

Design of an internally heat-integrated distillation column via an economic-based column energy profile approach

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ABSTRACT

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The internally heat-integrated distillation column (HIDiC) is considered one of several approaches for process intensification in chemical processes. Research on the design of the HIDiC has generated great interest during the past few decades. The design of an HIDiC could be carried out via various design approaches such as rigorous process simulation, mathematical programming, genetic algorithm, or H-xy and T-xy diagrams. In this study, an alternative approach based on an economic-based column energy profile was applied to the design of an HIDiC. The economic criterion for generating column energy profiles is the maximum energy saving per additional investment (MESAI). Each data point on the MESAI profile is generated by optimizing the heat load and by the additional investment required when adding a side exchanger at any stage. Aspen Plus simulation software was used in the profile generation and the HIDiC simulation. The resulting column profiles could help provide insights into the economic viability of the heat-integrated distillation column, aiding decision-making and reducing optimization efforts. The economic analysis conducted in this study reveals that the designs obtained from the MESAI profiles demonstrate lower costs compared to the design based on the H-xy and T-xy diagrams. Among the configurations studied, the best design from the MESAI profiles is the HIDiC with three side exchangers.

Keywords: internally heat-integrated distillation column, economic criterion, maximum energy saving per additional investment (MESAI)

1. INTRODUCTION

According to the 2030 United Nations Agenda for Sustainable Development and its Sustainable Development Goals (SDGs), energy is one of the most important topics that can strongly influence all other development goals (Department of Economic and Social Affairs, United Nations, 2021). To promote sustainable development activities in the energy sector, the key directions are the alteration of energy sources from fossil fuels to renewable

energy sources and the improvement in energy efficiency. In addition, these directions are also highly related to the reduction of global greenhouse gas (GHG) emissions. The energy inefficiency in various sectors, such as power generation, transportation, building, and industrial sectors, significantly contributes to global warming from GHG emissions (Seferlis et al., 2021). The energy efficiency improvement of any system must be managed not only for economic purposes but also for sustainability in the future. To achieve these goals, all aspects of process systems, i.e.,

design, integration, operation, and control, must be thoroughly considered. A comprehensive review of key technologies related to these aspects in various sectors was recently published (Seferlis et al., 2021).

Focusing on the industrial sector, the chemical and refining industries are undoubtedly the major energy consumers. Energy efficiency improvement in these industries will create substantial impacts towards the SDGs. Therefore, the efficiency improvement of energy-intensive units in chemical industries is mainly emphasized. Distillation is one of the most widely applied separation systems and the largest energy user in chemical industries. Even though distillation is a mature technology, it still has room for efficiency improvement. The application of advanced distillation processes, hybrid separation systems, and the design and optimization of distillation systems, including heat integration, should be concentrated in future research directions to achieve the efficiency improvement goal (Kiss and Smith, 2020). Considerable engineering effort and numerous research works have been dedicated to improving the energy efficiency in distillation systems and the heat integration among several distillation columns and their background process, or a combination of both. In a multicomponent separation system that involves several distillation columns, the column thermodynamic efficiency could be improved by introducing complex distillation schemes such as the fully thermally-coupled distillation or the Petlyuk column (Petlyuk et al., 1965). These complex columns have higher thermodynamic efficiency than an equivalent sequence of simple columns. As a result, the Petlyuk column could provide around 30% savings in energy requirement when compared to the sequence of simple columns performing the same separation task (Petlyuk et al., 1965). Moreover, the prefractionation and the main column sections in the Petlyuk scheme could be merged into a single column shell to create a dividing-wall column (DWC) which could save around 30% in capital investment (Triantafyllou and Smith, 1992). Nowadays, many DWCs have been successfully commercialized in various kinds of industries worldwide (Asprion and Kaibel, 2010; Dejanović et al., 2010; Yildirim et al., 2011).

Another attractive distillation scheme is the internally heat-integrated distillation column (HIDiC). It is an interesting alternative to the existing heat-pump-assisted distillation, or vapor recompression distillation (VRC) applied when separating a close-boiling mixture. The concept of HIDiC is based on combining VRC and heat integration between the rectifying and stripping sections of the same separation task. The advantage of this distillation scheme was illustrated by Mah et al. (1977). Since then, research has focused on the design and modeling of the HIDiC (Iwakabe et al., 2006; Nakaiwa et al., 2001; Olujić et al., 2006; Wakabayashi and Hasebe, 2013). The development of HIDiC has now reached the pilot plant stage in some countries (Olujić et al., 2009). Nevertheless, further research, both in terms of design and hardware development issues, is still needed before this application can be fully verified and accepted for commercial use. In the design of an HIDiC, the number, sizes, and locations of side exchangers are all significant factors. Several design tools, such as column energy profile, rigorous process simulation, mathematical programming, and genetic algorithms, have been implemented in various HIDiC design approaches. Here, some of them are briefly reviewed.

First, the column energy profile could be applied to the design of heat-integrated distillation systems. The concept of column energy profile has long been established. Initially, it was developed from the reversible distillation condition. For a column to become a reversible distillation column, the irreversibility occurring in the column must be decreased by operating the column in a diabatic manner in which heat transfer is allowed along column sections. As a diabatic column approaches the reversible condition, with no driving force at any point along the column, the column energy requirement will be at a minimum. At the reversible column condition, there must be no irreversibility due to mixing at the feed stage, no column pressure drop, and an infinite number of stages and side exchangers along the column sections (King, 1980). The reversible column condition is considered an ideal target in the design but has never been achieved in practice. Therefore, the primary benefit of allowing heat transfer along the column section in an actual column with a finite number of stages is better heat integration potential among different diabatic column sections and the background process rather than lowering the energy requirement in the column itself.

During the past several decades, many research works have been devoted to the evaluation of minimum energy requirements and also to the column energy profile for heat integration via the reversible distillation concept (Bandyopadhyay et al., 1998; Dhole and Linnhoff, 1993; Koehler et al., 1991; Terranova and Westerberg, 1989). Among all approaches used to generate reversible or near-reversible profiles, the column grand composite curve (CGCC) approach (Dhole and Linnhoff, 1993) is the most prevalent. It was applied in the design of heat-integrated distillation sequences (Chen et al., 2014; Douglas and Hoadley, 2006), heat-integrated complex distillation systems (Chen et al., 2021; Van Duc Long and Lee, 2013), or distillation systems with vapor recompression (VRC) (Gao et al., 2021). Additionally, it is also incorporated into the Aspen Plus® simulation software, which is widely used in the chemical industry. All reversible or near-reversible profiles have shown the outstanding feature of heat load targeting for any side exchanger. However, the heat load target obtained from these profiles is only an approximate value and cannot be immediately utilized in a real column without any iterations. Applying a heat load target at a selected side exchanger location obtained from a reversible profile could result in a heat load penalty encountered at the main condenser and reboiler. The stage temperature at the side exchanger installation will also be shifted from the value read from the reversible profile. Therefore, simulation and fine-tuning of a new column with an installed side exchanger are inevitable.

Apart from the works on the reversible profile, another approach was developed to generate a column energy profile based on a specific minimum driving force (Pinto et al., 2011). This profile is called the minimum driving force profile (MDFP). Unlike reversible or near-reversible profiles like the CGCC, the MDFP is a real column profile based on a finite number of stages. The heat load target at any particular stage in the rectifying or the stripping section is determined by adding some stages above the side condenser or below the side reboiler, respectively, until the exergy loss value around

the side exchanger stage is reduced to meet the specified exergy loss target. Since some stages are added to compensate for the lower exergy loss created by the side exchanger installation, the heat load target at a particular stage can be identified accurately from the MDFP without incurring any heat load penalty and temperature shift encountered when applying the CGCC approach. Another column energy profile generation approach was recently proposed (Jirojwong and Suphanit, 2019). The profile generation methodology is similar to that of the MDFP. However, the criterion used to determine the heat load target changed from an exergy loss criterion to an economic criterion. The economic criterion used in this approach is called the maximum energy saving per additional investment (MESAI) criterion. The obtained column energy profile is, therefore, called the MESAI profile.

Another design approach for a heat-integrated distillation system is the optimization of columns with a finite number of stages. Several design and optimization approaches were developed to deal with such complex systems. Alcántara-Avila et al. (2013) developed a three-level mixed-integer linear programming (MILP) optimization procedure to determine the optimal heat-integrated distillation sequence. The other type of mathematical programming approach, the mixed-integer nonlinear programming (MINLP), was applied to optimize an internally heat-integrated distillation column (HIDiC) (Harwardt and Marquardt, 2012). The genetic algorithm (GA) approach was successfully implemented in the optimization of the HIDiC by Shahandeh et al. (2014a, 2014b) and also extended to the integration of HIDiC in a distillation sequence by Khalili et al. (2020). Qiu et al. (2019) applied the data-driven analysis by collecting a large set of simulation results to evaluate the economic performance of an HIDiC. This extensive data set was used to train a radial basis function neural network (RBFNN) and set it as the fitness function of GA optimization. Although the mathematical programming and the stochastic optimization approaches could handle complex problems and cover large search spaces, the required computational resources were high, which could potentially increase, especially in a sizeable heat-integrated system involving several columns. The column energy profile approach, on the other hand, could offer designers more insight during the conceptual design stage while spending less computational resources when compared to the mathematical or stochastic-based approach. However, the column profiles developed in the past, such as the CGCC or the MDFP, were created on a thermodynamic basis. There is no economic consideration involved in their column profile generation.

