



Simulation-based heat performance evaluation of traditional and divided wall heat integrated distillation column for separation of BTX mixture

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To improve the effectiveness of the distillation process, a number of different approaches have been suggested, and the divided wall column is one of the techniques that have been taken into consideration. When dealing with multicomponent systems that demand high purity, it is common practice to employ an array of distillation columns for efficiently separating the components into multiple product streams. In order to limit the overall number of columns and space in this investigation, the simulation that is performed in the Aspen plus program makes use of four columns in a divided wall sequence. The current study investigates the process of separating benzene-toluene-p-xylene (BTX) utilizing the suggested design. In order to attain the highest possible product purity, the operating variables including the number of trays, reflux ratio, splitting ratio, and input composition have been optimized. Using Aspen Plus V8.8, the Sequential Quadratic Programming approach is used to optimize the parameters for optimal product purity. The vapour recompression approach has been utilized for heat integration in the divided wall column system. When compared to the standard distillation column, this technique results in a substantial decrease in the consumption of energy, particularly by 38.48%. The structure being discussed is referred to as a divided wall heat integrated distillation column (HIDIc). The results demonstrate that the product purity obtained with both configurations is 0.99 for benzene, 0.92 for toluene, and 0.97 for p-xylene.

Keywords: BTX, Divided wall column, Heat integration, HIDIc, Optimization, Thermal separation

Introduction

The search for methods of processing that not only conserve energy but also have positive environmental impacts is driven by the escalating costs of crude oil, which have become a consequence of the growing energy requirement and pollution levels. The periodic advancement in distillation techniques is a manifestation of global endeavours to achieve sustainable plant performance. Given the significant role of distillation in separation processes, ensuring its energy efficiency is of utmost importance. Consequently, reducing energy usage has been a central area of research for many years, with a particular emphasis on heat integration. By removing the prefractionator unit within the pseudo-Petlyuk column, we obtain an arrangement called the divided wall column (DWC), as depicted in Fig. 1. There are various applications for DWC beyond ternary separation. It plays a significant role in extractive and azeotropic distillation, in addition to multicomponent systems and reactive distillation. A vertical wall is inserted at an appropriate location within the DWC, dividing the central area into two halves. The DWC process has the capability to effectively segregate a

ternary mixture into three distinct streams, each containing a single pure product. The feed is directed towards the pre-fractionator side, while a side stream is extracted off the primary column. The intermediate boiling constituent of the ternary combination makes up the majority of the side stream. This technique effectively segregated the products from the liquid mixture.

Concepts were initially formulated in 1933, and Richard Wright invented the current idea in 1946¹. One major advantage of the DWC design is that it prevents the entry of high-boiling components into the top of the side column and the entry of boiling substances into the bottom of the side column. The processing of the middle and low middle boiling constituents occurs in the upper segment of the primary column, while the lower segment is responsible for separating the high boiling and intermediate boiling components.

Distillation has been utilized as a separating unit for over 150 years. The distillation operation in the petroleum and chemical sectors has relatively significant energy consumption, accounting for around 60-70% of the overall energy used. In order to improve

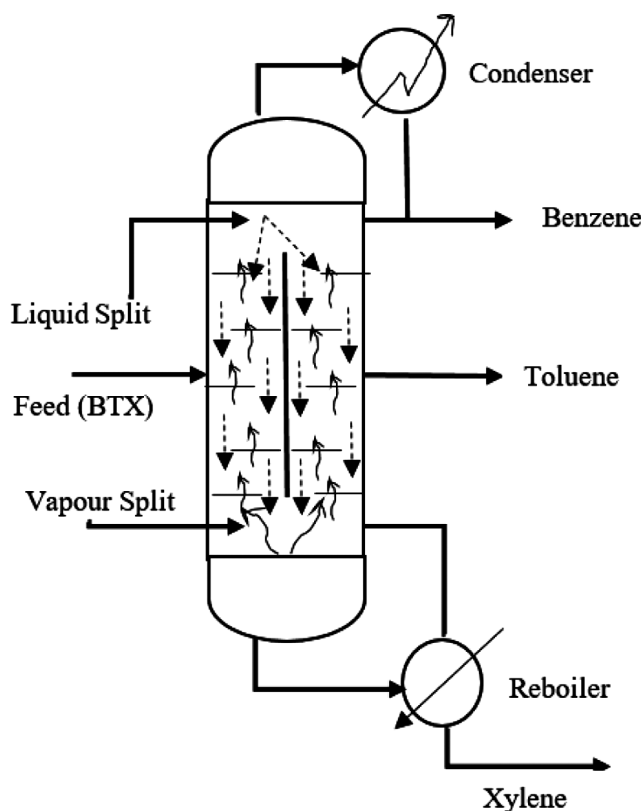


Fig. 1— Organized schematic of a divided wall distillation column

energy consumption and enhance purity, a hydrodynamic model consisting of heat-conduction equations, Navier-Stokes, and convection-diffusion was devised for the two-phase flow². According to reports, although having a low thermodynamic efficiency of approximately 5-10%³, they contribute roughly 3% of the overall energy usage. This necessitates the enhancement of its economic viability, energy efficiency, and emission level through the use of heat integration⁴. Heat integration technologies include vapour recompression-assisted divided wall column (DWC), internally divided wall heat integrated distillation column (HIDiC)⁵, and heat pump-assisted distillation⁶. DWC has emerged as a compelling option among all of these systems⁷. The DWC incorporates the prefractionator and the principal column of the Petlyuk arrangement into a unified shell, with the addition of a vertical wall⁸.

