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ANA PAULA R. PAIVA[1]
RAFAEL O. SANTOS[2]
MÔNICA P. MAIA[1]
DIEGO M. PRATA[1]

[1]**Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niterói, RJ, Brazil**

[2]**Chemical Engineering Program, COPPE, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil**

SCIENTIFIC PAPER

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IMPROVEMENT OF THE MONOCHLOROBENZENE SEPARATION PROCESS THROUGH HEAT INTEGRATION: A SUSTAINABILITY-BASED ASSESSMENT

Article Highlights

- Design and simulation of improved monochlorobenzene separation process through heat integration
- Design and simulation of utility plants for more realistic results
- Analysis in terms of water consumption, CO_2 emission, and utility costs
- An eco-efficiency comparison between the original and improved process
- Heat integrated process provides a 25% increase in eco-efficiency for the MCB process

Abstract

Chlorobenzene is an important chemical intermediate in the production of commodities, such as herbicides, dyestuffs, and rubber. In this work, a heat integration was proposed for a monochlorobenzene separation process. The conventional process structure and the proposed integrated one were designed and simulated. An optimization focused on minimizing the cooling and heating costs was performed to obtain the best-operating conditions for the heat integration. The simulation of a utility plant, including cooling water and steam generation sections, was also carried out for more accurate estimations of CO_2 *emissions, water, energy consumption, and operating costs. The processes were evaluated and compared in terms of their sustainable performances using the eco-efficiency comparison index method and environmental and economic indicators, such as* CO_2 *emission, water consumption, and utility cost, to assess the benefits of heat integration. The results demonstrated that the proposed strategy reduced around 57% of all environmental impacts and utility costs. As the composite evaluation index from the performance indicators showed, the proposed optimal heat integrated industrial plant significantly improved the initial processes' eco-efficiencies, up to 83%, proving a suitable strategy for a more sustainable process.*

Keywords: eco-efficiency, heat integration, monochlorobenzene, process simulation, sustainability indicators, utility plants.

In recent years, the impacts of rapid industrialization, economic competition, and rising energy demands, coupled with natural resource depletion and population growth, have been receiving attention globally from researchers, government, and economic agents, which shows that society has become more conscious about the ecosystem equilibrium. In this context, regulations, incentives, and goals have been discussed and proposed, such as the 2030 Agenda developed by the United Nations [1]. As part of the agenda, Sustainable Development Goals (SDGs) have been established as key goals for social, economic, and environmentally friendly development.

In this scenario, industries have evaluated their processes and performed improvement actions to reduce operating costs, risks, raw material consump-

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Correspondence: A.P.R. Paiva, Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niterói, RJ 156, 24210-420, Brazil.
E-mail: anapaiva@id.uff.br
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tion, and environmental impacts. Considering this last aspect, impacts, such as water and energy demand, greenhouse gas emissions, and wastewater generation, must be rigorously analyzed, specifically for the conceptual phase of the new process designs. Furthermore, increasing the efficiency of water and raw materials usage is also important to minimize industrial plant wastewater and solid residues.

Chemical products from biochemical and petrochemical industrial plants represent an important role in society [2]. These processes are mainly composed of raw materials extraction or conversion into the desired products, usually called the transformation industry. However, unconsumed raw materials and undesired subproducts can be found as a byproduct of these industrial processes, caused by the global conversion being less than 100%.

For these motives, purification and separation equipment, such as distillation columns, must obtain the main products at the desired commercial purity and recycle unreacted feedstock, increasing the overall process efficiency. Multiple conventional industrial plants employ these techniques: for example, the synthesis of methanol [3], butyl acetate [4], biodiesel [5], cumene [6], ethylbenzene [7], and maleic anhydride [8] addition, and purification processes focused on reutilization, such as the purification of acetic acid [9] and toluene-benzene, are also found in conventional industry. These processes have lower costs since the feedstocks are mixed with other contaminants. Nonetheless, the production costs should be further reduced to make the purified products more competitive.

Based on the concepts of sustainable development, improvement actions to increase the ecoefficiency of these processes are necessary. Many strategies can be performed to achieve this goal. For example, replacing the feedstock for ones with renewable sources, such as the use of biogas in energy generation and methanol synthesis [3,10], and the use of soy oil for biodiesel production [5], replacing a catalyst for another with greater efficiency in conversion and selectivity, as used in newer propylene polymerization plants [11], heat integration [4], single and multi-objective process optimization [5], and the development of process intensification techniques: reactive, double effect and dividing wall distillation [6,7,9,12], including membrane reactors [10].

The use of process simulation as a conceptual design and decision-making tool has been growing in recent years [12,13]. Process simulation is a mathematical model that provides the state of a determined system by numeric solution, starting from previously specified conditions: components, parameters, equipment sizing, flow rate, composition, pressure, temperature, and other operating conditions. Furthermore, to quantitatively evaluate the benefits of the chosen decision, indicators are commonly used to translate into metrics the economic, safety, and environmental aspects [12].

Thus, this work proposes a novel heat integration for the monochlorobenzene (MCB) separation process to reduce the environmental impacts and operating costs. The conventional and modified processes were simulated to evaluate this proposed concept. Also, eco-indicators were utilized to measure the change in water consumption, CO_2 emissions, and utility costs. The simulation of a utility plant, including cooling water and steam generation sections, was also carried out to achieve more realistic scenarios for water losses and energetic demand. Furthermore, a comparison between both processes was developed based on the eco-efficiency comparison index method to assess if the proposed modification achieves the goal of turning the process towards a more sustainable path.

MATERIAL AND METHODS

Process description

MCB separation process

Monochlorobenzene is an important chemical utilized as an intermediate in a diverse range of sectors such as the production of pesticides, herbicides, adhesives, repellents, degreasers, and pharmaceutical compounds. As a solvent, it has a high boiling point, resulting from the benzene (BEN) chlorination reaction, their main synthesis route. Benzene, an aromatic hydrocarbon, is used to synthesize aniline, cyclohexane, cumene, and mainly ethylbenzene, representing over 50% of benzene demand. In addition, benzene is primarily used in the production of styrene [14], although it can also be used as a fuel additive and a solvent. Both BEN and MCB are insoluble in water and are highly volatile.