Therefore, the objective of this study is focused on applying the MESAI profile (Jirojwong and Suphanit, 2019) to the design of an HIDiC. An economically optimum heat load at any stage could be identified from the MESAI profile. The design of an HIDiC could then be carried out by using the MESAI profiles and the pinch design method (Linnhoff and Hindmarsh, 1983). The successful implementation of the MESAI profiles in the HIDiC design is illustrated through a case study from past literature. The design result is then compared to the literature with respect to the design configuration and the economic performance. The details of the profile generation procedure, the case study, the economic bases, and design assumptions are described in the next section.

2. MATERIALS AND METHODS

The methodology for generating a column energy profile based on the economic criterion known as the MESAI approach (Jirojwong and Suphanit, 2019) is applied in this work. This section briefly describes the profile generation procedure for a simple column using the MESAI approach. Details of a case study from past literature used to illustrate the MESAI approach for a HIDiC design are then explained. Economic bases and design assumptions used in this case study are then given to complete this section.

2.1. MESAI approach

In this approach, generating a column energy profile starts by separately considering columns above and below the feed. Side condensers are only allowed in a rectifying section, while side reboilers are allowed in a stripping section. The overall procedures to create a heat source and a heat sink profile for a rectifying and a stripping section are illustrated as shown in Figure 1. At a particular stage in a rectifying section (stage i), the side condensing target at that stage can be determined by the simulation of a separate column section, starting from the condenser of the rectifying section of that stage, with an installed side condenser (Figure 1). The stream data of the internal vapor stream entering stage i (v_{i+1}) are taken from the base case simulation result as the input data of this separate section. There are two design specifications required in the simulation of this column section. The first one is the molar flow rate of the liquid product leaving stage i . This value is specified to be the same as the internal liquid flow leaving stage i (l_i) from the base case simulation. The other specification is the light key mole flow specification in the distillate stream (LK-spec). The simulation of the column section is first carried out by adding one stage above the considered stage. The simulation results are then checked against the stop criterion, in this case, an economic criterion. Some additional simulations may be required, with one stage added in each repetition until the stop criterion is satisfied. The heat load target ($\dot{Q}_i$) and the number of added stages required (K_i) at that particular stage temperature (T_i) can then be determined once the stop criterion is reached. There is no strict simulation order of the stages in the column section to determine the heat load target. However, stage i may begin with the stage below the condenser (stage 1). Subsequently, it can be moved downwards one by one until reaching the feed stage.

Similarly, at a particular stage in a stripping section (stage j), the side reboiling target can be determined by the simulation of a separate column section starting from the reboiler of the stripping section of that particular stage with an installed side reboiler (Figure 1). The stream data of the internal liquid stream entering that stage (l_{j-1}) are taken from the base case simulation results as the input data of this separate section. Two design specifications are also required in the simulation of this column section. The first one is the molar flow rate of the vapor product leaving stage j , which is specified to be the same as the internal vapor flow (v_j) from the base case simulation. The other specification is the heavy key mole flow in the bottom product stream (HK-spec). As with the rectifying section, the simulation of the separate stripping section is first carried out by adding one stage below stage j . The simulation results are then checked against the economic criterion. The simulation may be

repeated each time, with one more stage added until the economic criterion is satisfied. The heat load target ($\dot{Q}_i$) and the number of added stages required (K_i) at that particular stage temperature (T_i) in the stripping section can then be determined. Typically, the stage to be considered (stage j) may start at the bottom stage (stage n). After achieving the target heat load at any stage, the

stage to be considered can be successively moved upwards until reaching the feed stage. Finally, after obtaining the heat load targets at all stages, the column energy profiles for the rectifying and the stripping sections based on the economic criterion could be plotted on the same diagram.

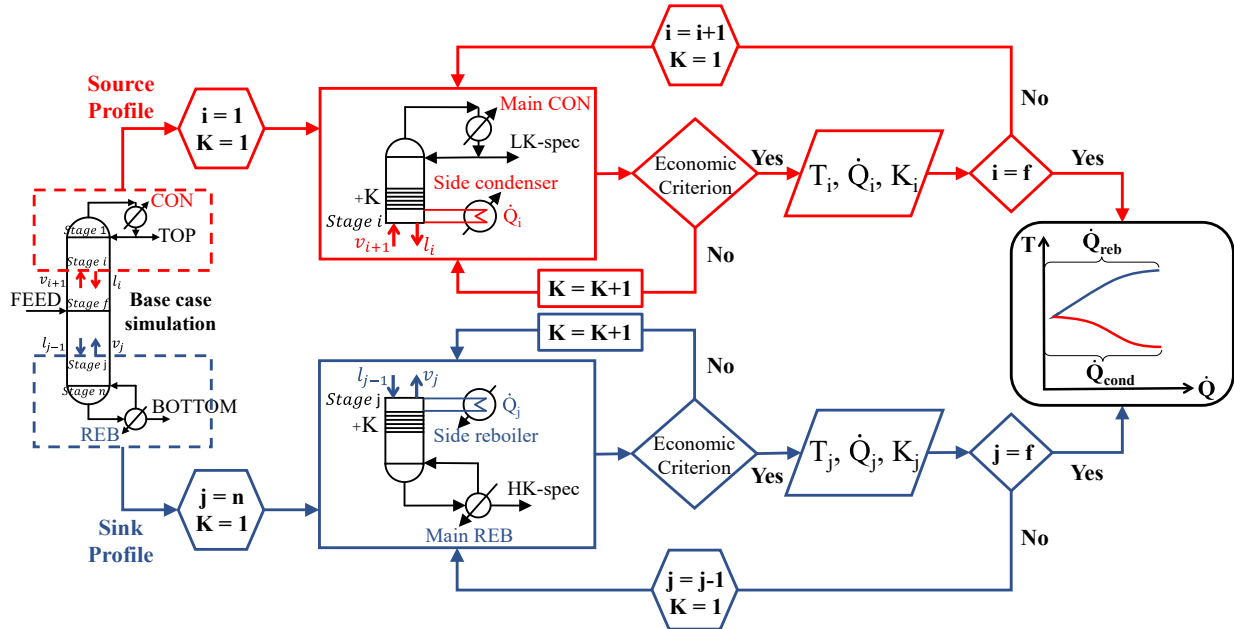


Figure 1. The methodology for generating an economic-based column energy profile by using simulation results from a base case column

Before proceeding to the details of the economic criterion, the economic effects of a side exchanger installation will be discussed. The installation of a side exchanger, along with some additional stages, could improve column thermodynamic efficiency, leading to a higher heat integration potential. On the other hand, it also affects the overall capital cost in many ways. For example, when installing a side reboiler in a column, the decrease in the column diameter in the section below the side reboiler

(Figure 2b) and a smaller size reboiler when compared to the base case column (Figure 2a) could provide some cost benefits. On the contrary, the increase in the overall tower height due to some added stages and a new side reboiler will impose some cost penalties on the system. Hence, an economic criterion considering both capital and energy aspects should be considered during the profile generation stage to obtain an economically optimum heat load target at any stage along the column section.

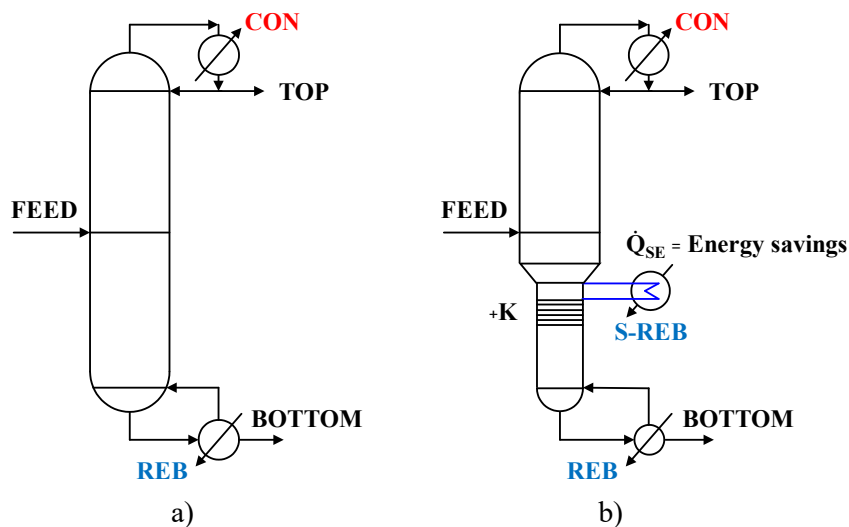


Figure 2. Comparison of column dimensions and exchanger sizes between (a) a base case column and (b) a column with a side reboiler

To account for both capital and energy costs when installing a side exchanger with some added stages, an economic performance indicator called the energy saving per additional investment (ESAI) is estimated, as shown in Equation (1). This is an indicator typically used in a retrofit problem in which the saving potential is traded off against the investment added.

$$ESAI = \frac{\text{Energy Saving}}{\text{Additional Investment}} = \frac{\dot{Q}_{SE}}{C_{GR,SE} - C_{GR,0}} \quad (1)$$

The energy saving is the side exchanger heat load ($\dot{Q}_{SE}$) at the stage being considered. It is assumed to be fully recovered by integrating with other heat sources or heat sinks in the process. The term additional investment is estimated from the difference between the capital cost of the column with a side exchanger and that of the base case column. Here, the grassroots cost (C_{GR}) defined by Turton et al. (2018) represents the capital cost estimate in each case. The capital cost of the base case column ($C_{GR,0}$) consists of the column, the main condenser, and the main reboiler costs. The capital cost of the column with a side exchanger ($C_{GR,SE}$) consists of the column, the main condenser, the main reboiler, and the side exchanger costs. The column cost will consider the new column height after stage addition. The column diameter between the side exchanger and its main exchanger will also differ significantly from the remaining section, as seen in Figure 2b. Therefore, the diameter used in the column cost estimation for the case with a side exchanger will be the average value of the diameters calculated from both sections of the column. The side exchanger cost is estimated from the required heat transfer area, considering the heat transfer between a side exchanger stream and its corresponding utility. The economic evaluation was done in a Microsoft Excel calculator block inside an Aspen Plus® simulation model. The estimated

column diameter and exchanger areas from the simulation were transferred to the calculator block to calculate the capital cost and the ESAI value.

