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Critical impacts of energy targeting on the sustainability of advanced biobutanol separation

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HIGHLIGHTS

➢ Adsorptive ABE separation coupled with distillation is highly energy intensive.

➢ Pinch technology can reduce heating and cooling energy by about 36%.

➢ Pumping energy is ignorable compared to those for adsorption and distillation.

➢ Employing multi-pressure distillation is critical for efficient energy saving.

➢ Over 98% decline in human health, ecosystem, and resource damage can be obtained.

GRAPHICAL ABSTRACT
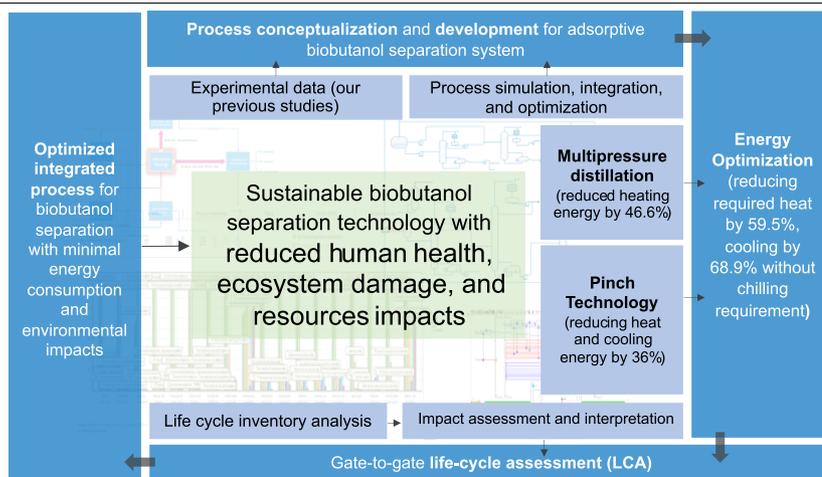
ARTICLE INFO

ABSTRACT

Biobutanol stands out as an advanced renewable biofuel, yet its production through fermentation yields a low butanol concentration, necessitating expensive and energy-intensive separation methods, particularly by distillation. Alternative approaches, including adsorptive separation, have emerged, with the 2-column zeolite-based process showing promise. This study employed Aspen Plus for simulating adsorptive separation, utilized Pinch technology for heat integration, and analyzed various alternatives using the life cycle assessment (LCA) approach. Compared to the base case, which relied on our previously acquired experimental data and further purification through atmospheric distillation, the adoption of indirect heating/cooling adsorption reduced heating energy demand by 59.5%. Additionally, cooling energy usage was increased notably by 68.9%, and chilling prerequisites were eliminated. The implementation of Pinch technology further reduced heating and cooling energy requirements by approximately 36%. Multi-pressure distillation was also explored, revealing its potential to reduce heating energy consumption by 46.6%, accompanied by a modest 6.2% increase in cooling energy demand. A gate-to-gate LCA framework was used to evaluate the environmental impacts. The results showed that the combination of indirect heating/cooling adsorption, multi-pressure distillation, and energy-efficient practices resulted in over a 98% reduction in damages related to human health, ecosystem well-being, and resource depletion compared to the base case. Prioritization of key performance indicators revealed that human health had the most significant influence, with prominent midpoint effects attributed to human toxicity and global warming. This study underscores the pivotal role of energy targeting in curtailing energy consumption and enhancing the sustainability of adsorptive biobutanol separation.

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Contents

Abbreviations	
ABE	Acetone, butanol, and ethanol
APOS	Advanced planning and optimization solutions
CHA	Chabazite
DALY	Disability-adjusted life years
EF	Environmental footprint
GHG	Greenhouse gas
ILCD	International reference life cycle data system
ISO	International organization for standardization
LCA	Life cycle assessment
LCC	Life cycle costing
LTA	Linde type A
NRTL	Non-random two-liquid
PVC	Polyvinyl chloride
RK	Redlich–Kwong
RED	Renewable energy directive
SC	Scenario
kPt	The key performance indicator prioritization technique
Wh	watt-hours

1. Introduction

Butanol has a wide range of applications in different chemical industries, including polymers and synthetic rubber, and it is also considered a promising alternative to gasoline and diesel fuel (Karimi et al., 2015; Amiri, 2020). It can play a major role in the transportation sector, as it has shown high performance when blended with gasoline, diesel, and jet fuel (Díaz et al., 2020; Adesanya et al., 2022). This could significantly reduce the environmental impacts of fossil-based fuels (Brito and Martins, 2017; Luo et al., 2020). Recently, biologically produced butanol, i.e., biobutanol, has attracted great attention (Riaz et al., 2022).

Biobutanol can be produced from various widely available and inexpensive resources, including municipal solid waste, agricultural residues, and lignocelluloses, through acetone, butanol, and ethanol (ABE) fermentation (Abo et al., 2019). However, butanol is a toxic component to ABE-producing bacteria, and thus, a low concentration of butanol (less than 15 g/L) is produced through fermentation (Amiri and Karimi, 2019). The low concentration of butanol results in costly and high-energy-demanding separation processes (Amiri and Karimi, 2019; Claessens et al., 2020b).

Distillation is among the processes that are commercially used for this purpose; however, at least five distillation columns with high capital cost and energy are required (Pereira et al., 2015; Chen et al., 2018). With the current energy prices, distillation is neither an economically feasible nor sustainable method for biobutanol recovery (Eloka-Eboka and Maroa, 2023). Thus, other alternatives, including gas stripping followed by adsorption-distillation, pervaporation-distillation, and dual extraction-distillation, were suggested (Mahmud and Rosentrater, 2020; Eloka-Eboka and Maroa, 2023).

Recently, adsorption has shown promising results and perspectives (Van der Perre et al., 2017; Claessens et al., 2020a). Among the adsorptive separation approaches for ABE separation, a two-column zeolite-based vapor-phase process has demonstrated excellent performance in terms of both product purity and recovery (Van der Perre et al., 2017). The system operates on the principle of stripping ABE from the fermentation broth, followed by selective adsorption and desorption of the ABE molecules. While both liquid and vapor-phase adsorptive systems can be utilized to purify butanol, the vapor-phase sequential adsorptive recovery of ABE through two columns offers several advantages over alternative recovery methods. Some of these advantages include high product purity, high product recovery, lower energy consumption (since it can be carried out at lower temperatures and pressures than other recovery methods), reduced waste (since vapor-phase adsorption does not generate any liquid waste, which can be an advantage from an environmental standpoint). Moreover, the reusability of adsorbents makes the process advantageous, as the zeolites employed in the vapor phase can be easily regenerated by heating, allowing them to be reused continuously for years.

Overall, the use of vapor-phase sequential adsorptive recovery of ABE through two zeolite columns is an efficient and cost-effective method for recovering ABE from fermentation broth (Van der Perre et al., 2017; Claessens et al., 2020a). This process includes two zeolite beds with complementary selectivity, one LTA-type zeolite adsorption column for biobutanol separation, and another CHA-type zeolite adsorption column for ethanol/acetone/water separation. Through this system, over 99% of butanol with high purity (>99.5%) is recovered. The system is capable of purifying butanol, whereas, for the purification of ethanol and acetone from the remaining chemicals and water, supplementary distillation is necessary (Van der Perre et al., 2017; Claessens et al., 2020b). However, the capacity and equipment required for the purification of ethanol and acetone after butanol recovery are less energy and costly processes than the separation of all products by distillation systems. Although the whole process, including

the two-stage adsorptive separation and following distillation, consumes much less energy than conventional distillation for ABE separation (Van der Perre et al., 2017; Claessens et al., 2020c), heat integration methods, e.g., Pinch technology, may be used to further reduce the energy consumption in the process.

Pinch technology is a powerful approach for reducing energy consumption in industrial processes. It involves analyzing the heat flows in a process and identifying areas where heat can be recovered and reused, reducing the need for external energy input (Kong et al., 2023). To do the heat integration through Pinch technology, the first step is identifying the heat flows in the process and determining where the heat can be recovered and reused. Once the Pinch analysis has identified areas where heat can be recovered, modifications to the process can be made to allow for heat integration. Then, heat exchangers can be installed to transfer heat between hot and cold streams, or process streams can be rerouted to maximize heat recovery. The final step in the Pinch analysis is to optimize the process to minimize energy consumption while meeting process requirements. This process involves balancing the heat flows and minimizing the temperature difference across the Pinch point. The main benefits of Pinch technology include energy savings, reducing both the amount of energy consumption and operating costs, process optimization by identifying areas for process optimization and efficiency improvements, and, consequently, environmental benefits (Joda and Ahmadi, 2019; Kong et al., 2023). The energy savings can be costly and environmentally beneficial for the process. Thus, the environmental benefits may be evaluated and quantified using the life cycle assessment (LCA) approach.

LCA is a valuable tool for optimizing and comparing different processes *via* a comprehensive evaluation of the environmental impact of a process (Khoshnevisan et al., 2018; Rahimi et al., 2018). The results of the LCA can be used to identify hotspots and areas where environmental impact is most significant and also to evaluate different scenarios for reducing impact (Khoshnevisan et al., 2018; Wang et al., 2021). To optimize a process using LCA, different process configurations, alternatives, and conditions can be compared to identify ways to reduce energy use, waste generation, and emissions to select the most environmentally friendly option (Khoshnevisan et al., 2018; Rahimi et al., 2018).

In this study, optimization of energy consumption was conducted for one of the recently developed and promising zeolite-based adsorptive ABE separation systems, followed by distillation. Pinch technology was used for energy optimization. Multi-pressure systems were employed for further energy saving. Moreover, the sustainability of the separation process was evaluated by a detailed LCA. Table 1 provides a summary of key papers focusing on the environmental analysis of ABE production, highlighting the originality and novelty of the present study.

2. Processes and Methods

2.1. Process description

The block flow diagram of the ABE separation process, providing an overview of the process, is shown in Figure 1. A mixture of ABE from the fermentation of municipal solid waste, containing 36.6% acetone, 83.9% butanol, and 20.8% acetone, is introduced into the separation process

Table 1.
Comparison of the most important papers published on the sustainability analysis of ABE production and the present study.