In the synthesis process of MCB, residual gases containing both MCB and benzene are released and are primarily connected to a number of contamination cases by inhalation [14]. MCB is also one of the main organic contaminants in soil, sediments, groundwater, and superficial water [15]. Benzene is also commonly found as a contaminant in soil and groundwater due to fuel storage tank leakage [16]. Both compounds are carcinogenic, mutagenic, and have a high potential for bioaccumulation, thus representing a high risk to health and ecosystems. Therefore, the MCB process directly impacts society and the environment.

The chlorination reaction of benzene occurs in the liquid phase at atmospheric pressure, over a temperature range between 27 °C and 37 °C, using iron chloride ($FeCl_3$) as a catalyst, as described by Eq. (1)

$$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl \tag{1}$$

The synthesis section of MCB produces a gaseous mixture composed of MCB, benzene, and hydrochloric acid. After scrubbing the hydrochloric acid from the product stream, a distillation unit is needed to separate the chlorobenzene from the benzene. It is important to guarantee that no acid is entering the distillation columns because this contaminant has high corrosivity and will harm the structure of the columns. The MCB separation process flowsheet, based on the works of Seider *et al.* [17], is described in Fig.1. The feed stream from the synthesis section consists mainly of MCB and benzene, with small amounts of HCl. This stream is heated in the HX1 by medium pressure steam and sent to the first flash separator F1. Next, the gas stream from the separator is sent to an absorber column A1, while the liquid is mixed with the bottom product of the absorber. The absorber A1 function removes the hydrochloric acid that persists inside the MCB process. The column is composed of 15 trays but only three theoretical stages. At the top of the absorber, HCl is removed with a purity of 95%, which can be recycled and used in the synthesis section. The upper stage of the absorber also receives a part of the bottom product of the distillation column D1. The mixture stream of the flash separator and the bottom product of the absorber still contains small amounts of HCl, which needs to be removed before the distillation column. For this reason, the stream is sent to a stripper unit T1, where the HCl is collected at the bottom of the treatment unit, and the acid-free stream is then sent to the distillation column. The column D1 is responsible for the separation of MCB from benzene. It has 30 trays corresponding to 20 theoretical stages, and the feed stream enters the column at the tenth stage. The benzene is produced in the distillate with a purity of 99.75%. The bottom product of the column is further cooled down before a fraction of the stream is recycled to the absorber. The product stream, composed of 99.999% of MCB, is represented by the stream S14.

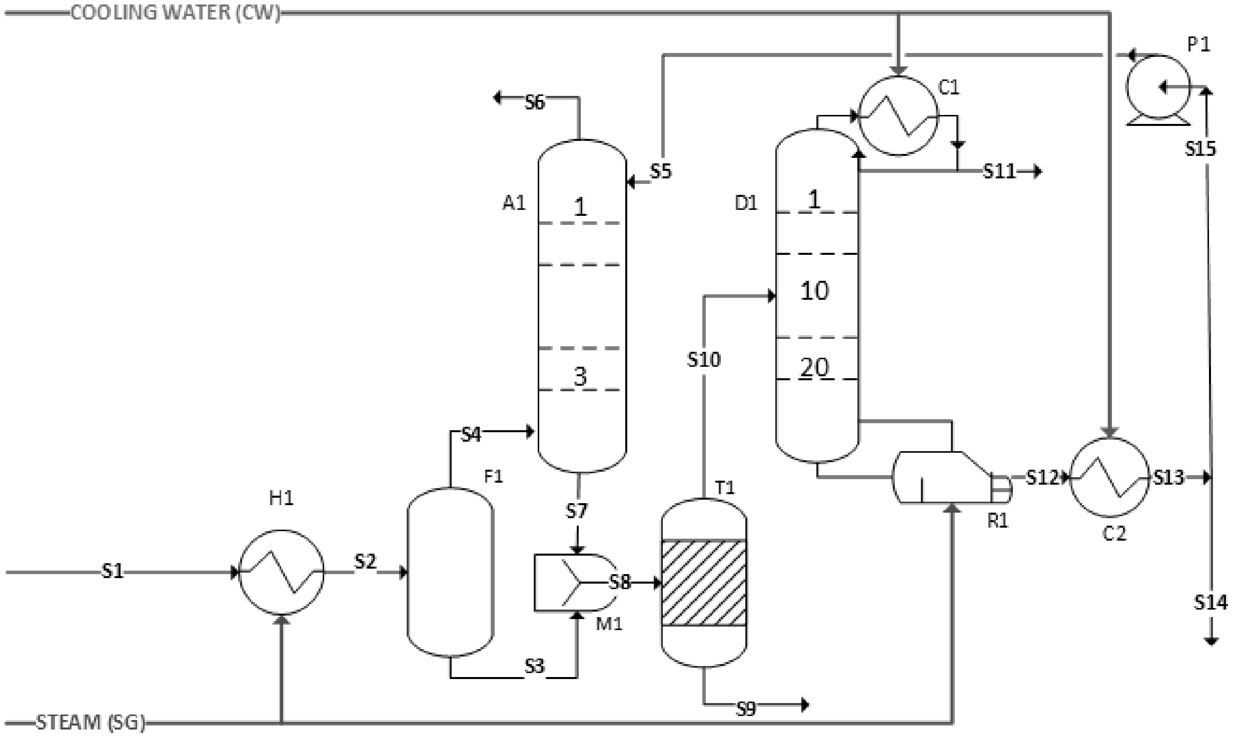

Figure 1. MCB separation process flowsheet.