The optimum heat load for a side exchanger installation at a particular stage could be determined by a simple optimization of ESAI values with respect to the number of added stages. The condition at the maximum ESAI value is chosen as the optimum condition for a side exchanger installation at the stage being considered. ESAI values could be optimized as a sensitivity analysis by following the methodology outlined in Figure 1. The ESAI value is repeatedly evaluated whenever another stage is added above a side condenser or below a side reboiler. Typically, the ESAI value will sharply increase when adding the first few stages. However, when the number of added stages is high, the increase in the ESAI value will be marginal. The ESAI value will finally reach a maximum point, as shown in Figure 3. If the number of additional stages is increased, further approaching the infinite value, the heat duty at that stage will reach a maximum value, which is a reversible heat duty found on a reversible distillation profile. At this condition, the ESAI value will approach zero as the investment cost becomes infinite from the infinite number of stages. Hence, a maximum point of ESAI will always be found. However, the number of additional stages at the optimum condition (maximum ESAI) will depend on the economic assumption of the capital investment. Here, the side exchanger duty evaluated at the maximum ESAI condition is chosen as a heat load target on a column energy profile. The number of added stages at that condition will be the number required to achieve the heat load target at that particular stage. Therefore, this economic criterion is called the MESAI criterion. In this work, the application of the MESAI approach for the design of an internally heat-integrated distillation column (HIDiC) is illustrated by a case study explained in the next section.

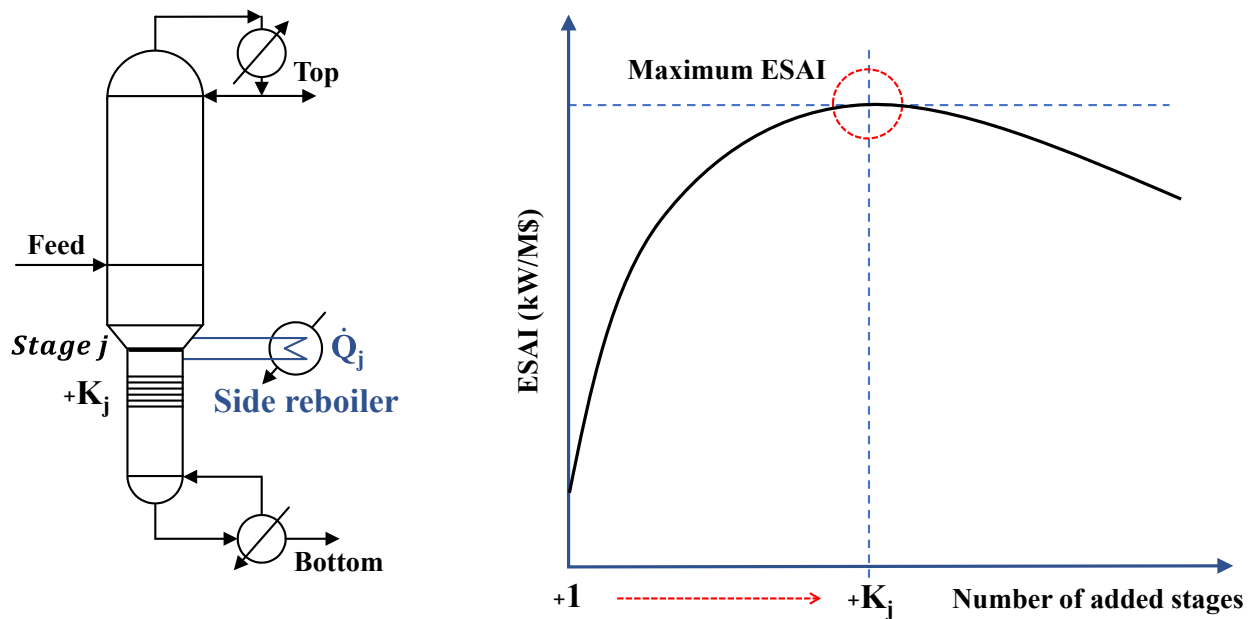


Figure 3. The optimization of ESAI with respect to the number of added stages in search of the optimum heat load target for a side exchanger installation at a particular stage

2.2. Case study: benzene/toluene separation

In this case study, a binary mixture of benzene and toluene is separated into two products by an HIDiC. The feed, product specifications, and other operating data from the reference literature (Wakabayashi and Hasebe, 2013) were adopted, as shown in Table 1. Similar to the reference

case in the literature, the RK-Soave property model was also applied here for the liquid-phase and the vapor-phase prediction. The recommended HIDiC design from the reference case for this separation was designed using H-xy and T-xy diagrams (Wakabayashi and Hasebe, 2013), as shown in Figure 4.

Table 1. Feed, product specifications, and other operating data of the reference case

Parameter	Value
Feed rate (kmol/h)	100
Benzene feed composition (mol%)	50
Toluene feed composition (mol%)	50
Liquid mole fraction in feed	0.5
Pressure in stripping section (kPa)	101.3
Pressure in rectifying section (kPa)	212.4
Compressor isentropic efficiency (%)	75
Benzene product purity (mol%)	99.9
Toluene product purity (mol%)	99.9

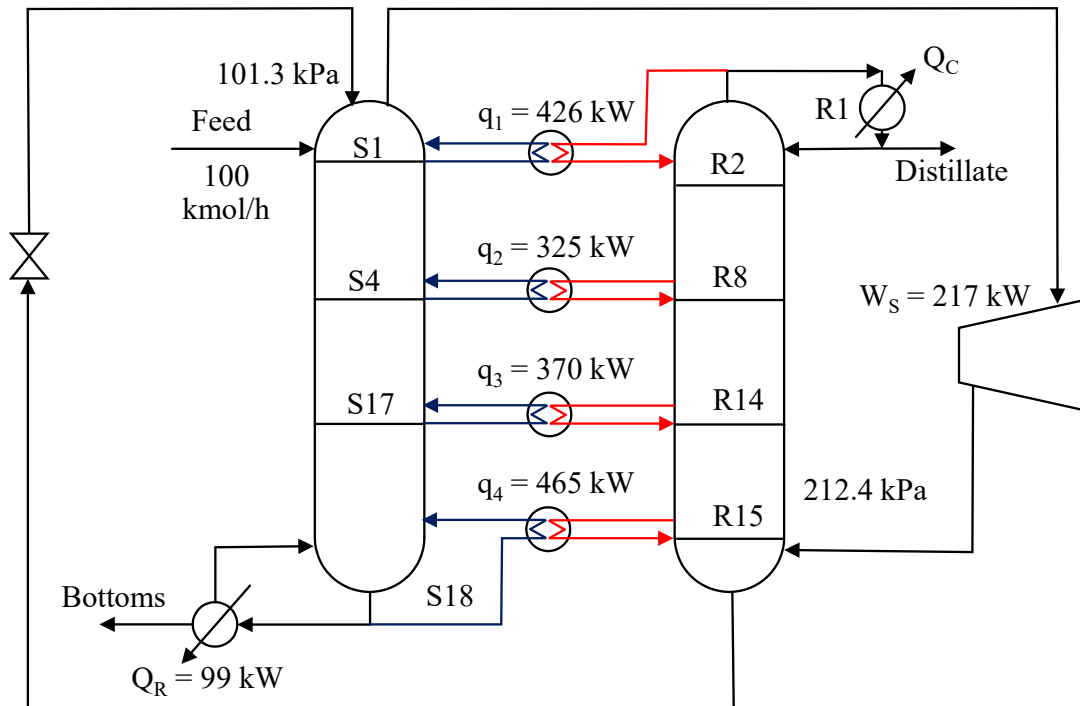


Figure 4. The flowsheet of the recommended HIDiC design for benzene/toluene separation from the reference case (Wakabayashi and Hasebe, 2013)

In this reference case, the HIDiC consists of 18 stages (including a reboiler) in the stripping section and 15 stages (including a condenser) in the rectifying section. Four side exchangers are installed to transfer heat between the stripping and the rectifying sections. The heat load of each side exchanger is shown in Figure 4. A trim condenser and a trim reboiler are required at the top of the rectifying section and the bottom of the stripping section, respectively. To create the base case structure for

MESAI profile generation, all side exchangers in the reference case (cf. Figure 4) were removed. The base case flowsheet without heat integration between sections, as shown in Figure 5, was then simulated to obtain all stage temperatures and internal stage flow data. These base case data were used in the MESAI approach outlined in the previous section to generate the MESAI profiles of the rectifying and the stripping sections, arbitrarily shown in Figure 6.