No.	Feedstock and Products	Separation of Products	LCA Method	Reference
1	ABE from corn and wheat straw	Distillation without heat integration/cooling was not considered	LCA using an economic allocation method/Impact assessment using IMPACT 2002+	Brito and Martins (2017)
2	ABE from the organic fraction of municipal solid waste	Distillation without heat integration/cooling was not considered	LCA using Simapro, following the guidelines by ISO 14040 to ISO 14044 /Impact assessment using IMPACT 2002+	Ebrahimian et al. (2023)
3	ABE from the organic fraction of municipal solid waste and lignocelluloses	Distillation without heat integration/cooling was not considered	LCA using GaBi following the guidelines by ISO 14040 to ISO 14044 /impact assessment only for global warming potential using IPCC 100-year	Meng et al. (2019)
4	ABE from agricultural wastes	Distillation without heat integration/cooling was not considered*	Cradle-to-gate LCA and LCC/Impact assessment using EF 2.0 method	Marzocchella et al. (2022)
5	ABE from corn and sugarcane	Distillation without heat integration/cooling was not considered	GHG emissions calculation using ISO 14040, GHG Protocol	Väisänen et al. (2016)
6	ABE from a mix of lignocellulosic materials available in México	Distillation with preliminary heat integration/cooling was not considered	Eco-indicator 99 methodology (EI99)	Quiroz-Ramírez et al. (2017)
7	ABE fermentation products	Separation of ABE by the liquid-liquid extraction and distillation using dividing wall columns	CO_2 emissions calculation	Segovia-Hernández et al. (2020)
8	ABE from microalgae	Distillation without heat integration/cooling was not considered	LCA using SimaPro based on ISO 14040 and 14044/ReCiPe endpoint scores	Wu et al. (2019)
9	ABE from barley straw	Extractive distillation using 8 distillation columns	GHG emissions calculation using RED methodology (that is a simplified method based on LCA).	Kuittinen et al. (2022)
10	ABE from the organic fraction of municipal solid waste	Distillation and Adsorptive separation with heat integration/cooling energy is considered	LCA using SimaPro based on ISO 14040 and 14044/ReCiPe endpoint and midpoint scores	**Current Study**

* Two different scenarios were investigated: a simple configuration of two distillation columns that enables recovery of butanol only and a 4 column for the separation of all ABE.

(Farmanbordar et al., 2018). Initially, ABE undergoes evaporation to produce a vapor stream that enters the vapor-phase adsorptive separation process. Initially, the vapor comprises water. Following this, the vapor undergoes a two-stage adsorptive separation process for butanol. Here, butanol is selectively adsorbed during the adsorption phase and desorbed during the subsequent desorption phase (Van der Perre et al., 2017; Claessens et al., 2020b).

A mixture of acetone and ethanol, along with water molecules, then enters the second adsorption process, where acetone, ethanol, and water are adsorbed during the adsorption phase and desorbed during the desorption phase. The product of the second adsorption process is a mixture of acetone, ethanol, and water that enters the distillation system to separate the water and purify acetone and ethanol. Thus, the final products of the distillation system are pure acetone and ethanol.
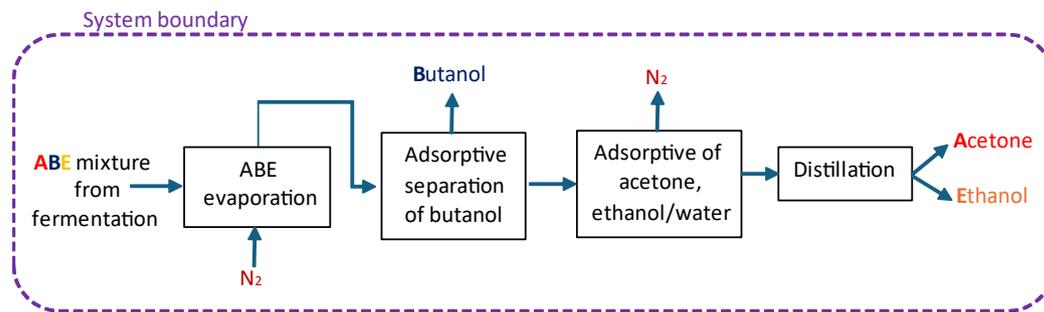
Fig. 1. Block flow diagram of ABE separation through the adsorptive separation system and system boundary considered for energy analysis and environmental impact analysis.

2.2. Plant capacity

The largest ethanol plant in Belgium, BioWanze, located in Wanze, Wallonia region, produces 300,000 m³ of ethanol annually from locally sourced grain and sugar beet obtained from farmers in the region. The ethanol manufactured at BioWanze is primarily used for blending with gasoline as a biofuel. Recognizing butanol as one of the most sustainable alternatives to ethanol (Amiri and Karimi, 2019), the present study assumes that the plant, with its current fermentation capacity, needs modification to produce butanol. This assumption aligns with the vision and strategy proposed by British Petroleum and Dupont as part of their joint venture, Butamax Advanced Biofuels company, for the future of US biofuel production (Butamax, 2019). As per assumption, the plant has the potential to produce 45,000 t/yr of acetone, 120,000 t/yr of butanol, and 14,000 t/yr of ethanol (refer to **Supplementary Data** for detailed calculations).

2.3. Process simulation

The process simulation was performed using Aspen Plus (V12, Licensed to VUB). The non-random two-liquid (NRTL) and Redlich–Kwong (RK) models were employed for predicting the thermodynamic properties of the liquid and gas phases, respectively.

2.4. Pinch methodology

The Pinch methodology is extensively applied in process industries to reduce energy consumption, accounting for process economy and adhering to process design constraints. This technique entails identifying heat sources and sinks, creating temperature-enthalpy diagrams, determining the minimum energy requirement, conducting heat integration, modifying designs, and optimizing. Aspen Energy Analyzer V12, licensed to VUB, is employed for this purpose (the data utilized for Pinch analysis is provided in **Supplementary Data**, **Table S5**).

2.5. Scenarios

- Base case

The base case relies on typical adsorption without heat integration, meaning that all heating and cooling requirements are provided by utilities (Van der Perre et al., 2017). The process flow diagram is shown in **Figure 2**, and all major equipment properties designed by Aspen Plus are presented in **Table 2**. After the adsorption of butanol on the zeolite, butanol is desorbed by hot N_2 gas. For the separation of butanol from the mixture of N_2 and butanol, the gas is chilled to -15°C in a heat exchanger (HX3); the liquid butanol is separated from N_2 gas in a vessel (V1), and then the separated butanol temperature is increased to 20°C and sent to the butanol product storage tank. The specifications, operating conditions, and energy consumption of pumps required for the process are presented in **Table 3**.

- Scenario 1 (Sc1)

All equipment in Sc1 is similar to the base case, except for the method used to separate butanol from the outlet gas in the first adsorber. In Sc1, this separation is accomplished through pressurization and condensation, in contrast to chilling, as in the Base case. The gas pressure is increased from 1 bar to 43.75 bar through a three-stage compression unit. To avoid over-temperature, a cooler and liquid separator are used after each compressor. The equipment properties are provided in **Table 4**, while the rest are similar to those of the Base case, as presented in **Tables 2** and **3**.

- Scenario 2 (Sc2)

Sc2 is founded on direct heating and cooling for adsorption/desorption processes without heat integration. In this scenario, each adsorption column is equipped with a heat exchanger. The desorption of adsorbed chemicals (specifically, butanol in the first adsorber and acetone, ethanol, and water in the second column) takes place by heating the respective column with steam through the internal heat exchangers. The equipment properties are presented in **Table 5**. ABE flash, HX1, and pumps are similar to Sc1.

- Scenario 3 (Sc3)

In Sc3, adsorption is based on direct heating and cooling for adsorption/desorption with heat integration (**Fig. 3**). In this scenario, all equipment and process flow diagrams are similar to Sc2, with the addition of heat integration using Pinch technology. The basis for Pinch technology is provided in the **Supplementary Data**.

- Scenario 4-6 (Sc4-Sc6)

In these scenarios, all equipment and the process flow diagram are similar to Sc2, with the addition of multi-pressure distillation and heat integration using Pinch technology (**Table 6**). The pressure of the first distillation column is set at 0.1, 0.05, and 2 bar in Sc4, Sc5, and Sc6, respectively.

2.6. LCA methodology

Considering ISO 14040 and 14044 standards (ISO 14040; ISO 14044), four distinct phases, i.e., goal and scope definition, life cycle inventory, LCA, and result interpretation, are involved in the LCA. Here, the first two phases are presented, and the last two phases are presented and discussed in the result section.

2.6.1. Goal and scope definition

The goal of this LCA study is to compare the environmental performance of various adsorptive ABE separation methods and identify opportunities for improving their environmental impact. The system boundary is illustrated in **Figure 1**. While the results are intended to support future decision-making, it is anticipated that the decision scope will be limited, leading to minor changes in the background system. Therefore, this study serves as a micro-level decision support analysis. To maintain simplicity, an attributional LCA is employed, following the ILCD Handbook (Joint Research Centre, 2010). The scope involves an attributional gate-to-gate analysis of ABE separation and purification units. It encompasses all energy and material inputs and outputs for the process, starting from receiving fermentation broth from ABE fermenters (based on our previous
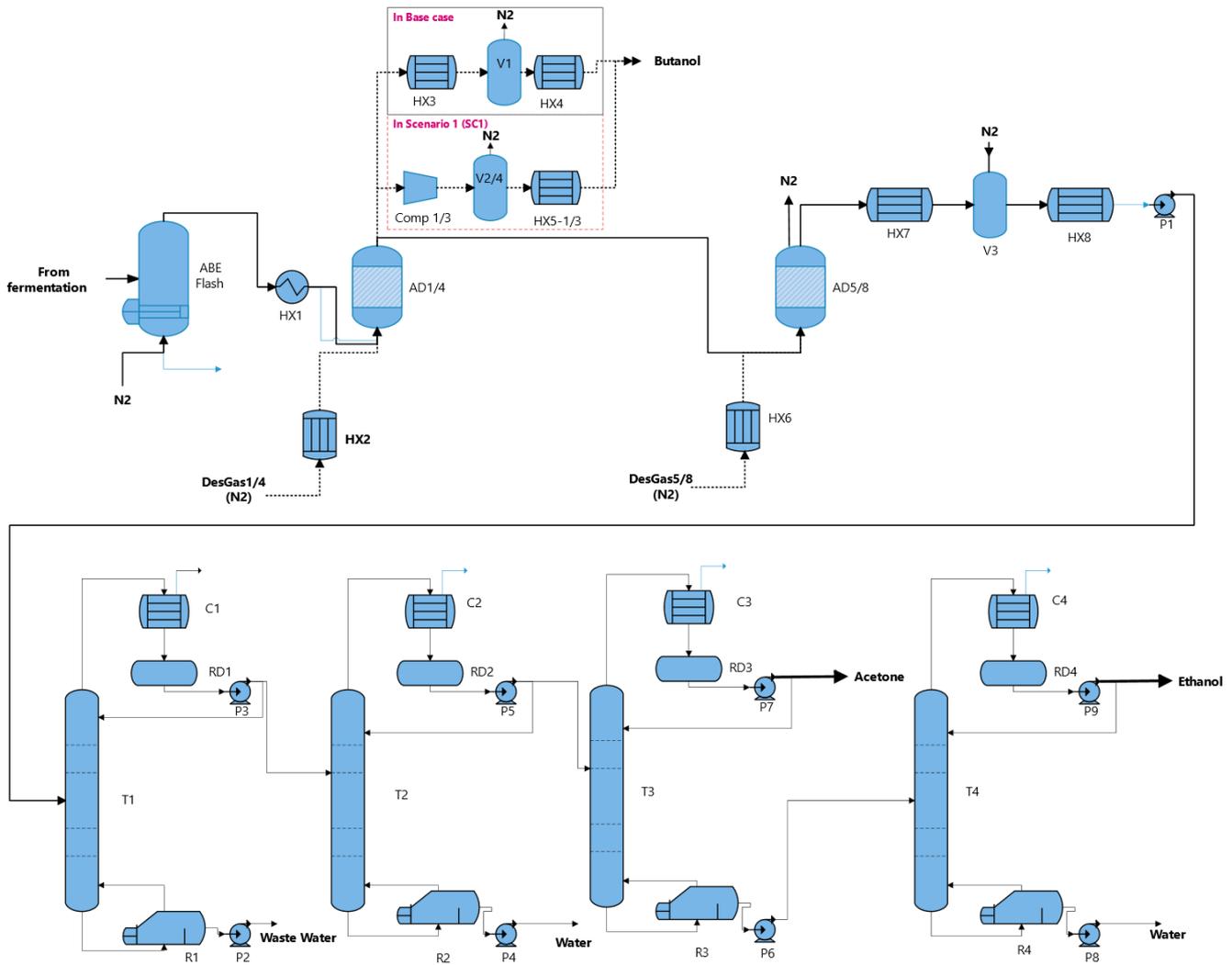
Fig. 2. Process flow diagram for direct heating and cooling adsorption without heat integration (Base case and Scenario 1).