Modified MCB separation process

The novel MCB separation process flowsheet, developed using heat integration concepts, is described in Fig.2. In the conventional process, the bottom product leaves the distillation columns at a high temperature, around 153 °C, and is cooled down until it reaches a temperature of 49 °C. Furthermore, the process feed stream is heated from 27 °C to 132 °C before being sent to the flash vessel. Based on these properties, a heat integration is proposed using these two streams. The FEHE, the feed effluent heat exchanger, harnesses the energy from the distillation column bottom product to heat the process feed stream, thus lowering the energetic demand for the heater H1 and the cooler C2.

Utility plant

The utility plant supplies auxiliary services such

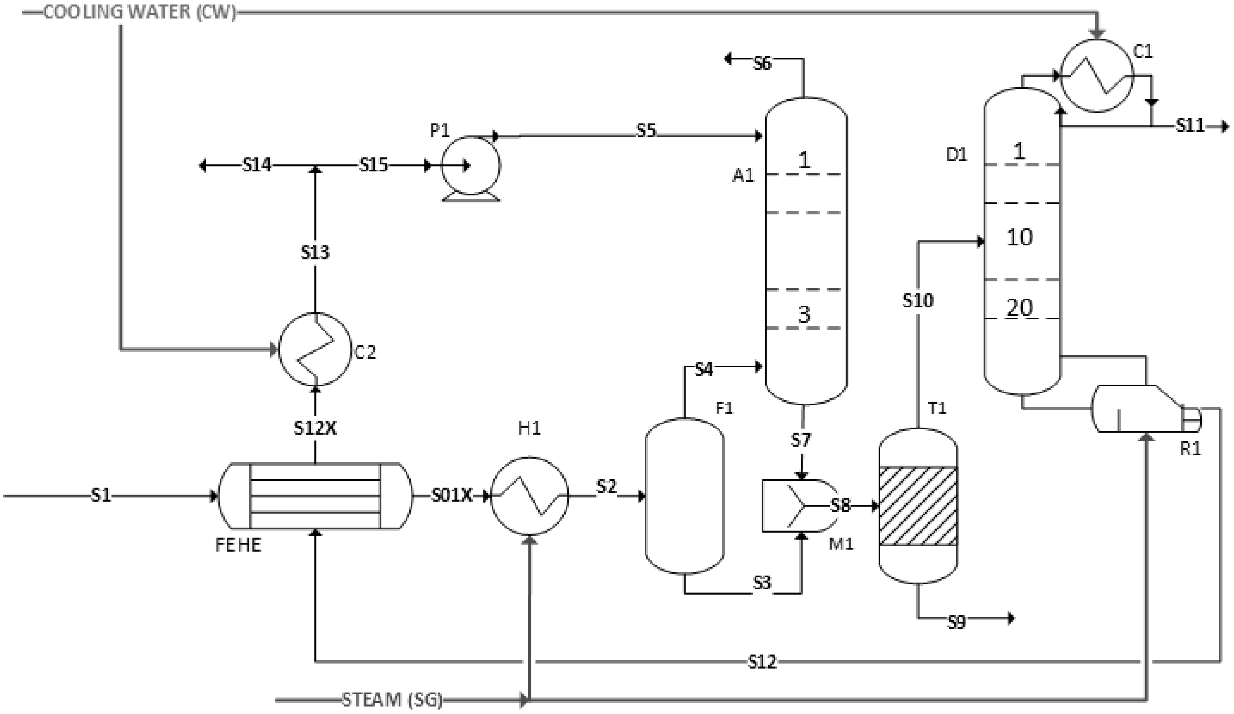

Figure 2. Modified MCB process flowsheet.

as electricity (by cogeneration), cooling water, steam, compressed air-fuel, and other necessary services for the operation of chemical process plants. Through simulations based on heuristics for water losses and equipment duties for this system, it is possible to obtain more realistic and trustworthy results for the total water and energy consumption of the process and, consequently, better estimate the CO_2 emissions and wastewater produced.

The utility plant modeled in this work is based on the system described by Turton *et al.* [18], and its flowsheet is illustrated in Fig.3. The energy cogeneration substation was not considered for the utility system. The water that returns from the cooling process is sent to the cooling tower in the cooling water section. The tower operates with an induced draft system, cooling the water to the desired temperature. A part of the water is lost by drift and another by windage. Furthermore, a blowdown must be done to avoid the accumulation of solids inside the utility plant. The fresh cooling water is then pressurized and recirculated into the cooling system.

In the steam generation section, fresh water passes through a pre-treatment unit composed of ion exchanger absorption beds and solid filters. Then, the treated water is sent to the deaerator, which is mixed with the returning condensate from the heating process. The water stream that comes from the deaerator is known as the boiler feeding water (BFW). Finally, the BFW is pressurized to the desired saturated steam pressure level and sent to the boiler.

The boiler heating can be divided into two sectors: the first sector, B1, represents the sensible heat exchange, which raises the pressurized water's temperature until the boiling point. The second sector B2 represents the latent heat needed to transform the liquid water into steam, which is then sent to the heating system. Like the cooling section, a blowdown must be done to avoid the accumulation of solids inside the utility system and reduce corrosion and water drift. Besides the boiler blowdown, water losses from the pre-treatment, the deaerator, and the process heating system must also be accounted for.

A makeup water stream is utilized to replenish the total water lost over the operation of the utility plants so that the system can continuously operate. The whole makeup water flow rate (m_{total}) is the sum of the flow rates for the cooling water section ($m_{CW¬}$) and steam generation section (m_{SG}). Moreover, Liew *et al.* [19] noted the importance of not neglecting the boiler-sensible heat in the process simulation since this can represent an estimation error of over 18% energy consumption.

