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Environmental assessment of the divided wall column in the separation of the BTX system

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ABSTRACT
In favor of the green economy, the concern for cleaner and more efficient technologies has been the focus of many researches regarding process intensification. In this context, the present work aims to present an energetic and environmental analysis for the separation of the ternary mixture Benzene-Toluene-Xylene (BTX) via a divided wall column (DWC), endorsing previous studies. The simulation results revealed that the application of this technique was able to reduce the total energy input, water consumption, and CO2 emissions by 15.78 %, 30.31 %, and 15.65 %, respectively. These findings indicate promising sustainability gains.

Keywords: Industrial growth, Energy sources, Clean technologies.

1 INTRODUCTION

Amid intense industrial growth, the demand for energy sources and raw materials has become more pronounced, leading to impacts that affect the entire society [1]. In this regard, environmental concerns have prompted the search for cleaner technologies that maintain productive competitiveness [2]. Thus, the intensification of processes has gained prominence, aiming to promote greater efficiency and sustainability in various industrial segments [3].

As a result, energy-intensive equipment, such as distillation columns, has been the focus of several studies in order to achieve better energy and water savings while also lowering CO_2 emissions and therefore promoting process eco-efficiency. In this context, the divided wall column (DWC) represents a significant advancement in multicomponent mixture separation [4]. The DWC is a modification of the Petlyuk layout in which the prefactionator and main column are combined into a single tower with a vertical wall dividing it into two portions [5]. DWC may also be used for extractive distillations, azeotropic separations, and reactive distillations, resulting in lower capital and operational costs [4].

In the industrial context, one of the processes that can associate economic progress with sustainability is the separation of the Benzene-Toluene-Xylene (BTX) system. This aromatic stream is often produced as a result of catalytic reforming of naphtha, steam cracking, and aromatization of liquefied petroleum gas (LPG). These chemicals major applications include the synthesis of petrochemical products and other organic compounds such as ethylbenzene and monochlorobenzene. As it is an important and large-scale chemical plant, its high energy demand encourages the use of intensification measures that have minor environmental consequences and encourage the efficient use of water in its operations.

Previous studies have suggested the DWC strategy to enhance the separation of the BTX system. Kim [6] showed that such an application could save about 35.8 % and 32.2 % of heating and cooling duties compared to the conventional counterpart. Such a result led to a reduction of 33.9 % in utility costs, favoring the financial return due to the increased investment. Meanwhile, Yuan et al. [7], Kiss and Rewagad [4], Ling and Luyben [8,9] focused on developing control structures for such separating system. An innovative design was proposed by Si et al. [10], which evaluated the alignment of DWC and vapor recompression (VRC) with the organic rankine cycle (ORC). It was shown that the ORC applied to the VRC-DWC could save up to 44.99 % of energy demand and 33.57 % in TAC expenditure while reaching an exergy efficiency of 0.15.

Nevertheless, none of the previous research attempted to assess the decrease in water usage and CO_2 emissions supplied by the DWC arrangement to the BTX separation, which is the purpose of this present work. Such an analysis is crucial in the sustainability evaluation as it provides further assistance for retrofitting and revamping current industry processes and aligns the production sector with the goals established in the 2030 Agenda [11].

2 OBJECTIVE

The current study attempts to replicate the two conformations (conventional process and DWC process) BTX separation process, as presented by Ling and Luyben [8]. An analysis of the energy and water consumption as well as the CO_2 emissions of such configurations was made to evaluate potential environmental and economic improvements, considering a utility plant for more realistic results.

