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Environmental assessment of the monochlorobenzene separation process through vapor recompression strategy

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ABSTRACT
Chlorobenzene is an important chemical intermediate in the production of commodities, such as herbicides, dyestuffs, and rubber. In this work, a vapor recompression intensification strategy was proposed to retrofit a real operating monochlorobenzene separation process. The conventional process and the intensification proposal were designed and simulated in UniSim Design Suite Software. A utility plant, including cooling water and steam generation sections, was also carried out for more realistic estimations of water and energy consumption as well as CO_2 emissions. The results revealed that the vapor recompression technique was able to reduce the total energy input, water consumption, and CO_2 emissions by 59.06 %, 56.33 %, and 67.23 %, respectively. These findings indicate promising sustainability gains.

Keywords: Thermodynamic efficiency, Energy consumption, Distillation.

1 INTRODUCTION

Distillation is a unit operation widely used in the chemical and petrochemical industries [1]. It is an energy-intensive process, under low thermodynamic efficiency, which requires high-quality energy consumption in the reboiler while rejecting a comparable quantity of waste heat to the condenser at a lower temperature [2,3], and represent high capital investment and operational utility costs [1,2,3].

In this context, several intensification process (IP) strategies have been developed to significantly reduce the energy demand and the respective carbon emissions as well as utility costs of modern separation and purification plants [1-4] in accordance to the 2030 Agenda for sustainable development [5]. The well-known PI strategies, including cyclic distillation [6], dividing-wall column [7,8], double-effect distillation (DED) [9,10,11-13], and vapor recompression (VR) [11-13,14,15], which account for around 50% [16], 30-40% [17], 30-45% [16], and 70% [1] of energy savings, respectively, among others, have been applied [1,2].

The literature reveals many important applications of VR as a PI strategy in the petrochemical industry. Luyben [14] designed a VR strategy for the ethylene-ethane separation system in order to save about 66% on the total energy demand. In turn, Kazemi et al. [15] explored the feasibility and effectiveness of this technology in eighteen distinct configurations for the propylene-propane system. Results showed that energy savings of between 80 % and 94 % were achieved. Recently, De Miranda et al. [18] applied the VR strategy to a cryogenic extractive distillation process for CO_2-ethane separation from natural gas. Results showed that the VR scheme applied between the depropanizer condenser and the deethanizer reboiler saved 24.2 % and 24.5 % of energy and water consumption, respectively, as well as 25.5 % and 21.4 % in CO_2 emissions and utility costs, respectively, which increased the conventional process's eco-efficiency by 41.9 %. Similarly, the VR scheme was applied to the cumene and ethylbenzene production processes. The results shown energy and CO_2 emissions savings of about 78% and 45%, as well as 76 % and 54 %, respectively [11,12]. In turn, Caxiano et al. [13] investigated the VR and DED intensification strategies for an acetic acid purification process. The VR design proved to be 67% and 44% more eco-efficient than the conventional counterpart and DED intensification scheme, respectively, mainly due to 80.5% of energy savings.

So far, few studies have paid attention to improve the industrial-scale monochlorobenzene (MCB) separation process, previously discussed in the Seider et al. [19] book. MCB is a chemical intermediate widely used in the production of several other compounds in the chemical, agrochemical, and pharmaceutical industries. In addition, it is used as a high-boiling solvent in both laboratory and industrial-scale applications [20,21,22]. Wang [20] investigated the optimization of an industrial MCB separation process represented by two distillation columns (a similar process to the one present in Seider et al. [19], besides the absorber tower) to save energy on both reboilers. The optimization was based on the design configurations and operational conditions, which include the number of stages as well as the reflux ratios and feed stage locations on both columns. Chen et al. [21] and Paiva et al. [22] committed their research toward the heat integration of the one-tower MCB separation process [19] based on optimization procedures to reduce operating costs. The former reduced 11.5% of the utility costs, while the latter reduced about 57% of all analyzed environmental impacts (energy and water consumption as well as CO_2 emissions). Recently, Figueiredo et al. [23] proposed a novel configuration based on heat integration and DED scheme as intensification proposal to revamping the one-tower MCB separation processes [19]. The new design proved savings of 60.15 % and 29.65 % in energy demand and total annualized cost (TAC), respectively. Complementary, savings of 61.79 %, 60.15 %, and 60.20 % in water consumption, CO_2 emissions and utility costs were achieved, respectively, which increased the process's eco-efficiency by 84.57 %.

This study is the continuation of the previous one [23] for investigating the performance of the VR scheme as a novelty to retrofit the MCB separation process. The conventional and proposed intensified processes were designed by computer simulation in UniSim software. Additionally, a utility plant with cooling water and steam generation sections was also considered to provide better estimates regarding energy and water consumption, as well as CO_2 emissions, to perform the environmental assessment.

2 OBJECTIVE

This work aims to design a proposal based on vapor recompression strategy. An analysis of the energy and water consumption as well as the CO_2 emissions of this configuration was made to evaluate potential environmental and economic improvements, considering a utility plant for more realistic results.

