



Investigation of energy-saving azeotropic dividing wall column to achieve cleaner production via heat exchanger network and heat pump technique

Ao Yang^a, Saimeng Jin^a, Weifeng Shen^{a,*}, Peizhe Cui^{b,**}, I-Lung Chien^c, Jingzheng Ren^d

^a School of Chemistry and Chemical Engineering, Chongqing University, Chongqing, 400044, PR China

^b College of Chemical Engineering, Qingdao University of Science and Technology, 53 Zhengzhou Road, Qingdao, 266042, PR China

^c Department of Chemical Engineering, National Taiwan University, Taipei, 10617, Taiwan

^d Department of Industrial and Systems Engineering, The Hong Kong Polytechnic University, Hong Kong, PR China

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ABSTRACT

A thermally coupled azeotropic dividing wall column (ADWC) configuration is explored for the separation of industrial wastewater to recycle the organic solvent tert-butanol. Heat pump technology is used to the ADWC configuration to improve the released heat duty quality of the condenser achieving the energy-saving. A gas preheater before the compressor is installed in the heat pump assisted ADWC configuration in increasing the temperature of the inlet vapour stream of the compressor that achieves effectively reducing the power and compression ratio of the compressor. To fully utilize a large amount of superheat energy produced in heat pump system indicated by the temperature-enthalpy and Grand Composite Curve diagrams, a green and sustainable Heat Integrated ADWC (HI-ADWC) separation configuration is proposed by the combined use of heat exchange network and heat pump implementations. Three indexes involving total annual cost, CO₂ emissions, and exergy loss are introduced to evaluate the economic, environmental and thermodynamic performances. The results illustrate that the TAC of the proposed green and sustainable HI-ADWC configuration is significantly reduced by 32.91% with a ten-year payback period compared to that of the existing configuration. CO₂ emissions are reduced by 86.43% and exergy loss of the HI-ADWC configuration by 36.72%. The proposed method for the green and sustainable HI-ADWC configuration could be widely extended to other industrial processes reduce energy consumption and related CO₂ emissions.

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1. Introduction

Distillation technology has been developed for separating and purifying of mixtures in the chemical industrial due to its advantages in the operation (Sharan et al., 2018) and control (Luyben and Chien, 2011). However, a drawback of the conventional distillation is required a great deal of energy consumption to achieve the separation task (Kiss and Ignat, 2012). In addition, a large amount of CO₂ emissions contribute to global warming (Wang et al., 2019b). Intensified distillation processes need to develop to overcome the above issues achieving the performance of energy-saving, cleaner

production and environmental protection (Matsuda et al., 2012).

To achieve the energy-saving, distillation processes with Heat Integration by changing operating pressure as technology is explored. For example, a novel pressure-swing extractive distillation configuration for separating acetone/methanol binary minimum-boiling azeotropic mixture is explored (You et al., 2017). The application of Heat Integration (Klemeš, 2013) for the extractive distillation process to separate tetrahydrofuran/water mixtures with lower operational pressure is then investigated (Gu et al., 2018). Design and optimization of ternary extractive distillation for separating acetonitrile/methanol/water was proposed by Wang et al. (2019a), and the calculation illustrates that total annual cost (TAC) of the lower operating pressure scheme can reduce by 47.0% than the operating at atmosphere pressure. Following that, the vacuum distillation scheme for low-sulfur biodiesel production was explored by Xie et al. (2019). A novel separation configuration as another

* Corresponding author.

** Corresponding author.

E-mail addresses: shenweifeng@cqu.edu.cn (W. Shen), cpzmagic@qust.edu.cn (P. Cui).

Nomenclature

ADWC	azeotropic dividing wall column	NRTL	non-random two liquid
C%	the carbon content of fuel, kg/kg	Q_{CW}	cold utility, kW
CCC	Cold Composition Curve	Q_{LP}	hot utility, kW
COM	compressor	Q_{fuel}	the heat requirement of fuel, kJ
COP	coefficient of performance	Q_{seq}	energy requirement, kJ
CYH	cyclohexane	S	entropy, kW
C_{TBA}	total cost of tert-butanol, US\$/y	HI-ADWC	Heat Integrated azeotropic dividing wall column
C_{Energy}	total cost of energy consumption, US\$/y	T_{inlet}	inlet temperature, °C
C_{RM}	total cost of raw material, US\$/y	T_{outlet}	outlet temperature, °C
C_{WT}	total cost of wastewater treatment, US\$/y	T-H	temperature-enthalpy
DWC	dividing wall column	TBA	tert-butanol
El	exergy loss, kW	T	temperature, °C
Ex	exergy, kW	TAC	total annual cost, US\$/y
GP-HP-ADWC	heat pump assisted azeotropic dividing wall column with a gas preheater	TCC	total capital cost, US\$
GCC	Grand Composite Curve	TOC	total operating cost, US\$/y
H	enthalpy, kW	TNR	total net revenue, US\$/y
HP	heat pump	T_R	reboiler temperature, °C
HP-ADWC	heat pump assisted azeotropic dividing wall column	T_C	condenser temperature, °C
HEN	heat exchanger network	x	molar composition, mol/mol
HCC	Hot Composition Curve	α	the molar mass ratio of CO ₂ and C
NHV	the net heating value of fuel, kJ/kg	λ_{seq}	latent heat of the steam, kJ/kg
		h_{seq}	enthalpy of the steam, kJ/kg
		η_C	Carnot efficiency

energy-saving technology has been investigated. A novel energy-saving extractive distillation with side-stream was studied by Tututi-Avila et al. (2017) for the separation of acetone/methanol mixtures using water as entrainer. Partial thermally coupled and double side-streams ternary extractive distillation sequences for acetonitrile/benzene/methanol separation are explored by Wang et al. (2018). In summary, energy consumption and CO₂ emissions of the process could be reduced via the intensified distillation configuration or Heat Integration scheme.

To further reduce the energy consumption, dividing wall column (denoted as DWC) configuration was explored by Petlyuk et al. (1965). BASF applied the first commercial DWC in 1985 at their Ludwigshafen site in Germany (Dejanovic et al., 2010). Kiss and Ignat (2012) reported that the steam cost of the DWC scheme could save up to 30% than the double-column separation sequence. DWC can be extensively applied to implement other processes (e.g., azeotropic, extractive and reactive distillations) with a dividing wall located at the bottom, top and middle of the operating unit. For example, Wu et al. (2014) proposed an energy-saving azeotropic-DWC (ADWC) separation configuration for heterogeneous azeotropic distillation. Yu et al. (2015) investigated the implementation of ethanol dehydration by employing ADWC. Wu et al. (2013) explored the energy-efficient potential of the extractive-DWC for heterogeneous distillation processes. The application of extractive-DWC for ethane recovery process is then studied (Tavan et al., 2014). Yang et al. (2018) studied the separation of ternary heterogeneous mixtures methanol/toluene/water with the multi-azeotrope system by using extractive-DWC with a side decanter configuration. Synthesis of tert-amyl methyl ether through a combination of the DWC with reaction distillation and pressure-swing configuration is proposed by Yang et al. (2017). Reactive-DWC scheme for the synthesis of triethyl citrate using multi-objective criteria is reported by Santaella et al. (2017). The above results show that the energy consumption of the DWC configuration could be further reduced than that of the conventional sequence.

DWCs separation technology can provide a vast potential to

effectively reduce the steam consumption. However, the heat duty of condenser has not been effectively utilized in the DWC sequence. Heat pump (HP) technology is employed to improve the released heat duty quality of the condenser to conform to the heat demand of the reboiler and is mainly utilized to reduce the energy required when the difference of temperature between the top and bottom of the column is small (Kumar et al., 2013). HP technique can be easily applied to existing processes because they can be installed externally and require little change to the existing designs (Olujić et al., 2006). For example, Long et al. (2015) proposed a novel self-heat DWC to improve the thermodynamic efficiency and production capacity of the column and the calculations illustrate that the self-heat configuration can effectively reduce the operating cost. Li et al. (2016) explored the energy-saving of three HP configurations for the ADWC, and the computational results show that the improved design configuration saves a TAC by 32.22% and CO₂ emissions by 63.79%. Xu et al. (2017) reported an approach to design intensified configurations involving the HP assisted DWC at the side product stage, and they illustrate that intermediate reboiler-side condenser HP assisted DWC scheme can reduce 8.57% of TAC. An improved, different pressure thermally coupled reactive-DWC for the synthesis of diethyl carbonate is proposed in author's recent work (Yang et al., 2019b) by using HP technique and the calculation illustrates that the TAC of the proposed scheme could be reduced by 20.52%. In summary, better environmental and economic benefits can be achieved in the DWC configuration because the latent heat of vaporization in the top vapour stream is effectively integrated via the HP technology.