The process of separating aromatic benzene, toluene, and xylene (BTX) compounds from reformates produced by catalytic cracking of heavy oil and naphtha involves a sequence of extraction and distillation steps⁹. The process involves first extracting the mixture of BTX compounds and then distilling the

extracted mixture. The reformate produced by the catalytic cracker consists of 13 significant components¹⁰, which can be classified into four groups: xylene and compounds with similar boiling points, toluene and hydrocarbons with comparable boiling points, benzene and compounds with similar boiling points, and lighter chemicals than benzene. Accurate and precise simulation of the DWC is essential in order to analyze its energy efficiency and responsiveness¹¹. Salten *et al.* proposed a transport phenomenon-based model for studying the impact of concentration and temperature on the column¹². Ensuring the safety and conducting a thorough risk analysis of a newly introduced design is always an absolute priority for any industry. A safety integrity label (SIL) for successive safety assignments has been established based on risk assessment. These features were integrated into an industrial control system (ICS), which is made up of a safety instrumented system (SIS) and a basic process control system (BPCS)¹³. According to Cui *et al.*, the explosion and fire threat category was determined to be medium. However, once compensatory measures were implemented, the degree of explosion and fire hazard became the safest, which aligns with the findings of the DYN-SIL analysis¹⁴. The DYN-SIL approach has the potential to be applied to actual production systems, especially the reactor-regenerator system.

Heat is the principal factor that drives the separation process in distillation, and it accounts for approximately 40% of the overall energy utilized by the chemical industry^{15,16}. The utilization of heat is inefficient when it is delivered to the bottom reboiler for evaporating a liquid combination at an elevated temperature, and is dissipated at a lower temperature during condensation at the very top of the column that performs distillation. Jian Zhai suggested using a heat pump and heat integration approaches for the pressure swing distillation column¹⁷. The primary focus of interest in the DWC is its controllability, which is crucial for energy conservation. In this regard, the authors recommend the use of modern and adaptive control approaches to regulate the purity of product¹⁸⁻²². Jiaxing Zhu introduced a method for separating dimethyl carbonate-methanol using aniline as a heavy entrainer. This method utilizes a vapour recompression-aided extractive dividing-wall column (EDWC-VRC) and incorporates intrinsic safety, environmental friendliness, and energy efficiency²³. The effectiveness of this methodology was evaluated

using a multi-criteria assessment. The Sargent column configuration is a better alternative configuration in comparison to the existing column configuration to separate and control the multi-component system from a single column with minimum energy utilization. The designs were obtained through rigorous simulations in Aspen Plus, linked to an optimization code using genetic algorithms in MATLAB. The optimization problem considers the total annual cost (TAC) minimization²⁴.

Heat integration is a fascinating field that many researchers have explored, focusing on the efficient use of energy within a system. One adaptable method for the heat integration process is vapour recompression. The vapour recompression device involves utilizing a compressor to increase the energy content of vapor that has been collected in the reboiler-condenser through a heat exchange with the bottoms. As indicated in Fig. 2, the condensate distillate is transferred into the reflux drum, whereas the bottom product is converted into vapour and sent into the column.

To facilitate the transfer of heat from the cooler overhead vapours to the hotter bottom product liquid, a temperature-driving force is established. This can be achieved by either condensing the overhead vapour at an elevated temperature through compression or by reducing the reboiler fluid pressure so that it boils at a reduced temperature. The vapour at the bottom of the

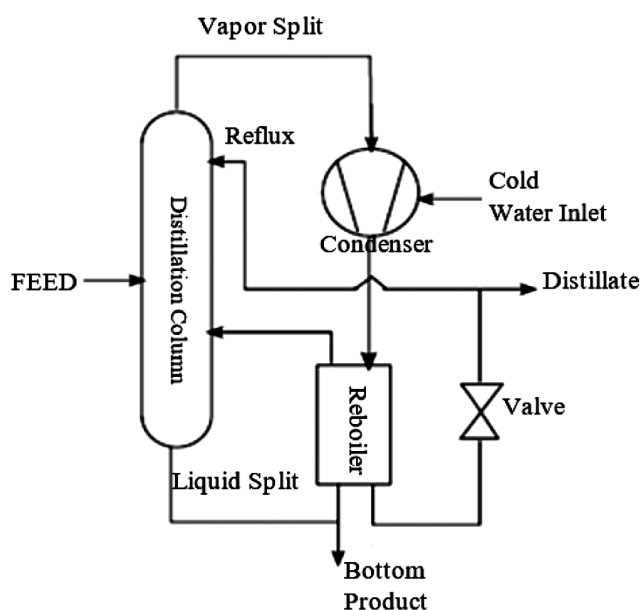


Fig. 2 — Organized schematic of a heat integrated distillation column (HIDiC)

column is then compressed until it reaches the pressure of the column. This type of column is commonly referred to as a HIDiC. Due to the complexity in the design of the column, internal mass transfer, and heat transfer coupling mechanism, the technical difficulties for the HIDiC process control are posed. The author gives his remark that due to the complexity of design, optimization, and manipulation of HIDiC, lots of research is required for large-scale industrialization²⁵.

Vapour recompression offers the benefit of efficiently transferring significant amounts of heat among the reboiler and condenser of the column using minimal energy input. Furthermore, it is possible to manipulate the temperature, and consequently the pressure, at any given location in order to attain optimal separation. This phenomenon is especially significant in cases when altering the pressure has an impact on the relative volatility²⁶⁻²⁸. The author has studied the performance of the heat-integrated column with a heat pump and concluded that the side vapour recompressed DWC (SVR-DWC) configuration is superior in terms of both energy consumption and payback time. Furthermore, the SVR-DWC provides a reduced complexity in compressor operation over the overhead vapor recompressed DWC (OVR-DWC)²⁹. Some other researchers have introduced the concept of a two-part heat-integrated dividing wall column with middle vapour recompression and proposed that the MVRC-DWCs have better energy and economic performance, and are more flexible than the VRC-DWCs, though the CSS-MVRC-DWC also has the same characteristics as the CRS-MVRC-DWC³⁰.