3 METHODOLOGY

The methodology here presented was developed by applying the UniSim software for process simulation and to gather the data requested for subsequent analysis. The upcoming subtopics will provide a more detailed understanding of the steps used in this research.

3.1 CONVENTIONAL PROCESS (CP) DESCRIPTION

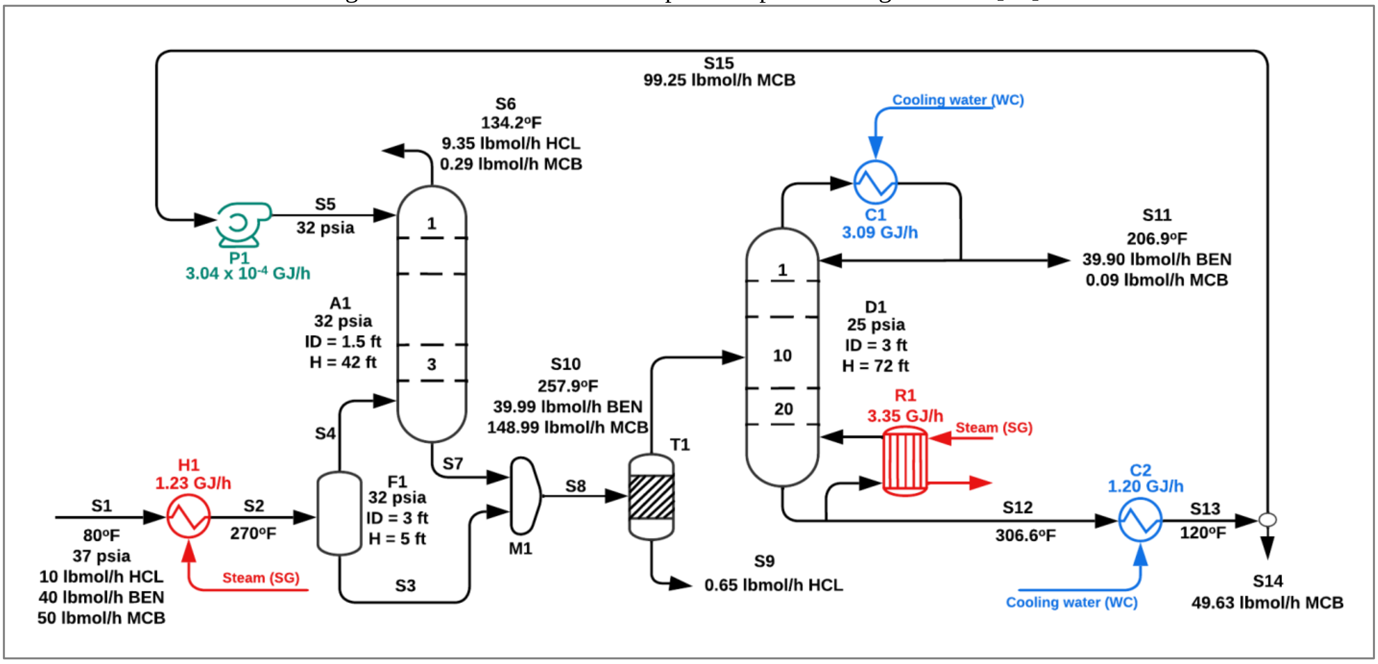
Many chemical compounds are produced through different reactions in an attempt to meet industry and society's demands. In particular, the synthesis of monochlorobenzene frequently entails the reaction of benzene (BEN) and chlorine catalyzed by a Lewis acid, usually iron chloride ($FeCl_3$), as portrayed in Eq. (1).

$$C_6H_6 + Cl_2 \xrightarrow{FeCl_3} C_6H_5Cl + HCl \tag{1}$$

The conventional separation process design of a real MCB operating plant located on the Gulf Coast of the United States, presented by Seider et al. [19], is described in Figure 1.

The feed stream S1 primarily consists of MCB and BEN, with minor amounts of hydrochloric acid (HCl). Before entering the flash separator F1, the feed is heated in the H1 heat exchanger using medium-pressure steam at 185.5 °C and 1136 kPa [24]. In F1, the vapor stream S4 is directed to an absorber A1 with 15 trays (equivalent to 3 theoretical stages) for removing a significant portion of the remaining HCl from the MCB process. The liquid phase S3 is combined with the bottom product from A1 and then sent to the stripper unit T1. The small amount of HCl remaining in stream S8 is collected at the bottom of T1, whereas the acid-free stream S10 enters the distillation column D1 at the tenth stage. This column has 30 trays (corresponding to 20 theoretical stages) and is responsible for separating MCB from BEN. Distillate stream S11 achieves a high purity of BEN, while the bottom product S12 is composed of 99.999% MCB (molar basis). Finally, S12 is cooled and divided into two streams: S14, the final product, and S15, which is recycled back to the absorber.