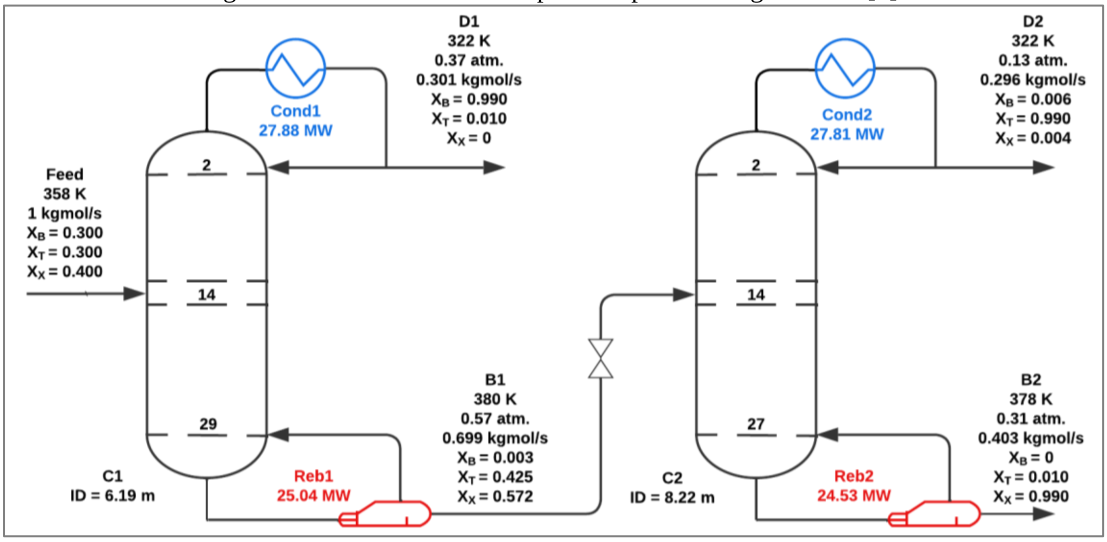
3 METHODOLOGY

The methodology used in this study was theoretical-computational performed in Unisim software.

3.1 CONVENTIONAL PROCESS (CP) DESCRIPTION

As proposed by Ling and Luyben [8], the conventional separation process with two distillation columns in series, represented in Figure 1, has a feed of 1 kmol/s composed (molar basis) of 30 % Benzene (X_B), 30 % Toluene (X_T), and 40 % ortho-Xylene (X_X) that enters the first column (with 30 stages; fed into the 14th stage; internal diameter of 6.19 m, spacing between plates of 0.601 m). In the output streams, the distillate (D1) has a high purity of benzene (99 % molar basis), while the bottom product (B1) passes through a valve and is subsequently sent to a second column (with 28 stages; fed in the 14th stage; internal diameter of 8.22 m, spacing between plates of 0.601 m). The separation resulting from the latter makes it possible to obtain a distillate (D2) rich in toluene (99 % - molar basis) and a bottom stream composed mainly of ortho-xylene (99 % - molar basis).

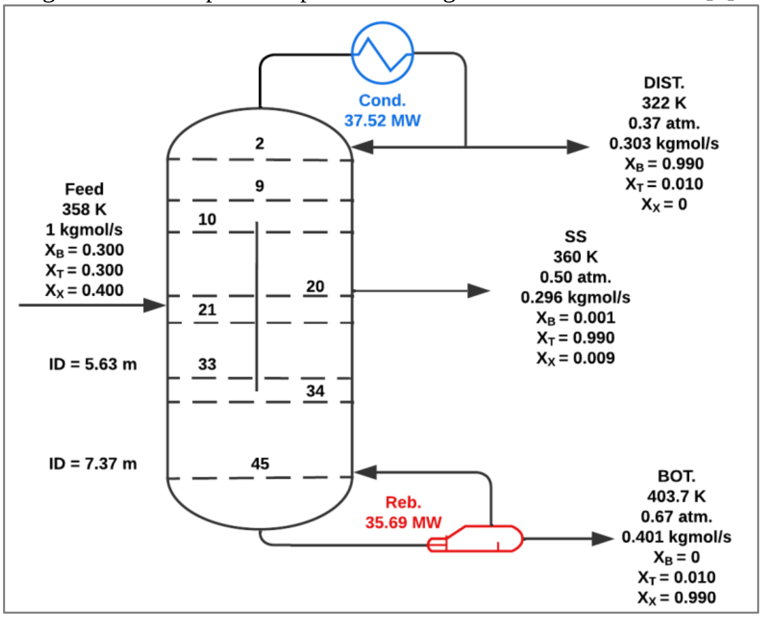
Figure 1: Conventional BTX separation process diagram flow [8].



3.2 DWC SEPARATION PROCESS DESCRIPTION

To improve the process's energy efficiency, the authors of the reference work [8] also proposed the separation through DWC, which is seen in further detail in Figure 2.

Figure 2: BTX separation process through DWC intensification [8].