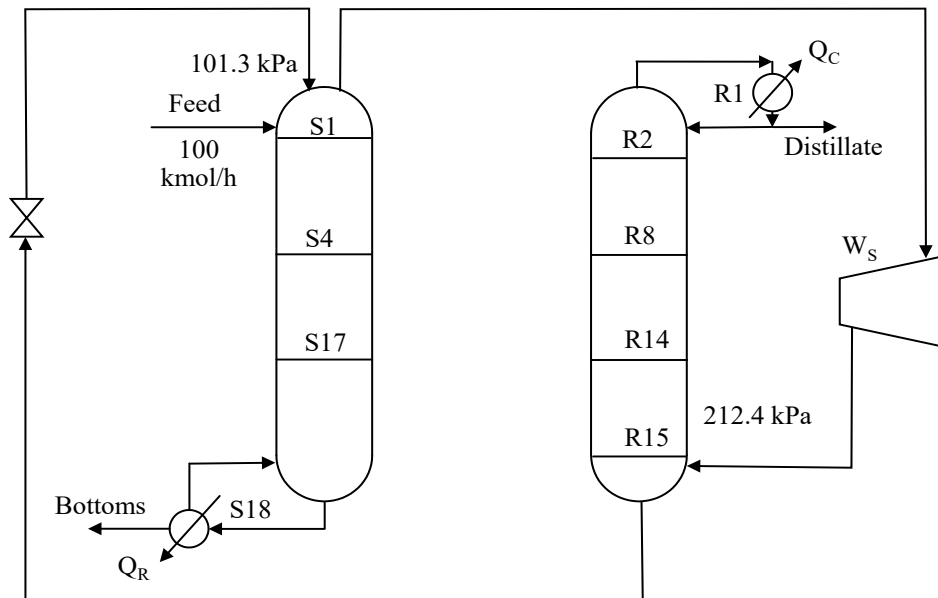


Figure 5. The base case flowsheet without heat integration for MESAI profile generation

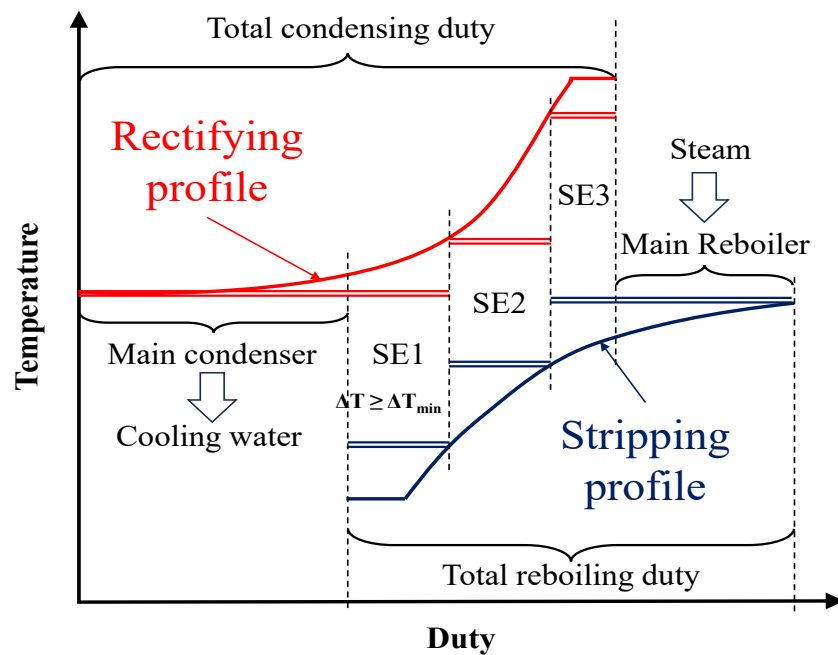


Figure 6. Design of side exchanger installation in an HIDiC using MESAI profiles

The rectifying profile is a heat source profile, while the stripping profile is a heat sink profile. The degree of heat recovery between column sections depends on the horizontal overlapping distance between both profiles. From Figure 6, the heat exchange between the heat source profile and the heat sink profile could be achieved using a certain number of heat exchangers. In this case, there could be many different numbers of heat exchangers to achieve the same amount of heat recovery. However, to achieve the desired heat recovery with the lowest investment, the desired number of heat exchangers should be kept at a minimum, while still satisfying a specified minimum temperature approach ($\Delta T_{\min}$) for a heat exchanger. This exchanger matching guideline is similar to that outlined in the pinch design method (Linnhoff and Hindmarsh, 1983).

The exchanger matching may start from either the left or the right side of the MESAI profiles. Each side exchanger's heat duty and location could then be easily determined from both profiles. In this work, the horizontal distance between the rectifying and the stripping profiles could be moved closer to or away from each other to obtain various HIDiC designs with different numbers of side exchangers. As both profiles are moved horizontally closer, the degree of heat recovery will be higher. However, the number of side exchangers required in the HIDiC design will also be higher. Hence, this exhibits a capital and energy cost trade-off problem in the design. Here, three different HIDiC designs with varying numbers of side exchangers were carried out and are discussed in section 3.2. The economic performances of all HIDiC designs were compared with one

another and to that of the reference case, as discussed in section 3.3. The economic performances of all HIDiCs were assessed based on the economic bases and design assumptions described in the next section.

2.3. Economic bases and design assumptions

The economic conditions were 8,322 operating hours per year, a 10% interest rate, and ten years of equipment lifetime. The equipment cost indices and utility costs are shown in Table 2. The capital cost estimates (see Appendix) were calculated from the grassroots cost (C_{GR}) correlations (Turton et al., 2018). The purchased equipment costs were based on the cost survey in 2001. The costs calculated from the models were adjusted to the costs in 2022 when accounting for inflation. Column sizing was estimated using the tray sizing option in the RadFrac block in Aspen Plus®. Based on a sieve tray with 0.6-m tray spacing on any section, the sizing was designed at 80%

flooding using Fair's correlation. All stages were assumed to be theoretical. For column costing, the construction material for both the shell and tray was considered to be carbon steel. The column cost had also considered the new column height after stage addition. The column diameter in the section between the side exchanger and its main exchanger will differ significantly from the remaining section as a result of the decrease in the vapor-liquid traffic in this column section (cf. Figure 2b). Therefore, the diameter used in the column cost estimation for the case with a side exchanger was the average value of the diameters calculated from both sections of the column. The side exchanger cost was estimated from the required heat transfer area, considering the heat transfer between a side exchanger stream and its corresponding utility. The overall heat transfer coefficient employed for side exchangers and reboilers was 1,150 W/m²·K, while the value of 1,500 W/m²·K was assumed for condensers.

Table 2. Equipment cost indices and utility costs

Parameter	Value	References
CEPCI (2022)	816	(Maxwell, 2020)
CEPCI (2001)	397	(Turton et al., 2018)
Steam cost (125°C) (\$/GJ)	2.03	(Turton et al., 2018)
Electricity cost (\$/GJ)	18.72	(Turton et al., 2018)
Cooling water (30°C to 40°C) (\$/GJ)	0.378	(Turton et al., 2018)

3. RESULTS AND DISCUSSION

3.1 MESAI profile generation

To create the MESAI profiles for this case study, all side exchangers in the reference case (cf. Figure 4) were removed. The base case flowsheet without heat integration between sections, as shown in Figure 5, was then simulated to obtain all stage temperatures and internal stage flow data. The light key (benzene) purity in the top product and the heavy key (toluene) purity in the bottom product are similar to those in the reference case, as shown in Table 1. These base case data were used to generate the MESAI profiles. The base case economics was the basis for calculating the ESAI at any simulation iteration. The MESAI profiles of both sections were created and plotted together on the same chart, as shown in Figure 7. Since the rectifying pressure was higher than the stripping pressure, the column heat integration potential could be observed from the overlapping region between the rectifying and the stripping profiles. The condenser and the reboiler duty for this base case were found to be 1,472 and 1,220 kW, respectively. The rectifying and the stripping profiles could be moved horizontally close to or away from each other to achieve various degrees of heat recovery between both sections. Subsequently, various HIDiC designs with different numbers of side exchangers could be established by adjusting the horizontal distance between both profiles. The shapes of the profiles around a few stages at the top of the rectifying profile and a few stages at the bottom of the stripping profile were relatively flat (Figure 7). By examining the feed stages on both profiles, the stage temperature changed rapidly. Both profiles could not be horizontally shifted to achieve a complete overlap without having negative temperature differences in some regions of the profiles. As a result, the total heat recovery between

the rectifying and the stripping sections could not be realized. Therefore, a trim condenser and a trim reboiler were required at the specified column operating pressures in this case study.

