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Adaptable downstream processing design for recovery of butanediols after fermentation

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ABSTRACT

The butanediols (BDOs), 2,3-, 1,4- and 1,3-butanediol, are platform chemicals that are mainly produced from fossil hydrocarbons but may be obtained through fermentation. However, low product concentration, by-product formation and high boiling temperatures of BDOs hinder downstream processing and increase overall fermentation costs. This study increases the competitiveness of industrial biotechnology by designing a large-scale process (broth processing capacity of 160 ktonne/y) for the final purification of BDOs after fermentation (recovery >99 %). It includes an initial preconcentration step in a vacuum distillation column to remove most water and light impurities. The initial removal of most of the water and the use of a heat pump system allowed significant energy reduction. At the heart of the process is an integrated dividing-wall column that can efficiently purify BDO from the remaining light and heavy impurities. Moreover, a single process design was proven effective in purifying different BDOs to > 99.4 wt%. This was cost-effective (total purification costs of 0.208 – 0.243 $/kg_{BDO}$) and energy-efficient (with primary energy requirements of 1.854 – 2.176 $kW_{th}h/kg_{BDO}$). The proposed purification sequence can be used for each BDO type, which offers flexibility in developing sustainable bioprocesses for BDO production.

1. Introduction

Despite the depletion of fossil resources, strict environmental regulations and concerns about energy security, many platform chemicals are predominantly produced via petrochemical routes. However, uncertainties related to the fossil fuel-based production drive interest in developing sustainable production processes. In that respect, fermentation presents a promising alternative for producing many biochemicals and biofuels (e.g. ethanol, isopropanol, butanol, 1,3-propanediol, butanediols, etc.). Among the perspective bioproducts that may be obtained through the fermentation process, butanediols (BDOs) are important platform chemicals with a wide variety of applications (Xiu and Zeng, 2008).

2,3-Butanediol (2,3-BDO) can be used as an intermediate for producing fuels, jet, diesel, high-octane gasoline, synthetic rubbers (Harvey et al., 2016), solvents (e.g. methylethylketone (MEK) (Sacia et al., 2015; Song et al., 2017)), drugs, cosmetics, lotions, softening agents, plasticizers, printing inks, fertilizers, etc. (Białkowska, 2016), with a global market estimated to be 270 million $ in 2022 and an expected growth rate of 3.5 % until 2031 (TransparencyMarketResearch, 2022a). Fermentative production of 2,3-BDO has recently been gaining attention due to higher productivity and lower toxicity compared to commonly produced monohydric alcohols (Haider et al., 2018b). LanzaTech, National Renewable Energy Laboratory (NREL) and BioPrincipia are some of the leaders in developing the production of 2,3-BDO from renewable sources (Köpke et al., 2011; NREL, 2022; Simpson, 2017)

1,4-Butanediol (1,4-BDO) is an important platform chemical commonly used as a solvent and for producing polyesters, polyurethanes, plastic fibers and pharmaceuticals (Satam et al., 2019). Its global market was estimated to be about 6.5 billion $ in 2022, with an expected growth rate of 9.4 % until 2032 (TransparencyMarketResearch, 2022b). Conventionally, 1,4-BDO is produced through the Reppe process (Luo and Li, 2021). Additionally, several different routes for 1,4-BDO production were developed: from 1,3-butadiene (Mitsubishi chemicals and Toyo Soda), propylene oxide (Lyondell) and butane (Davy Process Technology and BP). However, the Reppe process is dominant due to high yields and few steps (Satam et al., 2019). In addition to the fossil fuel-based processes, research attempts were made to produce 1,4-BDO by genetically engineered microorganisms (Burk et al., 2009). Genomatica and Novamont are leading the

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commercialization of sustainable 1,4-BDO production (Genomatica, 2016a, 2016b).

1,3-Butanediol (1,3-BDO) is also a commodity chemical commonly used as a solvent for food flavoring agents, as a hypoglycemic agent, in the production of polyester and polyurethane resins, biologically active compounds and liquid crystals, synthetic rubbers, resins and latex (Burgard et al., 2015). The global 1,3-BDO market was estimated to be 188.2 million $ in 2023, with a projected growth rate of 3.7 % (VerifiedMarketReports, 2024). Traditionally, 1,3-BDO is produced from acetylene or ethylene. Alternatively, 1,3-BDO can be obtained by microorganisms as patented by Genomatica (Burgard et al., 2015).

1,2-Butanediol (1,2-BDO) is used to synthesize polyester polyols, plasticizers, cosmetics and pharmaceuticals (Qin et al., 2024). Currently, it is dominantly produced from fossil-based n-butene via epoxidation and hydration reactions (Zhang et al., 2023). Alternatively, biomass may be used as a renewable feedstock for producing 1,2-BDO. However, the reported yields of converting biomass-derived substrates to 1,2-BDO have been low, while reaction pathways and catalytic mechanisms remain unclear (Zhang et al., 2023). Furthermore, the development of bioprocesses for direct production of 1,2-BDO has become a recent topic of interest. However, the obtained product concentrations are still relatively low (e.g. 0.15 g/L was obtained using genetically engineered Escherichia coli (Qin et al., 2024)) and additional improvements are needed to allow scaling up of this technology.

A significant research effort has been put into developing genetically engineered microorganisms that can produce different BDOs from renewable sources. Thus, fermentation of renewable carbon sources has an important potential to become a sustainable alternative to fossil hydrocarbon-based processes for the production of BDOs (Forte et al., 2016). Yet, the recovery of different BDOs after fermentation has not been as promptly addressed as the fermentation process. Therefore, the main goal of this study is to enhance the development of sustainable and competitive BDOs' fermentation processes by advancing downstream processing. In that respect, we propose a novel large-scale (broth processing capacity of about 160 ktonne/y) downstream processing design that may be easily adapted for the final purification of 2,3-, 1,4- or 1, 3-BDO after fermentation. The recovery of 1,2-BDO has not been included in the analysis due to the very low fermentation titers achieved so far. The block flow diagram of the complete bioprocess is presented in Fig. 1. As all BDOs are high-boiling fermentation products, initial filtration and ion exchange steps are required to remove biomass, biopolymers and inorganics before the final purification. Since these steps are conventionally used in industrial fermentation, they were not the focus of this work. Instead, our work focuses on the preconcentration and final purification parts of the recovery process.

2. Problem statement

Several challenges in the fermentation affect the downstream processing (e.g., low titers, presence of microorganisms, formation of by-products). Thus, the expenses of the separation process significantly contribute to the total production cost (Gawal and Subudhi, 2023). The existing studies on the recovery of BDOs after fermentation mainly focus on 2,3-BDO, while less work has been reported on the recovery of other BDOs. In that respect, various techniques have been proposed for separating high-boiling product from the fermentation broth. Solvent extraction has been limited to a small scale due to relatively low recovery and large required amounts of solvent. Similarly, salting-out extraction requires large amounts of salts and solvents, the recovery of which is energy-intensive. Salting-out (e.g. with K_2CO_3 (Afschar et al., 1993; Caballero-Sanchez et al., 2024)) requires complex pretreatment steps and significant amounts of salting-out agents (Gawal and Subudhi, 2023). Contrarily, sugaring-out extraction offers the possibility of reusing sugaring-out agents as substrates for microbes in the fermentation. However this method has resulted in lower product recoveries relative to salting-out extraction (Xie et al., 2022). Additionally, the potential toxicity of the solvent may pose a constraint when using extraction, salting-out extraction or sugaring-out extraction for product recovery. Reactive extraction with aldehydes and acidic catalysts (Koutinas et al., 2016) has the disadvantage of using mineral acids which generate a lot of waste, may cause corrosion issues and are expensive (Xie et al., 2022). Acidic anion-exchange resins have been proposed as an alternative to soluble acidic catalysts but proteins and salts from the broth decrease catalytic activity. Pervaporation has scaling-up limitations due to membrane fouling, equipment costs and process duration. Yet, all of these techniques require additional steps to obtain high-purity BDO product. Alternatively, as none of the BDOs form azeotropes with water and differences in boiling points are significant, distillation may be used for both the preconcentration and final purification. Distillation is a mature separation technology that can be easily operated on a large scale. Nonetheless, distillation implies evaporating large amounts of water which may lead to an energy-intensive process.