experimental data, Farmanbordar et al., 2018), separating CO_2 and water, and proceeding to purify acetone, butanol, and ethanol (Van der Perre et al., 2017).

In LCA, the environmental impacts of a system are quantified by defining the functional unit, which can be based on various criteria, including energy and mass. Given that the primary aim of this study is to obtain fuel-grade butanol, the functional unit is defined as 1 tonne of purified butanol exiting the system boundary. As the ratio between butanol, ethanol, and acetone remains similar across all scenarios, no allocation was considered in this study.

2.6.2. Life cycle inventory

To conduct an LCA, two types of data are required: background and foreground data. Background data for each scenario was obtained from the Ecoinvent 3 database, while foreground data were obtained from the mass and energy flows of process simulations conducted by Aspen Plus. As the purpose of this study is to compare different separation processes, the system boundary was defined to include the separation of components of the processes (Fig. 1). This boundary encompasses adsorption columns, distillation columns, separation vessels, compressors, and pumps. For comparison purposes, it is assumed that the environmental impacts of

equipment properties, adsorbents, and chemicals are similar for all scenarios. However, capital goods typically have a long lifetime, providing significant services over their lifespan. Hence, the total impact per tonne of products generated or ABE refined is very small. Accordingly, a cut-off approach is considered to exclude the impacts of capital goods.

2.6.3. Electricity data for LCA

Electricity is procured from the grid, utilizing the Belgian average generation mix. A dataset was generated, encompassing electricity inputs produced in Belgium, the transmission network, direct emissions to the air, and electricity losses during transmission (Table 7).

2.6.4. Heat from steam data for LCA

For the heat from steam data, the background information from Ecoinvent 3 (heat from steam in the chemical industry in the European region, APOS, S) was customized to Belgium. The original data in the database represented average data for the European region. Modifications were made using land occupation and water data specific to Belgium, including categories such as lake (natural origin), cooling, turbine use, well, and river.

Table 2.
Equipment specification and process data for direct heating and cooling adsorption without heat integration (Base case) obtained by simulation with Aspen Plus.

Equipment	Purpose	Specification and Operating Conditions	Energy Consumption (W)
ABE flash	Evaporation of ABE from fermentation broth	T inlet= 37°C; T evaporation=80°C; p=1 bar	6.87×10^8
HX1	Cooling the vapor to optimum adsorption temperature (40°C)	Inlet T=80°C; outlet T=40°C; p=1 bar	-4.14×10^7
AD1/4	Adsorption and desorption of butanol in 4 adsorption columns	Adsorption: 40°C; p=1 bar Desorption: 120°C; p=1 bar	Adsorption (40°C): 3.32×10^6; Desorption (120°C): 1.17×10^7; Cooling (120 to 40°C): 5.06×10^6
AD5/8	Adsorption and desorption of acetone/ethanol/water in 4 adsorption columns	Adsorption: 40°C; p=1 bar Desorption: 100°C; p=1 bar	Adsorption (40°C): 5.83×10^8; Desorption (100°C): 1.35×10^9; Cooling (100 to 40°C): 1.83×10^8
HX2	Desorption gas heater	T=20°C to 180°C; p=2 bar	3.13×10^7
Case I- HX3	Butanol and N_2 mixture chilling to condense butanol	T= 109°C to -25°C; p=1 bar	-2.88×10^7
Case I- V1	Liquid butanol separation from N_2 gas	T=-25°C; p= 1 bar	Adiabatic flash (0 W)
Case I- HX4	Heating butanol to ambient temperature	T=-25°C to 20°C; p= 1 bar	4.5×10^5
HX6	Desorption gas heater for second adsorber (AD5/8)	T=20°C to 120°C; p=1 bar	3.14×10^9
HX7	Chilling for separation of acetone and ethanol from desorption gas (N_2)	T=81°C to-40°C, p= 1 bar	4.45×10^9
V3	Separation of N_2 from acetone and ethanol	T=-40°C, p= 1 bar	Adiabatic
HX8	Distillation feed preheater	T=-40 to 20°C; p=1 bar	1.97×10^7
T1	Distillation column	Tray= 20; P=1 bar; Feed tray=5; T top= 61.5°C; T bottom= 99.6°C; boilup ratio: 0.2; Reflux ratio: 8.6	-
C1	Condenser of T1	T= 61.5°C; p= 1bar	2.62×10^7
R1	Reboiler of T1	T=99.6°C; p=1 bar	1.07×10^8
T2	Distillation column	Tray= 20; P=1 bar; Feed tray=2; T top= 59.2°C; T bottom= 92°C; Reflux ratio: 2; Boilup ratio: 4.1	-
C2	Condenser of T2	T= 59.2°C; p= 1bar	4.28×10^6
R2	Reboiler of T2	T=92°C; p=1 bar	4.39×10^6
T3	Distillation column	Tray= 25; P=1 bar; Feed tray=20; T top= 55.9°C; T bottom= 79.4°C; Reflux ratio: 3; Boilup ratio: 4.16	-
C3	Condenser of T3	T= 55.9°C; p= 1bar	3.09×10^6
R3	Reboiler of T3	T=79.4°C; p=1 bar	3.1×10^6
T4	Distillation column	Tray= 30; P=1 bar; Feed tray=15; T top= 77.7°C; T bottom= 95.6°C; Reflux ratio: 10; Boilup ratio: 13.9	
C4	Condenser of T4	T= 77.7°C; p= 1bar	4.66×10^6
R4	Reboiler of T4	T=95.6°C; p=1 bar	4.67×10^6

Table 3.
The specification, operating conditions, and energy consumption of pumps in the base case obtained by simulation with Aspen Plus.

Pump	Purpose	Specification and Operating Conditions	Energy Consumption (Electricity, W)
P1	T1 feed pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 79 J/kg; Fluid power= 5.9×10^4 W	8.6×10^4
P2	T1 bottom product pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 126 J/kg; Fluid power= 6.2×10^4 W	8.8×10^4
P3	T1 distillate pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 0.02 J/kg; Fluid power= 804 W	1.1×10^3
P4	T2 bottom product pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 79 J/kg; Fluid power= 5.9×10^4 W	8.6×10^4
P5	T2 distillate pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 33 J/kg; Fluid power= 667 W	953
P6	T3 bottom product pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 0.3 J/kg; Fluid power= 192 W	274
P7	T3 distillate pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 0.1 J/kg; Fluid power= 484 W	692
P8	T4 bottom product pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 24 J/kg; Fluid power= 39 W	56
P9	T4 distillate pump	Centrifuge pump; p out= 3.5 bar; pump efficiency= 70%; NPSH available= 0.3 J/kg; Fluid power= 153 W	219

Table 4.
Equipment specification and process for butanol recovery from desorbed gas from the first adsorber system obtained by simulation with Aspen Plus.

Equipment	Purpose	Specification and Operating Conditions	Energy Consumption (W)
Case II-Comp 1/3	3 stages compressors	First stage: 1 bar to 3.5 (109°C to 353°C) Second stage: 3.5 to 12.5 bar (30°C to 231°C); Third stage: 12.5 bar to 43.75 bar (30°C to 229°C)	First stage: 9.86×10^7 (Electricity) Second stage: 8.02×10^7 (Electricity) Third stage: 7.87×10^7 (Electricity)
Case II- V2/4	Liquid butanol separation from $_{N2}$ gas	First stage: (30°C, 3.5 bar Second stage: 30°C 12.5 bar Third stage: 30°C, 43.74 bar	Adiabatic flash (0 W)
Case II- HX5-1/3	After compressor cooler	HX5-1: 353°C to 30°C; 3.5 bar HX5-2: 231°C to 30°C; 12.5 bar HX5-3: 229°C to 30°C; 43.75 bar	HX5-1: -1.30×10^8 HX5-2: -8.27×10^7 HX5-3: -8.16×10^7

Table 5.
Equipment specification and process data for indirect heating and cooling adsorption without heat integration (Scenario 2) obtained by simulation with Aspen Plus*.