Methodology

Process simulation

The MCB separation process plant and its utility plant were simulated using the Honeywell Unisim Design Suite. Both simulations were carried out in steady-state. For the conventional MCB process, the

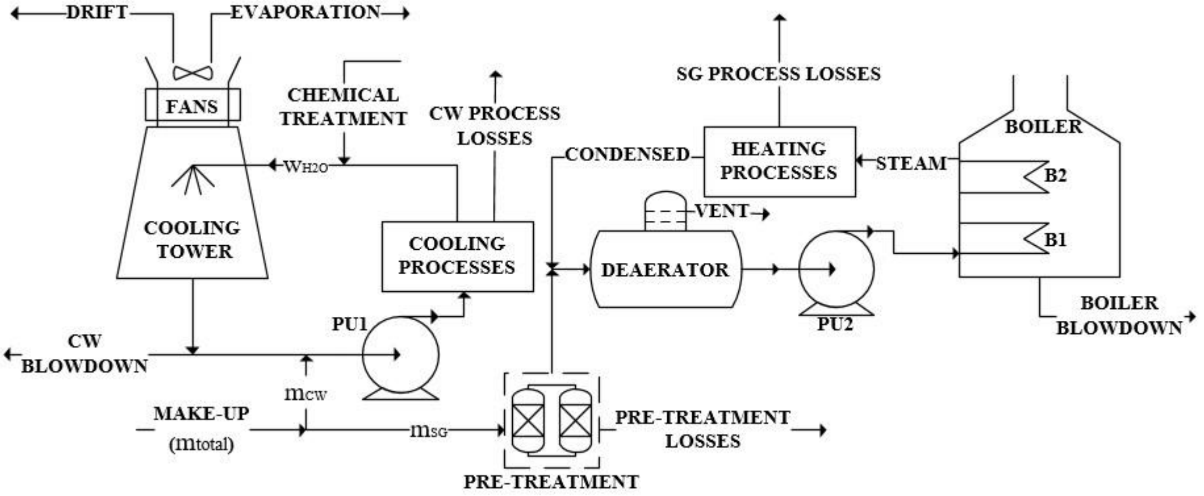

Figure 3. Utility plant flowsheet.

process configuration, main equipment, column specifications, operational conditions, and other parameters were implemented following the data provided by Seider *et al.* [17], to validate our simulation with existing literature data. In addition, the Wilson thermodynamic package was used for the simulation to correctly compare the present results with the reference work since the same thermodynamic model was employed. The Wilson thermodynamic package is an activity coefficient-based model recommended for non-ideal systems and thus, can better describe the phase equilibria inside the absorber and distillation column. The utility plant was simulated using the UNIQUAC thermodynamic package, as suggested by Turton *et al.* [18]. In addition, the energy duties data from the main MCB process were utilized as inputs to the utility plant model, thus obtaining more precise results.

Tables 1 and 2 summarize the heuristics for water losses and other operating, energy factors, and general assumptions used to simulate the utility system. It is important to note that the medium pressure steam pressure was selected as the desired steam class based on the temperature data from the heaters and distillation columns.

Table 1. Water losses heuristics for the utility plant

Parameter	Water loss (%)	Reference
Cooling tower blowdown	3	[17]
Evaporation losses	2.7	[24]
Water drift losses	0.3	[17]
Cooling system losses	1	[24]
Boiler blowdown	3	[17]
BFW pre-treatment losses	1	[24]
Condensate losses	10	[18]

Note: Vent losses from the deaerator were considered negligible.

Table 2. Utilities operating conditions and assumptions

Parameter	Value	Reference
Makeup water	101.3 kPa–30 °C	[18]
Cooling water (tower inlet)	516 kPa–45 °C	[24]
Cooling water (tower outlet)	216 kPa–30 °C	[24]
Medium pressure steam (MPS)	1136 kPa–185.5 °C	[18]
Boiler efficiency	80%	[17]
Boiler fuel gas - Natural gas	100% methane	[17]
Fan efficiency	99%	Assumed
Centrifugal pumps efficiency	75%	[17]
Heat exchanger temperature approach	10 °C	[18]

According to Caxiano *et al.* [9], the cooling tower fan duties can be calculated (in GJ/h) based on the cooling tower's circulating water volumetric flow rate by the following equation:

$$E_{fans} = w_{H_2O} \cdot 1.45222 \cdot 10^{-4} \tag{2}$$

Process simulation

The eco-efficiency is a common object of industries that aims for sustainability since the concept evaluates the relationship between the environmental impacts and the economic performance of the process, using tools that directly express this correlation called eco-indicators. According to Mangili *et al.* [13], an eco-indicator is a metric represented by the ratio between an environmental variable (energy and water consumption, CO_2 emissions, and others) and an economic variable (income or production). In this work, the production rate ($m_{production}$) was chosen for the eco-indicators.

For the evaluation of the ecoefficiency of the MCB separation process, three indicators were considered:

- Eco-indicator of water consumption, WC (m^3/t);
- Eco-indicator of CO_2 emissions, CDE (t_{CO2}/t);
- Specific utility cost, SUC (US$/t).

The reduction of water consumption, mitigation of greenhouse gas emissions, global climate action, and responsible production are all major objectives contained in the #6, #12, and #13 SDGs [1], which influenced the environmental indicators chosen for this study. In addition, the indicators of water consumption and CO_2 emissions (resulting emissions from fuel combustion in the boiler and the electricity consumption from the main process and the utility plant) are the most commonly used by works in the literature [13] and industrial process monitoring [20].

The chosen indicators must address the environmental consequences and the process economic performance for a more comprehensive evaluation of process ecoefficiency. As a result, the utility cost indicator was chosen as an economic indicator because it is directly related to the other metrics.