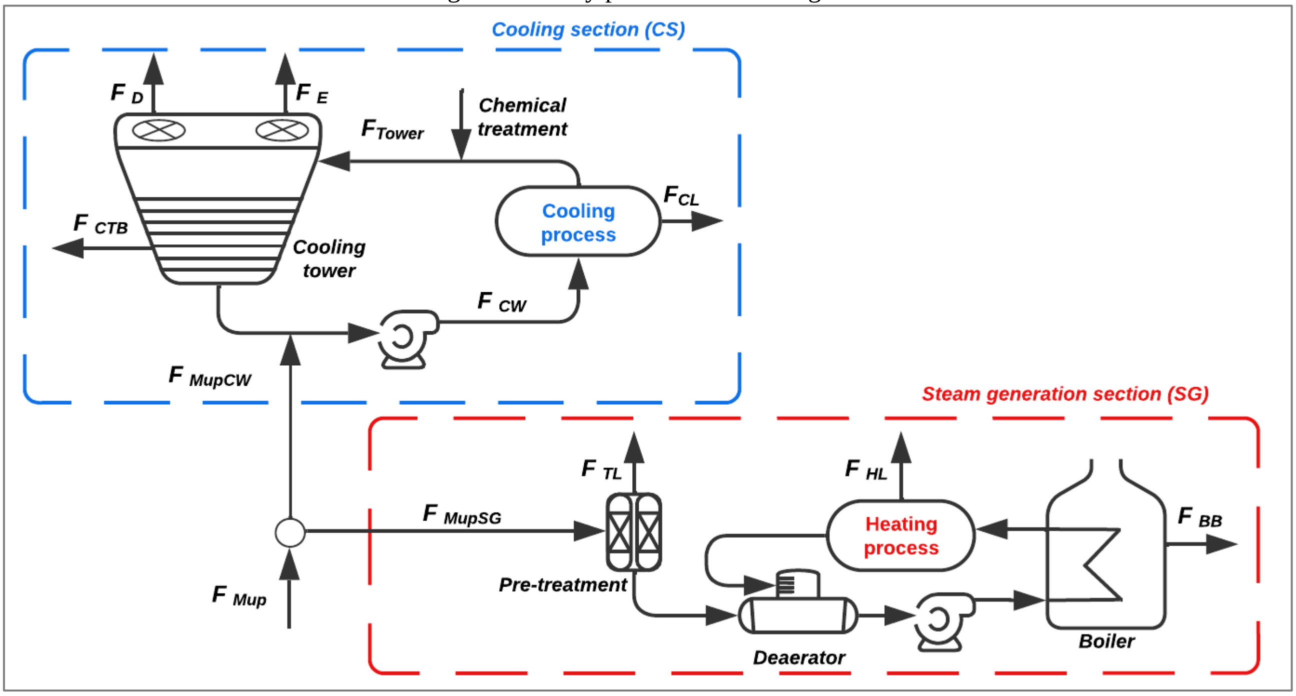
For this system, the input stream (Feed) is supplied to one side of the column with the same specifications as the conventional process, reaching the wall inside the tower (not necessarily in the center).

As a result of mass and heat transfer principals, the lighter species (benzene) goes mostly to the top of the column, leaving in the distillate (Dist.), while the heavy key (o-xylene) is directed to the bottom of the column, being removed almost entirely as a bottom product (Bot.). Furthermore, the toluene initially flows both to the upper part of the tower and to the lower part; however, when it reaches the extremes of the column, it starts to move on the other side of the wall, being recovered through the side stream (SS).

3.3 UTILITY PLANT

In order to provide more accurate and consistent estimates of the demand for utilities in the aforementioned processes, a simulation of the utility plant was also conducted. Such a plant consists of two subsystems primarily driven by water: the cooling (CS) and the steam generation (SG), as shown in Figure 3.

Figure 3: Utility plant flowsheet diagram.



The cooling section operates as an open system with recirculation, whereby the heated water streams, after thermal exchange, undergo chemical treatment and are then sent to the cooling tower (F_{Tower}). Within the tower, the fans facilitate the return of the water to its original supply temperature, enabling its reuse in the plant's refrigeration activities. Moreover, during this process, a makeup current (F_{MupCW}) is necessary to replace losses due to evaporation (F_E), drift (F_D), tower blowdown (F_{CTB}), and possible leaks in the equipment present in the operation (F_{CL}).