Figure 1: Conventional MCB separation process diagram flow [19].



3.2 VAPOR RECOMPRESSION INTENSIFIED PROPOSAL

Aiming for improvements in the MCB separation process, vapor recompression (VR) was explored as a PI strategy. The core concept of VR technology lies in exchanging utility streams, such as cooling and heating sourced externally, for the main plant process flows. This approach consequently reduces operational costs and elevates thermodynamic efficiency. Additionally, said technique is an external arrangement to distillation columns that provides no further changes in temperature or composition internal profiles [18] enhancing its potential application as a retrofitting design.

Within the petrochemical industry, VR is frequently evaluated for its impact on distillation performance. This technology essentially utilizes thermal energy lost in the column condenser to partially or completely fulfill the heat requirements of the column reboiler. However, due to the lower temperature maintained in the rectifying section, a compressor is employed to enhance the quality of the top vapor, thereby enabling heat exchange between this stream and the tower boilup [15].

Although VR offers numerous advancements and benefits, it is not always suitable for every chemical system separation. Pleşu et al. [25] proposed a mathematical equation that relates the viability of VR application to the Carnot cycle efficiency. Based on this, the coefficient of performance (COP) is introduced as shown in Eq. (2).

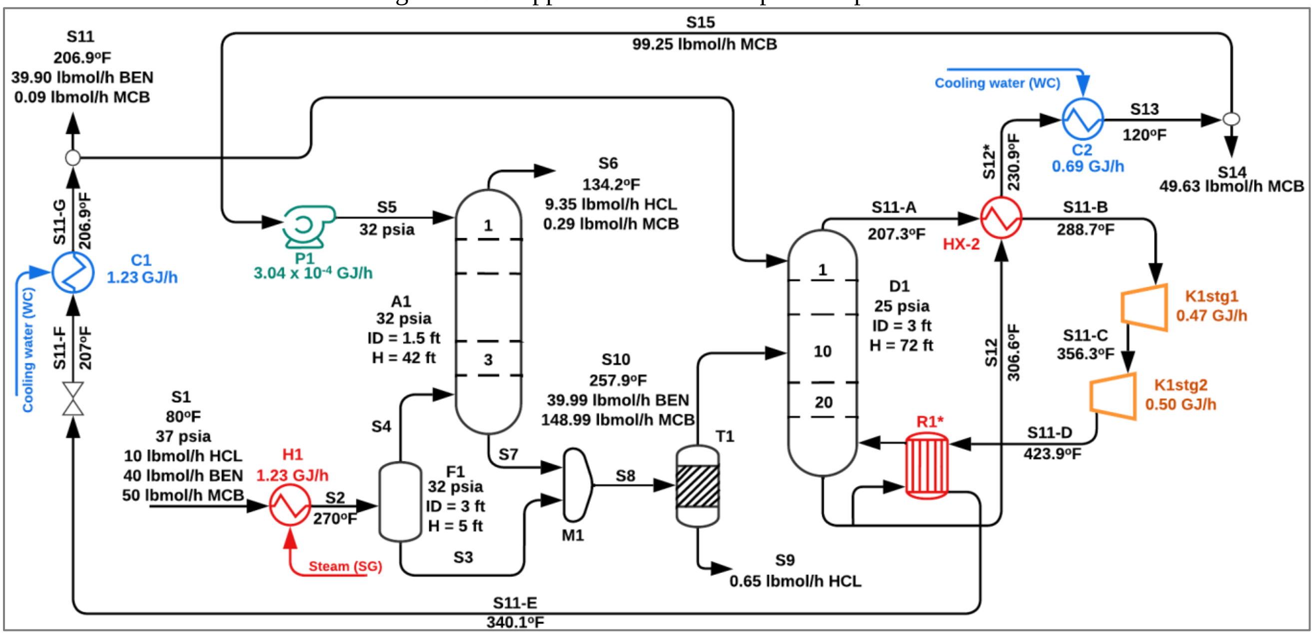
$$COP = \frac{1}{\eta_{Carnot}} = \frac{Q}{W} = \frac{T_c}{T_r - T_c} \qquad (2)$$

Where η_{carnot}, Q, W, Tc, and Tr represent, respectively, the Carnot cycle efficiency, reboiler duty, compression work, condenser temperature, and reboiler temperature. The last two temperatures are measured in Kelvin units. As shown by Eq. (2), VR is preferable to systems whose chemical species have relatively close boiling points.

For retrofitting purposes, the attractiveness of VR technology depends heavily on the system's COP. At a COP above 10, VR offers clear advantages. Between 5 and 10, the benefits are less clear and require further evaluation of other factors. Below 5, VR is generally not considered a feasible option. The COP value for the MCB separation process was 6.73, making it eligible for analysis.