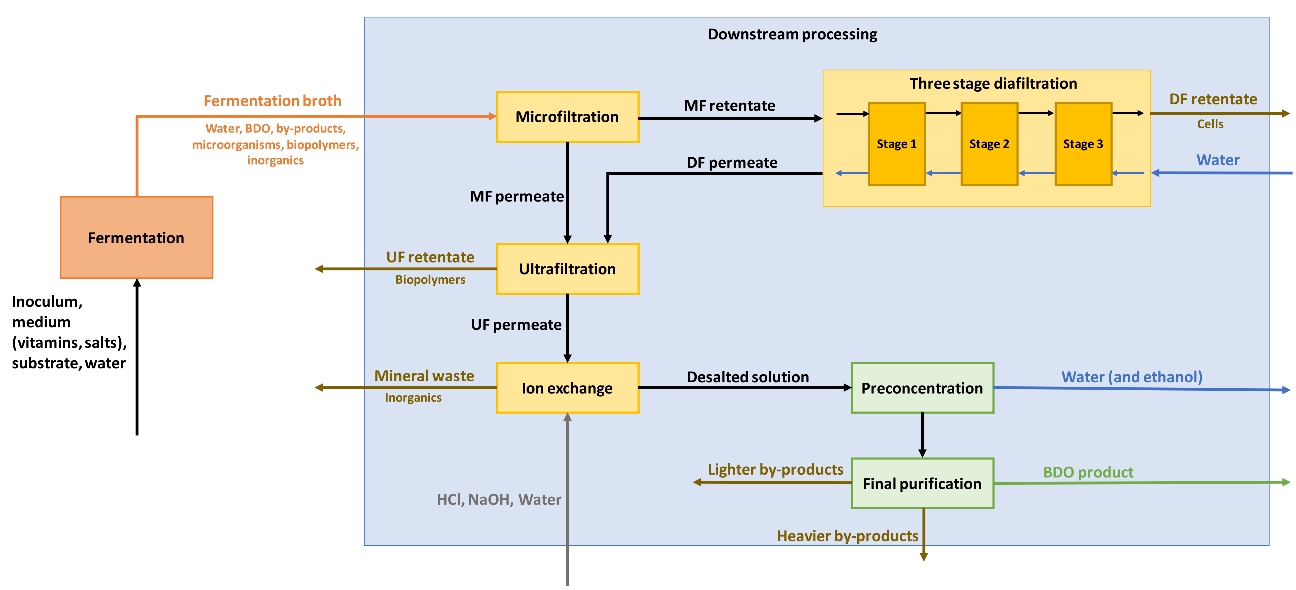

Fig. 1. Block flow diagram of the complete bioprocess (upstream and downstream), the focus of this work is on the preconcentration and final purification parts of the downstream processing.

Several distillation-based process configurations have been proposed for the final purification of BDOs (mainly 2,3-BDO) (Haider et al., 2018b; Hong et al., 2019; Van Duc Long et al., 2018). The total energy requirements for recovering 90 % of 2,3-BDO (product purity of 99.0 wt %) from fermentation broth (9.3 wt% 2,3-BDO) using these techniques are in the range of 3.2–8.6 $kW_{th}h/kg_{BDO}$. Extraction-assisted distillation processes using isobutanol, 1-butanol (Haider et al., 2018a) and oleyl alcohol (Harvianto et al., 2018) have been also studied. When these purification processes are used, about 3.1 – 6.5 $kW_{th}h/kg_{BDO}$ is needed to recover 90 % of 2,3-BDO from broth (9.3 wt% 2,3-BDO). Finally, a dividing-wall column (DWC) configuration was explored for recovering 2,3-BDO after the fermentation step. The proposed DWC design has its wall placed in the middle of the column and recovers the BDO product as a side stream. The top and bottom products from the DWC contain water with all light impurities and heavy impurities, respectively. A vapor recompression system has been proposed in which the top vapor from the DWC is compressed and used for partial evaporation of the feed stream to reduce the duty of the DWC's reboiler (Haider et al., 2020). In total, ~6.2 $kW_{th}h/kg_{BDO}$ is needed to recover 90 % of 2,3-BDO (product purity of 99 wt%) from the feed stream (9.3 wt%).

The novelty of this original study is twofold. Firstly, research on the downstream processing after the fermentation is expanded on the recovery of other BDOs besides 2,3-BDO. Additionally, the proposed advanced purification process improves cost-effectiveness and energy-efficiency of the BDOs' recovery. Process intensification principles were implemented as these were proven to significantly improve environmental impact (Vallejo-Blancas et al., 2022). The proposed final purification process consists of a heat pump-assisted preconcentration column that removes most water from the fermentation broth, and an integrated dividing-wall column (DWC) that efficiently recovers BDOs from all light and heavy impurities. Unlike the previously developed recovery processes including DWC, we propose separating most water and light impurities before DWC, using a heat pump-assisted distillation column. After this step, DWC may be used to purify BDO from the remaining light and heavy impurities. This process configuration can significantly reduce the equipment size and the thermal energy requirements of DWC because most of the water is separated in the first step. However, the preconcentration step is very energy intensive, and the use of a heat pump system is crucial for energy-efficiency. With the proper choice of operating parameters, the mechanical vapor recompression system applied to the first distillation column can drastically reduce total energy use and allow complete (green) electrification of this step.

3. Methods

3.1. Process design and simulation

Three fermentation processes were considered: case 2–3 (purification of 2,3-BDO), case 1–4 (purification of 1,4-BDO) and case 1–3 (purification of 1,3-BDO). Accordingly, compositions of the fermentation broths in these cases were taken from the published literature (Baldassarre et al., 2020; Haider et al., 2018b; Satam et al., 2019) and presented in Table 1. In all cases, the concentration of BDO is about 7 – 9 wt% while water makes most of the broth (87 – 91 wt%). Additionally, both light (ethanol, formic acid, acetic acid, 3-hydroxy-2-butanone (3-HB), 4-hydroxy-2-butanone (4-HB) and gamma butyrolactone (GBL)) and heavy by-products (lactic acid, succinic acid, 2-(4-hydroxybutoxy)-THF (HTHF), 2-pyrrolidone (PYR) and glucose) are present in this stream. To allow a fair comparison with the published literature and between different cases in this study, a feed flowrate of 20,000 kg/h was assumed in all cases, and it is assumed that prior steps for removing cells, biopolymers, and salts do not change this composition. Due to the mentioned similarities in the composition of the broth after the fermentative production of 2,3, 1,4- and 1,3-BDO, and similar thermodynamic interactions, it may be expected that one adaptable process design will be able to purify all three BDOs. This approach would enhance the flexibility of the bioproduction of BDOs. The flowsheets of these processes are presented in Fig. 2, Fig. 3 and Fig. 4, while the compositions and conditions of the main process streams are given in Table 2, Table 3 and Table 4. More detailed data on mass and energy balances are available in the Supplementary Information file.