Amount of sensible heat in the hot and cold streams has not always been used because the HP is applied in the distillation process. In order to comprehensively and effectively utilize the heat duty of cold and hot streams in the process, heat exchanger network (HEN) and Pinch Analysis (Klemeš et al., 2018a) are used to effectively decrease the requirements of steam and cooling water (Wang et al., 2009). A whole process with Heat Integration implementing HP was reported by Yang et al. (2016). In the proposed design, the steam and cooling water requirements are reduced by

61.5% and 20.6% compared to the conventional process. The HEN is employed to the Heat Integration design in the biodiesel production through the reactive distillation (Poddar et al., 2017) and they provided evidence that the operating cost of the Heat Integrated process is significantly reduced compared with the referenced process. Based on the listed studies, Xia et al. (2017) proposed a heat pump assisted pressure-swing distillation scheme with HEN matching, and they demonstrated that proposed process reduces TAC by 36.65% and 5.18% compared with the conventional and full Heat Integrated designs. The application of HEN can be employed to find a scheme with small energy consumption, TAC and CO₂ emissions.

According to the survey the existing ADWC and HP assisted ADWC (HP-ADWC1) configurations are explored to separate azeotropic mixture tert-butanol (TBA)/water (Luyben, 2016). In addition, an extractive distillation process for TBA dehydration is studied by Lo and Chien (2017). However, the application of both HEN and HP technologies to the ADWC configuration to achieve cleaner production has not yet been reported. As a consequence, in this work, a novel green and sustainable Heat Integrated ADWC (HI-ADWC) configuration is proposed by combining HP and HEN techniques for separating binary azeotropic mixtures TBA/water to achieve the purpose of cleaner production (i.e., energy-saving, reduction of CO₂ emissions and enhancing of thermodynamic efficiency). A conventional ADWC configuration is firstly simulated by the Aspen Plus V8.4 as a basic case. Following that, the ADWC with feed preheating (ADWC-FP) configuration is proposed to reduce the energy consumption of reboiler. HP assisted ADWC (HP-ADWC2) configuration is then proposed to further achieve energy-saving performance. A gas preheater before the compressor is installed to make further implemented reduce the power of the compressor. The HEN has been applied to achieve the optimal heat matching in the proposed green and sustainable HI-ADWC configuration.

2. Methodology

A systematic method is proposed for the design of the TBA dehydration process by combining the HP and HEN technologies into the ADWC scheme, as described in Fig. 1. In the first step, the energy analysis of the existing configuration is carried out to search for suitable alternative solutions. According to the analysis in the

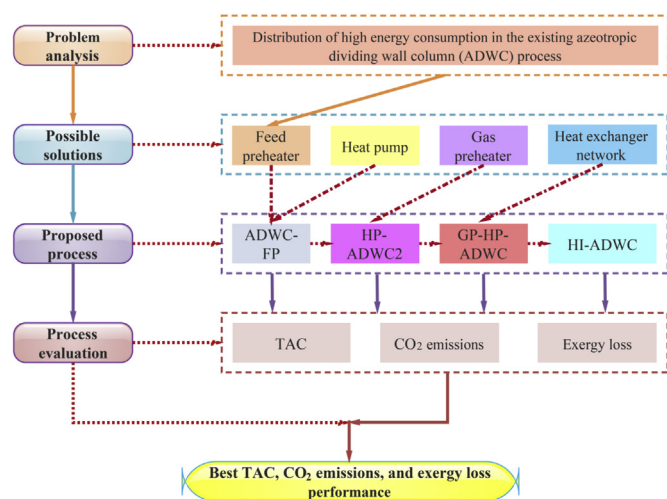


Fig. 1. The proposed framework of the HI-ADWC configuration design and evaluation (ADWC-FP: the ADWC with feed preheating; HP-ADWC2: heat pump assisted ADWC; GP-HP-ADWC: adding a gas preheater to the HP-ADWC; HI-ADWC: Heat Integrated ADWC; TAC: total annual cost).

first step, four possible solutions may be found to effectively reduce the energy consumption or improve the released heat duty quality of the condenser. In the solution step, feed preheater is used to heat the feed streams reducing the reboiler duty. Following that, HP is installed to further reduce energy consumption. A gas preheater before the compressor is added to effectively decrease the compressor ratio and power. Heat exchanger network is used to integrate the latent heat of vaporization and sensible for hot and cold stream achieving an optimal design. To validate the possible proposed solutions, four alternative configurations combining feed preheater, heat pump, a gas preheater for the compressor and heat exchanger network with ADWC configuration (i.e., ADWC-FP, HP-ADWC2, GP-HP-ADWC and HI-ADWC) are implemented via the Aspen Plus V8.4 (Aspen Technology, 2013a). Finally, three indexes involving TAC, CO₂ emission and exergy loss are introduced to find the best performance for the TBA dehydration process by alternative configurations and the existing configuration.

2.1. Existing azeotropic dividing wall column configuration

2.1.1. Azeotropic dividing wall column configuration

In this work, the existing ADWC configuration for separating binary azeotropic system TBA/water proposed by Luyben (2016) has been arranged. The existing ADWC configuration for TBA dehydration process is illustrated in Fig. 2. The fresh feed and the aqueous stream from the decanter are mixed and then fed into the column C2. High-purity water with 99.8 mol% is obtained at the bottom stream of column C1 while the top vapour stream and organic stream are sent to the middle and top sections of column C2. High-purity TBA with 99.8 mol% is obtained at the bottom of column C2 while the top vapour stream is condensed to the decanter. Finally, aqueous and organic phases are obtained via the decanter.

2.1.2. Evaluation, the feasibility of the HP, assisted ADWC

Pleșu et al. (2014) proposed a simple criterion coefficient of performance (denoted as COP) defining as in Eq. (1) to effectively evaluate the feasibility of an HP system.

$$\text{COP} = \frac{Q}{W} = \frac{1}{\eta_C} = \frac{T_C}{T_R - T_C} \quad (1)$$

where the reboiler duty is represented as Q , the requirement work of the compressor is denoted as W , Carnot efficiency is represented

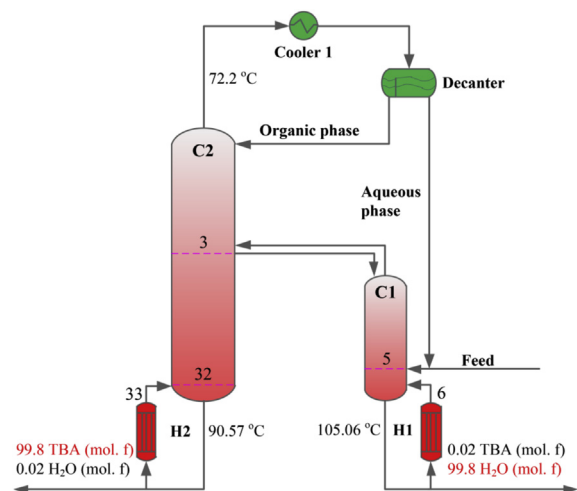


Fig. 2. Existing ADWC configuration for TBA dehydration.

as η_c , the reboiler temperature is represented as T_R ($^{\circ}\text{C}$), and the condenser temperature is denoted as T_C ($^{\circ}\text{C}$).

From the study of Luyben (2016) in Fig. 2, the temperature of the top vapour stream is 72.20°C while the temperatures of left and right reboilers are 105.06°C and 90.57°C . The calculation COPs of C1 and C2 are 10.51 and 18.80 (both higher than 10) indicating that the application of HP in C1 and C2 (or ADWC) configuration for separating TBA/water system is very favourable.

2.1.3. Energy analysis via the temperature-enthalpy diagram

In generally, the utility requirements of the chemical industrial process can be represented via the temperature-enthalpy (T-H) diagram as demonstrated by Yang et al. (2016). The overall hot and cold requirements are observed through the Hot Composition Curve (denoted as HCC) and Cold Composition Curve (abbreviated as CCC) in the T-H diagram (Poddar et al., 2017). The recovery heat of the process could be represented in the overlap region of HCC and CCC. In addition, the cooling water and steam requirements are the displacements of the CCC and HCC (Xia et al., 2017).

2.2. Four proposed alternative configurations

2.2.1. ADWC with feed preheating (ADWC-FP)

Fig. 3 illustrates the proposed alternative configuration ADWC with feed preheating (ADWC-FP) for TBA dehydration. To reduce the energy consumption of the ADWC scheme, two feed stream (i.e., S3 and S4) should be preheated to decrease the reboiler duty of column C1 (Xia et al., 2017). Compared with ADWC, the power consumption of compressor can be reduced when the HP is applied in the ADWC-FP. Following the suggestion of Xia et al. (2017), two product streams S5 and S12 should be cooled to 40°C . Of note is that the feed stream S9 is not preheated because this stream is fed to the first stage. The feed locations of S2 and S4 should be optimized because the thermal state of the feed has been changed.