The dynamic performance such as energetic, economic, and dynamic for the optimal HIDiC configuration was achieved for a range of relative volatility (α) from 1.12 to 2.4. The author concluded that HIDiC sequences have worse dynamic and control properties than the conventional columns³⁰.

The current study utilizes the Aspen plus simulator to evaluate the energy efficiency of BTX separation using both the traditional DWC and the suggested divided wall HIDiC. In the suggested heat integration concept, heat exchange combines the benefits of VRC. This intricate column arrangement provides a substantial level of energy preservation through internal heat integration. Heat transfer takes place between the stripping and rectifying. This updated version of HIDiC can be utilized for industrial applications.

Experimental Section

Simulation study

Aspen Plus software was used to study the temperature profile and the effect of different parameters on the product compositions. This simulation investigation focuses on the use of standard DWC for separating the ternary liquid system (BTX), as depicted in Fig. 3. The operational variables within the current investigation are specified in Table 1.

The DWC is a multifaceted column that can be broadly categorized into four distinct sections: aside column, stripper, rectifier, and prefractionator. For simulation reasons, it is depicted as four fictional columns, including a stripper with a kettle reboiler, one rectifier with a complete condenser, and two simple columns, as illustrated in Fig. 3.

In order to achieve the highest level of energy efficiency during the separation process, it is

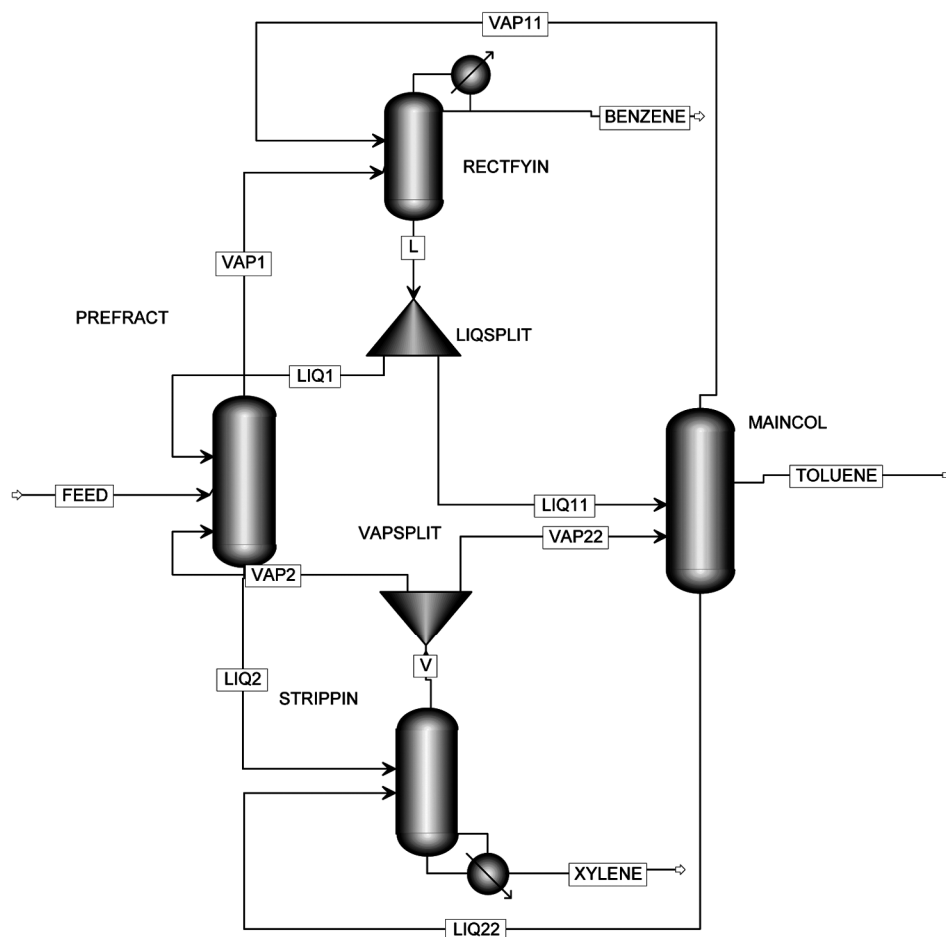


Fig. 3 — Simulation flow chart for a traditional divided wall distillation column

Table 1 — Operational parameters with their corresponding values

Parameters and conditions	Corresponding value of the parameter	Parameters and conditions	Corresponding value of the parameter
Feed flow rate	100 kmol/h	Bottom flow rate	60 kmol/h
Benzene	20 mol%	Side stream flow rate	15 kmol/h
Toluene	20 mol%	Side tray location	11
p-Xylene	60 mol%	Liquid split ratio	0.3
No. of trays in pre-fractionator column	20	Vapour split ratio	0.4
No. of trays in Rectifying section	15	Reflux ratio	6
No. of trays in stripping section	15	Boiling point of Benzene	81°C
No. of trays in post fractionator column	20	Boiling point of Toluene	110.6°C
Feed tray location	10	Boiling point of p-Xylene	138.4°C

important to minimize the presence of the mid-boiling component, toluene, in the feed. It is presumed that the DWS's vertical wall is located at the midpoint of the column. The feed stream's toluene content is 0.2 (mole fraction). As a result, it is assumed that the side column and the pre-fractionator have the same number of stages-20 steps each. To make things simpler, both the stripper and rectifier have an equal number of stages, specifically 15 stages each. Nevertheless, there is a decrease in pressure of 0.3 atm in the column, with the top stage having a pressure of 0.37 atm and the bottom stage having a pressure of 0.67 atm.