Equipment	Purpose	Specification and Operating Conditions	Energy Consumption (W)
STCo1**	Cooling water for heat removal during adsorption	Removing heat of adsorption at 40°C by cooling water	-3.32×10^6
	Steam for heating during desorption	Heating for desorption (from 40°C to 120°C) by steam	1.17×10^7
	Cooling water for heat removal after desorption	Cooling the column from 120°C to 40C for the next cycle by cooling water	-5.06×10^6
STCo2**	Cooling water for heat removal during adsorption	Removing heat of adsorption at 40°C by cooling water	-5.83×10^8
	Steam for heating during desorption	Heating for desorption (from 40°C to 100°C) by steam	1.35×10^9
	Cooling water for heat removal after desorption	Cooling the column from 100°C to 40°C for the next cycle by cooling water	-1.83×10^6
HX2	Butanol condenser	T= 120°C to 25°C; p=1 bar	3.32×10^6
T1	Distillation column	Tray= 20; P=1 bar; Feed tray=5; T top= 61.5°C; T bottom= 99.6°C; boilup ratio: 0.2; Reflux ratio: 30.9	-
C1	Condenser of T1	T= 61.5°C; p= 1bar	-8.75×10^7
R1	Reboiler of T1	T=99.6°C; p=1 bar	1.06×10^8
T2	Distillation column	Tray= 20; P=1 bar; Feed tray=2; T top= 59.2°C; T bottom= 92°C; Reflux ratio: 2; Boilup ratio: 4.1	-
C2	Condenser of T2	T= 59.2°C; p= 1bar	-4.28×10^6
R2	Reboiler of T2	T=92°C; p=1 bar	4.39×10^6
T3	Distillation column	Tray= 25; P=1 bar; Feed tray=20; T top= 55.9°C; T bottom= 79.4°C; Reflux ratio: 3; Boilup ratio: 4.16	-
C3	Condenser of T3	T= 55.9°C; p= 1bar	-3.09×10^6
R3	Reboiler of T3	T=79.4°C; p=1 bar	3.1×10^6
T4	Distillation column	Tray= 30; P=1 bar; Feed tray=15; T top= 77.7°C; T bottom= 95.6°C; Reflux ratio: 10; Boilup ratio: 13.9	-
C4	Condenser of T4	T= 77.7°C; p= 1bar	-4.66×10^6
R4	Reboiler of T4	T=95.6°C; p=1 bar	4.67×10^6

*ABE flash, HX1, and pumps are similar to SC1.
** In 4 adsorption columns.

2.6.5. Cooling data for LCA

A counterflow forced draft heavy-duty cooling tower equipped with a centrifugal fan filled with polyvinyl chloride (PVC) is employed to provide the cooling water utility. The foreground data is sourced from a commercial cooling tower offered by Baltimore Aircoil Company (Series V Cooling Tower) (Baltimore Aircoil Company, 2023). The input data for LCA is presented in **Supplementary Data**, **Table S1**. The data for makeup water (water, cooling, Belgium), steel (low-alloyed, Europe without Switzerland and Austria, steel production, APOS, S), PVC (Suspension polymerized, APOS, S), pumps (global, APOS, S), wastewater (average Europe without Switzerland, wastewater, APOS, S), electronics scrap (global, APOS, S), scrap steel (Europe without Switzerland, APOS, S), and PVC (waste treatment, global, recycling of PVC, APOS, S) were utilized. Additionally, for electricity used in the cooling water system (for pumps and fans) (Schulze et al., 2019; Baltimore Aircoil Company, 2023), the data on electricity mix for Belgium (as mentioned in the 2.7.3 section) was incorporated.
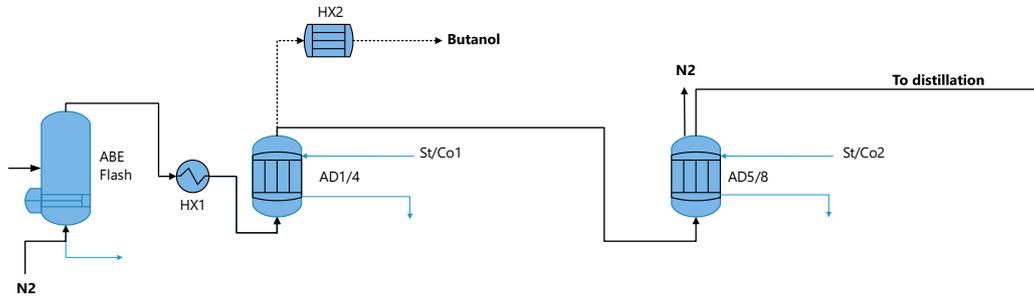
Fig. 3. Process flow diagram of adsorption parts for direct heating and cooling adsorption/desorption without heat integration (Scenario 2) (Distillation parts are similar to Sc1, presented in **Fig. 2**).

Table 6.
Specification and process data in Scenario 4-6 obtained by simulation with Aspen Plus (other equipment that are not mentioned in this table are similar to Sc2, presented in **Table 4**).

Scenario	Equipment	Purpose	Specification and Operating Conditions	Energy Consumption
Sc 4	T1	Distillation column	Tray= 20; P=0.1 bar; Feed tray=5; T top= 11.3°C; T bottom= 45.8°C; boilup ratio: 0.1; Reflux ratio: 212.8	-
	C1	Condenser of T1	T= 11.3°C; p= 0.1bar	-6.48×10^8
	R1	Reboiler of T1	T=45.8°C; p=0.1 bar	5.65×10^7
	T2	Distillation column	Tray= 20; P=1 bar; Feed tray=2; T top= 79.7°C; T bottom= 120.3°C; Reflux ratio: 2; Boilup ratio: 5.2	-
	C2	Condenser of T2	T= 79.7°C; p= 1bar	-4.56×10^6
	R2	Reboiler of T2	T=120.3°C; p=1 bar	5.27×10^6
Sc 5	T1	Distillation column	Tray= 20; P=0.05 bar; Feed tray=5; T top= -0.5°C; T bottom= 32.9°C; boilup ratio: 0.1; Reflux ratio: 211.6	-
	C1	Condenser of T1	T= -0.5°C; p= 0.05bar	-6.62×10^8
	R1	Reboiler of T1	T=32.9°C; p=0.05bar	5.7×10^7
Sc 6	T1	Distillation column	Tray= 20; P=0.1 bar; Feed tray=5; T top= 80.9°C; T bottom= 120°C; boilup ratio: 0.1; Reflux ratio: 212.8	-
	C1	Condenser of T1	T= 80.9°C; p= 0.1bar	-5.67×10^8
	R1	Reboiler of T1	T=120°C; p=0.1 bar	5.2×10^7
	T2	Distillation column	Tray= 20; P=1 bar; Feed tray=2; T top= 79.7°C; T bottom= 109.3°C; Reflux ratio: 2; Boilup ratio: 4.1	-
	C2	Condenser of T2	T= 79.7°C; p= 1bar	-4.3×10^6
	R2	Reboiler of T2	T=109.3°C; p= 1 bar	4.39×10^6

2.6.6. Chilling data for LCA

The background data for the absorption chiller operated with heat from a natural gas cogeneration unit, initially modeled for the rest of the world (APOS, S), was modified and utilized. The modification involved specifying Belgian data for land occupation and water (lake, natural origin, cooling, turbine use, well, and river), along with electricity data in Belgium.

2.6.7. Life cycle impact assessment methodology

To convert inventory data into potential environmental impacts for all scenarios, the ReCiPe Endpoint and Midpoint methods, modified by SimaPro 9.4 in 2022, were employed. ReCiPe is an advanced method developed by Radboud University, the Norwegian University of Science and Technology, and PRé Sustainability (Huijbregts et al., 2017). This method assesses a comprehensive set of midpoint environmental impacts (18 indicators) and categorizes them into three endpoint group impacts on human health, resource depletion, and ecosystem (Lamnatou et al., 2018; Hosseini et al., 2022). The assessment of human health employs the disability-adjusted life years (DALY) metric, which gauges the overall societal impact of disease or injury, considering both premature death and disability resulting from specific conditions or risk factors. Additionally, resource depletion, encompassing minerals, fossil fuels, and water, serves as a vital aspect of sustainable development, evaluated through its economic

impact by assessing the cost of natural resource consumption. In evaluating ecosystem damage, environmental impacts are quantified concerning habitat destruction, pollution, and climate change, using a unit of 100 species loss per year.

Normalization of midpoint impacts was carried out based on the average share of all emissions and resource use in the world during one year per person. Weighting was also applied to aggregate the different environmental impacts of scenarios into a single value based on their relative importance, facilitating the comparison of the total environmental impact of scenarios (Muhl et al., 2023).

3. Results and Discussion

The various processes for adsorptive-based ABE separation (including the base case and all scenarios) were simulated using Aspen Plus, and the required utilities were assessed. Subsequently, energy targeting was carried out using Pinch technology and multi-pressure distillation. The utilities were then utilized for LCA analysis in Simapro to assess the environmental impacts of each scenario. The results are presented and discussed here.

3.1. Energy consumption in each scenario

The energy required for each scenario, based on the recovery of 120,000 tonnes of butanol per year, was evaluated using Aspen Plus simulation.

Table 7.
Data for LCA analysis of 1 KW electricity in Belgium.

Input/output to Technosphere		Values in 2022*	Background Data Description Used in Simapro
Electricity	Nuclear	47.3%	Nuclear, pressure water reactor, Belgium, APOS, U
	Gas	26.9%	Natural gas, combined cycle power plant, Belgium, APOS, U
	Off-shore	7.5%	Wind, 1-3MW turbine, offshore, Belgium, APOS, U
	On-shore	5.0%	Wind, 1-3MW turbine, onshore, Belgium, APOS, U
	Solar	7.3%	Photovoltaic, 3kWp slanted-roof, multi-Si, panel, Belgium, APOS, U
	Biogas	2.4%	Heat and power co-generation, biogas, gas engine, Belgium, APOS, U
	Blast furnace gas	1.35%	Treatment of blast furnace gas, in power plant, Belgium, APOS, U
	Wood chips	1.41%	Heat and power cogeneration, wood chips, Belgium, APOS, U
	Oil	0.01%	Electricity from oil, Belgium, APOS, U
	Hydro	0.20%	Hydroelectricity, run-of-river, Belgium, APOS, U
	Hydro	0.63%	Hydroelectricity, pumped storage, Belgium, APOS, U
Transmission		$6,58\times10^{-9}$ km	Transmission network, market, APOS, U
		$3,17\times10^{-10}$ km	Transmission network, long-distance, construction, APOS, U
Emission to air	Dinitrogen monoxide	$5,0\times10^{-6}$ kg	Ecoinvent 3 database
	Ozone	$4,16\times10^{-6}$ kg	Ecoinvent 3 database

* Data obtained from www.elia.be, Belgium's 2022 electricity mix, 06 January 2023.

