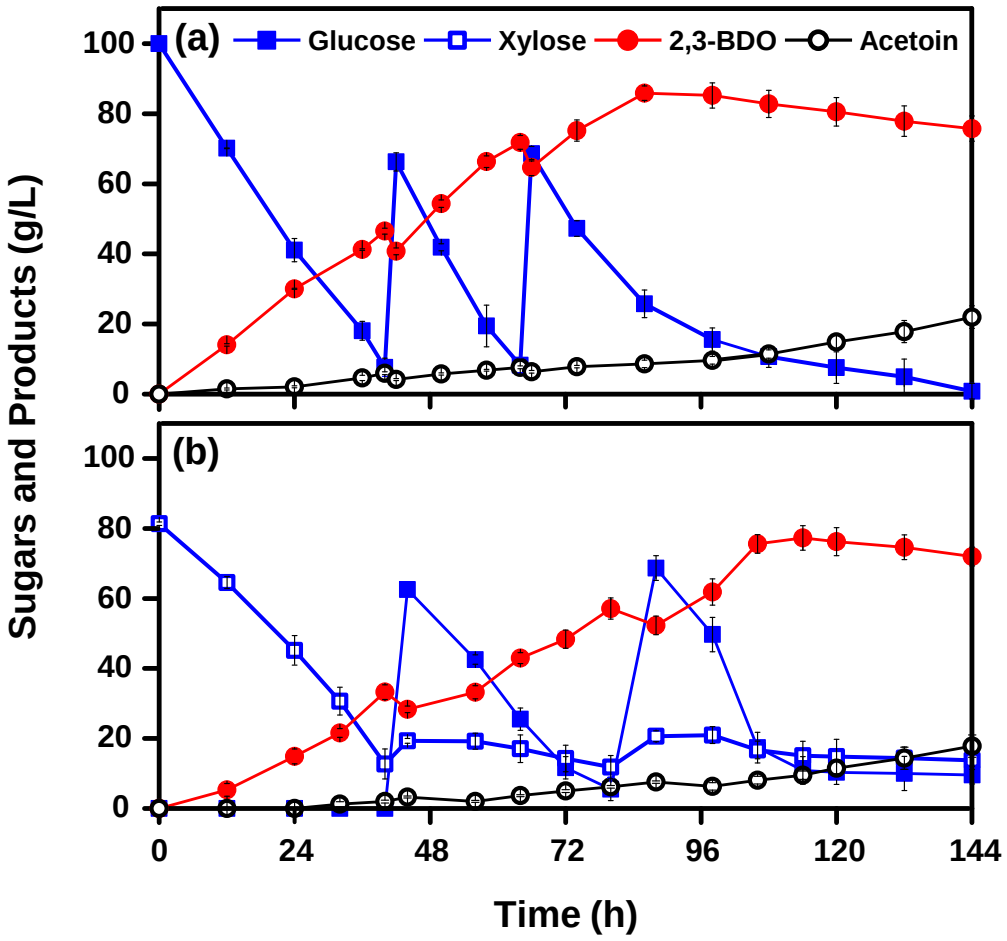

Fig. 3

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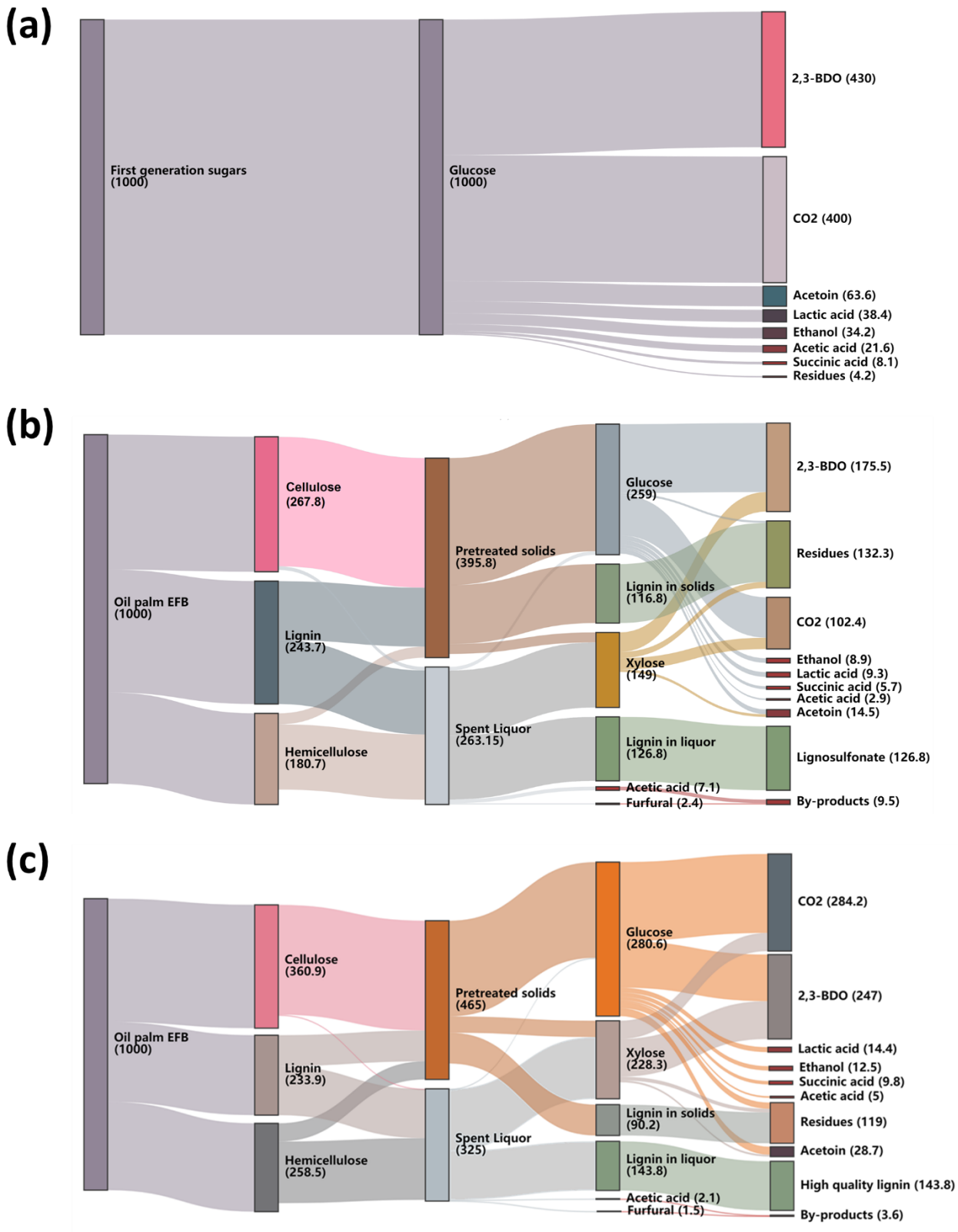