The indicators WC, CDE and SUC are defined by the Eqs. (3), (4), and (5), respectively.

$$WC = \frac{v_{H_2O,\, makeup}}{m_{production}} \tag{3}$$

$$CDE = \frac{E_{comb}\xi_{comb} + E_{ele}\xi_{ele} + m_{CO_2}}{m_{production}} \tag{4}$$

$$SUC = \frac{E_{comb}C_{NG} + E_{ele}C_{EE} + m_{total}C_{PW}}{m_{production}} + \frac{m_{CW}C_{CWT} + m_{SG}C_{SGT} + m_{WW}C_{WWT}}{m_{production}} \tag{5}$$

Specifications:

i. The production rate (in t/h), $m_{production}$, corresponds to the mass flow rate of stream S14 (MCB 99.9%). The streams S11 (BEN 99%), S06 (HCl 96), and S09 (HCl pure) are not considered a product stream because the benzene and HCl are recycled to the synthesis section of the MCB, which provides the feed stream of this separation process as a subproduct (fiscal tax).

ii. The $v_{H2O\, makeup}$ is the water makeup volumetric flow rate (in m^3_{H2O}) calculated from the sum of the water losses in the utility plant, considering both cooling water and steam generation sections;

E_{comb} and E_{ele} are, respectively, the energy by combustion consumed in the boiler and the electricity energy rate, both in GJ/h and calculated as described in Eqs. (6) and (7), where Q_{B1} and Q_{B2} correspond to the sensible and latent heat exchanged inside the boiler, respectively.

$$E_{comb} = \frac{Q_{B1} + Q_{B2}}{\eta_{comb}} \tag{6}$$

$$E_{ele} = \frac{E_{pumps}}{\eta_{pump}} + \frac{E_{fans}}{\eta_{fan}} \tag{7}$$

iv. η_{comb}, η_{pump}, and η_{fan} are the efficiencies for combustion and electric equipment (pumps and fan);

v. ξ_{comb} and ξ_{ele} are the CO_2 emission factors for direct and indirect sources: ξ_{comb} is equal to 0.0561 t_{CO2}/GJ, corresponding to the use of natural gas as fuel [21], and ξ_{ele} is equal to 0.0268 t_{CO2}/GJ [22], corresponding to the electricity use. This emission factor is based on the industrial plant locality. In this work, the emission factor corresponds to Brazil's average factor for the first semester of 2021.

vi. m_{CO2} (t_{CO2}/h) refers to the CO_2 emissions by fugitive sources. In this work, these emissions are considered negligible for standard operation mode (without shutting down and start-up events);

vii. The wastewater treatment cost refers to a secondary wastewater treatment facility composed of filtration and activated sludge.

viii. m_{WW} refers to the wastewater stream volumetric flow rate in m^3/h. Since the water lost by drift and evaporation in the cooling water can't be recovered, these are not considered for the total stream flow rate.

ix. C_{NG}, C_{EE}, C_{PW}, C_{CWT}, C_{SGT}, and C_{WWT} refers to the utility costs described in Table 3 [18,23]. C_{NG} is the natural gas cost ($/GJ), C_{EE} is the electricity cost ($/GJ), C_{PW}, refers to the process water cost ($/$m^3$), C_{CWT}, C_{SGT}, and C_{WWT} are the treatment costs for the cooling water, steam, and wastewater, respectively.

Table 3. Utilities cost

Utilities	Price	References
Natural Gas ($/GJ)	5.00	[23]
Electricity ($/GJ)	18.72	[18]
Process water ($/m³)	0.0157	[18]
Process water ($/GJ)	0.378	[18]
CW treatment ($/m³)	0.0347	[18]
SG treatment ($/m³)	0.1560	[18]
Wastewater treatment ($/m³)	0.0043	[18]

The ECI (Eco-efficiency Comparison Index) can be obtained from the normalized values of each indicator. These values are then plotted on a radar chart, allowing a visual representation of the performance of the processes relative to each category. The area S of each process' chart is then calculated using the Law of Sines, as described in Eq. (8), in which EI is the normalized value of each indicator and n is the total number of indicators utilized in the eco-efficiency analysis.

$$S = 0.5 \cdot \sin\left(2\pi/n\right) \cdot \left(EI_1 EI_n + \sum_{i=1}^{n-1} EI_i \cdot EI_{i+1} \right) \tag{8}$$

The ECI for the modified process is obtained by the ratio between the modified and conventional processes areas, as shown in Eq. (9), providing a quantitative metric for the eco-efficiency improvement by the heat integration [9].

$$ECI = 1 - \left(\frac{S_{modified}}{S_{conventional}} \right) \tag{9}$$

An optimization study was developed for the modified MCB separation process to obtain the best-operating conditions to minimize the heating and cooling costs. A preliminary analysis of the operating parameters was done to select the variables to be manipulated in the optimization. The temperature of the streams S01X, S02, S13, and the recycle ratio were the parameters suitable for optimization and chosen as decision variables. The optimization problem can be defined as:

$$\begin{aligned} \min_x F_{OBJ}(x) &= C_{NG}(Q_{HEATER} + Q_{REBOILER}) \\ &+ C_{PW}(Q_{COOLER} + Q_{CONDENSER}) \end{aligned} \tag{10}$$

In which x is the decision variables vector, Q_{HEATER}, $Q_{REBOILER}$, $Q_{COOLER0}$, and $Q_{CONDENSER}$ are the heater, reboiler, cooler, and condenser duties in GJ/h, respectively, and C_{NG} and C_{PW} are the cooling and heating utility costs in $/GJ.

The optimization procedure was developed in a python environment by a multistart algorithm that utilizes the Nelder-Mead method. The optimizer interacts with the software Unisim, giving the decision variables as inputs and receiving the objective function value as output.

RESULTS AND DISCUSSION

Process and utility plant simulation

Table 4 presents the results for the process streams data of the conventional MCB separation plant, and the simulation flowsheet is illustrated in Fig.4.

Table 4. MCB Conventional process results

Process stream	Temperature (°F)	Pressure (psia)	Molar flow (lbmol/h)	Molar Fraction MCB	Molar Fraction Benzene	Molar Fraction HCl
S1	80	37	50	0.5000	0.4000	0.1000
S11	207	25	0.1	0.0025	0.9975	0.0000
S14	120	25	49	0.9999	0.0000	0.0000

The simulation was validated by comparing the results obtained for the simulation with the data from Seider *et al.* [17]. The results were consistent with those from the base work, without any significant errors.