3.2 Design of HIDiCs via MESAI profiles

From the MESAI profiles obtained in the previous section, it could be seen that besides the horizontal distance between both profiles, which could affect the degree of heat integration between both sections and the design of the side exchanger installation, the specified value of ΔT_{min} is another significant factor affecting the number and size of side exchangers. According to the literature design result, the minimum temperature difference observed was around 6°C. To compare on the same basis, this value was chosen as the ΔT_{min} value in the HIDiC design using the MESAI profiles.

The HIDiC design could be carried out at various degrees of heat recovery between the rectifying and the stripping sections. However, there is no preference for the selection of the overlapping distance between both column profiles. In this work, the first HIDiC design was carried out by shifting the stripping profile horizontally to the left until the horizontal gap between both profiles on the left was 675 kW. To achieve the desired heat recovery with the lowest investment at this design condition, the desired number of heat exchangers should be kept at a minimum while still satisfying the specified ΔT_{min} (Linnhoff and Hindmarsh, 1983). The minimum number of side exchangers that could fulfill the specified ΔT_{min} was three side exchangers (Figure 8). The heat duty and location of each side exchanger are also shown on the diagram. This design is one of many possible designs in this condition. As both profiles are shifted closer to each other, the temperature difference between both profiles will be lower. To achieve side exchanger matchings

under the given $\Delta T_{\min}$ restriction, a large number of side exchangers will be required. This result is similar to what is normally found in the heat exchanger network design, especially around the pinch region where the temperature driving force is at the lowest level. Here, by shifting the stripping profile horizontally further to the left, another two HiDiC designs with 4 and 5 side exchangers were developed, as shown in Figure 9 and Figure 10, respectively. From the stage-pairing in the HiDiC designs with 3, 4 and 5 side exchangers, it could be seen that some feasible pairs, e.g., at the top (R1-S5) and at the bottom (R14-S18), are chosen in

all cases. They are all feasible since the temperature differences between the paired stages are at least equal to the $\Delta T_{\min}$ value. Shifting the stripping profile horizontally close to the rectifying profile does not alter the stage temperatures on both profiles. It is therefore feasible to select the same stage-pairing for various HiDiC designs under different degrees of heat recovery between the column sections. Moreover, the obtained side exchanger matching in each case is only one of many possible designs which may exhibit various heat load distributions among the side exchangers.

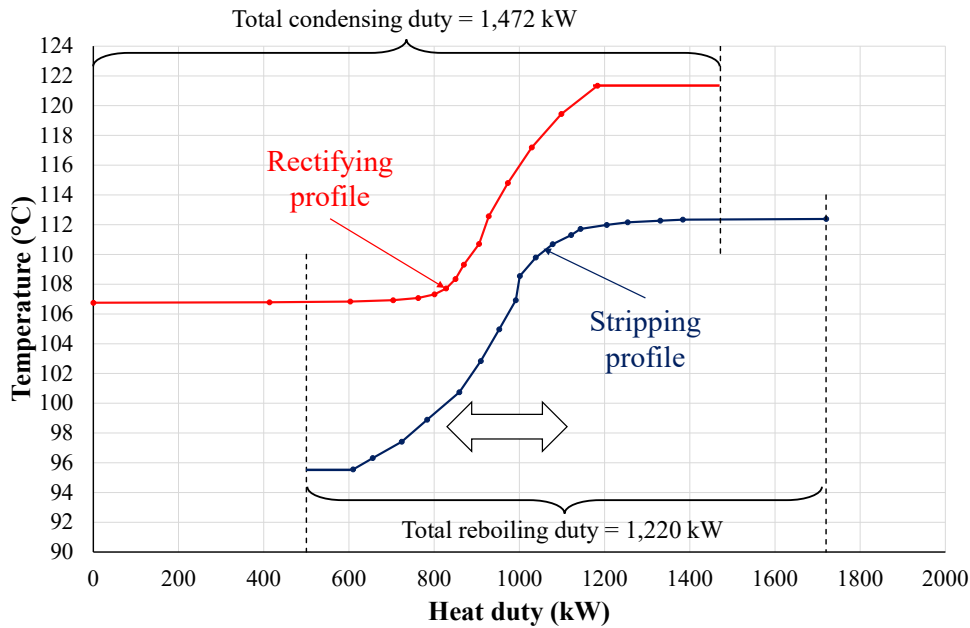


Figure 7. The MESAI profiles of the rectifying and the stripping sections in this case study

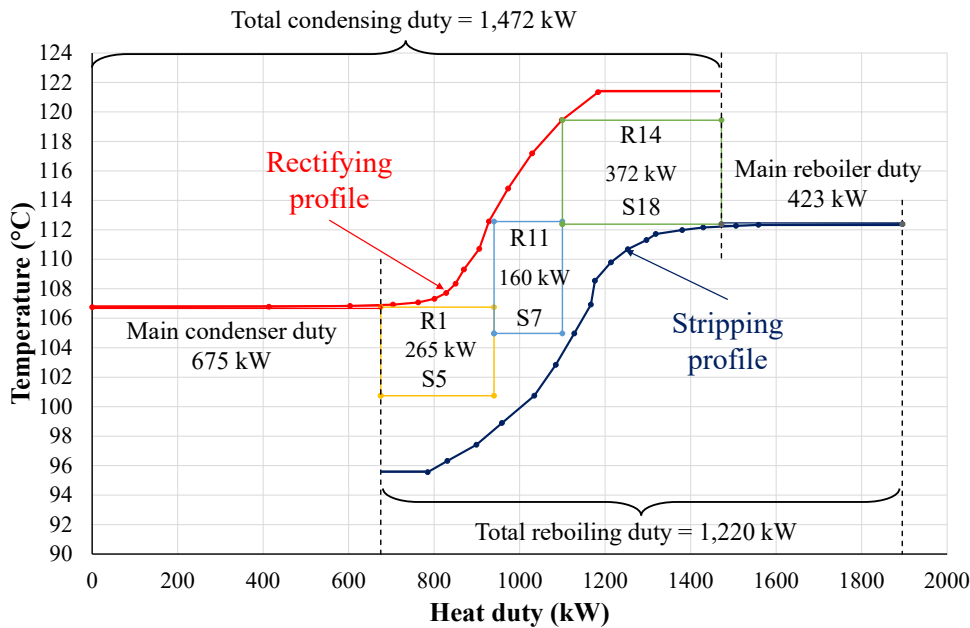


Figure 8. The heat duties and locations of the side exchangers for the HiDiC design with three side exchangers obtained from the MESAI profiles

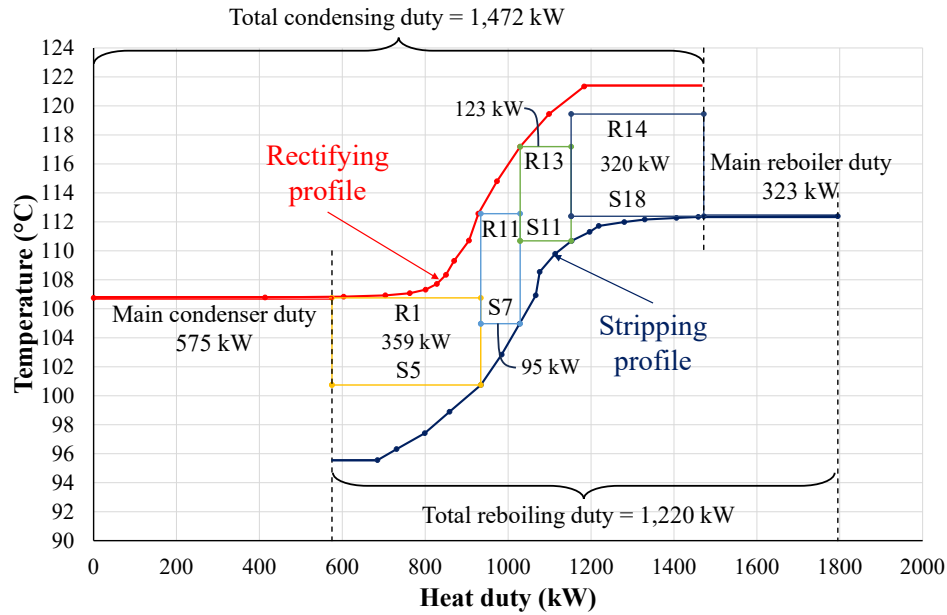


Figure 9. The heat duties and locations of the side exchangers for the HIDiC design with four side exchangers obtained from the MESAI profiles