In steam generation, water is initially treated in a cationic and anionic bed and sent to the boiler, where it acquires sensible and latent heat, shifting into the vapor state. In this way, the water, now heated, is made accessible to suit the demands of the industrial facility. Furthermore, analogous to the cooling process, losses are also present due to the boiler purge (F_{BB}), treatment (F_{TL}), and heating stage (F_{HL}). Therefore, a second makeup stream (F_{MupSG}) is introduced to compensate for the amount of water lost. It's important to emphasize that, in the SG section, different vapor classes can be generated [12], such as low-pressure steam (lps – 308 kPa and 134.5 ^{o}C), medium-pressure steam (mps 1136 kPa and 185.5 ^{o}C), and high-pressure steam (hps 4201 kPa and 253.8 ^{o}C). This present study used lps and mps as a utility for the CP and DWC processes, respectively, since these classes fulfill the minimum approach of 10 ^{o}C with the process streams to be heated in the reboiler, supporting the dynamic control of the main plant [13].

The heuristic values adopted during the simulation of the utility plants 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	[12]
Cooling tower inlet pressure	500 KPa	[12]
Cooling tower outlet temperature	30 ºC	[12]
Cooling process losses (F_{CL})	1 %	[14]
Drift losses (F_{D})	0.3 %	[14]
Evaporation losses (F_{E})[a]	1.8 %	[14]
Cooling tower blowdown (F_{CTB})	3 %	[14]

[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 %	[13]
Boiler blowdown (F_{BB})	3 %	[13]
Heating process losses (F_{HL})	10 %	[13]

Furthermore, in terms of energy consumption, the boiler's total demand (sensible and latent heat) must be corrected by its combustion efficiency of 80 %. [12] and since the duty of the cooling tower's fans cannot be retrieved directly from the UniSim software environment, they were calculated using Eq. (1) as suggested by Caxiano et al. [15]. Meanwhile, the energy requested by the utility pumps was calculated by the software, and the efficiency was set at 75 % [14]

$$\mathbf{W}_{\boldsymbol{Fans}}\left[\frac{\mathbf{GJ}}{\mathbf{h}}\right] = \frac{\left(\mathbf{F}_{\mathbf{Tower}}\left[\frac{\mathbf{m}^3_{\mathbf{H2O}}}{\mathbf{h}}\right]\right) \times \mathbf{2.432 \cdot 10^{-4}}\left[\frac{\mathbf{GJ}}{\mathbf{m}^3_{\mathbf{H2O}}}\right]}{\boldsymbol{\eta}_{\boldsymbol{Fans}}.} \quad (1)$$

In Eq. (1), W_{Fans} is computed using the specific area of the tower of 1.804 $ft^2/(m^3/h)$ and the fan power per area, whose value is 8.05×10^{-5} $(GJ/h)/ft^2$ [15, 16]. This adjustment uses the air wet bulb temperature of 26.7 °C (referent to Rio de Janeiro, Brazil) and accepts a cautious efficiency of 90 % for the tower's performance as well as 90 % for the electricity driven fans (η_{Fans}).

3.4 ENVIRONMENTAL ASSESSMENT

The purpose of the intensification techniques proposed for the BTX separation process is to boost its environmental performance, minimizing the emission of greenhouse gases and the generation of wastewater, as well as decreasing the expense of capital by reducing utility costs. In this context, the assessment of environmental, social, and operational impacts, especially in the initial stage of the project design, is essential to guarantee technical-economic feasibility and favor a future examination of eco-efficiency. Among the key metrics used to quantify prospective improvements to a process, those that account for water and energy consumption as well as CO_2 emissions stand out, being developed in this work to analyze and contrast the outcomes of the suggested configurations. Table 3 displays the equations used to evaluate the aforementioned metrics.