Figure 5 illustrates the modified MCB separation process simulation flowsheet. The results obtained for the optimized product streams, related to the mass flow rate and compositions, were the same as the conventional process.

Table 5 describes the energetic demand for the conventional original process (OP) and the modified heat-integrated process (HIP), including the main equipment and the duties of the utility plant.

Heat integration can reduce the energy demand of the cooler by up to 85%, the condenser by 52%, and the reboiler by 42%. Furthermore, the optimal conditions eliminate the need for the heater H1. As a result, the optimal duties lead to a total heating/cooling cost of 17.43 $/h, reducing more than 53% of the base case cost (36.59 $/h). Thus, the proposed modification

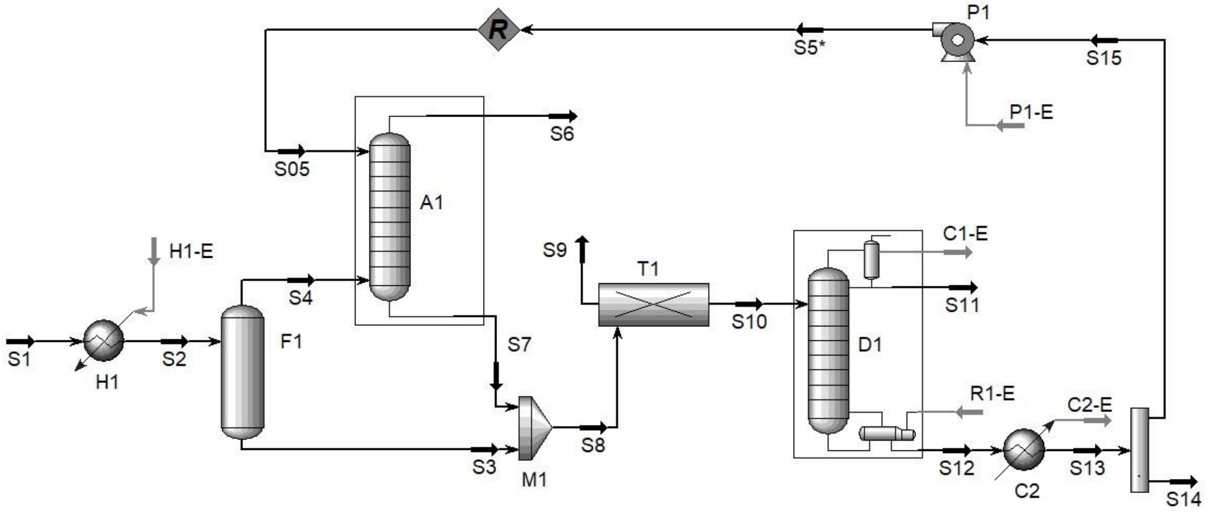

Figure 4. MCB conventional process simulation flowsheet.

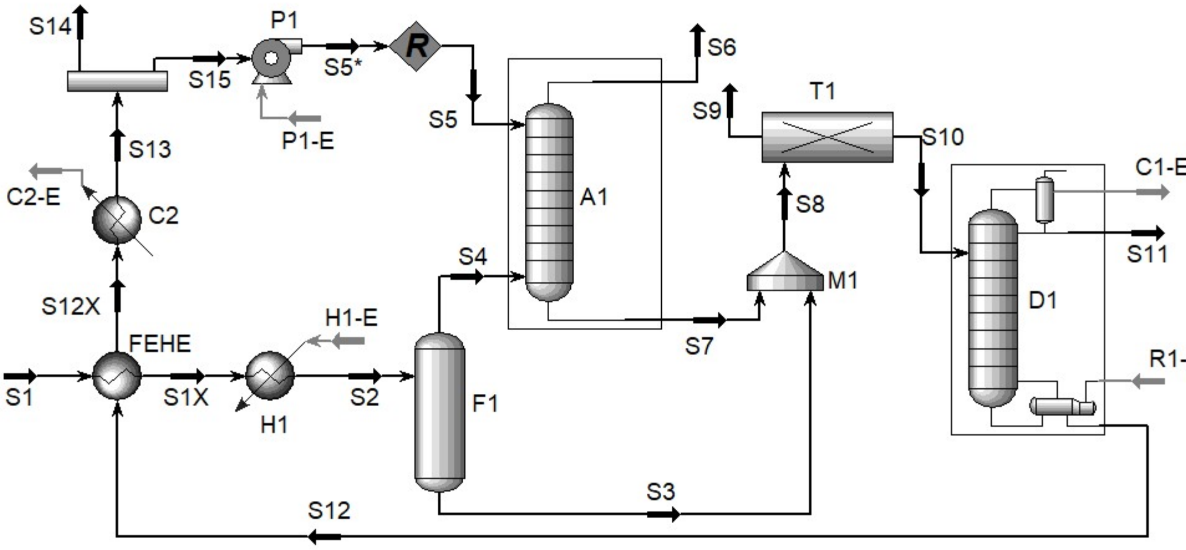

Figure 5. Modified MCB process simulation flowsheet.

achieves the goal of lowering heating and cooling demand.

The energetic duties of electricity-based equipment are significantly lower than the steam-based ones. Consequently, the CO_2 emissions are composed of a large factor of the emissions from the fuel combustion inside the boiler, as shown in Fig. 6.

The difference in scale between the emission sources shows the importance of choosing the right steam class for the process heating based on the operating temperature since it influences both latent and sensible heat portions of the boiler heat demand and, in turn, the process total gases emissions. Furthermore, the sensible heat section of the boiler composes around 17% of the boiler heating duty, in accordance with the results of 18% described by Liew *et al.* [19]. This part of the heat duty, commonly disregarded in other simulation works in the literature, can greatly affect the process energy profile. Changing the reboiler operating temperature, for example, can shift the necessary steam pressure class, allowing further manipulation of the total energy consumption. For example, the heat duties of the reboiler R1 is responsible for 37% and 53% of the process energy demand in the conventional and heat-integrated process, respectively.