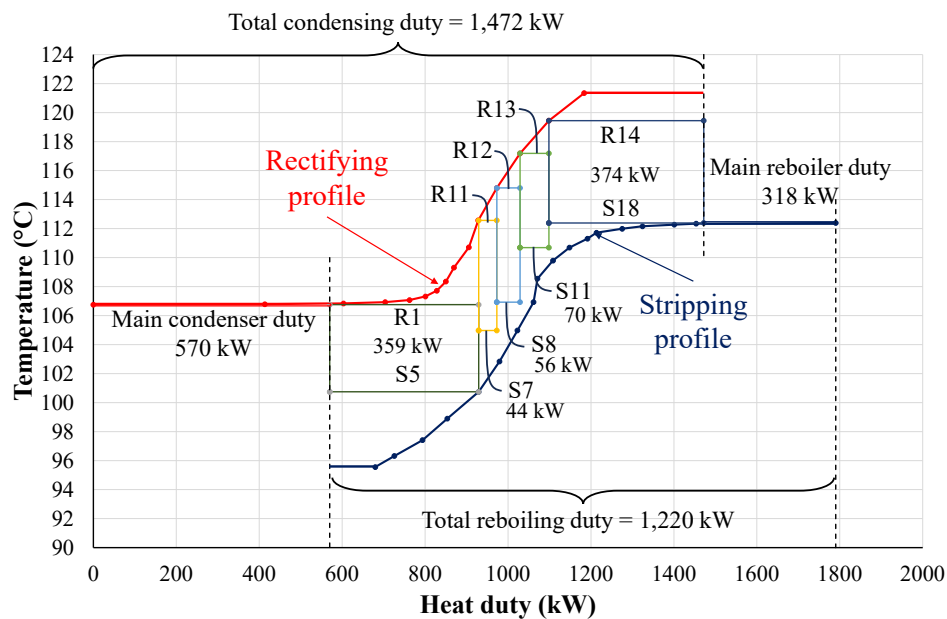


Figure 10. The heat duties and locations of the side exchangers for the HIDiC design with five side exchangers obtained from the MESAI profiles

The number of required added stages at each paired-stage location and the stage temperature difference between each pair are shown in Table 3. The HIDiC designs with 3, 4, and 5 side exchangers with the paired-stage locations, heat duties, and the number of added stages required, as obtained from the MESAI profiles, were then simulated under the same product purity specification as shown in Table 1. The stage temperature difference between each pair from the simulation was also compared to that from the MESAI profiles, as shown in Table 3. The results indicate discrepancies in the temperature differences from the simulation as compared to those found in the design using the MESAI profiles. Most of

the stage temperature differences from the simulation were lower than those from the MESAI profiles. Some temperature difference values were even below the specified $\Delta T_{\min}$ of 6°C. These discrepancies may have arisen from the changes in the compositions of the stream and flow at the connection of the rectifying and stripping sections through the compressor and the valve, which result in changes to total heat requirement or heat rejection. Therefore, to restore the violated temperature difference values to at least the specified $\Delta T_{\min}$ value, some adjustments to the number of stages added in rectifying and the stripping sections could be made.

Table 3. The stage temperature differences and the number of stages added, as obtained from the MESAI profiles, and the stage temperature differences from the simulation

Number of side exchangers	Paired stages	Number of stages added in the stripping section	Number of stages added in the rectifying section	ΔT on the MESAI profiles ($^{\circ}\text{C}$)	ΔT from HIDiC simulation ($^{\circ}\text{C}$)
3	S5-R1	7	-	6.0	5.8
	S7-R11	7	9	7.6	3.6
	S18-R14	-	9	7.1	7.2
4	S5-R1	7	-	6.0	3.2
	S7-R11	7	9	7.6	3.5
	S11-R13	6	9	6.5	6.3
	S18-R14	-	9	7.1	8.7
5	S5-R1	7	-	6.0	4.6
	S7-R11	7	9	7.6	7.5
	S8-R12	7	9	7.9	6.8
	S11-R13	6	9	6.5	6.7
	S18-R14	-	9	7.1	7.6

In this case study, adjustments to the number of stages added were carried out in the stripping section to compensate for the internal vapor and liquid flows, resulting in changes in the section temperature profiles. The results of the stage temperature differences at all paired stage locations after stage adjustments are shown

in Table 4. It can be seen that all stage temperature differences were above the specified $\Delta T_{\min}$. The economic performances of all HIDiC designs obtained from the MESAI profiles were then evaluated and compared to that of the reference case from the literature, as discussed in the next section.

Table 4. The stage temperature differences from the simulation after adjusting the number of stages added at the side exchanger locations

Number of side exchangers	Paired stages	Stages added in stripping (Adjusted)	Stages added in rectifying (Adjusted)	ΔT after stage adjustment ($^{\circ}\text{C}$)	Heat duty (kW)	Exchanger area (m^2)
3	S5-R1	9	-	6.3	265	34.1
	S7-R11	17	9	7.5	160	22.0
	S18-R14	-	9	7.2	372.1	46.3
4	S5-R1	13	-	6.1	359	51.1
	S7-R11	19	9	6.3	95	13.1
	S11-R13	6	9	6.2	123	17.4
	S18-R14	-	9	7.9	320.1	35.5
5	S5-R1	13	-	6.1	359.2	51.4
	S7-R11	7	9	7.5	43.8	5.1
	S8-R12	7	9	6.8	56.0	7.1
	S11-R13	6	9	6.7	69.6	9.0
	S18-R14	-	9	7.6	373.5	42.6

To evaluate the economic performance of the reference case for comparison with other HIDiC designs obtained in this work, the recommended HIDiC design from the reference case (Figure 4) was re-simulated by using Aspen Plus® V.10 under the economic bases and design assumptions outlined in section 2.3. The stage temperature differences between the paired stages at all side exchanger locations obtained from the re-simulation in this work are shown in Table 5. It should be noted that the stage temperature differences at some paired stages were lower than the specified $\Delta T_{\min}$. The violation in the stage temperature differences occurred due to the temperature shifts in the column sections when the side exchangers

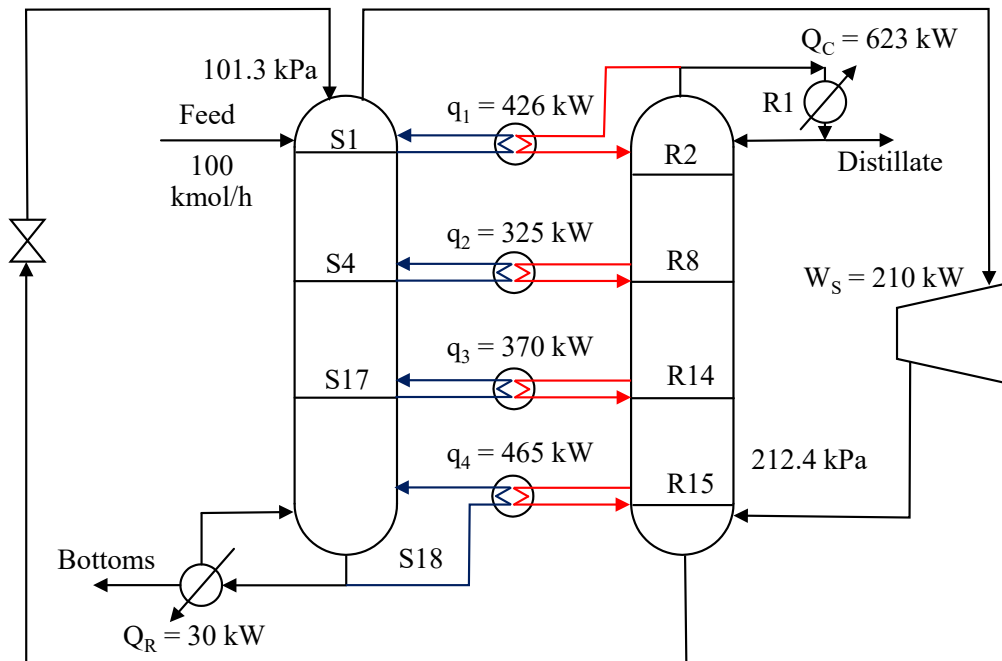
were installed without adding additional stages. The recommended HIDiC design from the reference case after the re-simulation is shown in Figure 11. The reboiler duty and the compressor work after the re-simulation were found to be different from those reported in the literature (Figure 4). These differences could be the consequence of using another simulator in this study, i.e., Aspen Plus® in this work vs PRO/II in the literature. The reference case after the re-simulation (Figure 11) was then used to evaluate economic performance for comparison with other HIDiC designs in the next section. All condenser, reboiler duties, heat transfer areas, and the compressor work in each case are summarized in Table 6.

Table 5. The stage temperature difference at each paired stage of the reference case (Figure 4) from the re-simulation

Side exchanger	Paired stage	Heat duty (kW)	Exchanger area (m ²)	Resulting ΔT between paired stages (°C)
1 st side exchanger	S1-R1	426	31.8	11.6
2 nd side exchanger	S4-R8	325	49.8	5.7
3 rd side exchanger	S17-R14	370	114.7	2.9
4 th side exchanger	S18-R15	465	70.4	5.7

Table 6. Heat duties, heat transfer areas of condensers and reboilers, and compressor work in each case

Case	Condenser duty (kW)	Reboiler duty (kW)	Condenser area (m ²)	Reboiler area (m ²)	Compressor work (kW)
Reference (Figure 11)	623	30	41.5	2.1	210
3 side exchangers (3SE)	651	130	43.4	9.0	138
4 side exchangers (4SE)	575	135	38.3	9.3	136
5 side exchangers (5SE)	568	44	37.8	3.1	138

**Figure 11.** The flowsheet of the recommended HIDiC design from the reference case after re-simulation

3.3. Economic comparison

In this section, the cost estimates of all major pieces of equipment in each case, i.e., column sections, a condenser, a reboiler, side exchangers, and a compressor, were calculated and annualized. The annualized equipment costs were divided into the column cost, the exchanger cost (including the main reboiler and the main condenser), and the compressor cost. The annualized utility cost consisted of the steam, cooling water, and electricity costs. Finally, the annualized equipment and utility costs were combined to estimate the total annualized cost in each case. The economic comparisons of all cases were carried out and discussed in each cost item.