Rigorous simulations for all process operations were performed in Aspen Plus. The complex interactions between different components in the broth were described using the NRTL (case 1–4) or NRTL-HOC (cases 2–3 and 1–3) thermodynamic property model. This model (Non-Random Two Liquid) uses binary interaction parameters to describe vapor – liquid (VLE) and liquid – liquid equilibrium (LLE) of highly non-ideal mixtures. HOC extension (Hayden-O'Connell) was used in cases 2–3 and 1–3 to describe complex interactions of polar components (e.g. carboxylic acids) in the vapor phase (Aspen Physical Property System, 2020). Validation of the used property model against available experimental data is presented in the Supplementary Information file.

Even though optimization of a chemical process is a non-convex mixed-integer nonlinear problem (MINLP) with no theoretical guarantee of a global optimum, minimizing energy requirements was the focus of process design. As energy costs are significant, this approach can be expected to reduce the total operating costs (OPEX) and consequently the total annual costs (TAC). Minimization of TAC was not considered the main goal during process design as previously suggested (Li et al., 2023). The problem with minimizing TAC is that it includes CAPEX for which there are no universal correlations. Additionally, CAPEX needs to be annualized and the ratio of OPEX and CAPEX depends significantly on the chosen payback period. The total number of trays in the columns, placement of the feed tray, reflux ratio, distillate-to-feed ratio, boilup ratio, vapor fraction, compression ratio, etc. are some of the decision variables considered in process development. Additionally, several constraints were taken into account, such as high recovery of all BDOs, high purity of BDO product streams, temperature limitations, and so on.

3.2. Economic analysis

The published NREL methodology (Humbird et al., 2011) was used

Table 1
Composition of the feed stream to downstream processing after different fermentation processes.

Case 2–3			Case 1–4			Case 1–3		
Component	Mass fraction	Boiling point (C)	Component	Mass fraction	Boiling point (C)	Component	Mass fraction	Boiling point (C)
Ethanol	0.0105	78.3	Ethanol	0.0021	78.3	Ethanol	0.0052	78.3
Water	0.8750	100.0	Water	0.9279	100.0	Water	0.9109	100.0
Formic acid	0.0003	100.6	GBL	4e−5	204.0	Acetic acid	0.0052	118.0
Acetic acid	0.0089	117.9	1,4-BDO	0.0697	228.0	3-HB	0.0052	143.0
3-HB	0.0093	143.0	HTHF	0.0002	246.8	1,3-BDO	0.0725	207.5
2,3-BDO	0.0930	180.7	2-PYR	3e−6	251.2	Glucose	0.0010	/
Lactic acid	0.0007	216.8	Glucose	2e−5	/*			
Succinic acid	0.0020	317.8						

* does not exist as a stable liquid that boils

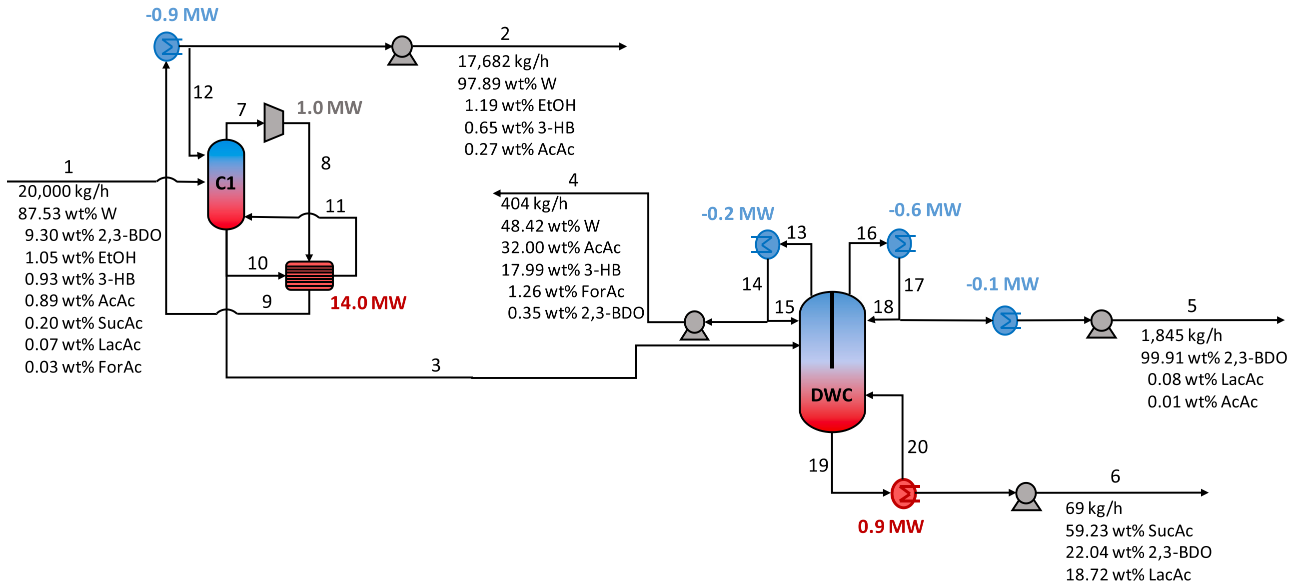

Fig. 2. Downstream process for the final purification of 2,3-BDO after fermentation (case 2–3), conditions and compositions of the numbered process streams are given in Table 2 (abbreviations: W – water, 2,3-BDO – 2,3-butanediol, EtOH – ethanol, ForAc – formic acid, AcAc – acetic acid, LacAc – lactic acid, SucAc – succinic acid and 3-HB – 3-hydroxy-2-butanone).

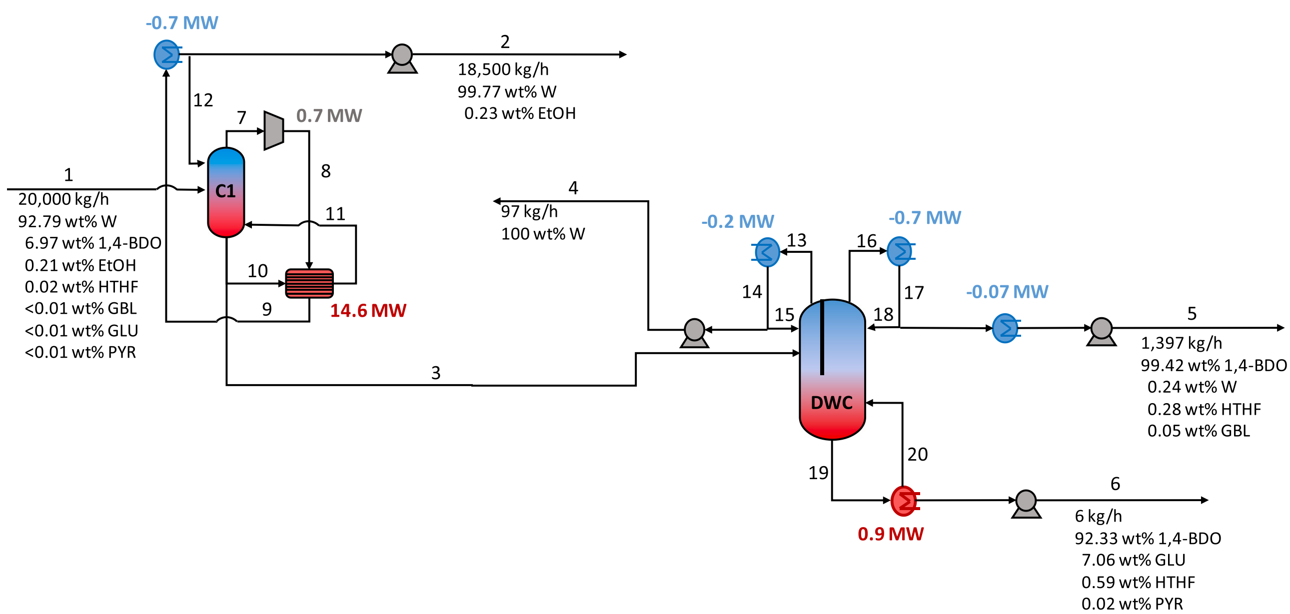

Fig. 3. Downstream process for the final purification of 1,4-BDO after fermentation (case 1–4), conditions and compositions of the numbered process streams are given in Table 3 (abbreviations: W – water, 1,4-BDO – 1,4-butanediol, EtOH – ethanol, GBL – gamma butyrolactate, HTHF – 2-(4-hydroxybutoxy)-THF, PYR – 2-pyrrolidone and GLU - glucose).