The results for the water consumption and water losses of each process obtained from the utility plant data are presented in Table 6.

As the total circulating water in the cooling water section is significantly larger than the steam generation section, the water losses from the cooling water plant

Table 5. Energy duties summary

Source	Duty (GJ/h)		Reduction
	OP	HIP	(%)
Main plant			
Condenser C1	3.09	1.50	51.45
Cooler C2	1.20	0.18	84.59
Heater H1	1.23	0.00	100.00
Reboiler R1	3.35	3.35	41.18
Pump P1	3.04E-4	4.12E-5	86.47
Utility plant			
Pump PU1	0.036	0.014	61.11
Pump PU2	0.003	0.001	66.67
Cooling tower fans	0.010	0.004	60.00
Boiler B1 (sensible heat)	1.194	0.514	56.98
Boiler B2 (latent heat)[a]	5.718	2.461	56.96
Cooling utilities	4.290	1.690	60.61
Heating utilities	6.912	2.974	56.97
Electricity consumption	0.050	0.020	60
Total energy consumption	11.252	4.684	58.37

[a] The boiler latent heat corresponds to the steam demand from the heater H1 and reboiler H1.

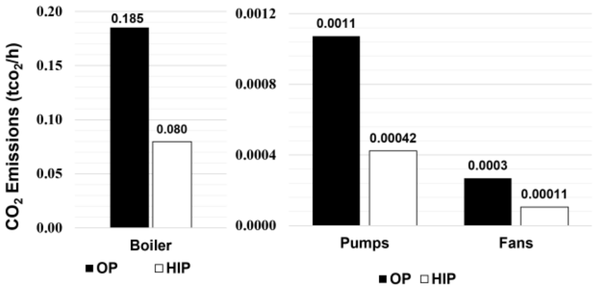

Figure 6. CO$_2$ emissions for the conventional (OP) and modified process (HIP).

Table 6. Water consumption results

Parameter	Flow rate (m^3/h)	
	OP	HIP
Cooling water losses	0.687	0.270
Cooling tower blowdown	1.978	0.778
Evaporation and drift losses	2.039	0.802
Boiler blowdown	0.071	0.031
Steam Generation losses	0.230	0.099
Treatment losses	0.003	0.001
Total water consumption	5.008	1.980

are the main component of the water consumption for both processes. As a result, the cooling water make-up stream represents over 93% of the total water consumption for the conventional and the modified processes.

The specific utility costs depend on both energy and water consumption. The lower heat duties attained from the heat integration cause a 57% lower cost for the modified MCB process than the conventional one. The utilities cost profiles for each process are shown in Fig. 7.

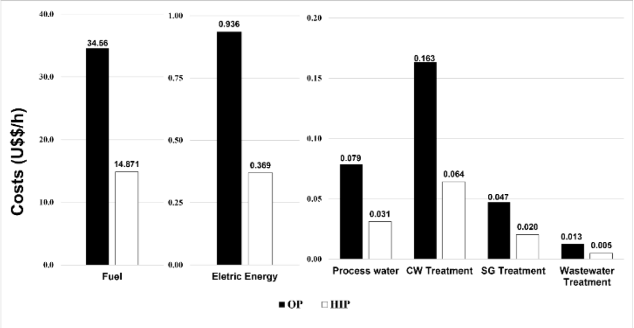

Figure 7. Breakdown of utility cost.

The fuel consumed in the boiler is the main component of the utility cost. However, the combined costs from electricity, wastewater, and water consumption represent lower than 4% of the costs for both processes. Hence, reducing the steam demand from the boiler provoked by the heat integration is responsible for the lower SUC.

Eco-indicators and ecoefficiency

The values of the indicators of water consumption, CO$_2$ emissions, and specific utility costs calculated for both MCB separation processes, coupled with the percentual reduction obtained by the heat integration, are shown in Table 7.

The indicators of the modified process are around 60% lower than those of the conventional plant. In accordance with the lower heat duties achieved for coolers and heaters, the heat integration provided a significant reduction of the environmental impacts of the MCB separation process.

The water consumption eco-indicator is lower than 2 m^3/t of product, a low value considering that the circulating water in the cooling tower has a value of 68 m^3/h for the conventional process and 27 m^3/h for the modified one. These flow rates are also lower than 4500 m^3/h, the maximum limit of the economic viability of a cooling system, as presented by Couper *et al.* [24].

Table 8 describes the results obtained for calculating the ECI from the normalized values of the indicators, and Figure 8 shows the radar charts elaborated for these indicators.

Table 7. Eco-indicators results

	Eco-indicators		Normalized indicators		Reduction (%)
	OP	HIP	OP	HIP	
WC ($m^3/t_{product}$)	1.977	0.781	1.000	0.430	60.47
CDE ($t_{CO2}/t_{product}$)	0.143	0.066	1.000	0.395	56.98
UC (U$$/$t_{product}$)	14.128	6.062	1.000	0.429	57.09

Table 8. ECI results

Eco-indicator x Eco-indicator	OP	HIP
CDE x WC	1.000	0.170
WC x UC	1.000	0.170
UC x CDE	1.000	0.185
Total	3.000	0.524
Chart area	1.299	0.227
ECI	0.0%	82.5%

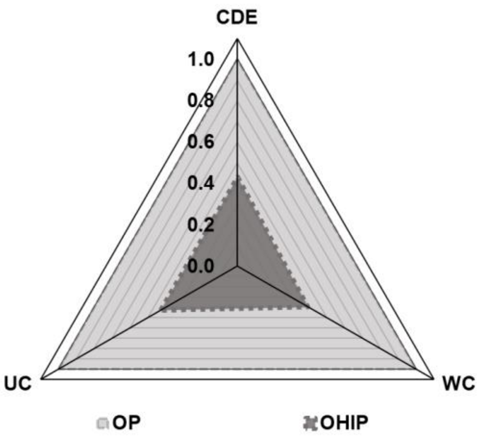

Figure 8. ECI radar chart for the MCB separation processes.