2.2.2. HP assisted ADWC (HP-ADWC2)

The proposed alternative configuration HP assisted ADWC (HP-ADWC2) for TBA dehydration is displayed in Fig. 4. To effectively utilize the latent heat of vaporization in the top vapour stream of column C2, a compressor is installed at the top of the column C2. The top vapour stream of the column C2 is compressed to a high temperature to provide heat duty for reboilers H1 and H2. In the simulation process, a new design specification is set by varying the outlet pressure of the compressor to satisfy the $T_{S15}-T_{R2} \geq 5^{\circ}\text{C}$ and $T_{S14}-T_{R1} \geq 5^{\circ}\text{C}$ (T_{S15} and T_{S14} represent the temperature of S15 and

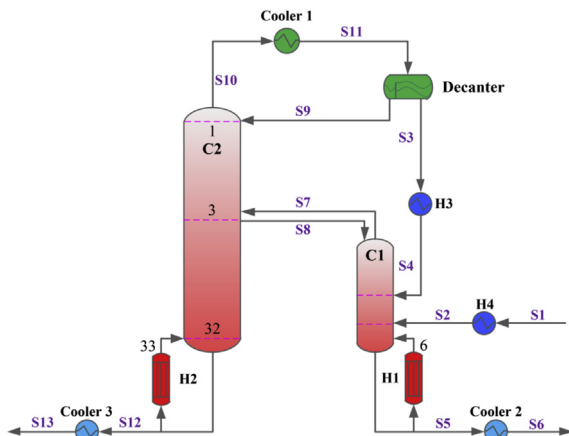


Fig. 3. Proposed alternative configuration ADWC-FP for TBA dehydration.

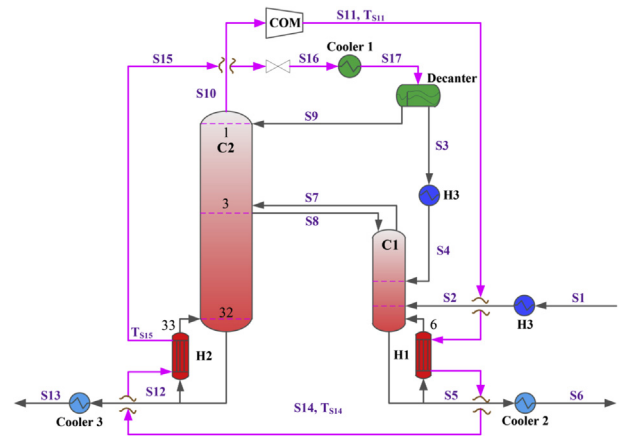


Fig. 4. Proposed alternative configuration HP-ADWC2 for TBA dehydration.

S14 streams). However, the condenser duty is lower than the sum of heat duty for H1 and H2 according to the study of Luyben (2016). To achieve exchange of heat, a higher temperature of compressed stream is required, which may cause a higher compression ratio for the compressor. A more energy-saving configuration should be proposed to further reduce the power consumption of compressor in the below section 2.2.3.

2.2.3. A gas preheater is installed before the compressor for the HP-ADWC2 (GP-HP-ADWC)

Following the suggestion of Li et al. (2016), a gas preheater before the compressor is installed in the HP-ADWC2 configuration (denoted as GP-HP-ADWC) as illustrated in Fig. 5, which could effectively reduce the power of the compressor. Compared with the HP-ADWC2 configuration, the compressor ratio (or outlet pressure) of the GP-HP-ADWC with a higher temperature of compressor inlet may be effectively reduced. The temperature of stream S18 should be optimized because it will affect the power of the compressor (W) and the outlet temperature of the compressed stream (T_{S11}). It is worth noting that heat input is needed for the gas preheater H5. In addition, the sensible heat of stream S15 and product streams S5 and S12 are not effectively utilized. The optimal heat matching will be shown in the below section 2.2.4.

2.2.4. Heat integrated ADWC (HI-ADWC) configuration

Following the study of Klemeš et al. (2018b), heat exchanger

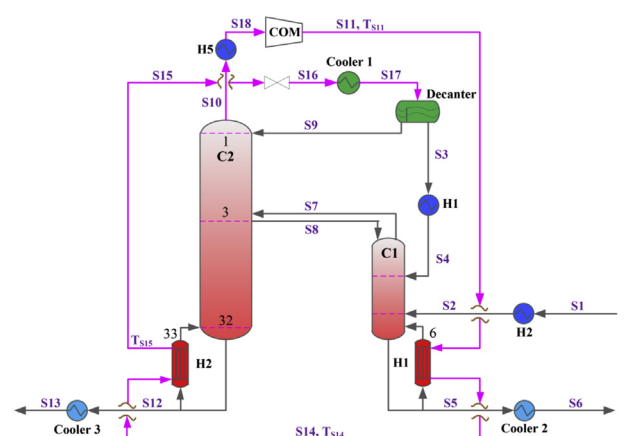


Fig. 5. Proposed alternative configuration GP-HP-ADWC for TBA dehydration.

network (HEN) should be used to match the hot and cold stream achieving the minimum energy consumption. To achieve the optimal and reasonable matching, Pinch Analysis (Klemeš et al., 2018a) and approach retrofit of HEN (Walmsley et al., 2018) are used, which is carried out in the Aspen Energy Analyzer V8.4 (Aspen Technology, 2013b). Fig. 6 demonstrates a conceptual design flowsheet of the optimal hot and cold stream matching. The heat duties of feed preheater (H1 and H2), reboiler 1 (H3), reboiler 2 (H4), gas preheater (H5), and coolers (cooler 1–3) and minimum Pinch Point Temperature should be determined in section 3.2.4. The energy-saving of the HI-ADWC should be re-evaluated because more capital investment is needed compared with the GP-HP-ADWC.

2.3. Economic, environmental and thermodynamic efficiency evaluations

In this investigation, three criteria (i.e., TAC, CO₂ emissions and exergy loss) are used to evaluate the economic, environmental and thermodynamic efficiency of the existing and proposed configurations.

2.3.1. Economic evaluation

TAC proposed by Douglas (1988) is introduced to assess the economics of the existing and the intensified designs, which consists of the total capital cost (TCC) and total operating cost (TOC). The computational formula of the TAC is illustrated as follow,

$$\text{TAC [US\$/y]} = \text{TCC/payback} + \text{TOC} \quad (2)$$

TCC involves the capital costs of shell, tray, decanter, condensers, reboilers, heat exchangers, and compressor.

The shell and tray costs of the column are calculated as follow,

$$\text{shell cost of column [US\$]} = (\text{M\&S})/280 \times D^{1.066} \times H^{0.802} \times C_{\text{SC}} \quad (3)$$

$$\begin{aligned} \text{tray cost of column [US\$]} &= (\text{M\&S})/280 \times 97.243 \times D^{1.55} \times H \\ &\times F_C \end{aligned} \quad (4)$$

where Marshall and Swift index (M&S) is assumed as 1,468.60 to the HP system (Feng et al., 2018); H [m] and D [m] represent the height and the diameter; coefficients of the shell cost for column and decanter (C_{SC}) is 3,919.32 (Olujić et al., 2006); correction factor

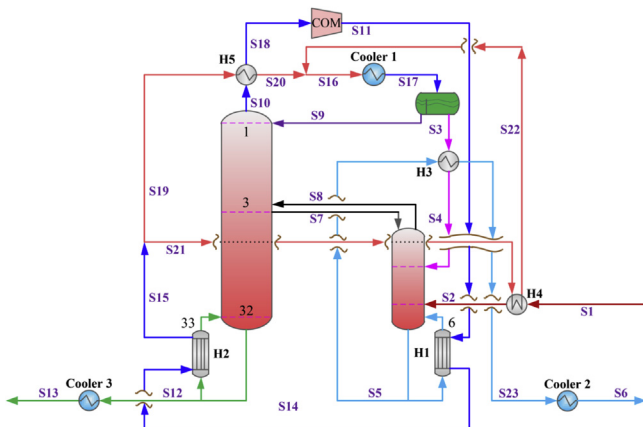


Fig. 6. Proposed alternative configuration HI-ADWC for TBA dehydration.

of the tray cost (F_C) is determined as 1.4 (Olujić et al., 2006).

Capital costs for the reboiler, condenser, and heat exchanger are obtained as follow,

$$\text{heat exchanger cost [US\$]} = (\text{M\&S})/280 \times A^{0.65} \times C_H \quad (5)$$

where A (m²) denotes the area of reboiler, condenser, and heat exchanger; coefficients of the kettle reboiler, condenser, and heat exchanger (C_H) are 1,775.26, 1,609.13, and 1,799.00 (Olujić et al., 2006).