Figure 2 shows a diagram of vapor recompression (VR) applied to the conventional monochlorobenzene (MCB) separation process. A two-stage compressor maintains a pressure ratio of four [19]. Likewise, two new heat exchangers were added to the flowsheet: HX-2 and R1*. The former pre-heats the column top vapor stream to prevent condensation during compression, which could damage the compressor. Meanwhile, the later serves as the column new reboiler, replacing the original one designed to use steam. After the compression and supplying heat to the column bottom stream, the overhead stream is directed to a throttle valve and to the condenser C1, reducing pressure and temperature, respectively, and returning to the distillate (S11) and reflux process conditions. In an attempt to reduce even more utility expenditures, the heated bottom stream was employed as a thermal energy source in HX-2 before being sent to the cooler C2.

Figure 2: VR applied to the MCB separation process.



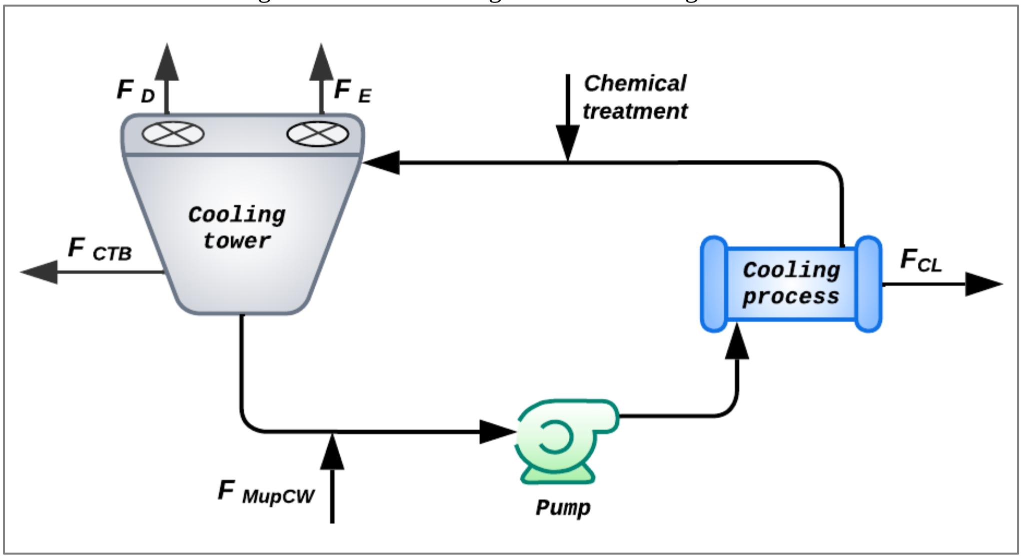
3.3 UTILITY PLANT

As industrial complexes grow and evolve, the demand for utilities rises rapidly due to their critical role in process operational running. In this sense, heating and cooling utilities must be considered for more realistic results, especially when energy-intensive equipment such as distillation columns are involved. The utility plant is a facility that provides auxiliary services to the main plant. It is composed of two sections, the cooling section (CS) and the steam generation section (SG), which are powered by water streams.

The CS is usually an open system with recirculation, as water can be reused, reducing the catchment volume [26]. Such an arrangement consists mainly of a cooling tower and a heat exchanger network connected by means of a pump [19], as seen in Figure 3. During this refrigeration process, the cold water supplied to the cooling facilities in the main plant is then heated and addressed to the cooling tower. Inside the tower, mechanical fans generate an air draft responsible for lowering the water's temperature once again [27].

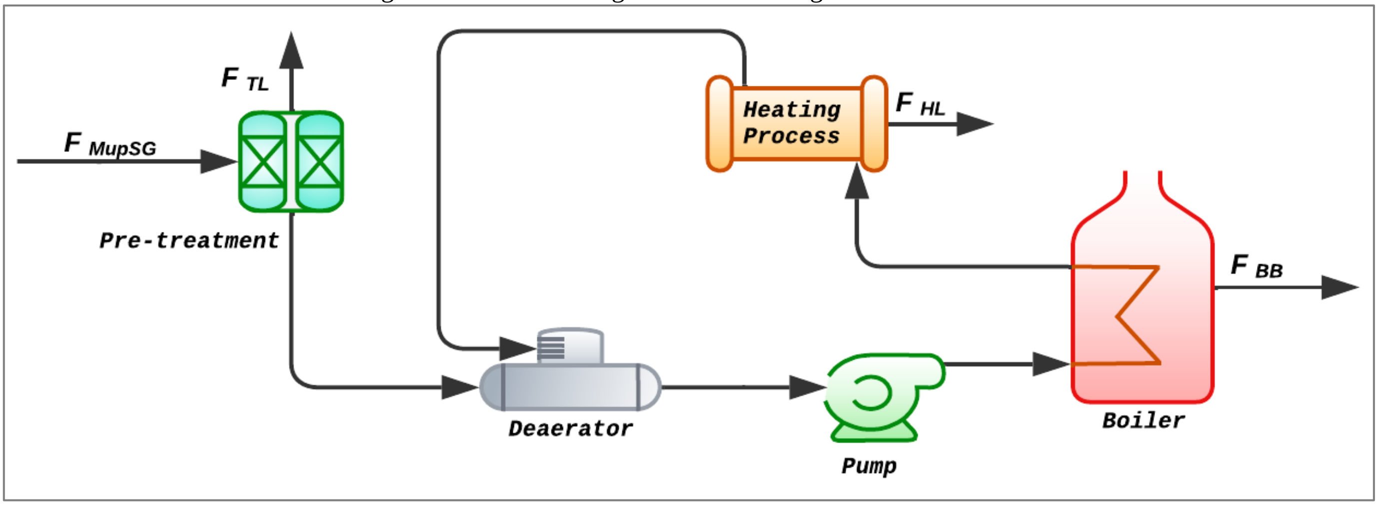
As a part of the aforementioned process, sources of water losses due to evaporation (F_E), drift (F_D), tower blowdown (F_{CTB}), and operation (F_{CL}) must be taken into account. The tower is in charge of the first three as a consequence of heat transfer between the cooling water and the surrounding air, entrained droplets, and the purging of untreated circulating streams, respectively [19]. Meanwhile, the last one refers to possible leaks in the system equipment. Thus, a make-up stream (F_{MupCW}) is required to replace the volume lost throughout the operation.