Achieving optimal parameter values

Aspen V8.8 provides a range of model assessment tools, including the ability to optimize variables in order to maximize or minimize a function by setting constraints on the variables. For this particular scenario,

an optimization with multiple objectives was conducted to achieve the highest possible purity of p-xylene, toluene, and benzene. This was accomplished by modifying several variables, including the flow rate of bottom steam and side product, the split fraction of vapour and liquid, and the portion of liquid returned as reflux. The software's limitations necessitate the use of toluene as the main focus for achieving maximum product purity. Xylene and benzene are classified as constraints, with a minimum requirement for their mole fractions to be 0.97 or higher. The optimum outcomes of product combination are acquired and listed in Table 2 after conducting a thorough simulation utilizing the sequential Quadratic Programming approach.

Composition analysis

The feed is introduced into the initial column at step 10. Fig. 4a shows that the mole fraction of p-xylene

Table 2 — Results of optimization for traditional DWC

Variable	Value of variable	Variable	Value of variable
Mole fraction of benzene	0.999	Liquid Split (L_{split})	0.366
Mole fraction of toluene	0.922	Vapour Split (V_{split})	0.549
Mole fraction of p-xylene	0.974	Side Stream Flow Rate (S_{flow})	20.022 kmol/h
Reflux ratio	5.465		

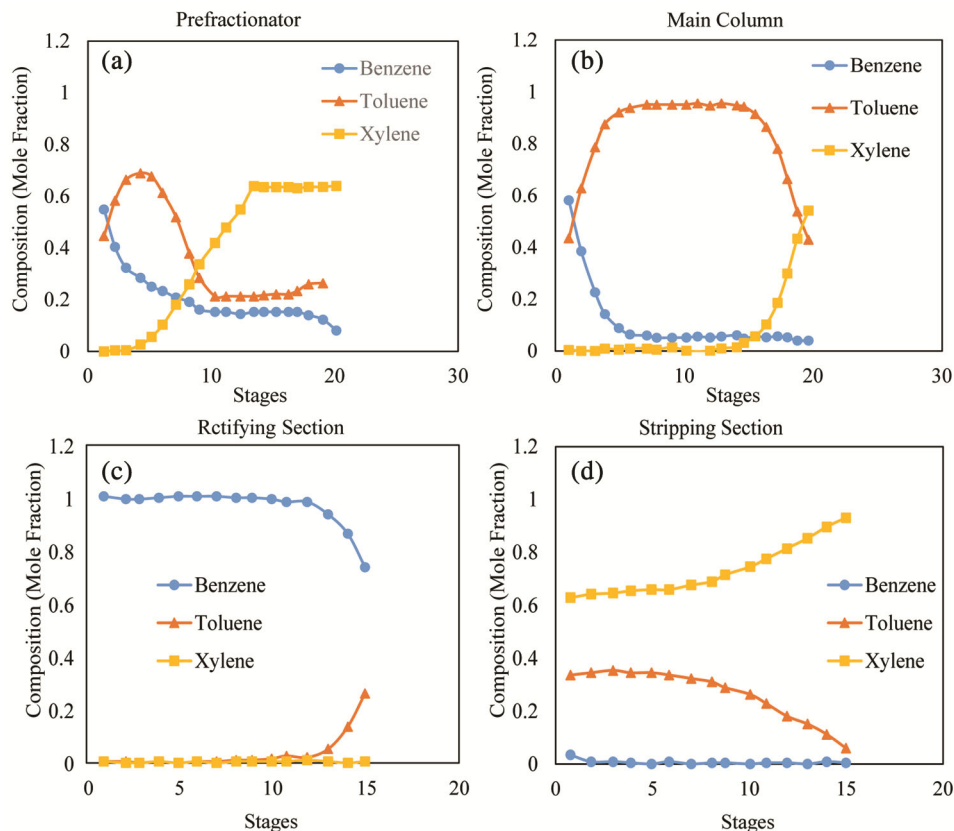


Fig. 4 — Composition of distinct constituents of BTX into different sections of DWC (a) pre-fractionator (b) main column (c) rectifier and (d) stripper

(a component with a high boiling point), declines above the feed stage while that of benzene (a component with a low boiling point) increases. Toluene, which is the component with a moderate boiling point, is evenly distributed along the column. The vertical wall located at the middle of the column, which acts as a separator between the main column and the pre-fractionator, makes this distribution in DWC possible. Because of variations in column temperature, the proportion of the heavier component gradually rises while the proportion of the lighter component gradually falls as we proceed down the column.

As indicated by the data in Fig. 4b, the toluene's proportion in the second column is significantly greater than compared to the other components. Furthermore, it is noteworthy that the highest level of purity is found in the central region of the column, which is a characteristic feature of a DWC having a vertical wall positioned in the middle. Along the column, benzene is barely noticeable, but at the bottom, there is a noticeable concentration of p-xylene. Thus, this analysis supports the decision to withdraw the side product stream from the mid-section of the column in order to achieve the optimum level of toluene purity. Fig. 4c clearly demonstrates that the upper section of the rectifier,

wherein the distillate is extracted, exhibits the largest concentration of benzene. This concentration gradually declines as we descend the column. Along the column, p-xylene (a heavier component) is barely noticeable, but at the bottom, there is a noticeable concentration of toluene. Fig. 4d illustrates that the highest proportion of p-xylene is found at the very end of the stripping column, which is the point from which the bottom product is extracted. The presence of benzene is minimal across the column, while the proportion of toluene substantially rises as we move upwards through the column.