to evaluate the performance of the developed recovery processes. Following this methodology, the total capital expenditure (CAPEX) account for costs of equipment purchase and installation, warehouse, site development, additional piping, prorateable expenses, field expenses, home office and construction, working capital, etc. The costs of equipment purchase and installation were estimated using the published cost correlations (Kiss, 2013), with a Marshall and Swift cost index of 1773.4 (end of 2021). According to the same methodology (Humbird et al., 2011), the operating expenses (OPEX) include costs of utilities, operating labor (BCcampus, 2023a, 2023b), maintenance, property insurance, waste treatment, etc. Thereby, the following approximations of the utility costs were taken into account: 60.48 $/MWh for electricity, 28.01 $/ MWh for low-pressure steam, 29.59 $/MWh for medium-pressure steam, 35.59 $/MWh for high-pressure steam and 1.27 $/MWh for cooling water (Kiss, 2013). The cost of operating labor includes labor burden and cost of supervisory and clerical labor. Furthermore, the following assumptions were made when calculating the cost of operating labor: 3 shifts per day, 3 free weeks per year for an operator and an average salary of 20 $/h for an operator. The wastewater treatment costs were calculated based on chemical oxygen demand (COD), using approximate costs of 0.09 $/kg COD (Humbird et al., 2011). The COD was determined following the published recommendations (Kerubo Oyaro et al., 2020). The cost of burning waste for energy was taken from the published literature (WRAP, 2023). The total annual costs (TAC) account for both CAPEX and OPEX with a payback period (PBP) of 10 years and were calculated from the following equation: TAC

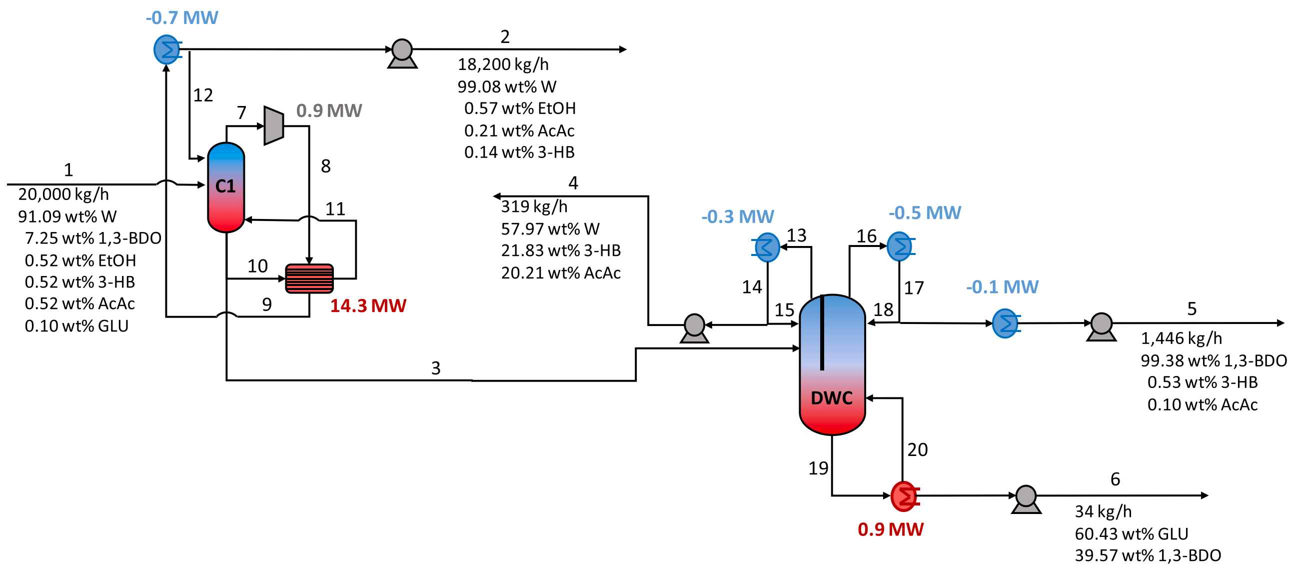

Fig. 4. Downstream process for the final purification of 1,3-BDO after fermentation (case 1–3), conditions and compositions of the numbered process streams are given in Table 4 (abbreviations: W – water, 1,3-BDO – 1,3-butanediol, EtOH – ethanol, AcAc – acetic acid, 4-HB – 4-hydroxy-2-butanone and GLU - glucose).

Table 2
Conditions and compositions of the main streams from Fig. 2 (Case 2–3).

Stream	1	2	3	4	5	6
Temperature [C]	30.0	50.1	70.7	47.5	30.1	149.2
Pressure [bar]	1.000	1.000	0.134	1.000	1.000	1.000
Flowrate [kg/h]	20,000	17,682	2318	404	1845	68
Mass fractions						
Water	0.8753	0.9789	0.0844	0.4842	0.0000	0.0000
2,3-BDO	0.0930	0.0000	0.8025	0.0035	0.9991	0.2204
Ethanol	0.0105	0.0119	0.0000	0.0000	0.0000	0.0000
3-HB	0.0093	0.0065	0.0314	0.1799	0.0000	0.0000
Acetic Acid	0.0089	0.0027	0.0559	0.3200	0.0001	0.0000
Succinic Acid	0.0020	0.0000	0.0175	0.0000	0.0000	0.5923
Lactic Acid	0.0007	0.0000	0.0061	0.0000	0.0008	0.1872
Formic Acid	0.0003	0.0000	0.0022	0.0126	0.0000	0.0000

Table 3
Conditions and compositions of the main streams from Fig. 3 (Case 1–4).

Stream	1	2	3	4	5	6
Temperature [C]	30.0	51.9	55.9	45.9	30.0	164.4
Pressure [bar]	1.000	1.000	0.134	1.000	1.000	1.000
Flowrate [kg/h]	20,000	18,500	1500	97	1397	6
Mass fractions						
Water	0.9279	0.9977	0.0672	1.0000	0.0024	0.0000
1,4-BDO	0.0697	0.0000	0.9293	0.0000	0.9942	0.9233
Ethanol	0.0021	0.0023	0.0000	0.0000	0.0000	0.0000
HTHF	0.0002	0.0000	0.0027	0.0000	0.0028	0.0059
GBL	< 0.0001	0.0000	0.0005	0.0000	0.0005	0.0000
Glucose	< 0.0001	0.0000	0.0003	0.0000	0.0000	0.0706
PYR	< 0.0001	0.0000	< 0.0001	0.0000	0.0000	0.0002

= CAPEX/PBP + OPEX. Furthermore, the influence of the PBP on TAC was analyzed.