Figure 3: Flowsheet diagram of the cooling section.



As for the SG, presented in Figure 4, water is initially treated in a cationic and anionic bed to remove possible contaminants before being passed to the deaerator to extract corrosive gases. A pump is then used to increase the pressure level. In this work, medium-pressure steam (185 °C and 1136 kPa) was adopted since the minimum approach of 10 °C was satisfied [28]. The stream, now pressurized, is sent to the boiler, where water is heated (sensible heat) and vaporized (latent heat). As a result of the accumulation of solids in this equipment, a purge is considered in the process, conserving the same heat transfer efficiency and avoiding corrosion. The steam produced is thereupon directed to the main plant exchangers and used as a heat utility.

Figure 4: Flowsheet diagram of the steam generation section.



Likewise, in the CS, SG has losses to be taken into account, such as treatment (F_{TL}) and heating losses (F_{HL}) as well as boiler blowdown (F_{BB}). Hence, another make-up stream (F_{MupSG}) is added.

The heuristic values adopted during the simulation process and their respective references are shown in tables 1 and 2.

Table 1 – Heuristic values adopted for the cooling section.

Property	Value	Reference
Cooling tower inlet temperature	40 ºC	[24]
Cooling tower inlet pressure	500 KPa	[24]
Cooling tower outlet temperature	30 ºC	[24]
Cooling process losses (F_{CL})	1 %	[19]
Drift losses (F_D)	0.3 %	[19]
Evaporation losses (F_E)[a]	1.8 %	[19]
Cooling tower blowdown (F_{CTB})	3 %	[19]

[a] Referring to a 10 ºC difference between the inlet and outlet of the cooling tower.

Table 2 – Heuristic values adopted for the steam generation section.

Property	Value	Reference
Treatment losses (F_{TL})	1 %	[28]
Boiler blowdown (F_{BB})	3 %	[28]
Heating process losses (F_{HL})	10 %	[28]

In addition, the boiler's 80% combustion efficiency must be considered in the overall demand for heat (sensible and latent) in order to calculate energy consumption [24]. Given the fact that the cooling tower's fans' duty cannot be obtained promptly from the UniSim software environment, Caxiano et al. [13] proposed Eq. (3) to compute it.

$$\mathbf{W}_{Fans}\left[\frac{\mathbf{GJ}}{\mathbf{h}}\right] = \frac{\left(\mathbf{F}_{\mathbf{Tower}}\left[\frac{\mathbf{m^3_{H2O}}}{\mathbf{h}}\right]\right) \times \mathbf{2.432 \cdot 10^{-4}}\left[\frac{\mathbf{GJ}}{\mathbf{m^3_{H2O}}}\right]}{\boldsymbol{\eta}_{Fans.}} \tag{3}$$

The fan power per area, 8.05×10^{-5} (GJ/h)/ft^2, and the specific area of the tower, 1.804 ft^2/(m^3/h), are applied to calculate W_{Fans} in Eq. (3) [13, 29]. This adaptation involves the use of an air wet bulb temperature of 26.7 ^{o}C (which is equivalent to Rio de Janeiro, Brazil) and accepts a conservative 90% efficiency for the functioning of the tower and for the electricity-driven fans (η_{Fans}).

3.4 ENVIRONMENTAL ASSESSMENT

Revamping and retrofitting existing processes often involve evaluating various sustainability indicators, such as energy demand, water consumption, and carbon dioxide (CO_2) emissions. This analysis is crucial for aligning production with environmental and social concerns, aiding stakeholders in their decision-making. Promising proposals identified through such analysis can then undergo further economic assessment to ensure overall project feasibility. In this context, to appraise the benefits addressed by the vapor recompression in the MCB separation process, the indicators previously mentioned were considered and computed by the equations presented in Table 3.