Subsequently, the utility amounts in Wh were calculated based on 8,500 operating hours per year, as reported in **Table 8**. The base case is centered on typical adsorption/desorption, utilizing experimental data obtained in our laboratory (Van der Perre et al., 2017; Claessens et al., 2020b), followed by conventional distillation. Based on simulation results, the amount of heat required for the separation of 120,000 tonnes of butanol per year is 5.34×10^{9} W, provided by medium-pressure steam (175°C). Considering 8,500 operating hours per year, the amount of heat per tonne of butanol is 3.78×10^{8} Wh, and the required cooling energy is 3.79×10^{8} Wh, provided by cooling water.

Table 8.
Utility consumption for purification of each tonne of butanol for all separation scenarios provided by Aspen Plus simulation.

Scenario	Total Required Heat (Wh)	Cooling Energy (Wh)	Chilling Energy (Wh)	Electricity (Wh)
Base case	3.78×10^{8}	3.79×10^{8}	3.17×10^{8}	1.86×10^{4}
Sc1	3.78×10^{8}	3.77×10^{8}	3.15×10^{8}	1.83×10^{7}
Sc2	1.53×10^{8}	6.40×10^{8}	-	1.86×10^{4}
Sc3	1.59×10^{7}	5.02×10^{8}	-	1.86×10^{4}
Sc4	1.69×10^{7}	1.69×10^{7}	4.59×10^{7}	1.86×10^{4}
Sc5	1.03×10^{7}	4.94×10^{8}	4.71×10^{7}	1.86×10^{4}
Sc6	8.49×10^{6}	5.33×10^{8}	-	1.86×10^{4}

N_2 is employed for the desorption of adsorbed butanol from the first adsorption column; thus, a mixture of N_2 and butanol exits the adsorption column. For the separation of butanol from N_2, chilling is required. Additionally, for the desorption of acetone and ethanol from the second adsorption column, chilling is required. In total, 3.17×10^{8} Wh of chilling energy is needed for the separation of each tonne of butanol. Electricity is mainly required for liquid pumping (1.86×10^{4} Wh), and the electricity for lightning and system control, which is negligible compared to electricity used in processing (i.e., pumping) (Peters et al., 2002), is ignored. Ebrahimian et al. (2023) studied the LCA of biofuel production from municipal solid waste and showed that for the separation of each tonne of

butanol by distillation, 2.5×10^{6} Wh electricity and 5.7×10^{6} Wh heat are required, neglecting cooling energy for purification.

In Sc1, heating energy, cooling energy, chilling energy, and electricity are 3.78×10^{8}, 3.77×10^{8}, 3.15×10^{8}, and 1.83×10^{7} Wh, respectively. The main difference between this case and the base case is related to the separation of butanol from the butanol and nitrogen vapor mixture after desorption (**Fig. 2**). In Sc1, where N_2 and butanol are separated by compression and condensation (without chilling), the amount of electricity consumption is higher compared to the base case (due to employing a 3-stage compressor), while slightly higher energy for chilling is required in the first case based on chilling. It is worth mentioning that for the separation of N_2, acetone, and butanol from the desorption of the second adsorption column, it is not possible to use compression due to the presence of high amounts of water; thus, chilling is used (HX7, **Fig.2**). In Sc2, based on direct heating and cooling adsorption/desorption without heat integration, the heating energy, cooling energy, and electricity are 1.53×10^{8}, 6.40×10^{8}, and 1.86×10^{4} Wh, respectively. Comparing Sc1 and Sc2 indicates that direct heating and cooling adsorption/desorption can significantly reduce energy consumption.

Sc3 is similar to Sc2, with heat integration using Pinch technology. **Figure S1** shows the optimized heat exchanger network for Sc3. The heat that should be removed during the desorption in the second adsorber ($STco_2$, which is 8.3×10^{9} W) is used to heat ABE flash; the heat needed for heating the first adsorption column desorption ($STco_1$, 1.17×10^{7} W), heat needs for heating during desorption of the second adsorption column ($STco_2$, 1.35×10^{9} W), and duty of T2 and T4 reboilers. As a result, the heat and cooling energies are reduced to 1.59×10^{7} and 5.02×10^{8} Wh, respectively. The pressure of the first distillation column significantly affects the separation energy demand (Chen et al., 2018). Thus, the pressure of the first distillation column is set to 0.1, 0.05, and 2 bar in Sc4, Sc5, and Sc6, respectively, while all equipment and process flow diagrams are similar to Sc2. Decreasing the pressure of T1 to 0.05 bar (Sc4) reduces the heat and cooling water required for the process; however, the processes need significant amounts of chilling energy ($>4\times10^{7}$ W). Increasing the pressure to 2 bars significantly reduces (8.49×10^{6} W) the heat required for the process, while cooling energy is reduced, and no chilling is required.

Overall, ABE separation is a high-energy-demanding process. Compared with distillation, the energy required for adsorptive separation is lower. One suggested solution is a fermentation–pervaporation integration process to increase the butanol concentration to over 190 g/L before sending it to the separation process (Chen et al., 2018). In that case, the energy for the

separation of each tonne of butanol can be decreased to 1.5×10^6 W; however, the integration of pervaporation to such high-capacity fermenters is costly and challenging. Meng et al. (2019) conducted a life cycle assessment based on the simulation of butanol and ethanol production processes from municipal solid waste. They used distillation for butanol purification. For gas stripping and distillation of each tonne of butanol, 3.9 Wh heat is required.

3.2. Energy saving by Pinch technology

In this study, employing Pinch technology (Sc2 vs. Sc3) results in a decrease of 89.6% in the steam and 21.6% in the cooling water required for the process. Overall, it saves around 35% of the total heating and cooling energy. Pinch technology is widely used for energy saving in distillation. In some studies, Pinch analysis could not help save high amounts of energy. For instance, Pavão et al. (2023) investigated heat integration of the ethanol production process, including a 4-column distillation system for the separation and purification of ethanol, to obtain a suitable heat exchanger network *via* the Pinch-based method. They showed that using a proper heat exchanger network, only 17% heat saving for the plant is possible, which is considerable at high-capacity plants.

In some studies, Pinch analysis has shown significant energy-saving effects. For example, Salina et al. (2021) used pinch technology for heat integration of a process to add fast pyrolysis of sugarcane into conventional ethanol production. Pinch analysis could help to reduce hot utility consumption by 56.0%. In another study, Fujimoto et al. (2011) studied the heat integration of bioethanol production from lignocelluloses and separation by distillation. Using Pinch analysis, they could decrease plant steam consumption by 66%.

Besides distillation, Pinch analysis could help save energy for the whole process and other separation processes than distillation. Petersen et al. (2015) compared fermentation-based processes for liquid biofuels from sugarcane bagasse with thermochemical processes (i.e., gasification and Fischer-Tropsch synthesis). They also used pinch technology for energy optimization and evaluated LCA. They showed that pinch could reduce energy consumption by around 28–30% and 37% for fermentation-based and thermochemical processes, respectively. Mailaram and Maity (2022) compared dual liquid-liquid extraction with distillation for butanol separation. While liquid-liquid extraction requires higher capital investment and is more complex compared to distillation, it is less energy-intensive. They used pinch technology for heat integration and showed that it is possible to reduce the energy consumption of the process based on lignocellulosic butanol production by 62% for distillation and 35% for liquid-liquid extraction using Pinch technology.

3.3. Multi-pressure distillation

Among the distillation columns, the first distillation column (T1) consumes the highest cold and hot utilities. The reboiler duty of T1 is 1.07×10^8 W, far higher than the duties of T2 (4.39×10^6 W), T3 (3.1×10^6 W), and T4 (4.67×10^6 W) (Base case, **Table 2**). For the condenser, T1 also has the highest cooling water demand.

Previously, it was found that the pressure of the first distillation column could significantly affect the energy demand of the whole separation system (Chen et al., 2018). As a matter of fact, decreasing the pressure can help evaporation and decrease the duty of reboilers. Thus, 0.1 bar (Sc4) and 0.05 bar (Sc5) could be selected to investigate the effect of lowering the pressure on the energy needed for the separation. However, decreasing the pressure in distillation means decreasing the column temperature (both condenser and reboiler). For instance, when the pressure of the first distillation column is decreased to 0.1 bar, the temperature of the condenser and reboiler are decreased to 11.3 and 45.8°C, respectively (Sc4). Further decreasing the pressure to 0.05 bar results in lower corresponding temperatures of -0.5 and 32.9°C (Sc5). Two issues now arise. The primary challenge arises from the fact that the condenser cannot be cooled by regular cooling water, as it requires cooling below 30°C. Therefore, it necessitates chilling water, as chillers are more energy-intensive and costly compared to cooling towers (Peters et al., 2002). The second issue is decreasing the temperature, since when the condenser temperature is very low (11.3°C in Sc4 and -0.5°C in

Sc5), the energy of the condenser cannot be used for heating the other process parts.

On the other hand, by increasing the first distillation column pressure, it is possible to increase the condenser temperature and use the condenser duty as a source of heating. In Sc6, the pressure is set to 2 bar, and consequently, the temperatures of the condenser and reboiler are increased to 80.9 and 120°C, respectively. The reboiler can be heated by low/medium pressure steam or the energy of any stream that has a temperature higher than 120°C. The energy of the condenser is hot enough (80.9°C) to heat the other part of the process. Thus, decreasing/increasing the pressure of the first distillation column has positive and negative effects on the energy consumption of the whole process. To further investigate its effect, first heat integration and then LCA are required.

3.4. LCA results

The inventory data, including total required heat, cooling energy, chilling energy, and electricity for all scenarios used in LCA, are depicted in **Table 8**. The life cycle inventories were converted to life cycle impact scores on the midpoint and endpoint levels using ReCiPe 2016, as shown in **Table 9**, **Figures 4** and **5**, and **Supplementary Data** (**Tables S3** and **S4**). This method implements the main three areas of protection factors: human health, ecosystem quality, and resource scarcity. The endpoint factors are derived from the 17 midpoint impact categories with a constant mid-to-endpoint factor (Huijbregts et al., 2017). In terms of human health, Sc6 and Sc1 exhibit the lowest and highest impacts, registering 0.1 and 8.7 DALY, respectively. The impacts of different scenarios on the ecosystem are also evaluated, with Sc6 showing the lowest ecosystem damage of 100 species loss per year. Moreover, there is a significant difference between the lowest and highest resource depletion among the scenarios. The lowest resource depletion of 4×10^{-4} belongs to Sc6, demonstrating that energy optimization had a significant effect on natural resource consumption.