By comparing the annualized column costs from all cases, as shown in Figure 12, it was found that the HIDiC from the reference case showed the lowest value, followed by the HIDiCs from the MESAI approach with 3, 4, and 5 side exchangers, respectively. As the number of side exchangers in the HIDiC design increased, the degree of heat recovery between the column sections also increased. However, some additional stages are required when installing side exchangers in the MESAI approach, which leads to an increase in the annualized column costs. For example, in the case of the HIDiC with five side exchangers, the number of stages increased from 18 to 51 stages and 15 to 51 stages in the stripping and the rectifying section, respectively.

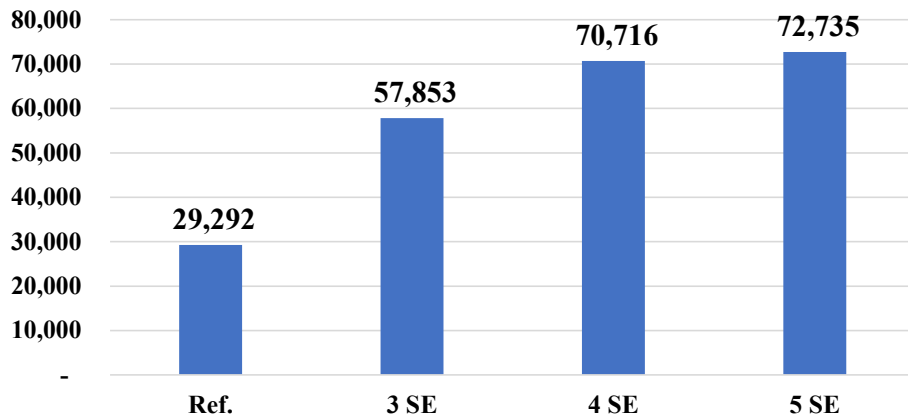


Figure 12. Annualized column cost (US\$/year) in each HIDiC design

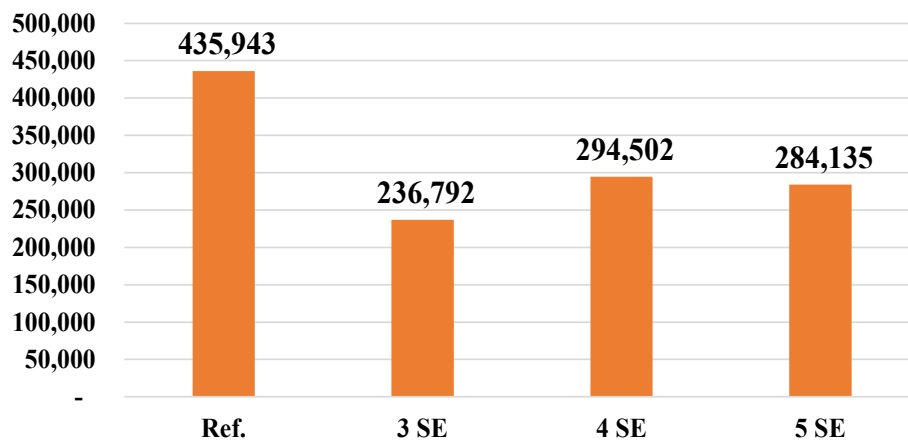


Figure 13. Annualized exchanger cost (US\$/year) in each HIDiC design

Generally, the exchanger cost depends on the number of exchangers in the system and the sizes of all exchangers, including all side exchangers, a condenser, and a reboiler in each case. It can be observed from Figure 13 that the HIDiC from the reference case exhibited the highest value of annualized exchanger cost, which was significantly higher than those from the MESAI approach. The reason behind the highest exchanger cost in the reference case was large side exchanger sizes resulting from small temperature differences ($\Delta T_{\min}$ violation) in some side exchangers (cf. Table 5). On the other hand, no HIDiC design from the MESAI approach showed a $\Delta T_{\min}$ violation in any exchanger, since some stages were added when installing side exchangers. The temperature profiles in both column sections were maintained; hence, the temperature difference values of all side exchangers could be kept above the specified $\Delta T_{\min}$ value. By comparing the HIDiC designs from the MESAI approach in Figure 13, it was found that the HIDiC with three side exchangers (3SE) had the lowest exchanger cost. The exchanger cost in the HIDiC from the MESAI approach increased as the number of side exchangers increased. However, the exchanger cost in the HIDiC with five side exchangers (5SE) was a slightly lower than that with four side exchangers (4SE) because of the larger temperature difference values found in some side exchangers in the middle section.

Compressor cost is another important cost contribution in both the capital investment and the operation. The compressor cost was estimated from the compressor power consumption, which depends on the pressure ratio and the vapor flow through the compressor. It can be seen from Figure 14 that the HIDiC from the reference case exhibited the highest annualized compressor cost, which was significantly higher than those from the MESAI approach. The HIDiC designs with 3, 4, and 5 side exchangers incurred approximately the same annualized compressor costs. Since the pressure ratio in all cases are equal in this case study, the compressor work depended on the vapor flow through the compressor. The vapor flow through the compressor was much higher in the reference case compared to the others, resulting in a significantly higher compressor work value of 210 kW in the reference case. The compressor work values of the 3SE, 4SE, and 5SE cases were 138, 136, and 138 kW, respectively.

The annualized utility costs in all cases are shown in Figure 15. In all cases, it can be seen that the annualized utility cost was dominated by the electricity required to operate the compressor. The electricity cost accounted for more than 80% of the cost in all cases. It can be seen from Figure 15, that the reference case required the highest annualized utility cost, followed by the 3SE, 4SE, and 5SE cases, respectively.

The total annualized cost (TAC) represented the sum of all costs mentioned above. As shown in Figure 16, all HIDiC designs from the MESAI approach exhibited much lower total annualized cost when compared to the reference case. The major cost contributors to the highest total annualized cost in the reference case were the exchanger, compressor, and utility costs (mainly electricity). Among the HIDiC designs from the MESAI

approach, the 3SE case showed the lowest TAC, followed by the 5SE and the 4SE case. Therefore, the best HIDiC design under the economic bases and design assumptions in this work is the HIDiC with three side exchangers (3SE). The column configuration, the side exchanger heat duties and locations, the number of additional stages, and all utility requirements of the 3SE case are summarized and shown in Figure 17.