Table 3 – Equations used for analysis of the simulation results

Metric	Equation	Unit
Energy consumption (EC)	$EC = \frac{W_{Comb.}}{\eta_{Comb}} + W_{Pump} + W_{Fans}$ [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} and W_{Fans} are already corrected by their respective efficiency

In Table 3, W_{Comb}, W_{Pump}, and W_{Fans} represent the energy consumption, in GJ/h, for combustion in the boiler, pumps, and fans, respectively, with η_{Comb} being the boiler efficiency (80%). Furthermore, W_{Comb} (natural gas combustion energy) and W_{Ele} (electricity consumption) are calculated according to Eqs. (2) and (3), respectively, while F_{Mup} considers the replacement water flows in the utility plant for the cooling system (F_{MupCW}) and steam generation (F_{MupSG}).

$$W_{Comb.} = \frac{Q_{sens} + Q_{lat}}{\eta_{Comb}} \tag{2}$$

$$W_{Ele.} = W_{Pump} + W_{Fans} \text{ [c]} \tag{3}$$

In Eq (2), Q_{sens} and Q_{lat} are, respectively, the portions related to sensible and latent heat in GJ/h. Q_{sens} is obtained directly by the utility plant.

Still in Table 3, ξ_{Comb} and ξ_{Ele} are the CO_2 emission factors from direct (combustion) and indirect (electricity) sources, respectively. The first has a set value of 0.0561 t_{CO2}/GJ [17] for natural gas as fuel. The second depends directly on the local energy matrix. Assuming the location of the processes in Brazil, this factor corresponds to the value of 0.0107 t_{CO2}/GJ, the average annual factor in this country for the year 2023 [18].

3.5 COMPUTATIONAL SIMULATION

To simulate the BTX proposed plants, the Unisim® R490 software was used under steady-state conditions. In the base article, the thermodynamic package used was the Chao-Seader, however, aiming for greater compatibility between data and smaller deviations, the Peng Robinson model was chosen (applicable for hydrocarbons at low pressures). For the utilities plant, the UNIQUAC model was adopted, as well as the heuristics listed in Tables 1 and 2.

Furthermore, it is not possible to simulate DWC setup using the Petlyuk column arrangement described by Luyben [19]. Thus, DWC was developed using four columns: two absorbers to represent the prefractionation and main columns (sections originated from the wall insertion), a column with a top condenser to represent the rectifying zone (above the wall), and another with a reboiler to represent the stripping section (below the wall).

Lastly, based on water and energy consumption data analysis as well as the selected efficiencies, the related metrics (EC, WC, and CDE) were determined through the Equations outlined in Table 3.

4 RESULTS

4.1 SIMULATION RESULTS

In the appendix, section A.1 presents a comparison of the process conditions, molar compositions, and energy inputs obtained via simulation with those of the reference article for the conventional process. Meanwhile, Section A.2 provides the same analysis, but regarding the DWC configuration.

From the data presented in the appendix, minor deviations in the compositions, temperatures, and pressures of the currents can be noted, considering the values and order of magnitude expressed in the article. Furthermore, divergences of up to approximately 9% and 6% were found for energies in the condenser and reboiler of the CP and DWC, in which a possible cause would be related to the different software used since the article uses Aspen Plus®. Such results (less than 10%) validate the base simulation for studies of intensification strategies.

4.2 ENVIRONMENTAL ASSESSMENT

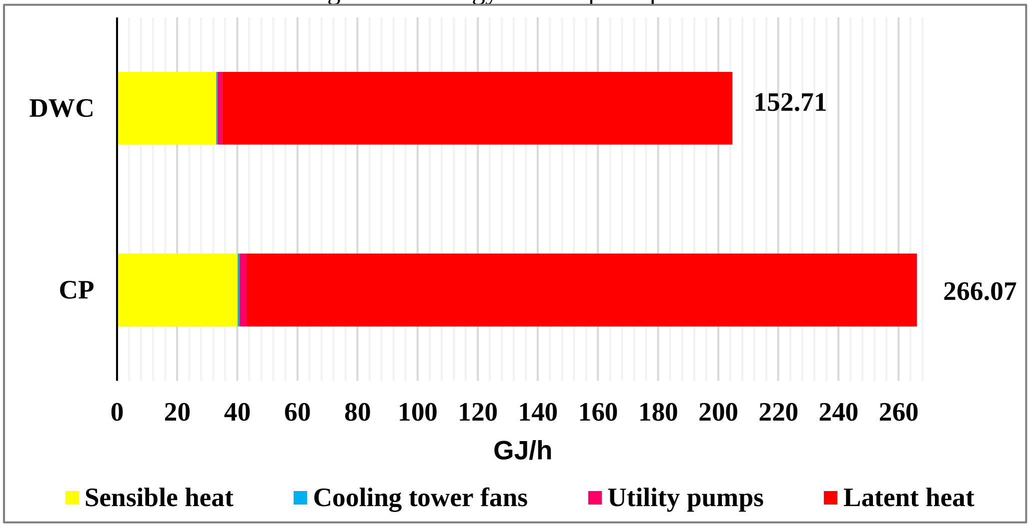
Table 4 presents the results for water and energy consumption for the simulated processes, considering the heuristics adopted for water losses, the total combustion demand with its respective efficiency and portions of heat (sensible and latent), as well as the electricity spent in each operating plant.