Table 9.
Data for LCA analysis of 1 KW electricity in Belgium

Scenario	Human Health	Ecosystem Damage	Resources Depletion
	DALY	Species Loss Per Year ($\times 10^3$)	USD ($\times 10^{-3}$)
Base case	8.6	7.8	25.7
Sc 1	8.7	7.9	26.0
Sc 2	1.5	1.8	6.5
Sc 3	0.2	0.2	0.7
Sc 4	0.9	0.7	1.8
Sc 5	0.9	0.7	1.6
Sc 6	0.1	0.1	0.4

Brito and Martins (2017) conducted a life cycle assessment for ABE production from corn, emphasizing that the highest impact of the process relates to ecosystem quality rather than human health and resource depletion. Mahmud and Rosentrater (2020) evaluated the LCA of adsorptive separation of ABE, focusing on single-stage butanol adsorption using activated carbon as an adsorbent. They showed that the ecotoxicity impact of this adsorptive separation is less than that of the separation of butanol by liquid-liquid extraction while having a higher global warming potential.

The key performance indicator prioritization technique (kPt) is a method used to identify and prioritize the most important environmental impact categories or indicators within an LCA study. kPt for endpoint impacts, presented in **Figure 4**, indicates that human health and resource depletion are the most and least effective of all separation processes, respectively. The minimum endpoint impacts are observed for Sc6, with values of 0.5 kPt for human health, 0.02 kPt for ecosystems, and 0.003 kPt for resources. These findings align with the results reported by Brito and Martins (2017), who obtained values of 0.5 kPt for human health, 1 kPt for ecosystem quality, and 0.25 kPt for resource impacts in ABE production from corn, using IMPACT 2002+ for impact assessment.

The major environmental impacts of the scenarios at the midpoint level are human non-carcinogenic toxicity, global warming (human health), human carcinogenic toxicity, global warming (terrestrial ecosystems), marine ecotoxicity, fine particulate matter formation, and fossil resource scarcity (**Fig. 5**). Human non-carcinogenic toxicity, i.e., the potential
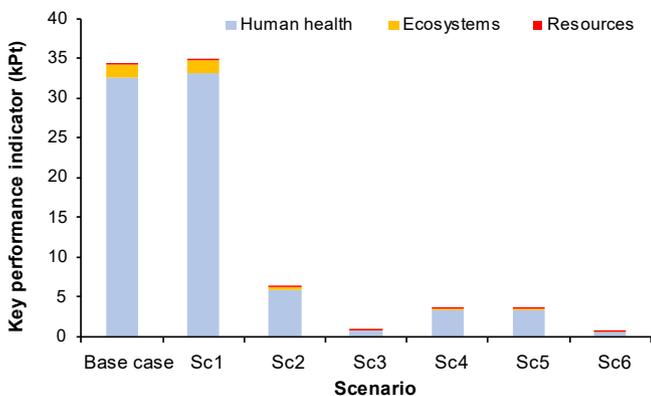
Fig. 4. Key environmental performance indicators for endpoint impacts.

adverse effects on human health not related to cancer, is identified as the most serious effect of the separation scenarios. The human non-carcinogenic toxicity of the base case is 17.5 kPt, which is reduced to 0.3 kPt and 0.2 kPt for Sc3 and Sc6, respectively. These results align with those presented by Wu et al. (2019) for ABE production from microalgae using distillation without heat integration. Their study indicates that among the 17 categories of LCA impacts analyzed by ReCiPe endpoint scores, human health damage due to climate change is approximately 20 kPt.

Despite the notable successes demonstrated in this study, certain limitations should be acknowledged. Firstly, the simulation model, while powerful, relies on certain assumptions and simplifications that may not perfectly represent the complexity of real-world processes. Utilizing pilot-scale data is suggested to improve the accuracy and reliability of the results. The study also focuses on the technological aspects of biobutanol separation, leaving out potential social and economic considerations. Additionally, implementing a parametric study could further enhance the understanding of the optimal conditions for adsorptive separation. These limitations highlight the need for further research, including experimental validation at the pilot scale and a more comprehensive consideration of the broader socio-economic context, to ensure the robustness and applicability of the findings in real-world scenarios.

3.4.1. Normalization and sensitivity analysis

Since the best results are achieved for Sc6, the contribution of damage vsources, namely heating, cooling, and electricity consumption, is monitored, followed by normalization of midpoint impacts. The results are presented in **Table S7** of the **Supplementary Data**. A sensitivity analysis was conducted to assess the impact of deviations of 5%, 10%, and 30% in the amount of consumed energies on the normalized endpoint impacts (see **Fig. 6**). It should be noted that the accuracy of process parameter calculations, including heating, cooling, and electricity consumption, may have deviations ranging from 5% to 30% (Peters et al., 2002).

The sensitivity of normalized endpoint environmental impacts to variations in heating, cooling, and electricity consumption in Sc6 is presented in **Table S7** of the **Supplementary Data**. The results show that among the damage sources, heating energy and electricity consumption had the highest and lowest effects, respectively. Thus, the impact is highly sensitive to changes in heating energy consumption, and the primary impact is on human health. Moreover, the sensitivity of global warming to these changes is evaluated (**Fig. S5**, **Supplementary Data**). The results indicate that heating has a critical impact on the global warming potential of the process. The findings align with those of a previous study by Ebrahimain et al. (2023), which indicated that ABE production's detrimental impacts are particularly sensitive to heat and electricity consumption in the process. Their research highlighted human health and resources as the most affected damage categories. According to their results, a 10% increase in electricity consumption resulted in a 22% rise in environmental impacts within the human health category, surpassing the impact of a 10.1% increase in electricity consumption on human health in this study.

4. Conclusions and Future Perspectives

The present study demonstrates a significant reduction in the energy requirements of the adsorptive separation process. Processes such as evaporation, adsorption, desorption, and distillation necessitate substantial amounts of heating, cooling, chilling, and electricity, with pumping energy being negligible in comparison. Pinch technology proves to be instrumental in markedly decreasing the energy needed for separation. The results offer perspectives for developing a sustainable separation process that prioritizes human and environmental well-being while minimizing resource depletion. In summary, this research outlines a sustainable approach to biobutanol separation based on adsorption, emphasizing the importance of energy conservation.
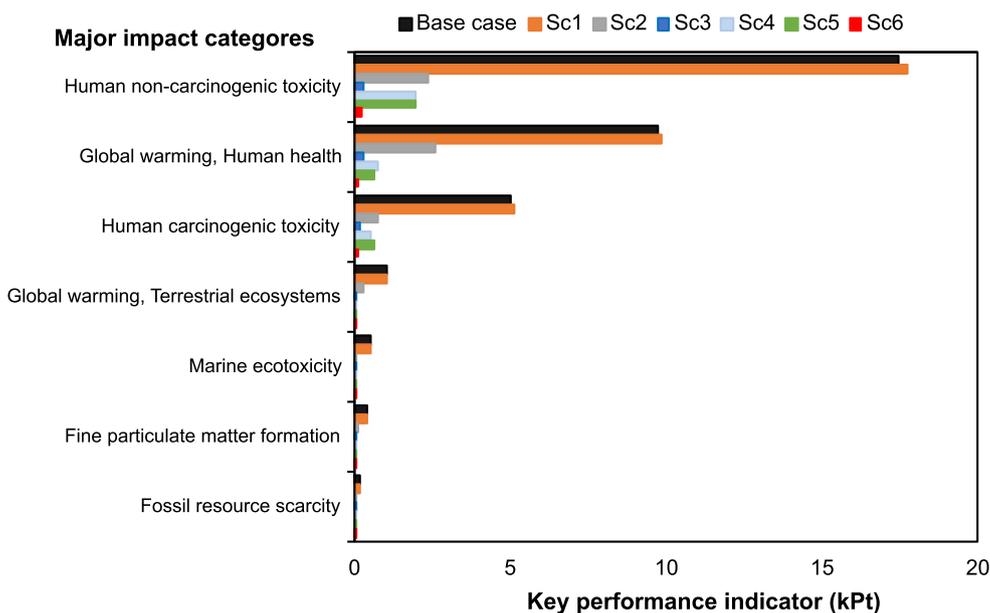

Fig. 5. Key environmental performance indicators for major midpoint categories.
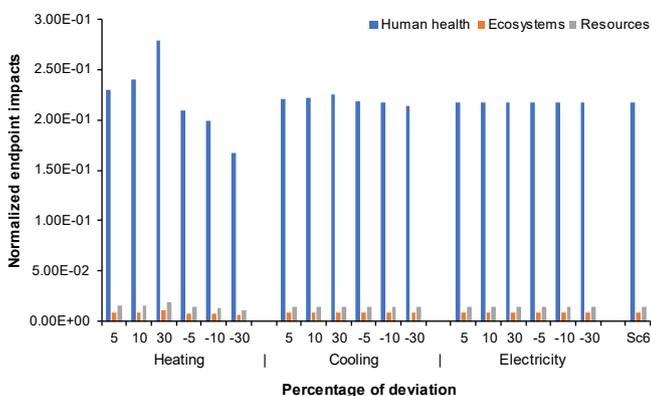
Fig. 6. Sensitivity of normalized endpoint environmental impact to variations in heating, cooling, and electricity consumption in Sc 6 (the best environmentally friendly scenario with minimum energy consumption).

Among the six scenarios evaluated and compared with the base case (typical adsorption/desorption process without heat integration), multi-pressure distillation with the first column pressurized to 2 bar demonstrates the lowest energy and environmental impacts, particularly on human non-carcinogenic toxicity and global warming. Reducing the first column pressure, typically in such distillation systems, could not contribute to reducing the heat required for the process. Implementing energy-saving measures through Pinch technology significantly enhances the environmental sustainability of ABE separation. Human health, ecosystem damage, and resource depletion have decreased from 8.6, 0.0078, and 25,700 to 0.1 (DALY), 0.0001 (Species loss per year), and 400 USD, respectively. Thus, this study establishes a crucial foundation for future investigations into the development of sustainable and environmentally friendly ABE separation technologies.

The practical implications of this study extend beyond biobutanol separation, encompassing biofuels and biochemicals. The adoption of adsorptive separation, especially with the innovative 2-column zeolite-based process, provides a promising alternative to traditional distillation methods. These findings underscore the significance of energy targeting, not only in curbing energy consumption but also in advancing the sustainability of adsorptive biobutanol separation. Future studies may focus on investigating potential social implications, including job opportunities, associated with adsorptive separation followed by a heat-integrated multi-pressure distillation system.