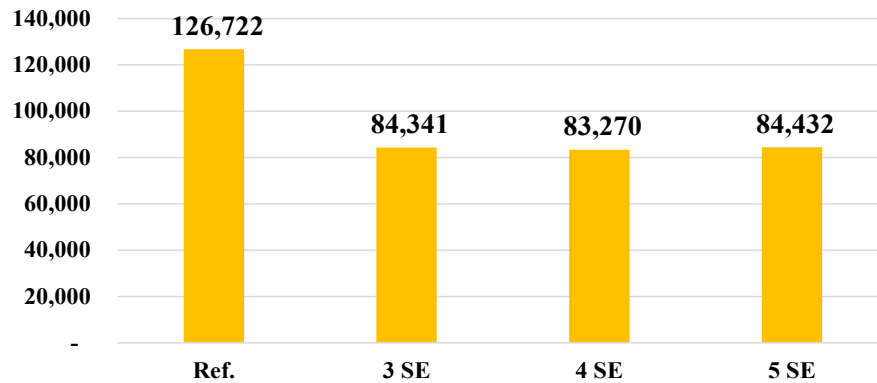


Figure 14. Annualized compressor cost (US\$/year) in each HIDiC design

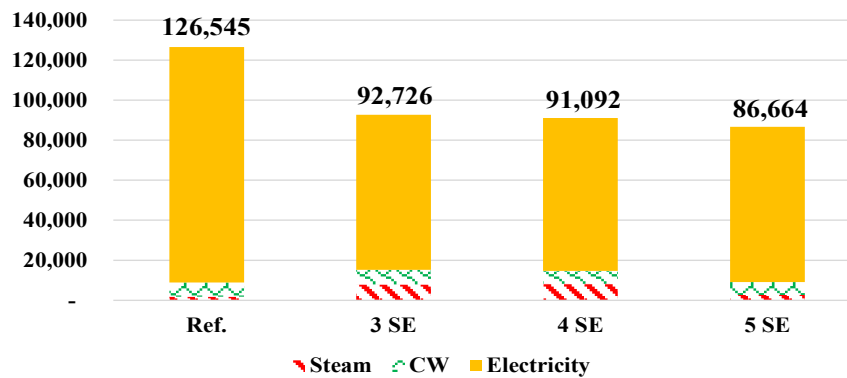


Figure 15. Annualized utility cost (US\$/year) in each HIDiC design

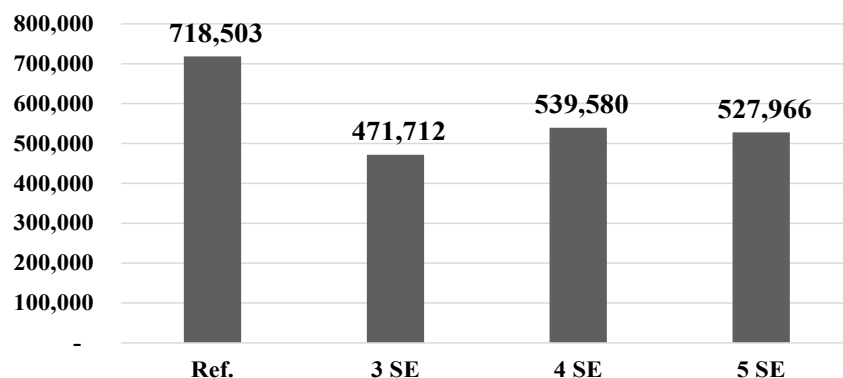


Figure 16. Total annualized cost (US\$/year) in each HIDiC design

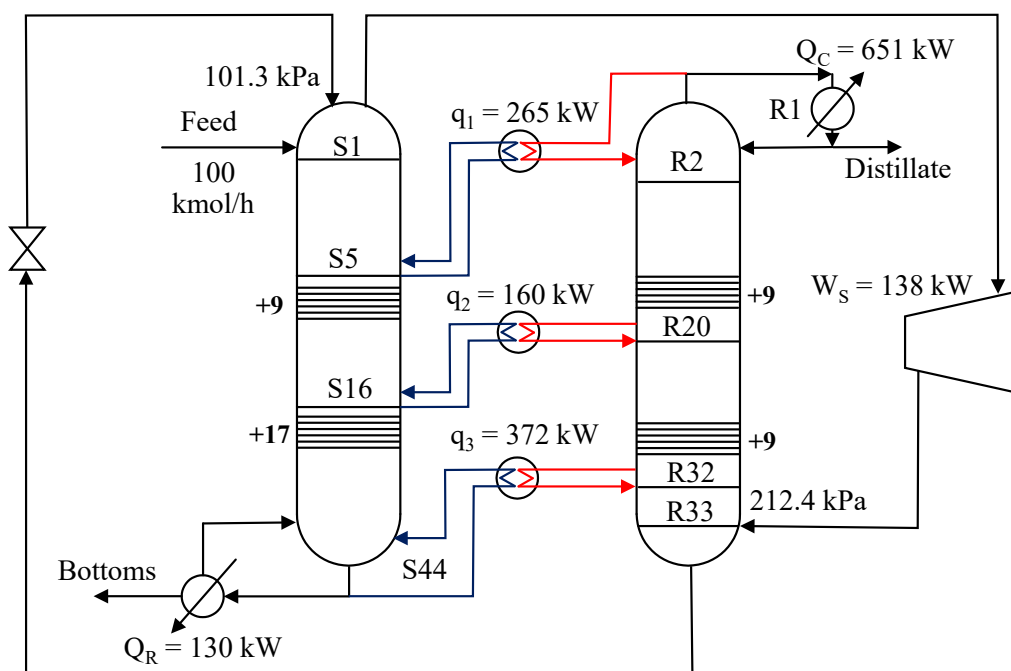


Figure 17. The flowsheet of the HIDiC design with three side exchangers from the MESAI approach

4. CONCLUSION

In this work, the economic-based column energy profile known as the MESAI profile was successfully applied to design an internally heat-integrated distillation column (HIDiC). The heat load and the location of the side exchanger were determined easily by using the MESAI profile and the pinch design method. The results could be used to set up an initial HIDiC design for further adjustment by rigorous simulation. The effort to achieve an economically viable HIDiC design can be reduced dramatically compared to other design approaches. This work compared the HIDiC design from the reference case based on the modified H-xy and T-xy diagrams to the designs from the MESAI approach. The HIDiC designs from the MESAI approach were found to be better economically. Unlike the HIDiC design from the reference case in which the numbers of stages in both columns were fixed, the amount of energy saving in the HIDiC from the MESAI approach could be realized directly from the MESAI profiles with less temperature shift. Although some stage adjustments were needed, the vapor flows through the compressor in all HIDiCs from the MESAI approach could be kept lower than the reference case, thereby saving the column utility consumption without incurring any workload penalty on the compressor. In the future, the MESAI profile could serve as a conceptual design tool for any complex heat-integrated distillation system consisting of several columns. The profile of each column in the system could be determined independently ahead of the design for heat integration, which could be further carried out by following the well-established pinch design guidelines.

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APPENDIX. CAPITAL COST ESTIMATION

The cost of each major piece of equipment was estimated using the cost models from Turton et al. (2018). The purchased equipment costs were based on the cost survey from May to September 2001 (CEPCI = 397). The costs calculated from the models were then adjusted for inflation to 2022 (CEPCI=816) (Maxwell, 2020). The purchased cost of the equipment, at ambient operating pressure and using carbon steel in construction, could be estimated by the following equation:

$$\log_{10}(C_p^0) = K_1 + K_2 \log_{10}(A) + K_3 (\log_{10}(A))^2 \quad (A.1)$$

where C_p^0 is the purchased equipment cost for base conditions (US\$). A is the capacity or size parameter of the equipment. K_1 , K_2 , and K_3 are parameters for each type of equipment. The values used in this study are given in Table A.1.

Table A.1 Constant parameters used in cost model Equation (A.1)

Equipment type	K_1	K_2	K_3	Capacity, Units	Min Size	Max Size
Sieve tray	2.9949	0.4465	0.3961	Area, m ²	0.07	12.3
Tower vessel	3.4974	0.4485	0.1074	Volume, m ³	0.3	520
U-tube exchanger	4.1884	-0.5277	0.3955	Area, m ²	10	1,000
Centrifugal compressor	2.2897	1.3604	-0.1027	Fluid power, kW	450	3,000

Table A.2 Constant parameters used in Equation (A.2) and (A.3)

Equipment type	C_1	C_2	C_3	Pressure range (barg)	$F_{M,CS}$	B_1	B_2
Tower vessel	0	0	0	$P < 3$	1	2.25	1.82
U-tube exchanger	0	0	0	$P < 5$	1	1.63	1.66
	0.03881	-0.11272	0.08183	$5 < P < 140$			
Centrifugal compressor	0	0	0	-	-	-	-

After evaluating the bare module cost (C_{BM}), the total module cost (C_{TM}) and the total grassroots cost (C_{GR}) can be estimated from Equation (A.4) and (A.5). C_{TM} is the cost of making small to moderate expansions or alterations to an existing facility, while C_{GR} represents an entirely new facility in which the construction is started on essentially undeveloped land, a grass field (Turton et al., 2018).

$$C_{TM} = 1.18C_{BM} \quad (A.4)$$

$$C_{GR} = C_{TM} + 0.5C_{BM} \quad (A.5)$$

Next, the total annualized cost of the distillation column was calculated by Equation (A.6). The economic assumptions were 8,322 operating hours per year, a 10% interest rate, and ten years of equipment lifetime.

$$TAC = C_{GR} \frac{i \times (1+i)^n}{(1+i)^n - 1} + C_{util} \quad (A.6)$$

where TAC is the total annualized cost (US\$/year), i is the interest rate of the distillation column (fraction), n is the equipment lifetime (years), and C_{util} is the annual cost of utilities (US\$/year).

Nomenclature

A capacity or size parameter in Equation (A.1)
 B constant parameters in Equation (A.2)
 C cost in the appendix or constant parameters in Equation (A.3)

The purchased equipment cost must be corrected with the bare module factor (F_{BM}), which accounts for the material (F_M) and pressure (F_P) factors in construction. The corrected value is now called the bare module cost (C_{BM}):

$$C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P) \quad (A.2)$$

where C_{BM} is the bare module cost of equipment (US\$). F_{BM} is the factor for calculating the bare module cost. For the centrifugal compressor, F_{BM} is 2.8. B_1 and B_2 are parameters for each type of equipment, as shown in Table A.2.

The pressure factor (F_P) in Equation (A.2) can be determined as follows:

$$\log_{10} F_P = C_1 + C_2 \log_{10}(P) + C_3 (\log_{10}(P))^2 \quad (A.3)$$

where F_P is the pressure factor for calculating the bare module cost. P is the operating pressure (barg) of equipment. C_1 , C_2 , and C_3 are parameters for each type of equipment, as shown in Table A.2.

F constant parameters in Equation (A.2), (A.3)
 i stage number in the rectifying section or fractional interest rate
 j stage number in the stripping section
 LK, HK light key, heavy key components
 K number of added stages or constant parameters in Equation (A.1)
 n bottom stage or equipment lifetime
 P pressure
 Q heat load
 T temperature
 U overall heat transfer coefficient
 v, l vapor, liquid flow

Subscripts

BM bare module
 CS carbon steel
 GR grassroots
 i, j stage number
 min minimum
 M material
 P pressure
 SE side exchanger
 TM total module
 util utility
 v, l vapor, liquid stream
 0 base case or reference

Greek letter

Δ difference

Abbreviations

CEPCI	Chemical engineering plant cost index
CGCC	Column grand composite curve
DWC	Dividing-wall column
ESAI	Energy saving per additional investment
HIDiC	Internally heat-integrated distillation column
MDFP	Minimum driving force profile
MESAI	Maximum energy saving per additional investment
TAC	Total annualized cost