Calculations of area and heat transfer temperature difference for the reboiler and heat exchanger are displayed as follow,

$$A_R [\text{m}^2] = \frac{Q_R}{(\Delta T_R \times U_R)} \quad (6)$$

$$\Delta T_R [\text{K}] = 160 - T_R \quad (7)$$

$$\Delta T_R [\text{K}] = \frac{(T_{\text{hin}} - T_{\text{cout}}) - (T_{\text{hout}} - T_{\text{cin}})}{\ln\left(\frac{T_{\text{hin}} - T_{\text{cout}}}{T_{\text{hout}} - T_{\text{cin}}}\right)} \quad (8)$$

where A_R [m²] represents the area of the reboiler and heat exchanger; Q_R is the reboiler duty; $U_R = 568 \text{ W/m}^2/\text{°C}$ is the heat transfer coefficient of the reboiler while U_R is $210 \text{ W/m}^2/\text{°C}$ for the gas preheater (Luyben, 2012); T_R [°C] are the reboiler temperature of the compressed vapour stream; ΔT_R [°C] in Eq. (7) denotes the heat transfer temperature difference of reboiler when the low-pressure steam is used; ΔT_R [°C] in Eq. (8) denotes the heat transfer temperature difference of heat exchanger while the reboiler input is provided via the compressed vapour stream; the inlet and outlet temperatures of the high-temperature stream denote as T_{hin} and T_{hout} ; the inlet and outlet temperature of the low-temperature stream represent T_{cin} and T_{cout} .

The calculations of area and heat transfer temperature difference for the condenser are shown as follow,

$$A_C [\text{m}^2] = \frac{Q_C}{(\Delta T_C \times U_C)} \quad (9)$$

$$\Delta T_C [\text{K}] = \frac{(T_{\text{hin}} - T_{\text{cout}}) - (T_{\text{hout}} - T_{\text{cin}})}{\ln\left(\frac{T_{\text{hin}} - T_{\text{cout}}}{T_{\text{hout}} - T_{\text{cin}}}\right)} \quad (10)$$

where A_C [m²] is the area of the condenser; Q_C [kW] is the condenser duty; $U_C = 852 \text{ W/m}^2/\text{°C}$ is the heat transfer coefficient of the condenser (Luyben, 2012); ΔT_C is the logarithmic mean temperature difference, which is calculated via the Eq. (10); T_{cin} and T_{cout} are 30 and 40 °C while the cooling water is used (Modla and Lang, 2013).

The capital cost and volume of the decanter could be obtained from the Eqs. (11) and (12) (Turton et al., 2008).

$$\text{decanter cost [US\$]} = (\text{M\&S})/280 \times D_d^{1.066} \times H_d^{0.802} \times C_{\text{SC}} \quad (11)$$

$$V_d [\text{m}^3] = F_V \times 2 \times 10/60 = \frac{\pi D_d^2}{4} \times H_d \quad (12)$$

where the height and the diameter of the decanter are abbreviated as D_d (m), and H_d (m); V_d [m³] is the volume of the decanter. The ratio of the H_d and D_d is assumed as 2 (Luyben and Chien, 2011).

Calculation of the capital cost for the compressor is illustrated in Eq. (13).

$$\text{capital cost of compressor [US\$]} = (M\&S)/280 \times 2047.24 \times [W/(0.9 \times 0.8)]^{0.82} \tag{13}$$

TOC includes the operating cost of steam, cooling and electricity, which could be calculated via the Eqs. (14)–(16).

$$\text{total steam cost [US\$/y]} = C_S \times Q_R \times 7200 \tag{14}$$

$$\text{total cooling water cost [US\$/y]} = C_W \times Q_C \times 7200 \tag{15}$$

$$\text{total electricity cost [US\$/y]} = C_E \times W/(0.9 \times 0.8) \times 7200 \tag{16}$$

where C_S (13.28 US\$/GJ), C_W (0.345 US\$/GJ), and C_E (16.8 US\$/GJ) are the cost of steam, cooling water, and electricity (Yang et al., 2019b); 7,200 h/y is determined as operating time.

Total net revenue (TNR, US\$) of the existing and the proposed schemes could be calculated via the Eq. (17) (Silva et al., 2017).

$$\text{total net revenue [US\$/y]} = C_{TBA} - C_{Energy} - C_{RM} - C_{WT} - \text{TCC/payback period} \tag{17}$$

where C_{TBA} , C_{Energy} , C_{RM} , and C_{WW} are the total cost of tert-butanol, energy consumption, and raw material wastewater treatment. Prices used in the net revenue analysis are illustrated in Table 1.

Although the HP system has a satisfactory performance to reduce the operating cost, it is hard to realize economic benefits in a short investment recovery period. The 10-year of payback period is determined to observe the energy-saving effect (Yang et al., 2019b).

2.3.2. Carbon dioxide emissions evaluation

The CO₂ emission is used to evaluate the environmental benefits of HP assisted distillation process (You et al., 2016) and it has been applied to assess the sustainability of the triple-column extractive distillation process (Zhao et al., 2018). The CO₂ emission is introduced to assess the environment and sustainability of the basic and proposed configurations (Tavan et al., 2014). However, the calculation of CO₂ emissions is a complex issue due to the energy required for the reboiler could be produced from the different raw materials, heavy fuel oil, natural gas, or coal. Gadalla et al. (2006) proposed a simplified calculation model of CO₂ emissions in Eq. (2) for the distillation system.

$$\text{CO}_2 \text{ emissions} = \left(\frac{Q_{\text{fuel}}}{\text{NHV}} \right) \times \left(\frac{C\%}{100} \right) \alpha \tag{18}$$

where the molar mass ratio of CO₂ and C (α) is 3.67, the net heating value (denoted as NHV) is 39,771 kJ/kg, and C% = 86.5 kg/kg is the carbon content of the fuel. The heat requirement of fuel (Q_{fuel}) is calculated as follows,

$$Q_{\text{fuel}} = \frac{Q_{\text{seq}}}{\lambda_{\text{seq}}} \times (h_{\text{seq}} - 419) \times \left(\frac{T_F - T_0}{T_F - T_S} \right) \tag{19}$$

where energy requirements in kJ and latent heat and enthalpy in kJ/kg of the steam are denoted as λ_{seq} , h_{seq} and Q_{seq} . $T_F = 2,073.15$ K is the flame temperature, $T_S = 433.15$ K is the stack temperature, and the ambient temperature T_0 is 298.15 K. Following the suggestion of Waheed et al. (2014), CO₂ emission of the compressor is 184 kg/h while the power requirements of a compressor are 1,000 kW.

2.3.3. Thermodynamic efficiency evaluation

To evaluate the proposed configurations, energy efficiency is another significant indicator (Yang et al., 2019c). For a given system, the exergy loss (El) is defined as Eq. (20), which exhibits the difference value between total input and output of exergy (Sun et al., 2013).

$$\text{El} = \sum \text{Ex}_{\text{input}} - \sum \text{Ex}_{\text{output}} \tag{20}$$

Exergy (Ex) is calculated for a given specified system by the enthalpy (H) and entropy (S), which is illustrated in Eq. (21) as follow,

$$\text{Ex} = (H - H_0) - T_0 \cdot (S - S_0) \tag{21}$$

where the enthalpy difference between the system and the reference state is denoted as $H - H_0$, the $S - S_0$ illustrates the entropy difference between the system and the reference state, and the $T_0 = 25$ °C is the reference temperature.

3. Computational results

In the real plant, TBA is always obtained from the direct hydration of isobutene in a reactive distillation process (Lei et al., 2009). Following that, downstream azeotropic mixture (i.e., TBA and water) of the reactive distillation is explored by Yu et al. (2015) to obtain the high-purity of TBA. Chen et al. (2019) investigated the heterogeneous azeotropic distillation to separate TBA/water while an energy-saving extractive distillation in vacuum for the separation of TBA/water binary azeotrope (see Fig. A1) is proposed by Lo and Chien (2017). In this work, the proposed alternatives configurations are studied based on the heterogeneous heat pump assisted ADWC (HP-ADWC1) configuration by Luyben (2016) due to its advantage in operation.

3.1. Existing ADWC configuration

3.1.1. Residue curve maps

In the ADWC configuration, the vapour-liquid and liquid-liquid equilibriums of the ternary azeotropic system TBA/water/cyclohexane (CYH) could be well described via the built-in non-random two liquid (NRTL) model (Luyben, 2016) of the Aspen Plus V8.4 while all interaction parameters are summarized in Table 2.

Table 1
Product and energy costs for the tert-butanol dehydration process.

Product	Price	Units	Reference
Tert-butanol	1,000	US\$/t	PHC, (2016)
Raw material	300	US\$/t	Information provided by specialists
Low-pressure steam	13.28	US\$/GJ	Yang et al. (2019b)
Cooling water	0.345	US\$/GJ	Yang et al. (2019a)
Electricity	16.8	US\$/GJ	Yang et al. (2019b)
Wastewater treatment	1.20	US\$/t	Kim et al. (2009)

Table 2
Interaction parameters of the NRTL model for the azeotropic distillation system.

Component i	TBA	TBA	Water
Component j	Water	CYH	CYH
Temperature units	°C	°C	°C
A _{ij}	-0.6868	-1.3739	13.1428
A _{ji}	7.0893	1.0691	-10.4585
B _{ij}	203.4190	559.5210	-1,066.9800
B _{ji}	-1,372.3800	245.1070	4,954.9000
C _{ij}	0.3000	0.4700	0.2000

Residue curve maps and material balance lines for TBA/water/CYH system are illustrated in Fig. 7. It is found that three additional azeotropes are formed while the entrainer CYH is added into the TBA/water system. A ternary TBA/water/CYH minimum azeotrope point is located in heterogeneous ranges with an azeotropic temperature of 65.2 °C. Another two azeotropes TBA/CYH and CYH/water are also formed with azeotropic temperatures of 71.9 °C and 69.5 °C.