Table 3 – Equations used for analysis of the simulation results

Metric	Equation	Unit
Energy consumption (EC)	$EC = \frac{W_{Comb.}}{\eta_{Comb}} + W_{Pump} + W_{Comp.} + W_{Fans}$ [b]	$\frac{GJ}{h}$
Water consumption (WC)	$WC = F_{Mup} = F_{MupCW} + F_{MupSG}$	$\frac{m^3_{H2O}}{h}$
CO_2 Emissions (CDE)	$CDE = (W_{Comb.} \cdot \xi_{Comb}) + (W_{Ele} \cdot \xi_{Ele})$	$\frac{t_{CO2}}{h}$

[b] W_{Pump}, $W_{Comp.}$, and $W_{Fans.}$ are already corrected by their respective efficiency

Table 3 displays the energy consumption in GJ/h for combustion in the boiler, pumps, compressor, and fans as W_{Comb}, W_{Pump}, $W_{Comp.}$, and W_{Fans}, respectively. The boiler efficiency is represented by η_{Comb} and is 80%, while the pumps and compressor energy were obtained directly from the UniSim software, where their efficiency was set at 75% [19]. W_{Comb} (natural gas combustion energy) and W_{Ele} (electricity consumption) are determined using equations (4) and (5), respectively. F_{Mup} accounts for the replacement water flows in the utility plant’s cooling system (F_{MupCW}) and steam generation (F_{MupSG}).

$$W_{Comb.} = \frac{Q_{sens} + Q_{lat}}{\eta_{Comb}} \quad (4)$$

$$W_{Ele.} = W_{Pump} + W_{Comp.} + W_{Fans}{}^{\text{c}} \quad (5)$$

Already corrected by the efficiency.

Q_{sens} and Q_{lat} in Eq (4) represent the sensible and latent heat components in GJ/h, respectively. Q_{sens} is acquired straight from the utility facility.

In Table 3, ξ_{Comb} and ξ_{Ele} represent the CO_2 emission factors from combustion and electricity sources, respectively. The first has a predetermined value of 0.0561 t_{CO2}/GJ [30] for natural gas as fuel. The second is directly dependent on the local energy matrix. Assuming the processes are located in Brazil, this factor equates to a value of 0.0234 t_{CO2}/GJ, which is the average value for the years 2021 and 2022. [31].

3.5 COMPUTATIONAL SIMULATION

During the computer-aided process, version 490R of the software UniSim was used. In such a procedure, all the specifications and conditions were set according to Seider et al. (2016). The conventional and intensified schemes were simulated under steady-state conditions by applying Wilson's package. As seen in Figueiredo et al. [23], this thermodynamic model is a good fit for the system, describing appropriately the phase equilibria inside the absorber and distillation column.

Concerning the utility plant, the UNIQUAC package was chosen, using the ideal vapor model specification. The reproduction of said plant was developed as presented in Section 2.3 by employing the literature recommendations shown in Tables 1 and 2.

Moreover, heuristics regarding compression ratio (mentioned in Section 2.3), equipment efficiency, and a minimum approach of 10 °C in heat exchangers [28] were adopted for more reliable results. As a final point, the given outcomes were analyzed by the equations displayed in Table 3 for the evaluation of further sustainable improvements.

4 RESULTS

4.1 SIMULATION RESULTS

Section A of the appendix contains UniSim flowsheets for both, the conventional process and the VR proposal, used in this study.

Regarding the CP simulation findings, close agreement (within 5%) was found between the simulation results and the specifications in Seider et al. [19] for the operational conditions, stream compositions, and energy duties. This consequently confirms the successful replication and potential for further intensification of the MCB separation process.

4.2 ENVIRONMENTAL ASSESSMENT

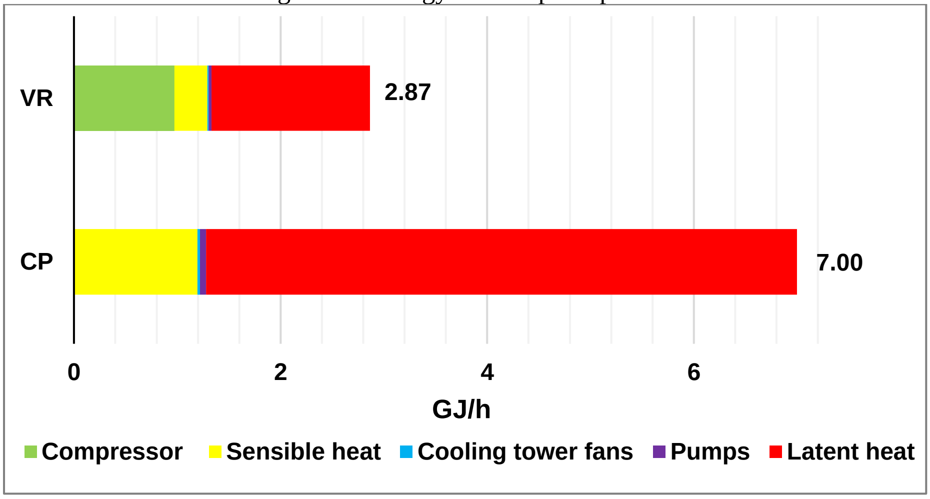
The findings for water and energy consumption in the simulated processes are presented in Table 4. This includes water consumption, heuristics in the established estimates for water losses, as well as details on overall combustion demand and its efficiency. Additionally, the table breaks down heat consumption into both sensible and latent parcels, alongside the electricity used by each operational plant analyzed.