Fig. 4

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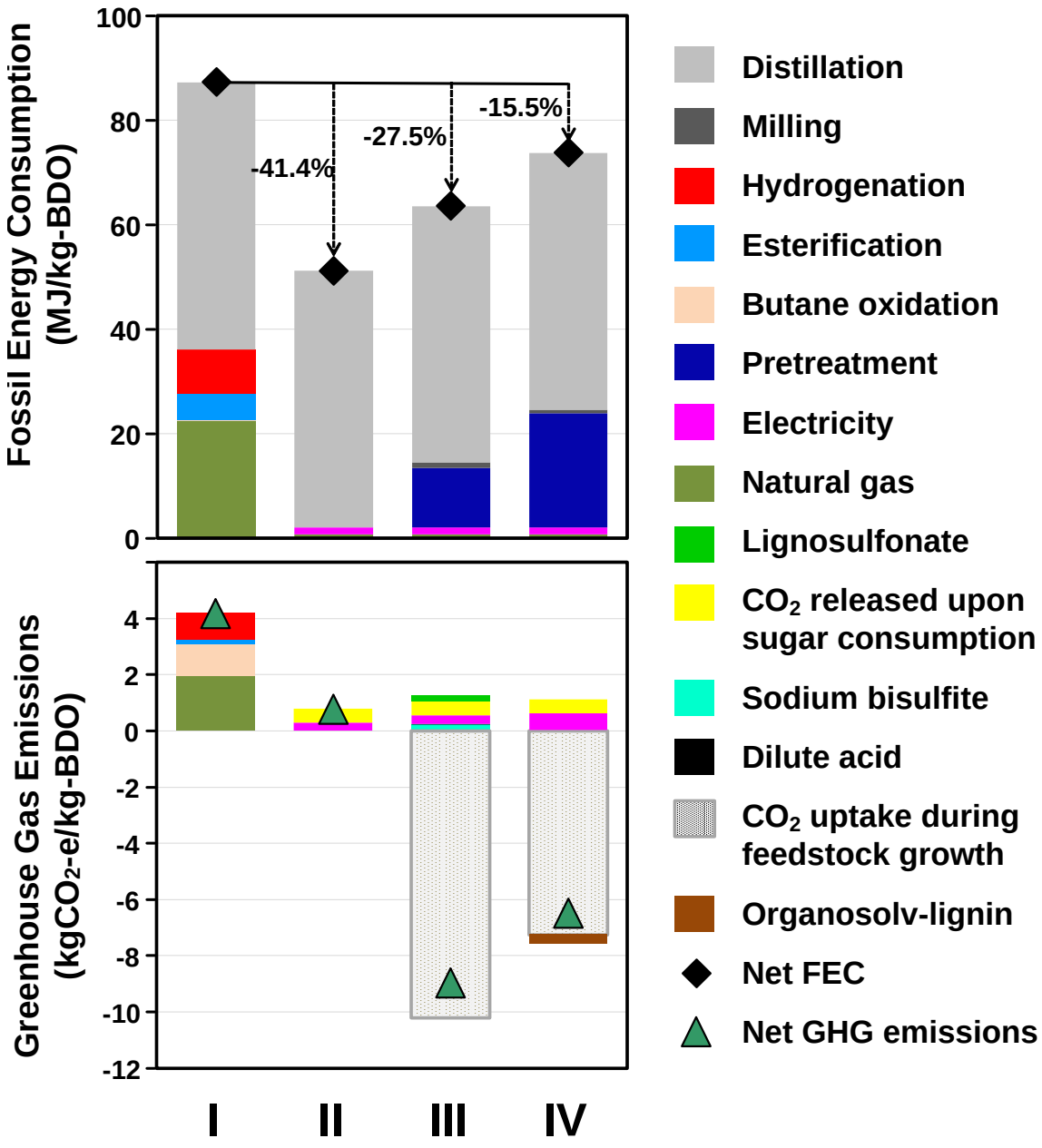