Columns temperature profile

Fig. 5 displays the temperature distribution within the column. Based on the simulation findings, it was observed that the increased presence of higher boiling constituents causes the pre-fractionator column's temperature to rise as the feed stage descends (Fig. 5a). In the same manner, the temperature beyond the feed phase is reduced due to a greater concentration of low boiling constituents. While the temperature rises as we move down from the top level in the primary column, it maintains rather steady in the middle stages and then advances again in the bottom stages (Fig. 5b).

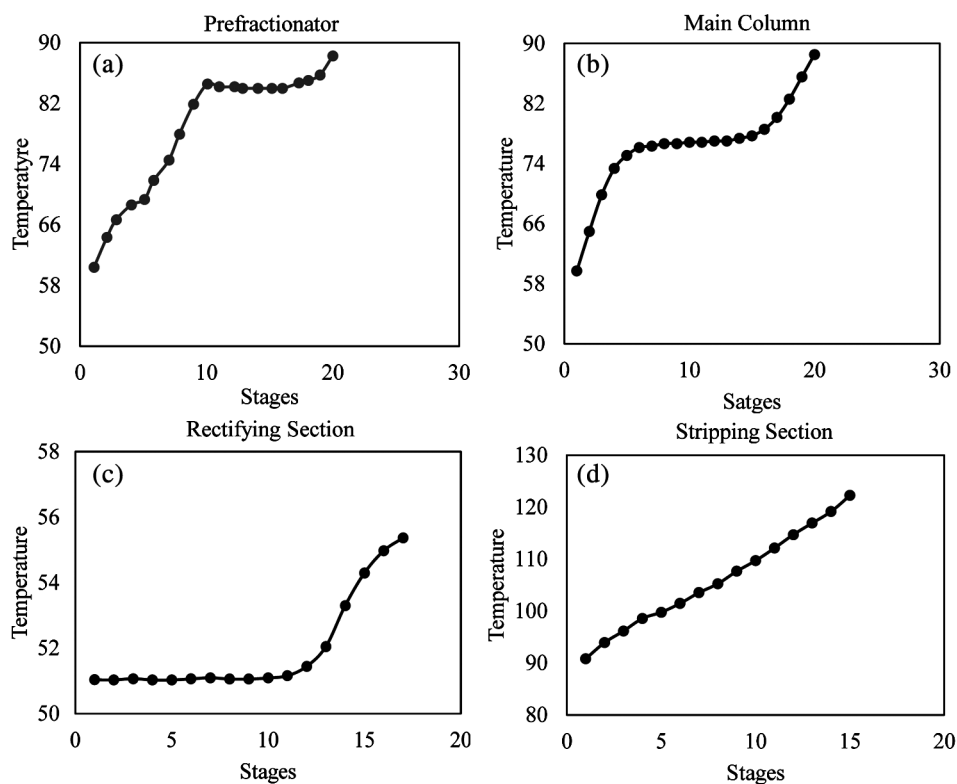


Fig. 5 — Temperature distribution with feed stages within the different sections of DWC (a) pre-fractionator, (b) main column, (c) rectifier and (d) stripper

Starting at the top stage, the rectifier's temperature rises slowly; however, it climbs sharply beginning in stage 8 and continues along the remaining column (Fig. 5c). In addition, the temperature change in the stripper column follows a linear pattern as one moves downward (Fig. 5d).

HIDiC using vapour recompression

In order to significantly cut down on energy usage, the BTX mixture was separated using a divided wall column using the vapor recompression technology. Fig. 6 illustrates the suggested heat integration flowsheet. An isentropic compressor, also known as a COMP, is designed to process the overhead vapours that are produced by the rectifying section's top stage. The vapours thus obtained (0.37 atm) are compressed to 3.115 atm. The high-temperature liquid discharged from the lower stage of the stripping segment is transported via a liquid splitter (SSPLIT). To maximize product purity, a split fraction of 0.5086 is employed. The HOTIN stream, emanating through the compressor,

is sent via a shell and tube heat exchanger to raise the temperature of the COLDIN stream that originates from the splitter. This process alters the phase of the stream, resulting in a vapour portion 1. Upon exiting the heat exchanger, the COLDOUT stream proceeds to the bottom stage's stripping portion.

The stream HOTOUT exists in a state of liquid-vapour phase. The steam's temperature has been further reduced using a condenser, resulting in its transition to a liquid phase with a zero vapour fraction. Afterwards stream S1 is directed to a liquid splitter called DSPLIT. The split fraction, which is 0.8582, is utilized in Eq. (1) to calculate the reflux ratio.

$$\frac{RR}{(RR+1)} \quad \dots (1)$$

Where RR represents the optimal reflux ratio utilized in the simulation of traditional DWC. The purity of the distillate is significantly impacted by this reflux ratio, which can be managed by modulating the flow rate of distillate in the manufacturing unit.