From the data displayed in Table 4, the VR proposal showed a great reduction of 59.06% in the total energy demand compared to its conventional counterpart. A graphic visualization of this results is given by Figure 5. As expected, the demand for electricity increased for the intensified scheme as an electric-driven device, the compressor, was added to enable thermal exchange between the rectifying and stripping sections. Given this, no medium-pressure stream was needed to power the D1 column reboiler. In addition, the heat available in the bottom product stream was used as a pre-heating fluid, which did not lead to a rise in the need for burning natural gas and provided further savings in the cooling utilities required in the cooler C2.

Table 4 – Outcomes found for energy and water usage.

Process	**CP**	**VR**
Boiler latente heat(GJ/h)	5.72	1.53
Boiler sensible heat (GJ/h)	1.19	0.32
Electricity (GJ/h)	0.09	1.01
Total energy demand (GJ/h)	**7.00**	**2.87**
Condenser (GJ/h)	3.09	1.23
Cooler (GJ/h)	1.20	0.69
Total cooling demand (GJ/h)	**4.29**	**1.91**
Cooling process losses (m^3/h)	1.03	0.46
Evaporation and drift (m^3/h)	2.14	0.96
Cooling tower blowdown (m^3/h)	2.10	0.94
Losses in the cooling water system (m^3/h)	**5.27**	**2.35**
Boiler blowdown (m^3/h)	0.07	0.02
Treatment losses (m^3/h)	0.003	0.001
Heating process losses (m^3/h)	0.23	0.06
Losses in the steam generation system (m^3/h)	**0.30**	**0.08**
Total water consumption(m^3/h)	**5.58**	**2.44**

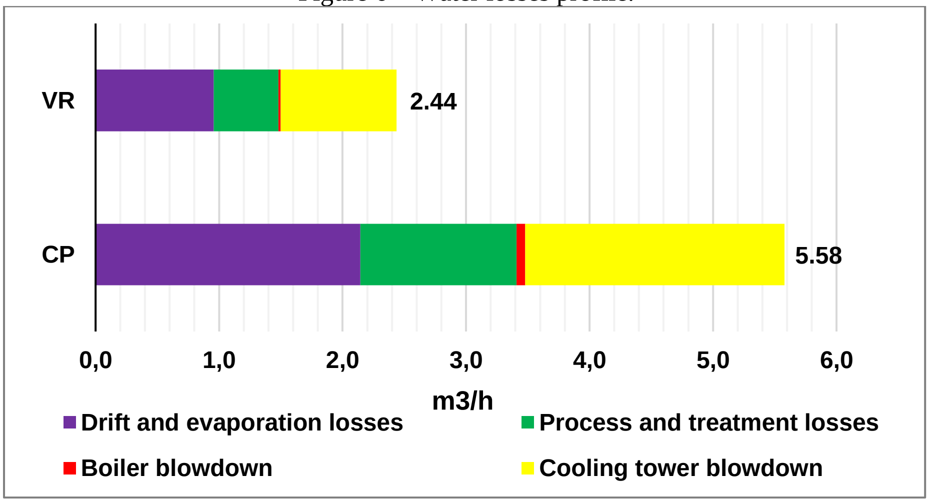
Figure 5 – Energy consumption profile.



As demonstrated in this work and in Figueiredo et al. [23], sensible heat is critical in the energetic evaluation, accounting for over 17% of the total energy required in the boiler for the MCB separation process. Many studies do not consider this type of heat since, in simulation software, credit is only taken for the latent heat. Consequently, deviations in the energy analysis are found, leading to errors that reflect in the acquisition and purchase of utilities.