The ECI values, calculated from the chart areas, demonstrate that the heat-integrated process is 83% more eco-efficient than the conventional process. It corroborates the importance of heat integration in developing a more sustainable process. As no data was found for the indicators in previous works on the MCB-benzene separation process, it is believed that this work can hopefully provide a framework for reference for future analysis of the monochlorobenzene separation in the literature.

CONCLUSION

This study proposed a heat integration strategy for monochlorobenzene separation process to increase sustainability performance compared to the original process presented in Seider *et al.* [14]'s work. Both processes were designed via computer simulation based on process data provided in the reference work and a utility plant simulation for more accurate estimations of water and energy consumption and, consequently, the CO_2 emissions.

The optimal heat integrated process reduced over 57% of the utility cost, thus significantly increasing the process' economic performance. Furthermore, the modified configuration, composed of changes to recycle ratio and heat exchangers' temperatures, removes the necessity of a heater before the absorber column.

Results showed that the proposed design provided 60% and 57% lower water and energy consumption and around 57% lower CO_2 emissions than the original process. These lower indicators align with SDGs #6, #12, and #13 of the 2030 Agenda [1]. Thus, the optimal heat integrated design provided an 83% increase in its eco-efficiency compared to the original process.

The results of this work demonstrate the potential of the process heat integration strategy in reducing environmental impacts and improving economic performance. These findings can also help engineers weigh the economy against the environmental impacts for selecting the suitable process intensification. Future works should also consider process intensification studies on distillation columns (vapor recompression, double-effect distillation, etc.) to further increase the eco-efficiency performance.

NOMENCLATURE

BEN	Benzene
BFW	Boiler feeding water
C_{CWT}	Treatment costs for the cooling water
CDE	Eco-indicator of CO_2 emissions
C_{EE}	Electricity cost

C_{NG}	Natural gas cost
C_{PW}	Process water cost
C_{SGT}	Treatment costs for steam
C_{WWT}	Treatment costs for wastewater
ECI	Eco-efficiency Comparison Index
E_{comb}	Energy by combustion consumed in the boiler
E_{ele}	Electricity energy rate
E_{fans}	Cooling tower fan duties
EI	Normalized value of each indicator
$FEHE$	Feed effluent heat exchanger
$Fobj$	Objective function
HIP	Process through heat integration
MCB	Monochlorobenzene
m_{CO2}	CO_2 emissions by fugitive sources
$m_{CW}\neg$	Flow rate of the cooling water section
$m_{production}$	Production rate
$m_{production}$	Sum of the mass flow rates of streams S06, S09, and S14
m_{SG}	Flow rate of the steam generation section
$v_{H2O,makeup}$	Sum of the makeup flow rates for the cooling water and steam generation sections of the utility plant
m_{WW}	Wastewater stream volumetric flow rate
N	Total number of indicators utilized in the eco-efficiency analysis
OP	Original process
Q_{B1}	Sensible heat exchanged inside the boiler
Q_{B2}	Latent heat exchanged inside the boiler
Q_{COOLER}	Cooler duty
$Q_{CONDENSER}$	Condenser duty
Q_{HEATER}	Heater duty
$Q_{REBOILER}$	Reboiler duty
S	Area of each process' chart
$S_{conventional}$	Conventional process area of ECI chart
$SDGs$	Sustainable Development Goals
$S_{modified}$	Modified process area of ECI chart
SUC	Specific utility cost
WC	Eco-indicator of water consumption
x	Decision variables vector
w_{H2O}	Circulating water volumetric flow rate of the cooling tower
η_{comb}	Combustion equipment efficiency
η_{fan}	Fans efficiency
η_{pump}	Pumps efficiency
ξ_{comb}	CO_2 emission factor for combustion using natural gas as fuel
ξ_{ele}	CO_2 emission factor for electricity

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ANA PAULA R. PAIVA[1]
RAFAEL O. SANTOS[2]
MÔNICA P. MAIA[1]
DIEGO M. PRATA[1]

[1]Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niterói, RJ, Brazil

[2]Chemical Engineering Program, COPPE, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ, Brazil

NAUČNI RAD

POBOLJŠANJE PROCESA SEPARACIJE MONOHLOROBENZENA KROZ INTEGRACIJU TOPLOTE: PROCENA ZASNOVANA NA ODRŽIVOSTI

Hlorobenzen je važan hemijski intermedijer u proizvodnji herbicida, boja i guma. U ovom radu je predložena integracija toplote za proces separacije monohlorobenzena. Projektovana je i simulirana konvencionalna struktura procesa i predložena integrisana. Izvršena je optimizacija usmerena na minimiziranje troškova hlađenja i grejanja, kako bi se postigli najbolji uslovi rada za integraciju toplote. Simulacija postrojenja, uključujući sekcije za proizvodnju rashladne vode i pare, sprovedena je za preciznije procene emisije CO_2, vode, potrošnje energije i operativnih troškova. Procesi su procenjeni i upoređeni u smislu njihovih održivih performansi korišćenjem metode poređenja indeksa eko-efikasnosti i ekoloških i ekonomskih indikatora, kao što su emisija CO_2, potrošnja vode i operativni troškovi, kako bi se procenile prednosti integracije toplote. Rezultati su pokazali da je predložena strategija smanjila oko 57% svih uticaja na životnu sredinu i operativnih troškova. Kao što je pokazao kompozitni indeks evaluacije iz indikatora učinka, predloženo optimalno toplotno integrisano industrijsko postrojenje značajno je poboljšalo ekološku efikasnost početnih procesa, do 83%, dokazujući odgovarajuću strategiju za održiviji proces.

Ključne reči: ekološka efikasnost, toplotna integracija, monohlorobenzen, simulacija procesa, indikatori održivosti, postrojene.