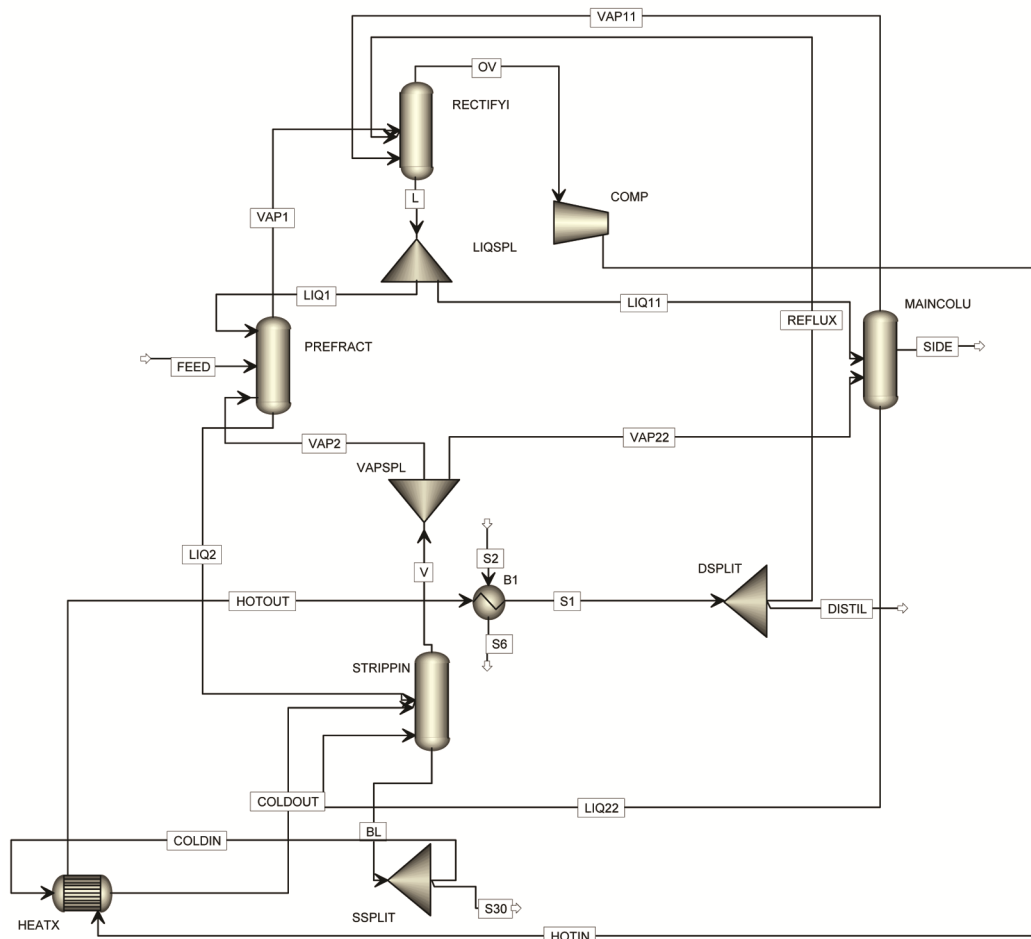


Fig. 6 — Divided wall HIDiC flowsheet

Table 3 — Results of optimization following heat integration

Variable	Value of variable	Variable	Value of variable
Benzene (mole fraction)	0.999	L_{split}	0.366
Toluene (mole fraction)	0.922	V_{split}	0.549
Xylene (mole fraction)	0.976	Side Stream flow	20.022 kmol/h
Compressor pressure	3.115 atm	Bottom flow rate	60.00 kmol/h
S_{SPLIT}	0.529	S_{FLOW}	14.921 kmol/h
Reflux ratio	5.465		

The residual stream, DISTIL, is extracted as the product stream and the refluxed stream is routed back to the rectifying section's top stage. To summarize, the stripping section's bottom liquid was heated using a heat exchanger and compressor to create vapours by harnessing the heat from the overhead vapours. Thus, it is an altered iteration of reboiling instead of employing a reboiler in the traditional procedure.

Optimized parameters for maximum purity

In order to optimize the purity of p-xylene, toluene, and benzene in the product, several factors were considered. These included varying the rate of flow of the side product stream (SFLOW), redirecting a fraction of the stripper's bottom liquid to the heat exchanger (SSPLIT), and adjusting the discharge pressure of the compressor (COMP).

The goal of the optimization was to enhance the quality of the toluene while ensuring that the mole fractions of p-xylene and benzene were larger than or equal to 0.97, as stipulated by the constraints. The findings obtained from the optimized simulation are presented in Table 3.

Results and Discussion

An essential aspect of comprehending the process involves examining how the quality of the product constituents is affected by different conditions and parameters. Various parameters were selected for variation, including the side stream flow rate, number of stages in the pre-fractionator, vapour split fraction, liquid split fraction, and reflux ratio. Theoretical analysis has been conducted to provide a comprehensive explanation for the observed trend. This analysis aims to improve our comprehension of the conditions and procedure of separation. In addition, the study examined the impact of adjusting the reboiler duty on the product purity. This was done by inputting the reboiler duty into the stripper column rather than the bottom flow rate. The goal was to assess the energy efficiency of the divided wall column process.