3.3. Sustainability assessment

Environmental impact of the developed recovery processes was estimated by determining several key sustainability metrics (energy intensity, water consumption, greenhouse gas emissions, material intensity, wastewater intensity, pollutant and toxic emissions) (Schwarz et al., 2002; Sheldon, 2018).

- Energy intensity is the amount of total energy required to recover a kilogram of product (Schwarz et al., 2002), with a distinction between the types of used energy. Thermal and electrical energy requirements stand for the specific amounts of used thermal and electrical energy, respectively. The primary energy requirements account for both thermal and electrical energy through an electrical-to-thermal conversion factor (a conservative value of 2.5 was used (BP, 2021)).
- *Greenhouse gas emissions* represent the amount of carbon dioxide (CO_2) that is emitted per kilogram of product (Schwarz et al., 2002). These emissions are related to energy usage and were calculated

Table 4
Conditions and compositions of the main streams from Fig. 4 (Case 1–3).

Stream	1	2	3	4	5	6
Temperature [C]	30.0	50.6	66.5	47.1	30.1	155.5
Pressure [bar]	1.000	1.000	0.134	1.000	1.000	1.000
Flowrate [kg/h]	20,000	18,200	1800	319	1446	34
Mass fractions						
Water	0.9109	0.9908	0.1029	0.5797	0.0000	0.0000
1,3-BDO	0.0725	0.0000	0.8060	0.0000	0.9938	0.3957
Ethanol	0.0052	0.0057	0.0000	0.0000	0.0000	0.0000
3-HB	0.0052	0.0014	0.0430	0.2183	0.0053	0.0000
Acetic Acid	0.0052	0.0021	0.0366	0.2021	0.0010	0.0000
Glucose	0.0010	0.0000	0.0115	0.0000	0.0000	0.6043

using the published literature (Kiss and Suszwalak, 2012; Mantingh and Kiss, 2021). Lastly, a distinction was made between the source of electricity: green (renewable electricity) and grey (electricity from fossil fuels).

- Water consumption indicates the amount of water needed per kilogram of recovered product. This metric accounts for 7 % loss of cooling water (Schwarz et al., 2002) and 70 % recovery of condensate in the steam cycle (Lieberman and Lieberman, 2022).
- *Material intensity* is the amount of waste (excluding wastewater) that is formed per kilogram of recovered product (Schwarz et al., 2002).
- *Wastewater intensity* measures water that needs to be sent to wastewater treatment per kilogram of product (Sheldon, 2018).
- *Pollutant and toxic materials* stand for the amount of formed pollutants and toxic materials per kilogram of recovered products (Schwarz et al., 2002).

4. Results and discussion

4.1. Initial water removal

Due to the high concentration of water, presence of many by-products and microorganisms, several steps are required in the downstream processing. After the initial filtration and ion exchange steps (not included in this study), the fermentation broth is still very dilute. Thus, a preconcentration step can be implemented to remove most of the water with some light by-products before the final purification. This step may be performed in distillation column C1 (see Fig. 2, Fig. 3 and Fig. 4), whereby most of the water with light by-products is separated as the top product while BDO with heavy by-products and the remaining light components is obtained at the bottom. Reduced pressure operation in this column can facilitate separation, decrease energy requirements and avoid high temperatures that may lead to degradation of components. The operating pressure of 0.130 bar (top pressure) was chosen to minimize reboiler duty while allowing the usage of inexpensive cooling utilities (e.g. cooling water) in the condenser. The structured packing type Mellapak 250 with a pressure drop of 0.225 mbar per theoretical stage was defined for internals due to the reduced pressure operation (Sulzer, 2023).

Practically, all components lighter than BDO can be separated as the top product from column C1. However, the temperature difference between the top and the bottom of the distillation column would be too high to use heat pumps because the bottom product would become concentrated with high boiling components. Due to the high water content of the feed stream, the preconcentration step is very energy-intensive (reboiler duty of over 12 MW). Thus, energy-saving opportunities in this step are crucial for the energy-efficiency of the complete purification process. In that respect, the proper choice of operating parameters should allow the use of a heat pump system that would significantly reduce energy requirements for the complete downstream processing. More precisely, not separating all light components in the distillate of column C1 decreases the temperature difference between the top and the bottom of this column allowing the implementation of mechanical vapor recompression (MVR). This heat pump system involves compressing the top vapor from the distillation column and using it instead of external heating utility in the reboiler. Consequently, the electrical energy used to power the compressor replaces much higher thermal energy (Kiss and Infante Ferreira, 2016). If the temperature difference between the top and bottom of the distillation column is too large, hot compressed vapor cannot provide sufficient heat to evaporate the bottom liquid. The measure of the obtained energy savings with heat pump systems may be expressed through the coefficient of performance (COP). COP is equal to the ratio between exchanged thermal energy (between compressed top vapor and bottom liquid) and the required electrical energy to power the compressor (Kiss and Infante Ferreira, 2016). COP values higher than 2.5, which is a conservative value of the electrical-to-thermal conversion factor (BP, 2021), prove the energy efficiency of the installed heat pump system. COP values of the proposed MVR systems are > 14. Thus, the installed heat pump systems resulted in significant energy savings while allowing complete (green)electrification of the preconcentration step.

Finally, the top product from column C1 contains most of the water with some light impurities (case 2–3: 98.0 wt% water, 1.2 wt% ethanol, 0.6 wt% 3-HB and 0.3 wt% acetic acid; case 1–4: 99.8 wt% water and 0.2 wt% ethanol; case 1–3: 99.1 wt% water, 0.6 wt% ethanol, 0.2 wt% acetic acid and 0.2 wt% 3-HB). Due to their small amounts, valorization of by-products from this stream was not considered. Instead, this stream was sent to the wastewater treatment, the costs of which were included in further economic and sustainability analysis. If the small amounts of by-products do not interfere, this stream may be used upstream to reduce fresh water demand.

To the best of our knowledge, the published studies on the purification of BDOs after fermentation have not included a multistage preconcentration step in which most of the water and light components are removed without losing BDO product. Some studies considered an evaporation step in a flash unit before the final purification (Haider et al., 2020, 2018b). However, smaller amounts of light components are removed in this step while most of these components are sent to the final purification. Consequently, larger equipment units with higher thermal energy requirements are needed in the last step. Moreover, water with light by-products is removed as the top product, heavy by-products are obtained at the bottom and BDO product is recovered as a side stream. Thus, the temperature difference between the top and the bottom of the column is too large, and the heat pump system can only be used to preheat the feed stream but not to evaporate the bottom liquid. Alternatively, removing all light components in a flash evaporator unit was suggested before the final distillation. The top vapor from the distillation column is compressed and used to partially heat the evaporator unit (Van Duc Long et al., 2018). However, one-stage separation resulted in a loss of BDO. Furthermore, the installed heat pump system could not provide sufficient heat in the flash unit. On the contrary, we propose a multi-stage preconcentration step in the heat pump-assisted distillation column C1 in which most light components are removed without losing BDO product. Thus, the reboiler duty and equipment size in the final purification step will be smaller due to the significantly reduced flowrate of the feed stream to this step. Additionally, the MVR system in column C1 can completely cover the thermal energy requirements of the pre-concentration step. As this operation is very energy-intensive, the implemented heat pump system drastically reduces the energy requirements of the total downstream process.