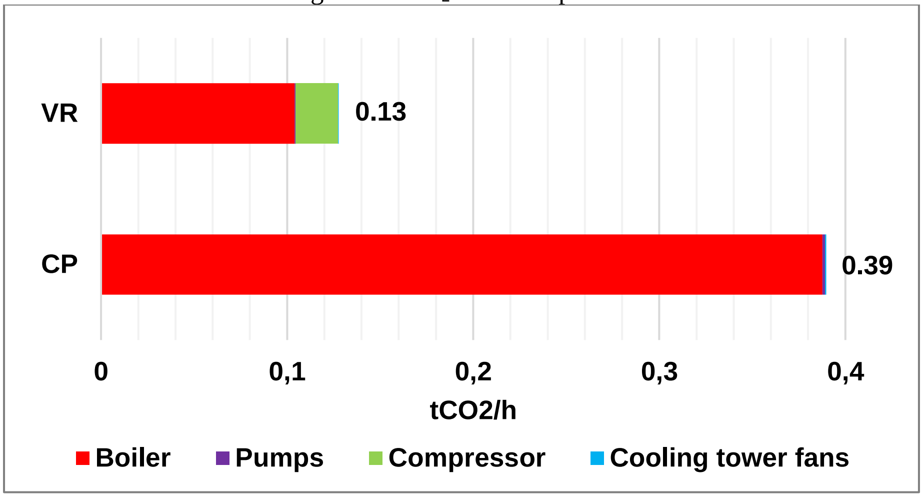
In accordance with the decrease in energy input in the intensified process, less water is necessary to fulfill the cooling and heating plant demand. Due to this, smaller quantity of water circulates in the utility facilities, reducing up to 56.33% of the water losses, as shown in Table 4 and Figure 6.

Figure 6 – Water losses profile.



VR technology shows promise for reducing CO_2 emissions, as illustrated in Figure 7. This effect is driven by two factors: its energy consumption profile and the local power generation mix. VR reduces natural gas usage but increases electricity demand. Consequently, locations with a high share of renewable energy in their power grid will experience significantly lower CO_2 emissions compared to conventional processes reliant on natural gas. Countries like Brazil, which heavily invest in clean energy, are likely to benefit most from this strategy, potentially achieving a reduction of around 67% in emissions.

Figure 7 – CO_2 emission profile.



5 CONCLUSION

This study investigated the environmental advantages of a vapor recompression intensification approach in the monochlorobenzene original separation process. A utility plant was contemplated to produce more realistic results. The outcomes revealed that this technique achieved reductions in all of the metrics evaluated when compared to the conventional process, lowering up to 59.06% in energy demand and 56.33% in water use, as well as decreasing CO_2 emissions by 67.23%. Given the present issue of aligning production with the goals outlined in the 2030 Agenda [5], the findings indicate some positive effects on sustainability. However, to guarantee economic viability, the expense of purchasing a compressor, as well as the local cost of process utilities, must be measured. These data may assist in ensuring the benefits of this design and supporting its incorporation in MCB separation facilities around the world.

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APPENDIX

A. UniSim PDF Flowsheets

Figure A.1 – PC diagram in the UniSim interface.

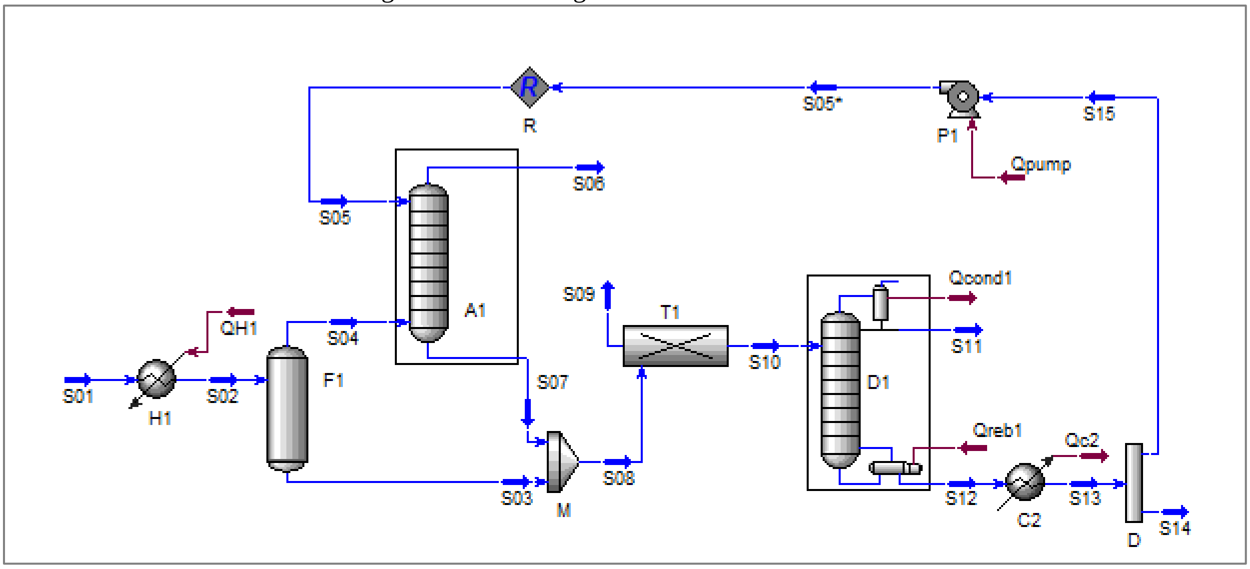

Figure A.2 – VR diagram in the UniSim interface.