Influence of reflux ratio on the purity of a product

The rectification section's operating line gradient increases with the reflux ratio, reaching a maximum

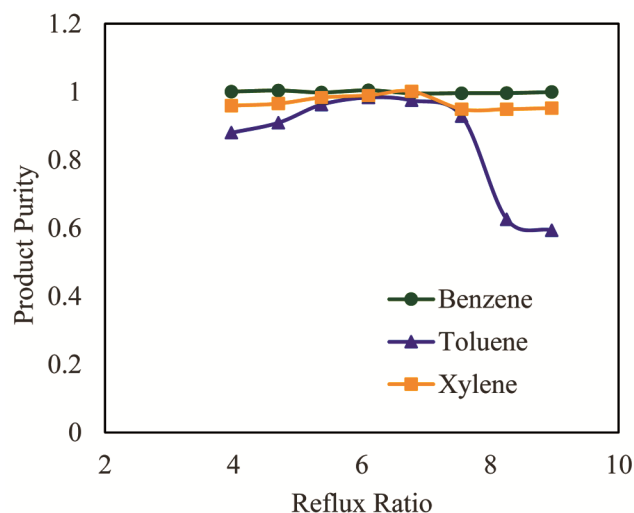


Fig. 7 — Influence of reflux ratio on the purity of a product

value of 1. Fig. 7 demonstrates that boosting the reflux ratio to 5.46 results in a corresponding rise in the overall purity of the top product (benzene). The impact of raising the reflux ratio on the bottom product's purity is diminishing, reaching its highest level at the optimal reflux ratio and subsequently experiencing a minor decline. The impact of reflux ratio (RR) on the side stream (toluene) was not conclusive as the purity remained relatively unchanged up to a reflux ratio of 5.46. However, beyond this point, the purity of toluene significantly decreased due to the highest purity of the bottom and top products. Based on the analysis, it can be established that a reflux ratio of 5.46 is the most suitable for conducting additional simulation studies.

Influence of liquid split fraction on the purity of a product

The liquid split fraction in a DWC is a crucial parameter that determines the amount of liquid that enters the pre-fractionator column extracted from the rectifier's bottom stage. When supplying feed to the pre-fractionator, the amount of liquid redistributed from the rectifier is supposed to be lower than that in the primary column or post-fractionator. This is done to ensure that the liquid hold-up is maintained in both segments. Consequently, as the split fraction increases, the purity of toluene and benzene declines

dramatically, whereas the purity of p-xylene experiences a slight variation (Fig. 8). At a split factor of 0.45, all three constituents reach their highest purity, making it the ideal value for this parameter.

Influence of vapour split fraction on the purity of a product

The vapour split fraction is a crucial parameter that quantifies the proportion of vapour originating from the stripping section's top stage and stepping into the main and pre-fractionator column. Fig. 9 demonstrates that increasing the vapour split fraction leads to an initial increase in the purity of toluene and benzene, reaching a maximum, and then progressively decreasing. Nevertheless, the p-xylene purity remains rather stable until a vapour split fraction of 0.55, beyond which it gradually diminishes. The maxima point corresponds to the optimal value of the vapour split fraction (0.55) for achieving maximum product purity.

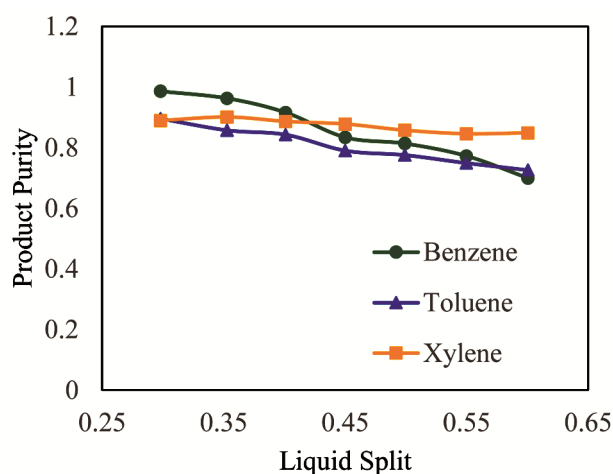


Fig. 8 — Influence of liquid split fraction on the purity of a product

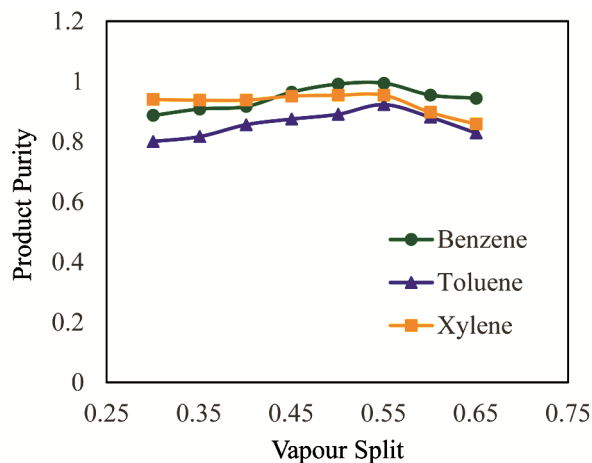


Fig. 9 — Influence of vapour split fraction on the purity of a product

Influence of the number of stages in the pre-fractionator on the purity of a product

Fig. 10 revealed that the purity of the bottom (p-xylene) and top (benzene) products was not significantly affected by the number of stages in the pre-fractionator, with the exception of a little alteration in the purity of the mid constituent (toluene).

Influence of side steam flow rate on the purity of a product

Despite the rise in the flow rate of the side stream, the purity of benzene remains rather stable. The p-xylene's purity remained constant and did not exhibit any significant variation. However, it reached its highest level at the optimal value of side stream flow. Nevertheless, as depicted in Fig. 11, the level of purity in toluene declined as the flow rate increased. The ideal flow rate is about 20 kmol/h, as the intermediary product toluene is greatly influenced by the flow rate of the side stream.