Fig. 5

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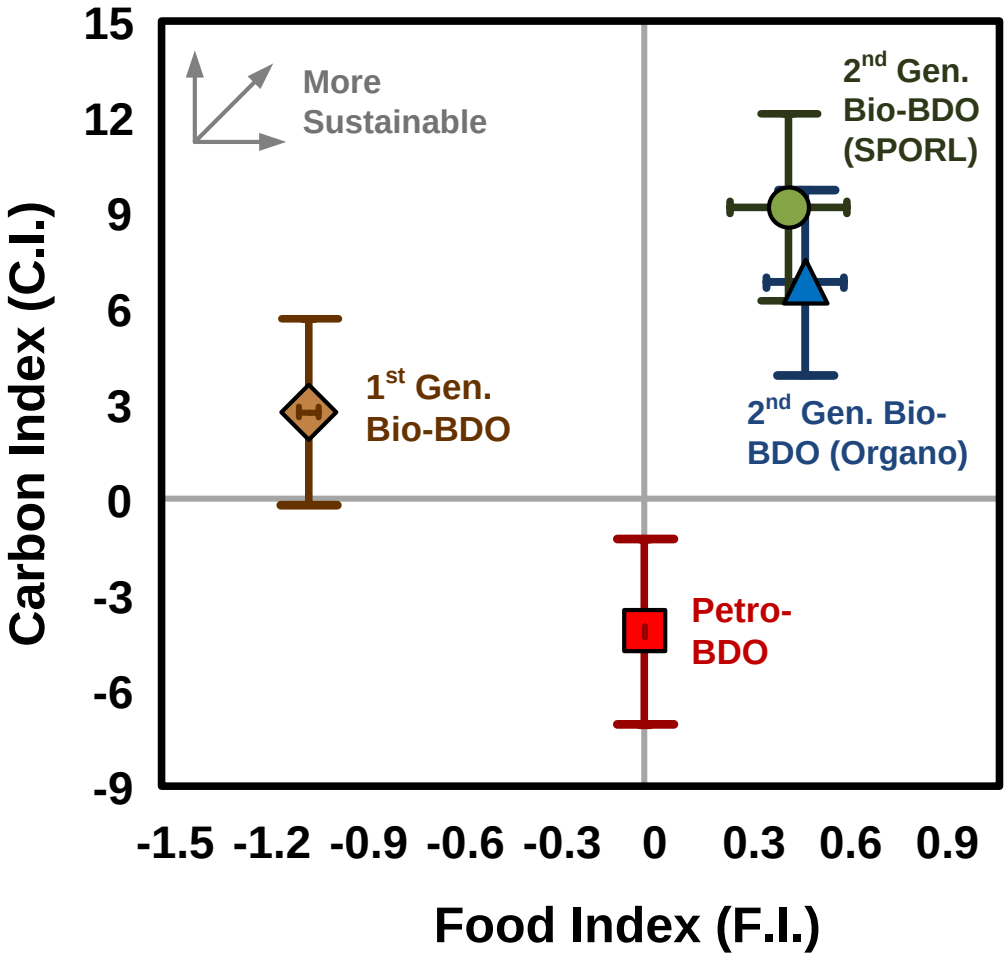

Fig. 6

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Table 1. Comparison of sustainability index of 2,3-BDO production with other studies.

Feedstock	Yield (g/g)	Productivity (g/L/h)	Titer (g/L)	Strain	Data Source	Sustainability Index	
						Food index	Carbon index
Wheat straw	0.33	0.45	32.5	*Paenibacillus polymyxa* DSM 365	[1]	0.516	6.316
Soybean hull	0.44	0.55	20.5	*Pantoea agglomerans*	[2]	0.467	8.409
Corn cob	0.5	0.59	35.7	*Klebsiella oxytoca ACCC 10370*	[3]	0.494	5.520
Sugarcane bagasse	0.39	0.29	21	*Enterobacter aerogenes* EMY-22-galP	[4]	0.617	6.789
Wood	0.29	0.27	13.3	*Klebsiella pneumoniae*	[5]	0.243	8.894
Oil palm EFB	0.45	0.72	77.3	*Klebsiella pneumoniae* PM2	This study	0.497	6.799

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