Acknowledgments

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Prof. Keikhosro Karimi is a luminary in the realm of bioprocess and process development, boasting a rich scholarly portfolio that includes over 250 peer-reviewed journal papers, 10 book chapters, and over 100 conference papers. With a substantial h-index of 75 and cumulative citations surpassing 20,000 on Google Scholar, he stands as a distinguished figure in his field. His recognition extends globally, acknowledged as one of the Worldwide Highly Cited Researchers by Web of Science (2020-2023) and among the World's Top 1% Scientists by Clarivate (2022). In his role as an educator and mentor, he has supervised five postdocs, 20 Ph.D., and 35 MSc students, demonstrating his commitment to nurturing the next generation of researchers. Dr. Karimi has also spearheaded an Industrial Biotechnology Group at IUT, where he led various initiatives, including idea development, proposal preparation, fund acquisition, programming, project planning, and management across 14 impactful projects. His research profile is available at Google Scholar.

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Supplementary Data

Calculation of Plant Capacity

Belgium's largest ethanol plant, BioWanze, Wanze, Wallonia, Belgium, annually produces 300,000 m^3. Ethanol is primarily used as a biofuel additive for gasoline. However, butanol is seen as a more sustainable alternative to ethanol. In this study, the possibility of modifying the fermentation capacity of the plant to produce butanol was explored. This approach is a widely accepted concept, previously explored by British Petroleum and Dupont (Butamax, 2019). The yield of ethanol production is 0.48 g ethanol per g consumed sugar, while 0.25 is the typical butanol yield (g butanol/g consumed sugar) (Amiri and Karimi, 2019).

The following relation was used to calculate the BioWanze plant capacity for biobutanol production:

Butanol production capacity = 300,000 (m^3 ethanol/year) / 0.789 (ethanol density, m^3/ton) × 0.25 (g butanol/g sugar) / 0.48 (g ethanol/ g sugar) ≈ 120,000 (tons/year)

For the concentration of acetone, butanol, and ethanol, as well as amounts of acetone and ethanol, experimental data conducted by Farmanbordar et al. (2018) were used.

Pinch Technology Heat Exchanger Networks (Grid Diagrams)
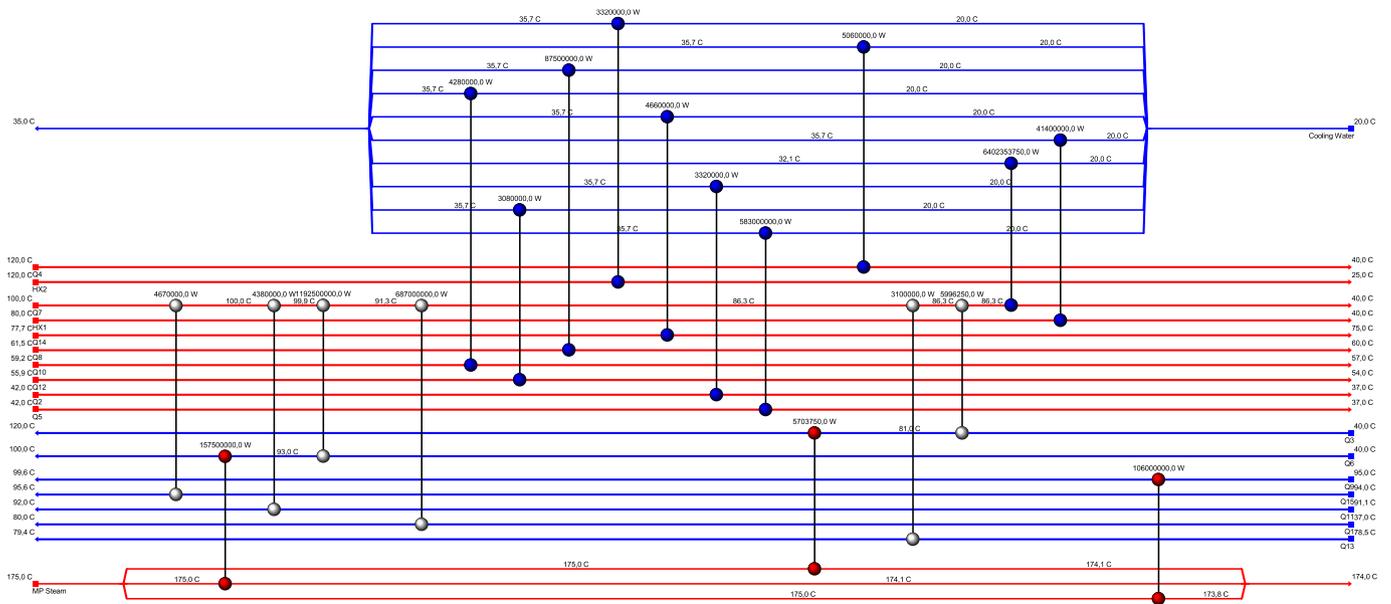
Fig. S1. Grid diagrams for Sc3.
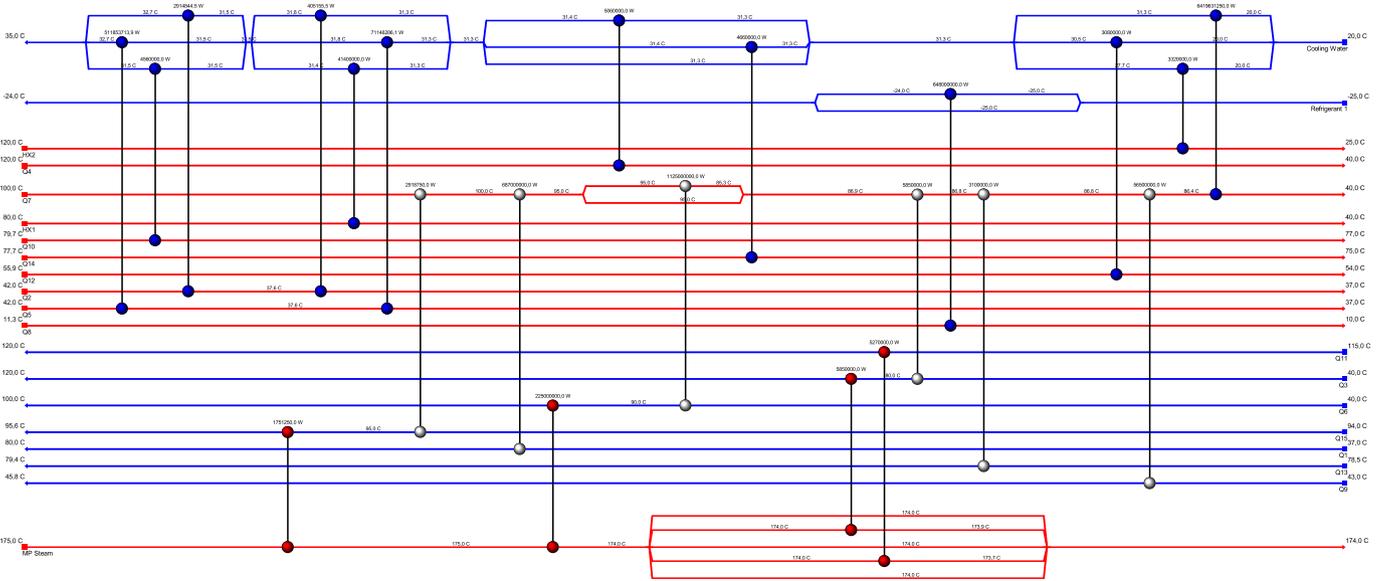
Fig. S2. Grid diagrams for Sc4.
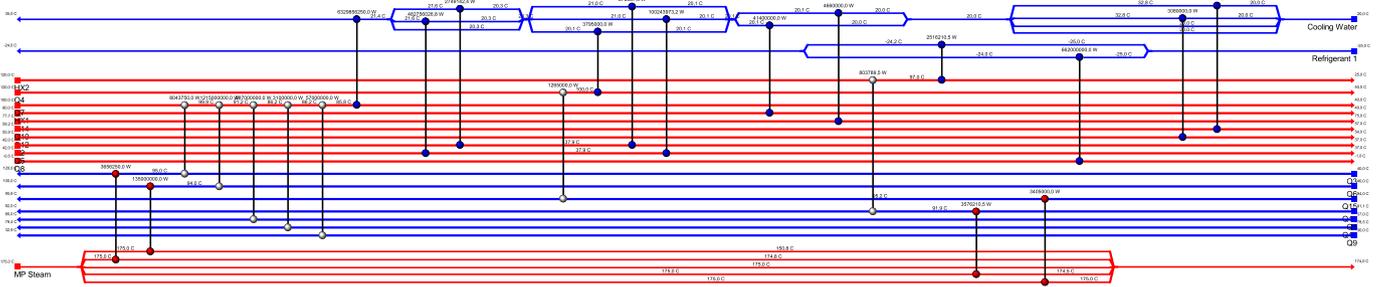
Fig. S3. Grid diagrams for Sc5.
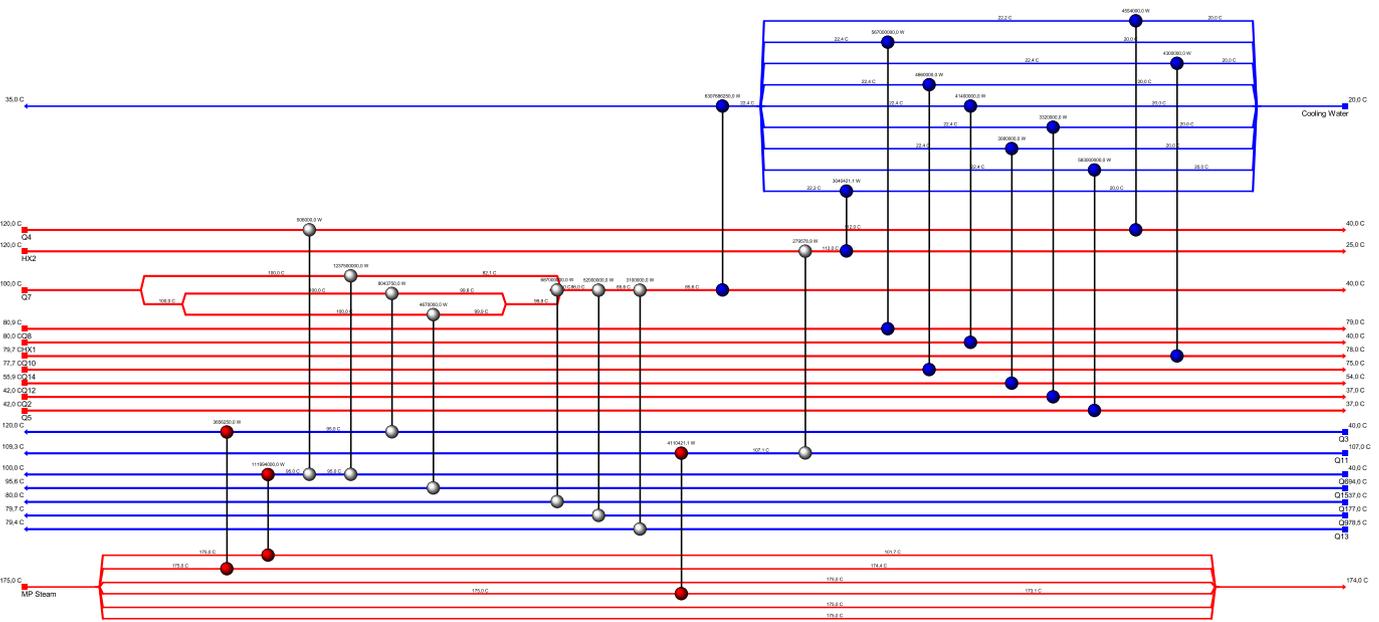
Fig. S4. Grid diagrams for Sc6