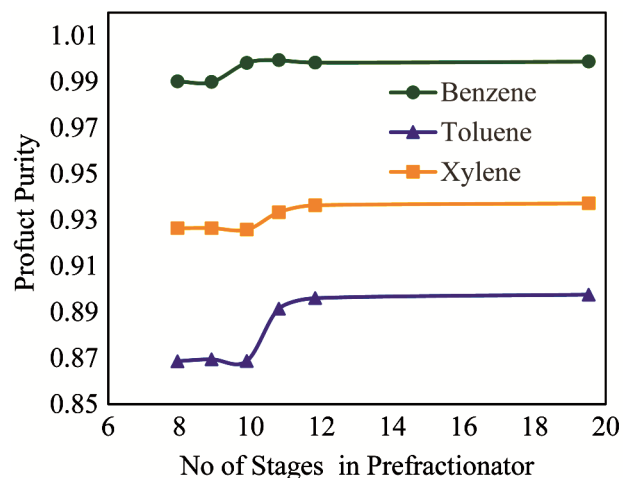


Fig. 10 — Influence of number of stages in the pre-fractionator on the purity of a product

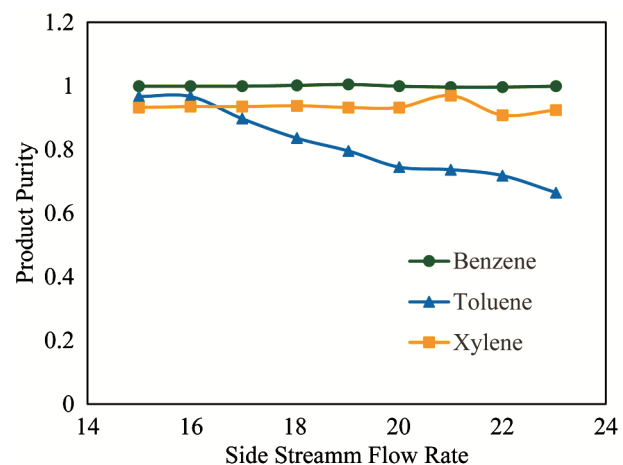


Fig. 11 — Influence of side steam flow rate on the purity of a product

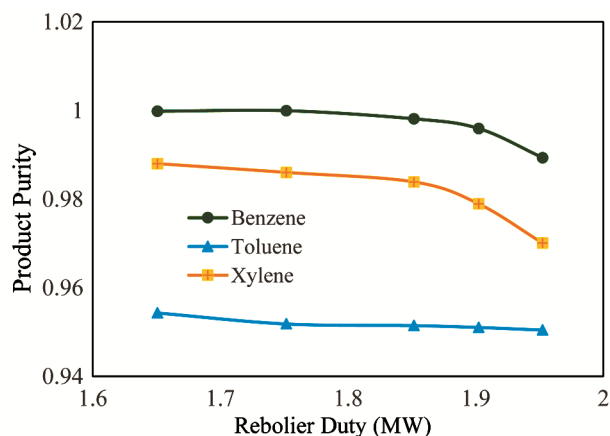


Fig. 12 — Influence of reboiler heat duty on the purity of a product

Table 4 — Comparison of Energy consumption between HiDiC and conventional DWC

Component	Heat duty of conventional DWC process (kW)	Heat duty of HiDiC Process (kW)	% Energy Saving
Heat exchanger	-	763.905	2.19%
Compressor	-	318.005	
Reboiler	1106.16	-	
Condenser	1164.68	314.997	72.95%
Total	2270.68	1396.907	38.48% (overall)

Influence of reboiler heat duty on the purity of a product

In order to investigate the DWC energy efficiency, the heat duty of the reboiler in the stripper column was adjusted within the range of 1.650 MW to 1.950 MW, as illustrated in Fig. 12. There was no noticeable alteration in the purity of none of the extracted products, including the side, bottom, and top streams. The data demonstrates that a DWC exhibits comparable efficiency while consuming less energy. The dynamic functioning of the column is not impacted by the amount of energy utilized. Hence, the ideal power usage for achieving the highest level of product purity is 1.65 MW.

Comparison of HiDiC and the traditional DWC system

In contrast to the HiDiC architecture, which consists of four splitters, one heat exchanger, one condenser, and four columns to attain equivalent purity with lesser energy usage, the standard DWC system consists of two splitters, one stripper with kettle reboiler, one rectifier with a total condenser, and two columns. The reboiler of the divided wall column is substituted with a tube heat exchanger, a shell, and an isentropic compressor in HiDiC. The total heat and work duty of this replacement is 1081.91 kW, which is 2.19% lower than that of the reboiler. Table 4 clearly demonstrates

the energy consumption of each design. It is evident that by employing the vapour recompression technique in a divided wall column, energy savings of up to 38.48% can be achieved. Additionally, the condenser duty had a reduction of 72.95%.

Conclusion

A simulation was conducted for a BTX (benzene–toluene–p-xylene) mixture using a divided wall column (DWC), yielding high product purities of 0.99 for benzene, 0.92 for toluene, and 0.97 for p-xylene under optimized conditions. The study further investigated how varying operating parameters affect product purity. Results confirm that DWCs can achieve high separation efficiencies with relatively low energy consumption. To enhance energy performance, vapour recompression was integrated into the DWC system. This heat-integrated configuration reduced total energy consumption by 38.48% compared to the conventional DWC setup for a feed composition of 0.2 benzene, 0.2 toluene, and 0.6 p-xylene (mole fractions). Specifically, the energy requirement dropped from 2270.68 kW in the standard DWC to 1396.91 kW in the heat-integrated process. The reboiler energy usage decreased by 72.95%, while the condenser showed a 2.19% reduction. In regions with limited water availability, minimizing cooling water usage becomes critical. Therefore, strategies that reduce condenser energy demand are especially valuable in such scenarios.

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