The fresh feed (x_F), aqueous phase (x_{AQ}) and liquid sidestream (x_{L1}) are mixed at x_{M1} point and then is separated at a close TBA/water binary azeotropic mixture with a composition x_{V1} and a high purity of water with a composition x_{B1} in the column C1. Following that, the organic phase (x_{OR}) and the top vapour stream x_{V1} of column C1 are mixed at x_{M2} point. A ternary azeotropic mixture (x_{V2}) and a high purity of TBA with a composition x_{B2} are obtained based on the lever rule of the C2. The top vapour stream of the C2, x_{V2} , is cooled to a liquid and then it is separated into aqueous and organic phases (i.e., x_{AQ} and x_{OR}) via a decanter.

3.1.2. Process design

Fig. 8 illustrates the modified ADWC configuration without heat pump for separating TBA/water azeotropic system by Luyben (2016) while the modified heat pump assisted ADWC (HP-ADWC1) configuration is illustrated in Fig. A2. Total theoretical stages of two columns C1 and C2 are 6 and 33. Two columns are both operated at atmospheric pressure while the per tray pressure drop is 0.7 kPa. The aqueous phase and fresh feed are mixed and fed to the column C1, where the mixed stream is separated into high-purity water in the bottom stream and a ternary azeotropic mixture in the top vapour stream. Following that, the top vapour of column C1 and the organic phase stream are fed to the middle and top section of the C2. A high-purity of TBA with 99.8 mol% and a ternary azeotropic point TBA/water/CYH mixture are obtained in the column C1 based on the lever rules. The 99.8 mol% of water is obtained at the bottom stream of C2. The reboiler duties of columns C1 and C2 are 1,539.67 kW and 1,663.03 kW.

3.2. Proposed alternative configurations for TBA dehydration

3.2.1. ADWC with feed preheating (ADWC-FP) configuration

Following the suggestion in section 2.2.1, the feed locations of the ADWC-FP configuration should be optimized, and the

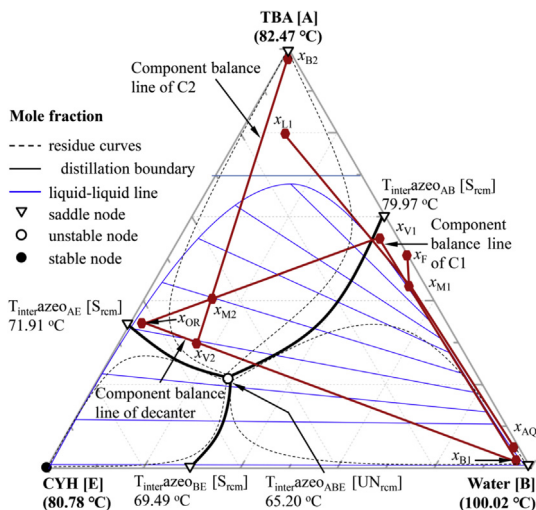


Fig. 7. Residue curve maps and material balance lines for TBA/water system using entrainer CYH.

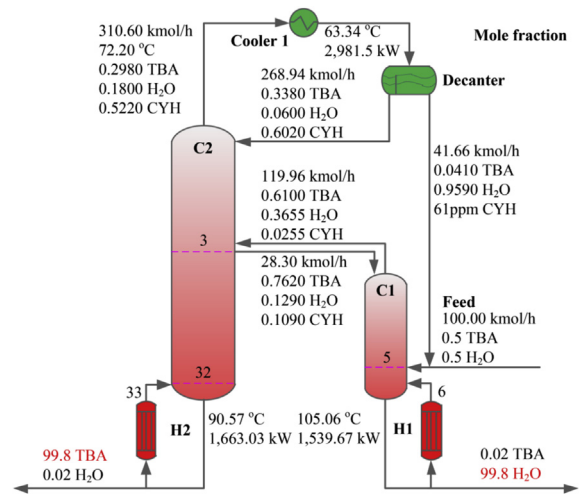


Fig. 8. Scheme of the existing ADWC with detailed parameters by Luyben (2016).

optimizations of feed locations of the aqueous phase and fresh feed are illustrated in Figs. 9 and 10. To achieve the specification products purities with minimum total reboiler duty, the fifth stage is determined as a feed location for aqueous phase and fresh feed.

Fig. 11 shows the ADWC-FP scheme for the separation of TBA/water system by using CYH as a heterogeneous entrainer. The aqueous phase (S3) and fresh feed are preheated at 73.68 °C and 87.50 °C via the preheaters 1 and 2 (H3 and H4). Reboiler duty of column C2 (H2) is 1,663.03 kW while 1,345.67 kW of H1 in ADWC-FP is obtained compared with the 1,539.67 kW of the existing configuration, which is consistent with the assumptions in Section 2.2.1. Finally, the product streams S12 and S5 are cooled at 40 °C via the coolers 2 and 3. The condensation required in coolers 2 and 3 is 187.17 and 72.32 kW.

Fig. 12 illustrates the T-H chart of the ADWC-FP configuration, where the blue and red lines demonstrate the CCC and HCC. In the ADWC-FP configuration, Q_{LP} is the low-pressure steam consumption of H1-H4 and Q_{CW} indicates the cooling water requirements of coolers 1–3. From Fig. 12, the overlap region (yellow zone) is small between lines of HCC and CCC, indicating that heat recovery is small. The low-pressure steam and the cooling water requirements of the ADWC-FP configuration are 3,045.4 and 3,130.63 kW. In addition, 158.33 kW can be recovered by the observation of the heat recovery zone.

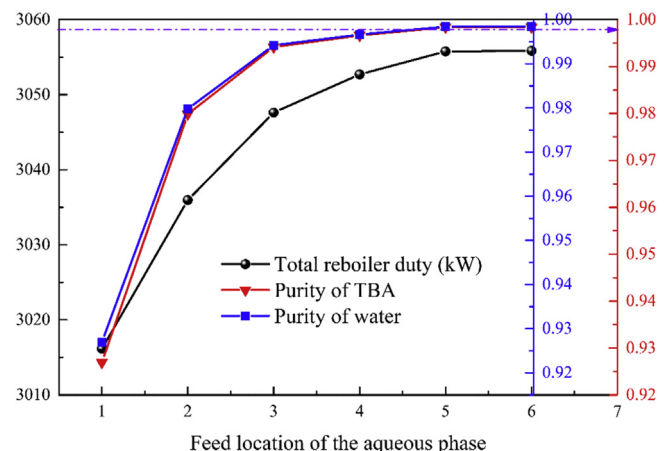


Fig. 9. Effect of the feed location of aqueous phase on total reboiler duty.

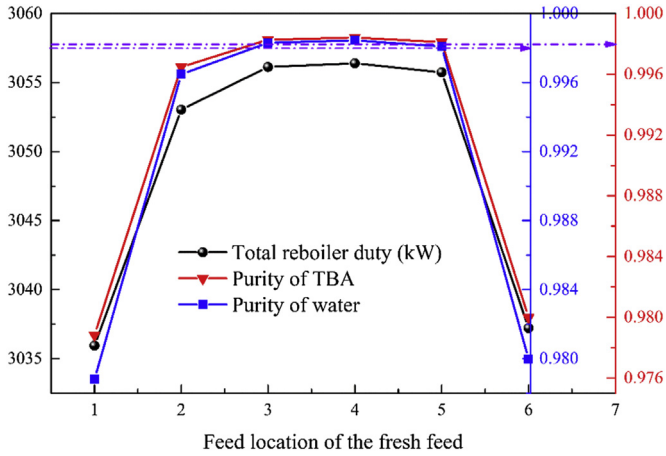


Fig. 10. Effect of the feed location of fresh feed on total reboiler duty.

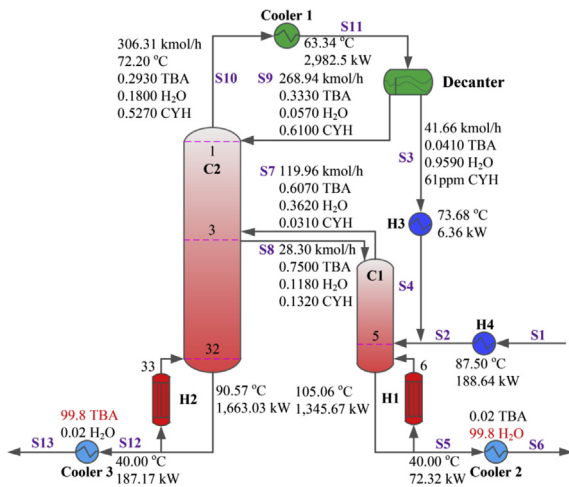


Fig. 11. Flowchart of the ADWC with feed preheating.