4.2. Final purification in a dividing-wall column

After the preconcentration step, a final purification is required to obtain a high-purity BDO product. Firstly, the remaining water and light impurities may be removed as the top product of the next distillation column. The bottom product from this column would contain BDO and heavy impurities. To obtain the final product, an additional distillation step is required. The top product from this column would be purified BDO, while all heavy impurities would be separated as the bottom product. Thus, a sequence of at least two distillation columns is required to separate BDO from light and heavy impurities. Alternatively, a dividing-wall column with a divided overhead section and common bottom section (DWC) may be used for the final purification (Fig. 5). This is a highly integrated system that merges two distillation columns into one shell and reduces the number of heat exchangers that are required (one reboiler and two condensers). As the DWC unit is not available in Aspen Plus, it was simulated as a thermodynamically equivalent sequence of two distillation columns (Fig. 5). Left and right parts of DWC are presented as DWC_L and DWC_R, respectively. The number of stages, location of the feed stage, reflux ratio, distillate-to-

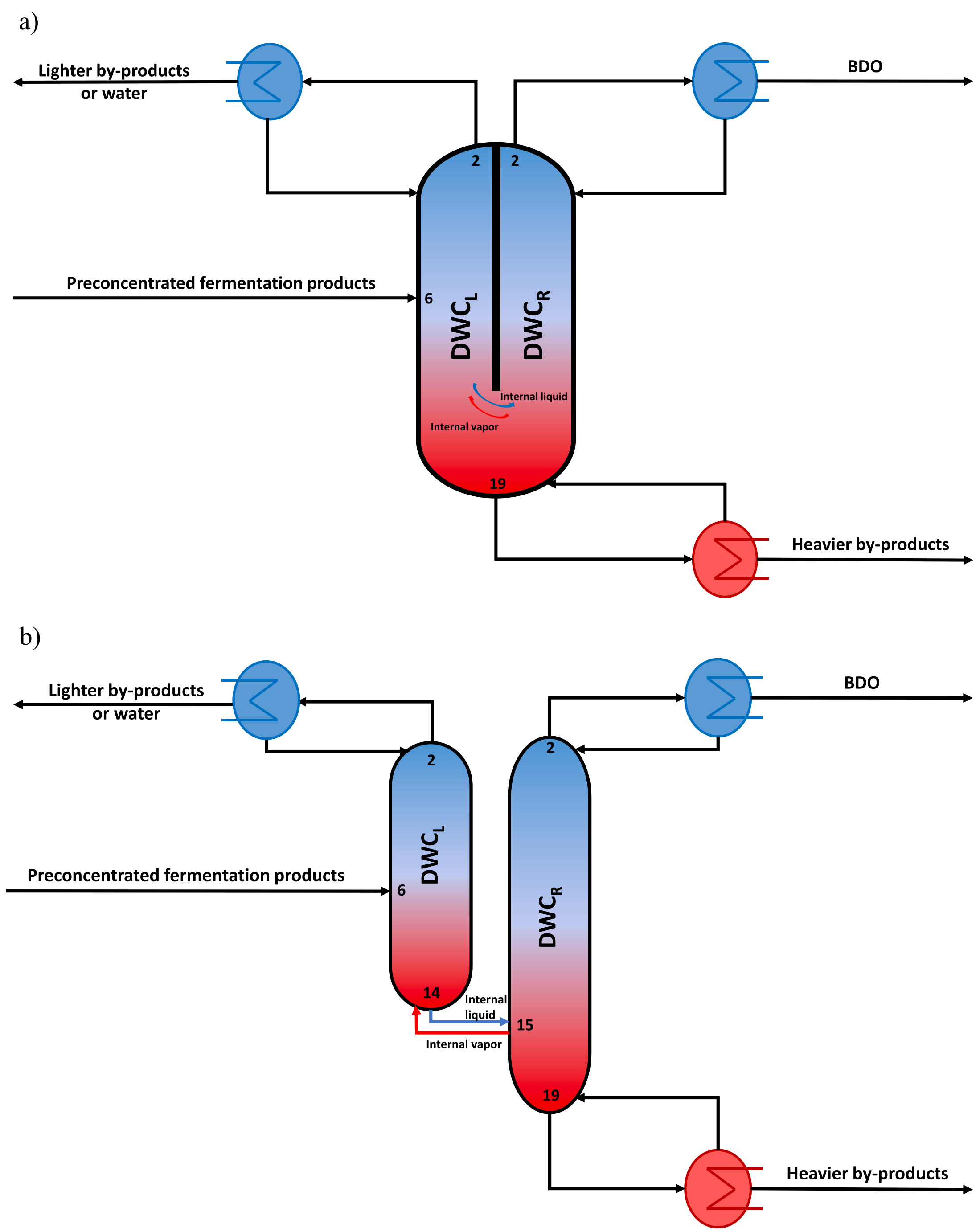

Fig. 5. DWC design (a) and the equivalent sequence of distillation columns (b) - the numbers in the column indicate the column tray number.

feed ratio and vapor split were varied to allow high recovery of high-purity BDO product while minimizing energy requirements. More details about the design of DWC are presented in the Supplementary Information file. In short, DWC has 20 stages in total, whereby the first and the last stages are condenser and reboiler by the convention in Aspen Plus. The wall is placed in the top 14 stages (13 excluding the condenser). Due to the large temperature difference between the two top products (BDO and light impurities), thermal insulation will be needed to ensure the energy efficiency of DWC. Temperature profiles of DWC in all cases are presented in the Supplementary Information file. The bottom liquid from DWC_L is sent to DWC_R, while the part of the rising vapor from DWC_R is directed to DWC_L to ensure sufficient vapor flow. Due to the similarities in the fermentation broth composition, a similar vapor split is required for recovering high-purity BDO products in all cases (about 23 – 42 % of the rising vapor from DWC_R is sent to DWC_L). Likewise, a similar ratio of DWC_L and DWC_R's cross-section areas (position of the wall) is needed (DWC_L and DWC_R's surface areas are 24 – 34 and 66 – 76 % of the total DWC's surface area). Consequently, the operation of the same DWC unit may be easily adapted to purify different BDOs (BenitM, 2024). The DWC operates at reduced pressure (top pressure of 0.1 bar) to avoid high temperatures that may lead to decomposition while allowing the usage of less expensive heating and cooling utilities (medium-pressure steam in reboiler and cooling water in condensers). Due to the required vacuum, structured packing type Mellapak 250 with a pressure drop of 0.225 mbar per theoretical stage was chosen for the DWC's internals (Sulzer, 2023).

Liquid composition profiles of the DWC in all cases are presented in the Supplementary Information file. Summarizing, the concentration of BDO increases towards the bottom of DWC_L and the top of DWC_R. Concentrations of water and light impurities are high at the top of DWC_L, while being negligible at the bottom of DWC_L and in DWC_R. Contrarily, concentrations of heavy impurities are insignificant in DWC_L but increase towards the bottom of DWC_R. Finally, high-purity BDO product (>99.4 wt%) is obtained as the top product from DWC_R in all cases. Due to the relatively small amounts, none of the by-products was purified. The top product from DWC_L contains the remaining light impurities (water, acetic acid, formic acid, 4-HB, 3-HB and GBL). As for the top product of column C1, it was assumed that this stream would be sent to wastewater treatment. The bottom product from DWC_R contains fermentation by-products heavier than BDO (succinic acid, lactic acid, HTHF, PYR and glucose). It was assumed that these streams could be burnt for energy and the appropriate gate fee was included in the economic analysis.