Table 4 – Results regarding energy and water consumption.

Process	CP	DWC
Boiler latente heat(GJ/h)	223.00	169.62
Boiler sensible heat (GJ/h)	40.08	33.00
Electricity (GJ/h)	2.98	2.06
Total energy demand (GJ/h)	**266.07**	**204.68**
Condenser (GJ/h)	184.53	127.62
Total cooling demand (GJ/h)	184.53	127.62
Cooling process losses (m^3/h)	43.93	30.38
Evaporation and drift (m^3/h)	91.33	63.16
Cooling tower blowdown (m^3/h)	127.72	88.33
Losses in the cooling water system (m^3/h)	**262.98**	**181.87**
Boiler blowdown (m^3/h)	2.56	2.11
Treatment losses (m^3/h)	0.11	0,09
Heating process losses (m^3/h)	8.28	6.81
Losses in the steam generation system (m^3/h)	**10.95**	**9.01**
Total water consumption(m^3/h)	**273.93**	**190.89**

The data presented in Table 4 indicates that DWC achieved a reduction in energy demand of approximately 15.78% when compared to its conventional counterpart, as can be seen with further details in Figure 4. Such a result is due to DWC operating conditions that minimize the entropy of the mixture, besides having only one reboiler and condenser instead of two [20]. A disadvantage of the DWC arrangement regarding energy consumption is the higher temperature required in the reboiler in contrast with the CP process, which is linked with the pressure distribution in the column internal [21] and leads to the necessity of higher-class vapor utility.

Figure 4 – Energy consumption profile.



Although Kim [6] showed a further improvement of over 30 % in the energy amount needed for cooling and heating demands, such a process was slightly different as it considered a feed stream that had aromatics and non-aromatics, enhancing the necessity for an extraction process that is highly energy intensive due to the solvent's high boiling point. As a consequence, DWC was applied to such process to reduce extraction loads, provide energy savings, and reduce operational costs. In contrast, Ling & Luyben [8] focused only on the separation of the BTX aromatic compounds, leading to distinct results from the ones presented in this paper, as already expected.

In terms of water consumption, as energy demands were lowered for the DWC configuration, the amount of water needed for cooling and heating in the column's condenser and reboiler was also minimized, leading to less circulating water in the utility plant. As a consequence, losses due to evaporation, drift, process, treatment, cooling tower blowdown, and boiler blowdown were diminished, reducing the make-up flow acquisition by 30.31 % when compared to the conventional process. Additional details regarding this outcome are provided in Table 4 and graphically depicted in Figure 5.

Concerning CO_2 emissions, it is clear that such a measure results in a decrease that is comparable to the energy consumption findings, since no electric power equipment, such as big compressors, were included in the evaluated intensification. Because the combustion energy demand in the boiler accounts for almost 99% of the total power required in such an operation, the reduction was mostly attributable to the decrease in natural gas consumed in the DWC system. This, along with a little drop in electricity use, resulted in a 15.65% reduction in CO_2 emissions for the suggested alternative, displayed in Figure 6.

Figure 5 – Water losses profile.