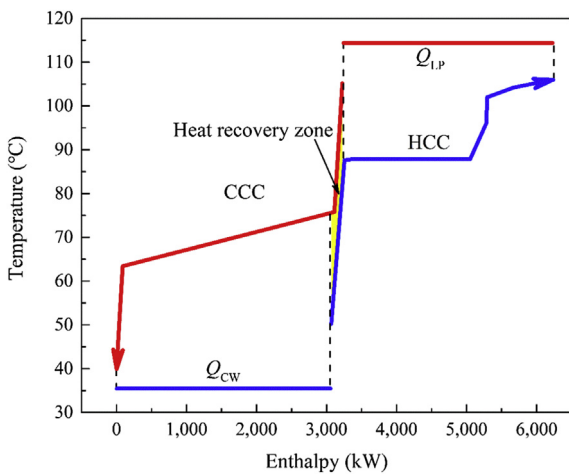


Fig. 12. The T-H diagram of the ADWC-FP configuration.

From the observation T-H diagram of Fig. 12, a lot of utilities are required in the ADWC-FP with preheated feed. All because, the 2,982.5 kW of the condenser (i.e., cooler 1) has been not effective utilized in the ADWC-FP configuration (Fig. 11). To effectively utilize

the heat duty of the condenser and reduce the energy consumption of reboilers, HP approach is promising in saving the cost of ADWC-FP systems. The applications of HP, a gas preheater for the compressor, and HEN to the ADWC-FP configuration are further investigated to improve the released heat duty quality of the condenser to meet the heat demand of the reboiler and reduce the cost.

3.2.2. Heat pump assisted ADWC (HP-ADWC2)

Two proposed design specifications in section 2.2.2 are carried out by varying the outlet pressure of the compressor to satisfy the $T_{S15}-T_{R2} \geq 5 \text{ }^\circ\text{C}$ and $T_{S14}-T_{R1} \geq 5 \text{ }^\circ\text{C}$ in Aspen Plus V8.4. The obtained HP-ADWC2 configuration with detailed information to separate TBA/water system using entrainer CYH is demonstrated in Fig. 13. The top vapour stream of the column C2 is compressed to a higher temperature by a compressor (COM). The compressed stream can provide the duty to the reboiler of the columns C1 (H1) and then give the duty to the reboiler of the column C2 (H2). Finally, its pressure can be reduced by a valve and then is cooled by the cooler 1.

The temperature of the stream S15 (i.e., 95.6 °C) is lower than the saturated vapour temperature. A massive compressor power 615.85 kW is required to achieve the heat exchange for H1 and H2. Following the suggestion in Section 2.2.3, TAC of the HP-ADWC2 may be reduced by increasing the temperature of compressor inlet (reducing the compressor power).

As is evident in Fig. 14, Q_{LP} and Q_{CW} of the HP-ADWC2 scheme are 16.7 kW and 705.00 kW. In addition, 3,167.22 kW can be recovered by observation of the heat recovery zone. On the basis of the presented analysis, the HP-ADWC2 configuration can save much more energy compared to the ADWC-FP configuration. However, a larger compressor power is needed to improve the energy quality. As such, a further energy-saving configuration should be proposed to effectively reduce the compressor power via the installation of a gas preheater.

3.2.3. Adding a gas preheater to the HP-ADWC (GP-HP-ADWC)

From Fig. 13, the temperature of the recompressed stream by the compressor is high after heating the reboiler in the proposed HP-ADWC2 configuration, which causes the energy is wasted directly when this stream enters the cooler 3. Therefore, HP system improvement is happening in the HP-ADWC2 to reduce energy losses. A gas preheater before the compressor is installed in the HP-ADWC2 configuration (denoted as GP-HP-ADWC) to effectively reduce the energy consumption of the compressor, which is

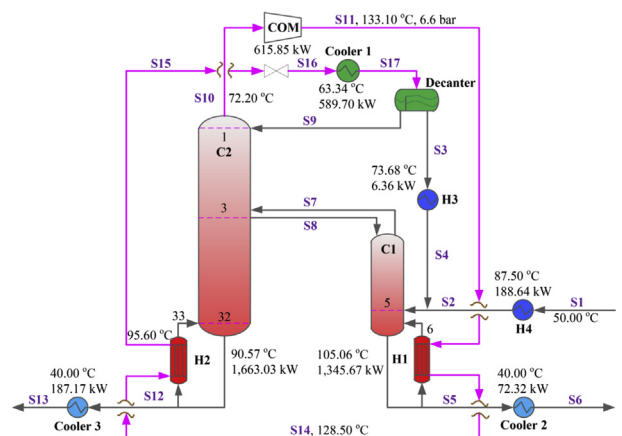


Fig. 13. Flowsheet of the proposed HP-ADWC2 configuration.

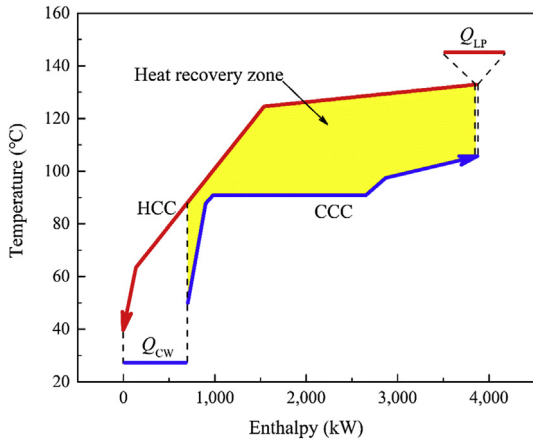


Fig. 14. T-H diagram of the HP-ADWC2 configuration.

suggested by section 2.2.3. Fig. 15 demonstrates the effect of temperature of a preheater on TAC, power of a compressor, the temperature of reboiler and preheater and compressor ratio. The results show that the temperature of the preheater is determined as 89.9 °C to provide adequate temperature difference (ΔT) for

reboiler H1.

Fig. 16 shows the GP-HP-ADWC configuration for separating the TBA/water system with CYH as an entrainer. A gas preheater before the compressor is added to heat the vapour stream from the C2. Preheated vapor stream is then fed to the compressor achieving a

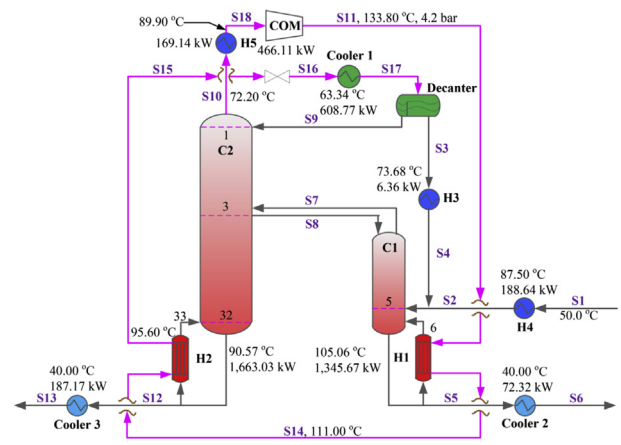


Fig. 16. Flowsheet of the GP-HP-ADWC configuration.