4.3. Economic analysis

The results of the performed economic analysis are summarized in Table 5 and presented in Fig. 6. The influence of PBP on TAC is presented in Fig. 7. The installed equipment cost is 5141, 4612 and 4984 k$ in cases 2–3, 1–4 and 1–3, respectively. In all cases, the largest contributor to the total equipment cost is the cost of heat exchangers (about 39 – 42 %) and compressors (about 30 – 36 %), followed by the cost of distillation columns (about 21 – 23 %). In comparison, the cost of pumps is significantly lower (about 4 – 5 % of the total equipment costs). Slightly lower equipment costs when recovering 1,4-BDO (case 1–4) are mainly due to the marginally lower cost of distillation columns and compressor in the MVR system. Since installed equipment cost makes up the largest part of CAPEX (about 55 %), CAPEX are slightly lower in case 1–4 (8419 k$) compared to cases 2–3 (9402 k$) and 1–3 (9111 k$).

Calculated OPEX for the final purification of BDO are 2340, 1471 and 1903 k$/y in cases 2–3, 1–4 and 1–3, respectively. Expressed per kilogram of BDO product, the total OPEX are 0.159, 0.132 and 0.164 $\$/kg_{BDO}$. The largest contributors to OPEX are the labor costs (30 – 48 %), the cost of wastewater treatment and handling heavy impurities (5 – 33 %) and the electricity cost (20 – 23 %). The costs of medium-pressure steam, cooling water and other operating costs are much lower (about 10 – 15 %, <1 % and 6 – 8 %). Lower OPEX in case 1–4 is mainly because of lower wastewater treatment (due lower amounts of light impurities) and electricity expenses (due to lower required compressor power in the MVR system).

Finally, TAC, which include both CAPEX and OPEX with a PBP of 10 years, are 3280, 2313 and 2814 k$/y, or 0.222, 0.208 and 0.243 $\$/kg_{BDO}$ in cases 2–3, 1–4 and 1–3, respectively. Since CAPEX and OPEX are the lowest when recovering 1,4-BDO (case 1–4), absolute TAC are also the lowest in this case. Nonetheless, TAC for the final purification of BDO in all cases is lower than 0.3 $\$/kg_{BDO}$ with a PBP of 10 years. However, TAC do not increase drastically even with shorter PBP (see Fig. 7). For example, with a PBP of three years or only one year, TAC are 0.371 – 0.430 and 0.796 – 0.958 $\$/kg_{BDO}$. The net unit production cost of 2,3-BDO from sugarcane bagasse was determined to be 1.13 – 2.28 $/kg, with the minimum selling price of 1.86 – 3.99 $/kg (Gadkari et al., 2023). Moreover, the minimum selling price of 2,3-BDO produced from sucrose, molasses or glycerol was estimated to be about 4 – 5.2 and 3.7 – 5.7 $\$/kg_{BDO}$ for production capacities of 10 and 20 ktonne/y, respectively (Koutinas et al., 2016). Considering the significant contribution of downstream processing to total production costs (Gawal and Subudhi, 2023), the proposed cost-effective and adaptable process for the final purification may represent a major advancement toward competitive fermentative production of BDOs.

Table 5
Key performance indicators in terms of economics and sustainability for the final purification of BDOs.

	Case 2–3	Case 1–4	Case 1–3
Economic indicators			
CAPEX [k$]	9402	8419	9111
OPEX [k$/y]	2340	1471	1903
OPEX [$\$/kg_{product}$]	0.159	0.132	0.164
TAC [k$/y]	3280	2313	2814
TAC [$\$/kg_{product}$]	0.222	0.208	0.243
Sustainability metrics			
Thermal energy requirements [$kW_{th}h/kg_{product}$]	0.506	0.662	0.615
Electrical energy requirements [$kW_eh/kg_{product}$]	0.539	0.502	0.624
Primary energy requirements [$kW_{th}h/kg_{product}$]	1.854	1.917	2.176
Water consumption [$m^3_w/kg_{product}$]	0.145	0.145	0.161
Water loss [$m^3_w/kg_{product}$]	0.010	0.011	0.012
CO_2 emissions, grey electricity [$kg_{CO2}/kg_{product}$]	0.319	0.324	0.373
CO_2 emissions, green electricity [$kg_{CO2}/kg_{product}$]	0.073	0.096	0.089
Wastewater intensity [$m^3_{waste\ water}/kg_{product}$]	0.010	0.014	0.013
Material intensity [$kg_{waste}/kg_{product}$]	0.037	0.004	0.024
Pollutant emissions [$kg_{pollutant}/kg_{product}$]	0	0	0
Toxic emissions [$kg_{toxic\ materal}/kg_{product}$]	0	0	0

4.4. Sustainability assessment

The determined key sustainability metrics are summarized in Table 5.

- *Energy intensity*: The thermal energy requirements are 0.506, 0.662 and 0.615 $kW_{th}h/kg_{BDO}$ in cases 2–3, 1–4 and 1–3, respectively. As DWC's reboiler duty is similar in all cases (~0.9 MW_{th}), the lowest thermal energy requirements in case 2–3 are due to the largest product flowrate. The electrical energy requirements are 0.539, 0.502 and 0.624 kW_eh/kg_{BDO} in cases 2–3, 1–4 and 1–3. The largest electricity demand in case 1–3 is for powering the compressor in the MVR system applied to column C1. Thus, the total primary energy requirements for the final purification of BDO are 1.854 $kW_{th}h/kg_{BDO}$ in case 2–3, 1.917 $kW_{th}h/kg_{BDO}$ in case 1–4 and 2.176 $kW_{th}h/kg_{BDO}$ in case 1–3. To the best of our knowledge, the published