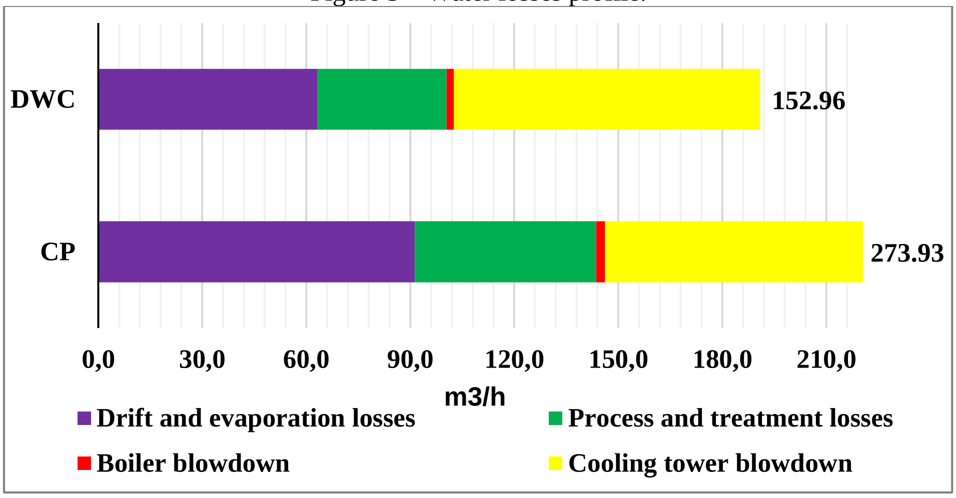
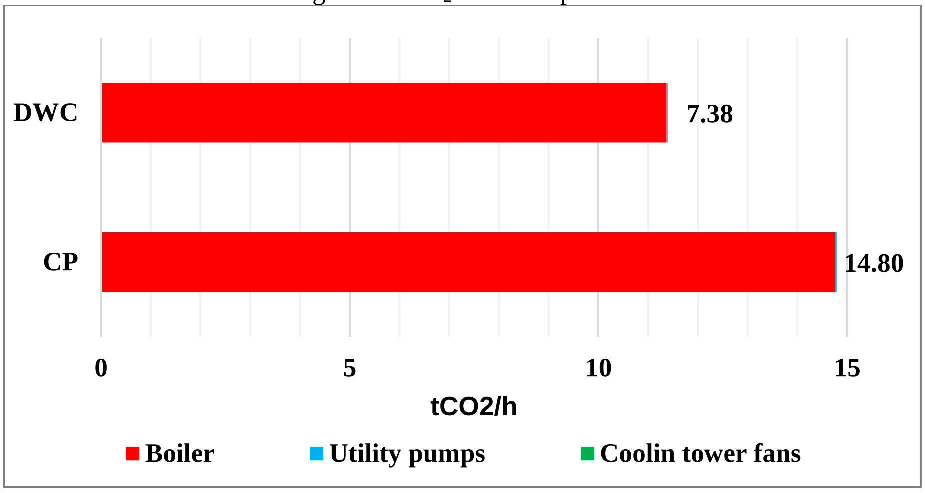


Figure 6 – CO_2 emission profile.



5 CONCLUSION

In this work, a study was carried out to investigate the reductions in energy, water consumption, and CO_2 emissions from the intensification of the conventional BTX separation process through the implementation of the divided wall column. A utility plan was considered to obtain more realistic results. The results showed that this strategy presented reductions for the three metrics studied when compared to the conventional process, saving up to 15.78% in energy demand and 30.31% in water consumption, as well as reducing CO_2 emissions by 15.65%. The outcomes demonstrate certain sustainability advantages that are consistent with the goals outlined in the 2030 Agenda [11]. When combined with a future review of the DWC's economic feasibility, these findings can validate the benefits and advocate for this configuration to be implemented in BTX separation plants operating worldwide.

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APPENDIX

A.1. Conventional Process

The given results of the conventional process throughout the simulation in the software UniSim are presented in Table A.1.1 and A.1.2 as well as their comparison with the data provided by Ling & Luyben (2009). Meanwhile Figure A.1 shows the conceptual flowsheet of the CP in the simulation environment.