The sensitivity of total global warming, including human health, terrestrial ecosystems, and freshwater ecosystems global warming, to variations in heating, cooling, and electricity consumption in Sc 6 are calculated and presented in **Figure S5**.
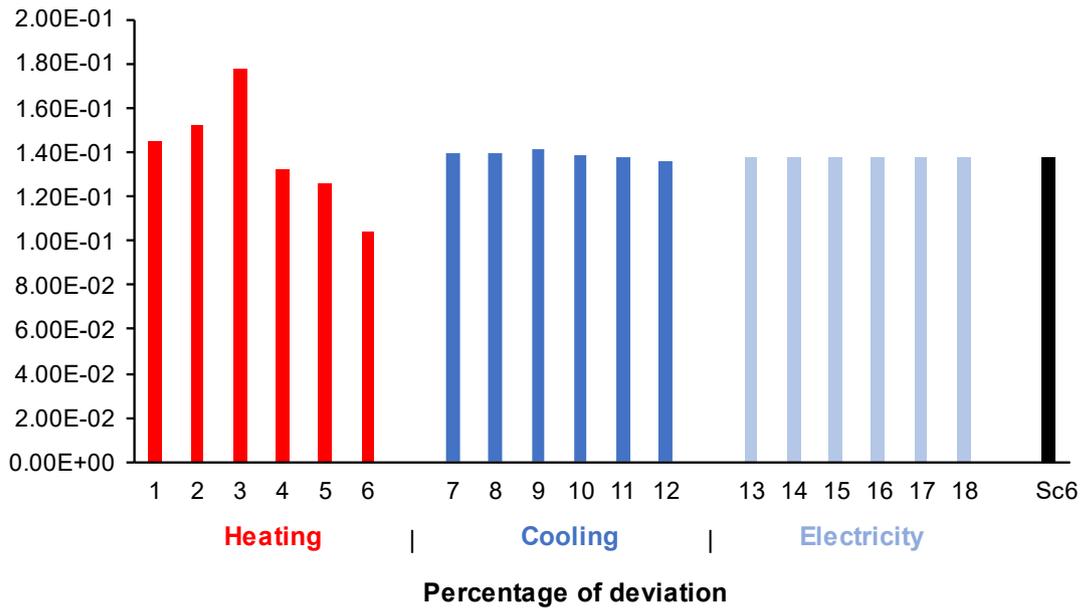
Fig. S5. Sensitivity of normalized global warming potential to variations in heating, cooling, and electricity consumption in Sc 6 (the best environmentally friendly scenario with minimum energy consumption)

**Cooling tower data for LCA**

A counterflow-forced draft cooling tower with a centrifugal fan is used to provide the cooling water utility. Data from a commercial cooling tower from BAC is used. The cooling tower is a heavy-duty system with a fan drive and is filled with polyvinyl chloride (PVC). The input data for LCA are presented in **Table S1**.

Table S1.
Data for LCA analysis of 1 KW electricity in Belgium (Schulze et al., 2018 and 2019; Baltimore, 2023).

Life cycle stage	Objective	Amount	Unit
Manufacturing and raw materials	Stainless steel	850	kg
	PVC	192.3	kg
	Pumps (2, 18kW electric motors)	600	kg
	Fan (5 kW, electric motor)	135	kg
Usage	Fresh water consumption	63740000	kg
	Electricity consumption	864	Wh
	Blowdown water	21246000	kg
End of life	Electric scrap (2 pumps+1 fan)	735	kg
	Stainless steel scrap	850	kg
	Waste PVC	192.3	kg

Adsorption column data

The first adsorption column is packed with LTA-type zeolite monolith, and the second is packed with CHA-type zeolite monolith. The properties are presented in **Table S2**.

Table S2.
Adsorption column properties (Van der Perre et al., 2017; Liu et al., 2019).

Adsorption Column	Property	Amount	Unit
First adsorption column	Superficial velocity	5	m/s
	Total gas volume flow rate	984	m^3/s
	Area	196.8	m^2
	Zeolite adsorption capacity for butanol	0.108	kg butanol/kg zeolite
	Bulk density	0.684	kg/L
	Amount of zeolite	308	m^3
	Heat capacity of zeolite	0.9	J/g.C
Second adsorption column	Superficial velocity	5	m/s
	Total gas volume flow rate	9904	m^3/s
	Zeolite adsorption capacity for water	0.25	kg water/kg zeolite
	Bulk density	0.684	kg/L
	Amount of Zeolite	15,014	m^3
	Heat capacity of zeolite	0.9	J/g.C

Table S3.
Midpoint damage categories for human health and resource depletion.

Impact Category	Unit	Base case	Sc1	Sc2	Sc3	Sc4	Sc5	Sc6
Global warming, Human health	DALY	2.554819	2.5788607	0.6861848	0.073265	0.200817	0.176728	0.040308
Stratospheric ozone depletion	DALY	0.0001313	0.00013647	2.45E-05	3.56E-06	1.32E-05	1.36E-05	2.51E-06
Ionizing radiation	DALY	0.0001639	0.00027706	4.48E-05	5.42E-06	1.30E-05	1.20E-05	3.36E-06
Ozone formation, Human health	DALY	0.0002345	0.00023719	6.46E-05	7.30E-06	1.81E-05	1.63E-05	4.25E-06
Fine particulate matter formation	DALY	0.1123255	0.11309934	0.0281409	0.003217	0.009388	0.008677	0.001896
Human carcinogenic toxicity	DALY	1.3145121	1.3532704	0.2079664	0.045579	0.145569	0.16761	0.038915
Human non-carcinogenic toxicity	DALY	4.5730245	4.6511313	0.6232909	0.085437	0.513821	0.52248	0.058184
Water consumption, Human health	DALY	-0.000706	-0.0005812	-0.0009239	-0.00077	-5.94E-05	-0.0008	-0.00082
Mineral resource scarcity	USD	76.615396	80.105645	5.3934737	1.324514	9.974281	10.87067	1.171751
Fossil resource scarcity	USD	25658.415	25920.803	7120.9871	751.6582	1957.88	1694.518	408.41

Table S4.
Midpoint damage categories for ecosystem damage (Species loss per year).

Impact Category	Base case	Sc1	Sc2	Sc3	Sc4	Sc5	SC6
Global warming, Terrestrial ecosystems	0.0051094	0.00515749	0.0013723	0.000147	0.000402	0.000353	8.06E-05
Global warming, Freshwater ecosystems	1.39E-07	1.41E-07	3.74E-08	4.00E-09	1.10E-08	9.64E-09	2.20E-09
Water consumption, Terrestrial ecosystem	-1.42E-06	-6.58E-07	-1.39E-06	-1.34E-06	-1.91E-07	-1.52E-06	-1.44E-06
Water consumption, Aquatic ecosystems	2.85E-09	2.88E-09	-2.40E-10	-2.07E-10	4.22E-10	2.33E-10	-2.21E-10
Ozone formation, Terrestrial ecosystems	3.42E-05	3.46E-05	9.39E-06	1.06E-06	2.66E-06	2.39E-06	6.17E-07
Terrestrial acidification	0.0001001	0.00010072	2.81E-05	3.19E-06	7.63E-06	6.85E-06	1.87E-06
Freshwater eutrophication	2.39E-05	2.42E-05	5.86E-06	1.14E-06	2.16E-06	2.56E-06	9.30E-07
Marine eutrophication	6.81E-09	7.10E-09	5.62E-09	3.96E-09	5.28E-10	4.21E-09	4.17E-09
Terrestrial ecotoxicity	6.50E-06	6.59E-06	1.09E-06	1.27E-07	6.75E-07	6.58E-07	7.61E-08
Freshwater ecotoxicity	3.58E-06	3.64E-06	2.33E-07	3.67E-08	4.64E-07	4.80E-07	2.72E-08
Marine ecotoxicity	0.0025343	0.00257837	0.0003394	4.64E-05	0.000286	0.000291	3.16E-05
Land use	2.45E-05	2.60E-05	7.05E-06	8.28E-07	1.83E-06	1.66E-06	5.00E-07

Table S5.
Parameters used in Pinch Technology analysis (Schulze et al., 2019; Peters et al., 2002).

Properties		Values	
Process utilities	Cooling water	Inlet temperature: 20°C	Outlet temperature: 35°C
	Medium pressure steam	Inlet temperature: 175°C	Outlet temperature: 174°C
Pinch rate of return (ROR)		10%	
Plant life (PL)		20 yr	
Annualization factor[*]		0.1175	
ΔT min		5°C	
Operating hours		8500 h/yr	

[*] AF= [(ROR/100)*(1+ROR/100)^PL]/[(1+ROR/100)^PL-1]

Table S6.
Pinch temperatures detected by Aspen Energy Analyzer.

Scenario	Pinch Temperatures	
	Hot (°C)	Cold (°C)
Sc 3	100	95
Sc 4	100	95
	25	20
	11.3	6.3
Sc 5	100	95
	25	20
	-0.5	-5.5
Sc 6	100	95

Table S7.
Normalization of Endpoint impacts for SC6.

Damage Category	Endpoint Impacts		
	Heating	Cooling Water	Electricity
Human health	**0.7827**	**0.5383**	0.0017
Ecosystems	0.0502	0.0094	0.0001
Resources	0.0141	0.0005	0.0000

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