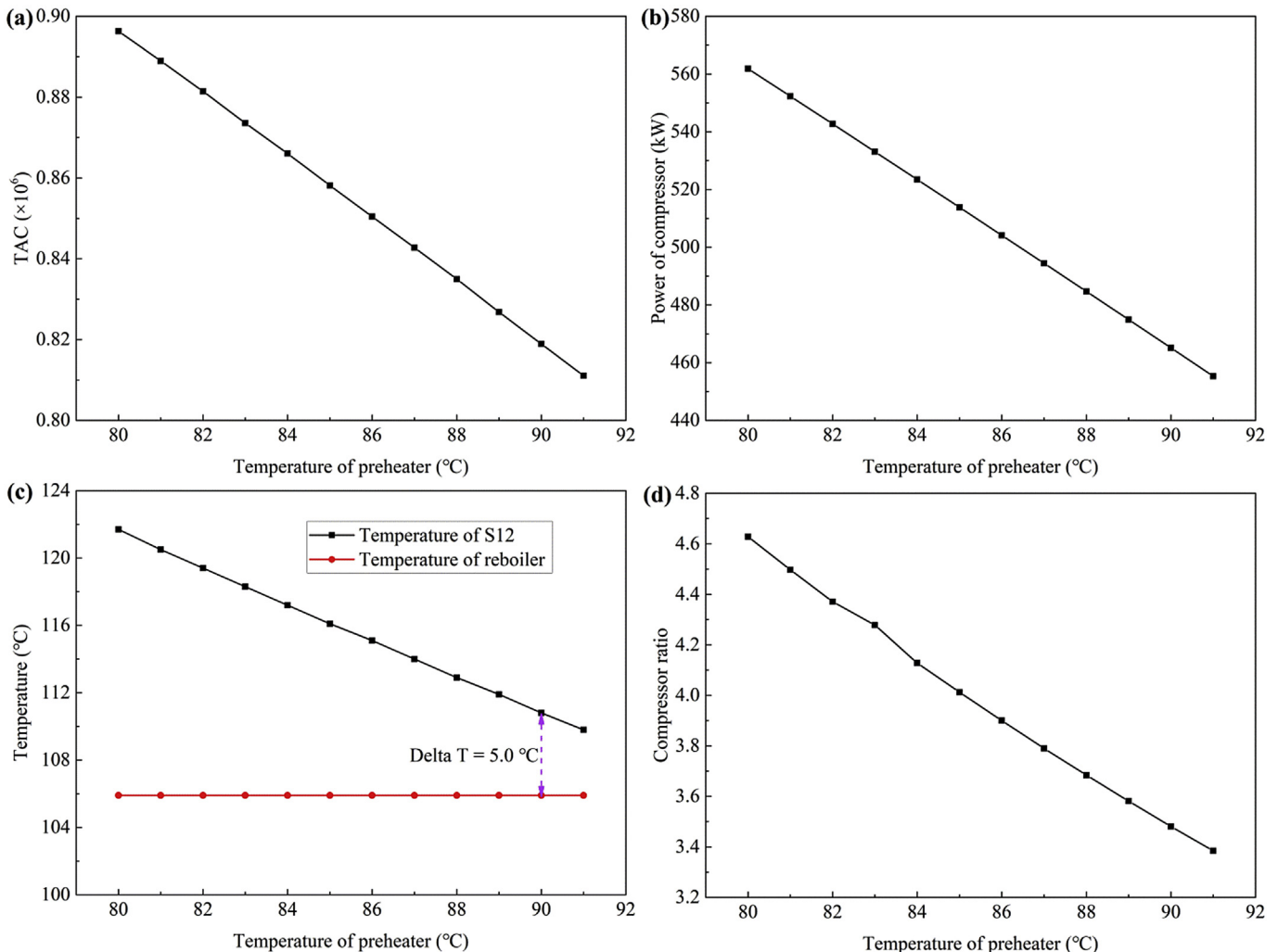


Fig. 15. Effect of temperature of a preheater on (a) TAC, (b) power of compressor, (c) temperature of reboiler and preheater and (d) compressor ratio.

higher temperature to provide heat duty for the two reboilers (H1 and H2).

As is depicted in Fig. 17, the cooling water demands of the GP-HP-ADWC design are 505.68 kW while no need additional steam in the GP-HP-ADWC configuration. Also 3,248.06 kW can be recovered by the observation of the heat recovery zone (i.e., yellow region).

The heat recovery and utility demands at each temperature of the GP-HP-ADWC configuration could be analyzed via another effective tool Grand Composite Curve (GCC). The minimum cooling water requirement Q_{CW} is the bottom residual of the GCC. Additionally, the yellow shaded area is heat recovery pockets where the heat can be circulated from hot streams to cold streams. Fig. 18 displays the GCC of the GP-HP-ADWC configuration. Obviously, there is no need to provide steam for the GP-HP-ADWC configuration. The minimum cooling requirements Q_{CW} in this configuration is 505.68 kW.

3.2.4. Heat integrated ADWC (HI-ADWC) configuration

A large amount of superheat energy is observed via the T-H and GCC diagrams of GP-HP-ADWC configuration when the HP technology is used. The Heat Integrated ADWC (HI-ADWC) is proposed based on the GP-HP-ADWC configuration to fully utilize the superheat energy. To design an energy-saving HI-ADWC configuration, the heat exchanger network (abbreviated as HEN) is an effective tool (Liu et al., 2018).

All detailed information of the hot and cold streams in the GP-HP-ADWC configuration are presented in Table 3. The minimum heat transfer temperature difference 5°C is determined to achieve the minimum TAC, which is obtained by the Aspen Energy Analyzer V8.4.

The optimal HEN of the GP-HP-ADWC configuration with eight heat exchangers is presented in Fig. 19. Among eight heat exchangers, heaters H1-H5 are self-heat exchangers; coolers 1–3 are coolers by using cooling water. The heating demand in the HEN is not needed while the cooling duty of only 505.68 kW is needed.

The final configuration, combined with the optimal HEN, is illustrated in Fig. 20. In this work, the electric power of 466.44 kW is needed to achieve the self-heating. The reboilers H1 and H2 are heated by the compressed streams S11 and S14. Additionally, the sensible heat of the streams S19 and S21 can be used to provide the heat duty of H5 and H4. The stream S3 is heated by the stream S5 (i.e., heat exchanger H3). Finally, cooling water is used in coolers 1–3 to cool the S16, S23, and S12 streams.

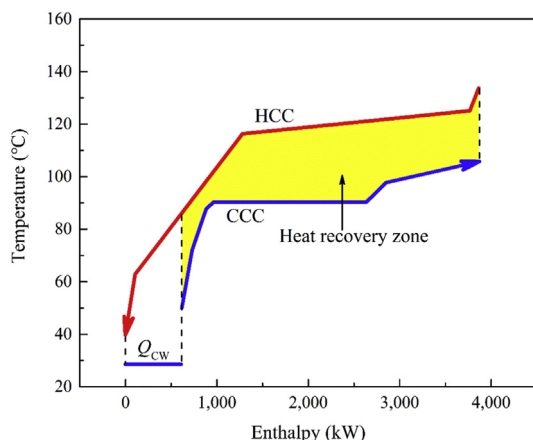


Fig. 17. T-H diagram of the GP-HP-ADWC configuration.

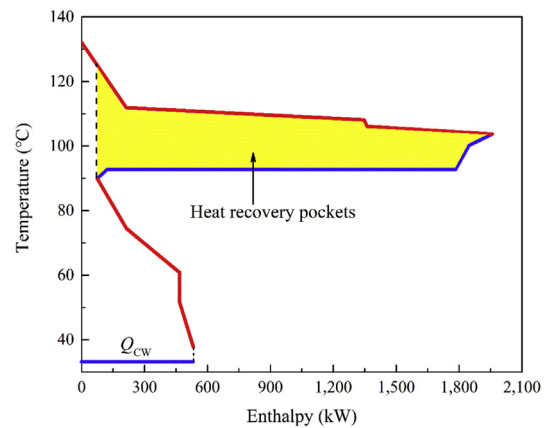


Fig. 18. Grand Composition Curve for the GP-HP-ADWC configuration.

Table 3

Thermodynamic data for hot and cold streams in the GP-HP-ADWC configuration as calculated by Aspen Plus.

Stream	Stream type	T_{inlet} ($^\circ\text{C}$)	T_{outlet} ($^\circ\text{C}$)	Heat duty (kW)
To H1@C1_To_S5	Cold	87.8	105.9	1,345.67
To H2@C2_To_S12	Cold	90.5	90.6	1,663.03
S10_To_S18	Cold	72.2	89.9	169.14
S1_To_S2	Cold	50.0	87.5	188.64
S3_To_S4	Cold	67.4	73.7	6.36
S11_To_S17	Hot	133.8	63.3	3,618.88
S5_To_S6	Hot	105.9	40.0	72.32
S12_To_S13	Hot	90.6	40.0	187.17

3.3. Performance evaluations

3.3.1. Economic evaluation

The economic comparisons between the four proposed designs and the two existing configurations are summarized in Table A1 and Fig. 21. It is obvious that the capital cost of the HP assisted ADWC configurations (HP-ADWC1, HP-ADWC2, GP-HP-ADWC, and HI-ADWC) are higher than that of the ADWC configurations (ADWC and ADWC-FP) because the capital cost of the compressor is expensive. However, TAC involves energy and capital investments. The application of compressor makes full use of the latent and sensible heat of the compressed and product streams to provide the heat for reboiler and preheater, leading to reduce the operating cost of HP assisted ADWC configurations. Compared with the existing HP-ADWC1 design, the intensified HI-ADWC configuration can save 56.51% of TOC. Compared with the existing HP-ADWC1 scheme, TAC of the HI-ADWC configuration can save 32.91% with ten years payback period.

In addition, the total capital cost of the extractive distillation by Lo and Chien (2017) is 804,300 US\$, and the re-calculation total operating cost is 787,000 US\$. The total annual cost is 867,400 US\$ with ten years payback period, which is far higher than the 662,400 US\$ of the proposed HI-ADWC configuration.

Table A2 gives the comparison of the TNRs of the existing and proposed designs. TNRs of tert-butanol dehydration process are 14,607,700 US\$, 15,042,600 US\$, 14,595,500 US\$, 15,083,600 US\$, 15,236,600 US\$, and 15,362,900 US\$ for ADWC, HP-ADWC1, ADWC-FP, HP-ADWC2, GP-HP-ADWC, and HI-ADWC configurations. TNR of the HI-ADWC configuration is 2.13% and 5.17% higher compared to the existing ADWC and HP-ADWC1 configurations.