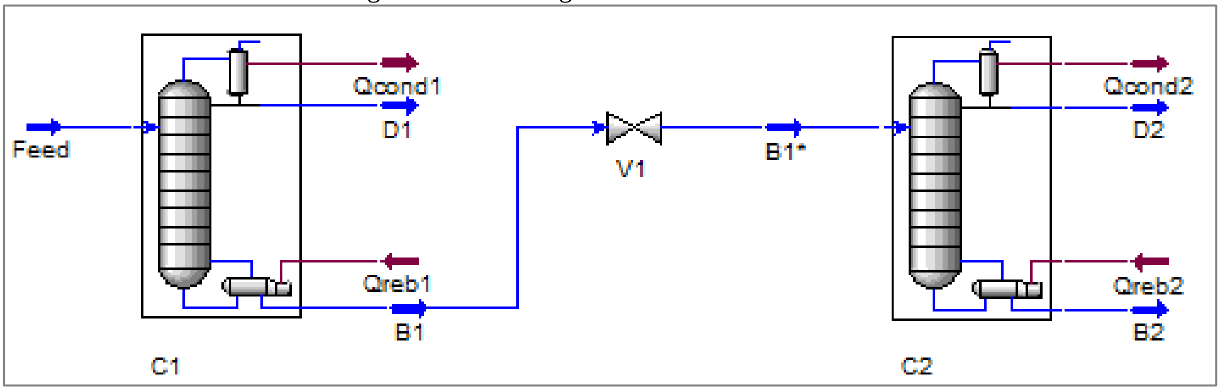
Table A.1.1 – Analysis of CP process flow streams condition.

Streams		T	P	Flow	Molar fraction		
		(K)	(atm.)	(kgmol/s)	B	T	X
D_1	Ling e Luyben	322.0	0.37	0.3010	0.990	0.010	0.000
	UniSim	323.8	0.37	0.3010	0.990	0.010	0.000
	Deviation (%)	0.56	0.00	0.00	0.00	0.00	0.00
B_1	Ling e Luyben	380.0	0.57	0.6990	0.003	0.425	0.572
	UniSim	378.2	0.57	0.6990	0.003	0.425	0.572
	Deviation (%)	0.47	0.00	0.00	0.00	0.00	0.00
D_2	Ling e Luyben	322.0	0.13	0.2960	0.006	0.990	0.004
	UniSim	323.5	0.13	0.2961	0.006	0.990	0.004
	Deviation (%)	0.47	0.00	0.03	0.00	0.00	0.00
B_2	Ling e Luyben	378.0	0.31	0.4030	0.000	0.010	0.990
	UniSim	376.5	0.31	0.4028	0.000	0.010	0.990
	Deviation (%)	0.40	0.00	0.05	0.00	0.00	0.00

Table A.1.2 – Analysis of CP energy streams.

Stream		Equipment	Energy (MW)	Deviation (%)
Q_{cond1}	Ling e Luyben	Condenser of column C1	27.88	8.86
	UniSim		25.41	
Q_{reb1}	Ling e Luyben	Reboiler of column C1	25.04	6.31
	UniSim		26.62	
Q_{cond2}	Ling e Luyben	Condenser of column C2	27.81	7.05
	UniSim		25.85	
Q_{reb2}	Ling e Luyben	Reboiler of column C2	24.53	6.48
	UniSim		22.94	

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



A.2. DWC Process

The given results of the DWC process throughout the simulation in the software UniSim are presented in Table A.2.1 and A.2.2 as well as their comparison with the data provided by Ling & Luyben (2009). Meanwhile Figure A.2 shows the conceptual flowsheet of the DWC in the simulation environment.

Table A.2.1 – Analysis of DWC process flow streams condition.

Streams		**T**	**P**	**Flow**	**Molar fraction**		
		(K)	**(atm.)**	**(kgmol/s)**	**B**	**T**	**X**
Dist.	Ling e Luyben	322.0	0.37	0.303	0.990	0.010	0.000
	UniSim	323.8	0.37	0.303	0.990	0.010	0.000
	Deviation (%)	0.56	0.00	0.00	0.00	0.00	0.00
SS	Ling e Luyben	360.0	0.50	0.296	0.001	0.990	0.009
	UniSim	360.6	0.50	0.296	0.001	0.990	0.009
	Deviation (%)	0.17	0.00	0.00	0.00	0.00	0.00
Bot.	Ling e Luyben	403.7	0.67	0.401	0.000	0.010	0.990
	UniSim	401.5	0.67	0.401	0.000	0.010	0.990
	Deviation (%)	0.54	0.00	0.00	0.00	0.00	0.00

Table A.2.2 – Analysis of DWC energy streams.

Stream		**Equipment**	**Energy (MW)**	**Deviation (%)**
Q_{cond1}	Ling e Luyben	Condenser of DWC	37.52	5.52
	UniSim		35.45	
Q_{reb1}	Ling e Luyben	Reboiler of DWC	35.69	5.60
	UniSim		37.69	

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