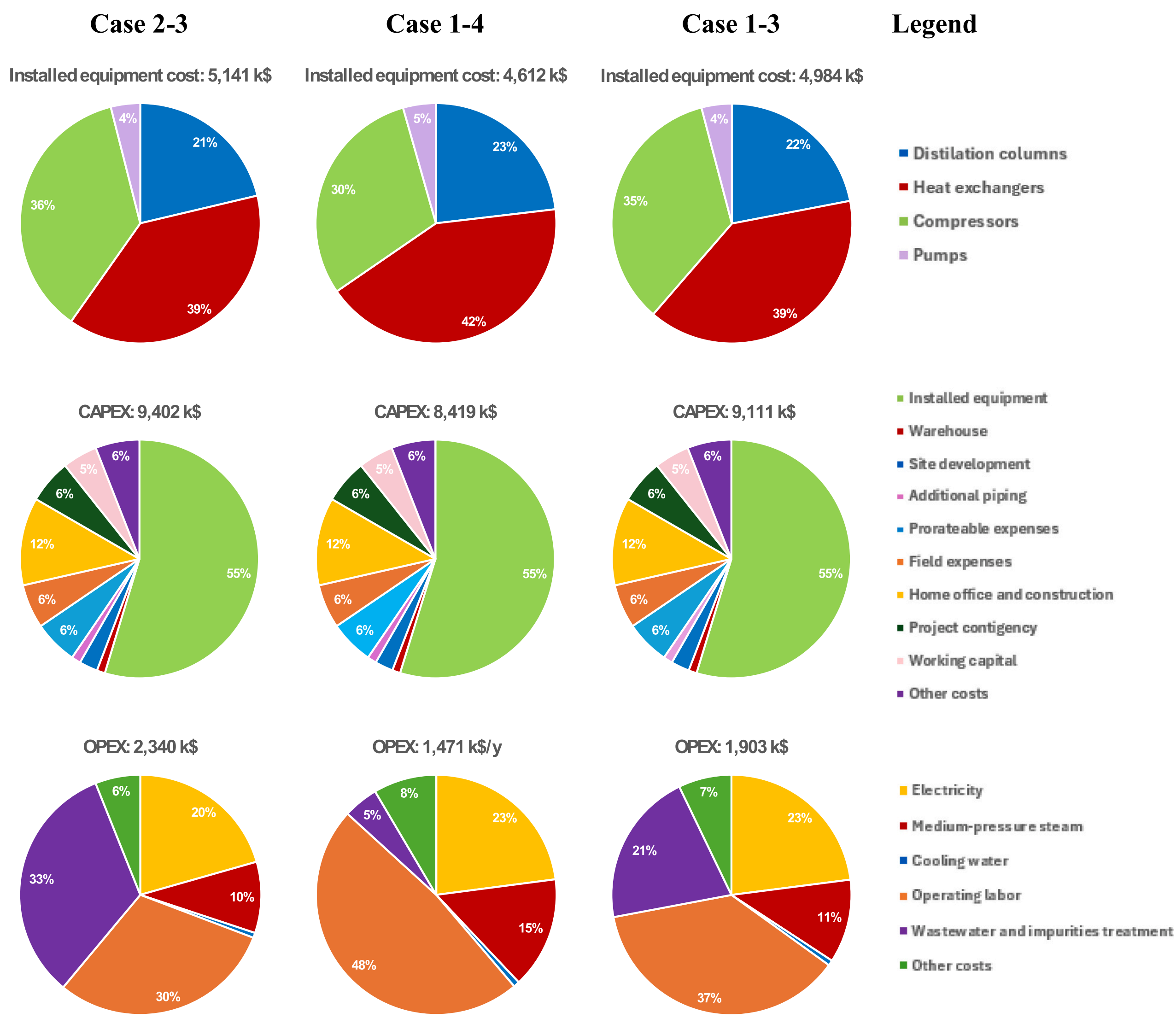

Fig. 6. Comparison of economic indicators of the final BDO purification in cases 2–3, 1–4 and 1–3.

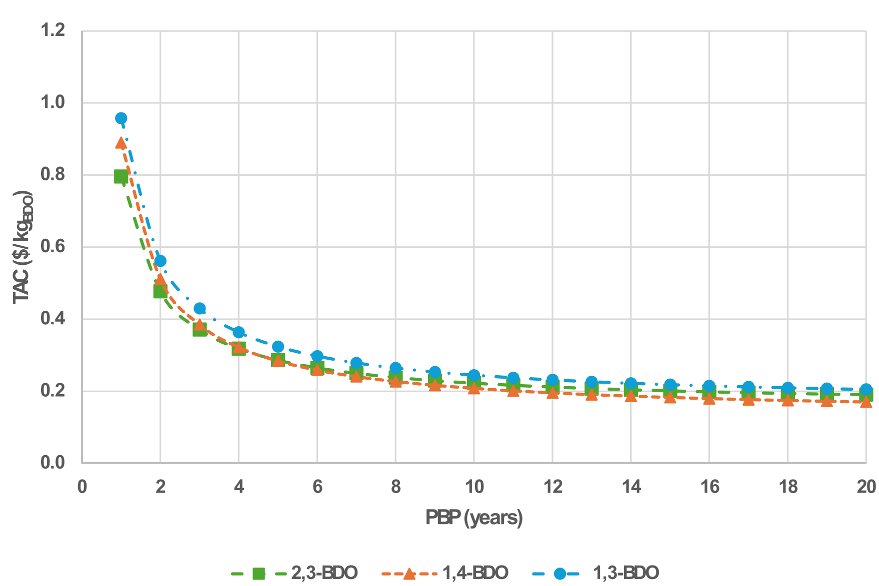

Fig. 7. Influence of the payback period (PBP) on the specific total annual costs (TAC) for purification.

processes for the recovery of BDO after fermentation have energy requirements ranging from approximately 3.1 to 8.6 $kW_{th}h/kg_{BDO}$ (Haider et al., 2018b, 2018a; Harvianto et al., 2018; Hong et al., 2019; Van Duc Long et al., 2018), with the process using DWC requiring approximately about 6.2 $kW_{th}h$ to recover 1 kg of BDO (Haider et al., 2020). Thus, our process allows a more energy-efficient purification of BDO after fermentation.

- *Greenhouse gas emissions*: Being related to energy usage, CO_2 emissions follow the same trend as energy requirements: 0.319, 0.324 and 0.373 kg_{CO2}/kg_{BDO} if grey electricity is used, or 0.073, 0.096 and 0.089 kg_{CO2}/kg_{BDO} if green electricity is used. Considering that the total climate effect of fossil-based and bio-based 2,3-BDO production was estimated to be 7.36 and 4.03 kg CO2 eq (Ebrahimian and Mohammadi, 2023), the proposed purification process can reduce the total emissions.
- *Water consumption*: By decreasing thermal energy requirements with installing the heat pump system, water consumption (0.145 – 0.161 m^3_{water}/kg_{BDO}) and water loss (0.010 – 0.012 m^3_{water}/kg_{BDO}) are significantly reduced.
- *Material intensity:* Since the top streams from column C1 and DWC_L were accounted for in the wastewater treatment metrics, only the bottom product of DWC was considered in the calculation of the material intensity. Thus, the obtained values are 0.037, 0.004 and 0.024 kg_{waste}/kg_{BDO}. Significantly lower values in case 1–4 compared to cases 2–3 and 1–3 are due to the less heavy by-products in the fermentation broth.
- *Wastewater intensity*: The top products from column C1 and DWC_L would be sent to the wastewater treatment. Since the fermentation broth is very dilute, large water flowrates need to be treated. Thus, the values of wastewater intensity metrics are 0.010, 0.014 and 0.013 $m^3_{waste\ water}/kg_{BDO}$ in cases 2–3, 1–4 and 1–3, respectively.
- *Pollutant and toxic materials*: Since pollutants and toxic materials are not formed, values of these metrics are equal to zero in all cases.

5. Conclusion

The proposed downstream processing design enables eco-efficient large-scale (broth processing capacity of 160 ktonne/y) purification of BDOs from a dilute fermentation broth (initial BDO concentration ranging from 6.97 to 9.30 wt%). Due to the similarities in thermodynamic properties and broth composition when producing 2,3-, 1,4-, and 1,3-BDO, a single process configuration was proven to effectively purify different BDOs after fermentation, offering additional flexibility in developing competitive bioprocesses for BDO production. To significantly reduce the overall energy requirements, a preconcentration step in a heat pump-assisted vacuum distillation column may be implemented before the final purification. Removing most of the water and light impurities in this step significantly decreases reboiler duty and equipment size in the final purification. A proper choice of operating parameters allows the use of a mechanical vapor recompression heat pump system to the preconcentration column, drastically reducing overall energy requirements and minimizing dependence on external steam for heating. The final purification of BDO product from the remaining light and heavy impurities may be effectively performed in an integrated dividing-wall column. Finally, this downstream processing configuration was proven to cost-effectively (total purification costs of 0.208 – 0.243 $\$/kg_{BDO}$) and energy-efficiently (total energy requirement of 1.854 – 2.176 $kw_{th}h/kg_{BDO}$) recover over 99 % of BDO as a high-purity product (> 99.4 wt%).

CRediT authorship contribution statement

Tamara Janković: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Data curation, Conceptualization. **Adrie J. J. Straathof:** Writing – review & editing, Validation, Methodology, Formal analysis. **Siddhant Sharma:** Writing – review & editing, Visualization, Validation, Software, Methodology. **Anton A. Kiss:** Writing – review & editing, Writing – original draft, Validation, Supervision, Resources, Methodology, Investigation, Formal analysis, Conceptualization.

Declaration of Competing Interest

The corresponding author, Anton Kiss is an editor for the journal Chemical Engineering Research and Design, but has had no access to, or involvement in, the peer review process for this paper or its handling by the journal at any point.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cherd.2024.12.011.

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