3.3.2. Environmental evaluation

The CO_2 emissions of the ADWC, HP-ADWC1, ADWC-FP, HP-

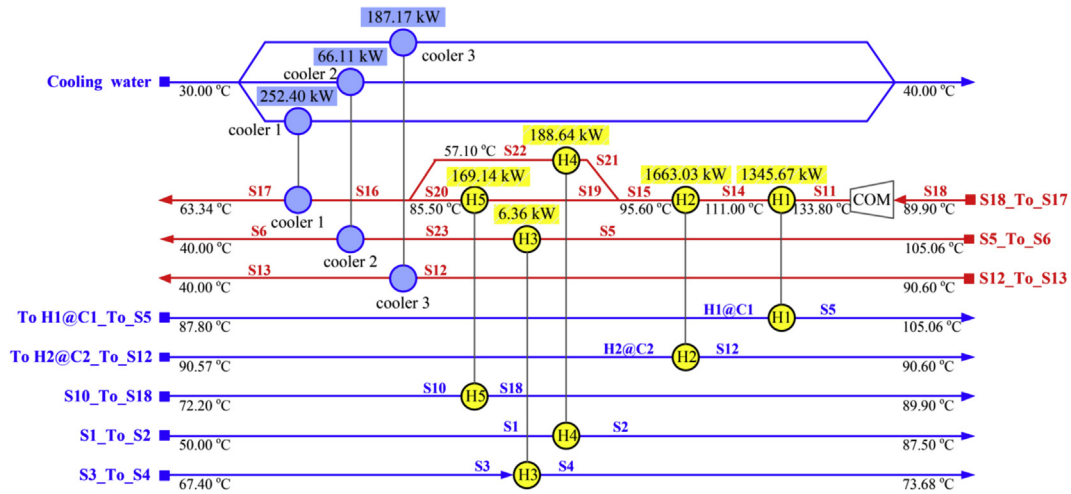


Fig. 19. Heat exchanger network for the HI-ADWC configuration.

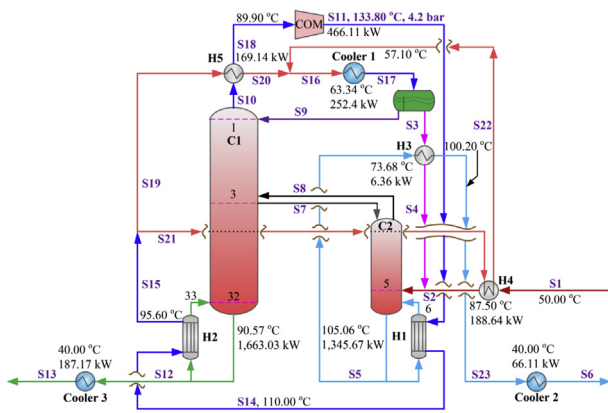


Fig. 20. Flowsheet of the proposed sustainable HI-ADWC configuration.

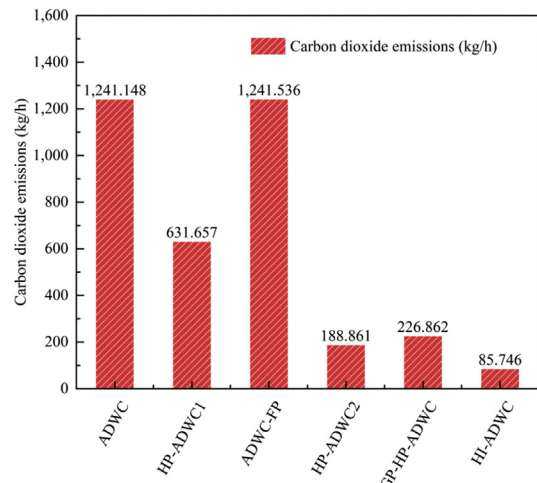


Fig. 22. Environmental comparisons of ADWC, HP-ADWC1, ADWC-FP, HP-ADWC2, GP-HP-ADWC and HI-ADWC configurations.

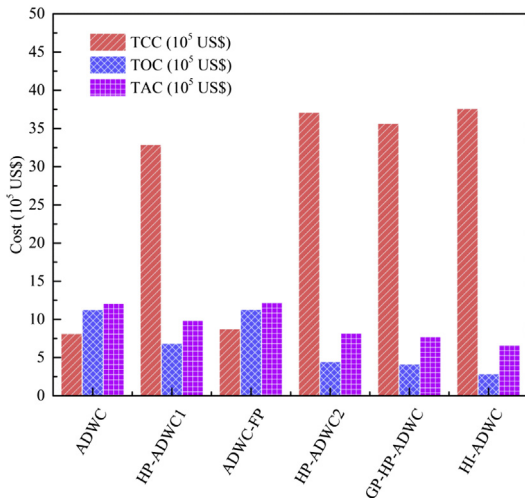


Fig. 21. Economic comparisons of ADWC, HP-ADWC1, ADWC-FP, HP-ADWC2, GP-HP-ADWC and HI-ADWC configurations.

ADWC2, GP-HP-ADWC and HI-ADWC configurations are 1,241.148 kg/h, 631.657 kg/h, 1,241.536 kg/h, 188.861 kg/h, 226.862 kg/h and 85.746 kg/h (see Fig. 22 and Table A3). Compared

with the existing HP-ADWC1 configuration, the CO₂ emissions of the proposed HP-ADWC2, GP-HP-ADWC and HI-ADWC configurations are reduced by 70.10%, 64.08% and 86.43%. The proposed intensified HI-ADWC configuration shows advantages in the reduction of CO₂ emissions.

3.3.3. Thermodynamic efficiency evaluation

The exergy loss of the existing and four proposed configurations are illustrated in Fig. 23 and Table A4. It indicates that the exergy loss of the existing configurations and four proposed configurations are 824.684 kW, 501.023 kW, 851.013 kW, 486.566 kW, 421.036 kW and 317.055 kW. Compared with the existing HP-ADWC1 configuration, the exergy loss of the HI-ADWC configuration is reduced by 36.72%.

In summary, the proposed HI-ADWC configuration is demonstrated to be more attractive in green and sustainable from the comparison of economic, thermodynamic, and environmental performances.

4. Conclusion

A novel green and sustainable Heat Integrated azeotropic

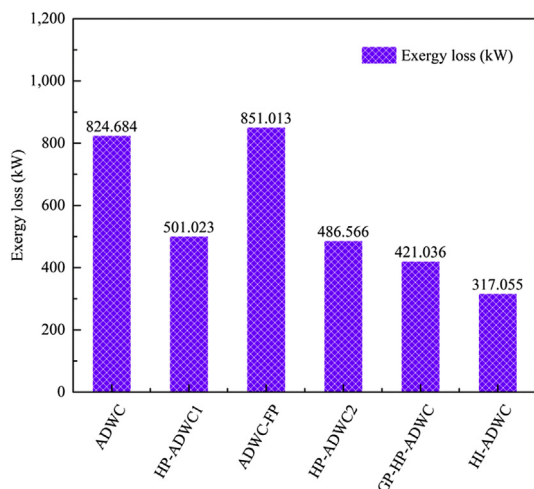


Fig. 23. Exergy loss comparisons of the existing and proposed configurations.

dividing wall column (HI-ADWC) configuration for separating azeotropic mixtures tert-butanol/water is proposed to achieve the performance of energy-saving, reduction of CO₂ emissions and enhancing of thermodynamic efficiency. The temperature-enthalpy and Grand Composite Curve diagrams are used to analyze the energy consumption of the proposed configurations. The heat exchange network is utilized to design the optimal heat matching of the HI-ADWC configuration. ADWC-FP, HP-ADWC2 and GP-HP-ADWC configurations are also designed to compare the economic, environmental and thermodynamic performances. The results demonstrate that total energy investment of the HI-ADWC configuration can be reduced by 56.51% compared with the HP-ADWC1 configuration. However, the total capital investment of the HI-ADWC configuration is increased with the compressor is installed. The HI-ADWC configuration can save 32.91% of total annual cost compared with the HP-ADWC1 scheme when the payback period is set as ten-year. The net revenue of the HI-ADWC configuration can improve 320,300 US\$ compared with the existing HP-ADWC1 configuration. The exergy loss of the proposed configuration is reduced by 36.72% compared with the existing HP-ADWC1 configuration by Luyben (2016). As a consequence, the proposed HI-ADWC configuration show promising not only on economic but also significantly improves thermodynamic efficiency, thereby achieving the performances of sustainable development and cleaner production.

There have three constraints that need to be considered when applying the proposed HI-ADWC configuration. Firstly, the temperature difference between the condenser and reboiler should be lower than 30 °C or COP of the column exceeds 10. Secondly, the difference in heat duty between reboiler and condenser should be small enough. Thirdly, it should be the case that the amount of waste heat is not fully utilized.

Once the above constraints are met, the proposed method for the HI-ADWC configuration could be widely extended to other processes such as azeotropic, reactive, and extractive dividing wall column to effectively utilize the heat duty of condenser achieving a reduction in TAC and sustainable development. The results of the analysis revealed that the CO₂ emissions of the proposed HI-ADWC configuration can reduce 86.43% compared with the existing HP-ADWC1 configuration.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jclepro.2019.06.224>.

Notes

The authors declare no competing financial interest.

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