



Synergy of electrification and energy efficiency improvement via vapor recompression heat pump and heat exchanger network to achieve decarbonization of extractive distillation

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ARTICLE INFO

Keywords:

Carbon neutrality
Electrification
Renewable energy sources
Vapor recompression heat pump
Extractive distillation

ABSTRACT

Considering ongoing energy transition and zero-carbon electricity, distillation processes as end-user sector need to rethink energy use, and eventually substitutes fossil fuel sources by renewable energy sources. Hence, in this article, we design several ensemble configurations for extractive dividing wall column (EDWC) as wide-boiling systems to investigate the role of energy efficiency improvement and electrification based on renewable energy sources in the decarbonization of distillation processes. Vapor recompression heat pumps play a dual role to achieve decarbonization of distillation process via efficiency improvement and electrification. The intermediate heating methods (i.e., intermediate reboiler, IR and feed evaporator, FPH) can reduce payback times of heat pump via reducing temperature quality of heat source. Heat exchanger network can comprehensively and effectively recovery waste energy to achieve energy efficiency improvement. To achieve complete decarbonization of distillation process, a novel multistage heat pump is proposed by combination of heat exchange network and intermediate heating methods (EDWC-MHP-FPH-IR-HEN). The economic assessment shows the payback period of EDWC-MHP-FPH-IR-HEN is 4.53 years and compared with original EDWC, it achieves only 4.83% TAC reduction and can achieve significant (44.97%)TAC reduction with five-year and ten-year payback period, respectively. This result demonstrates long pay period still impede the complete electrification of distillation and only in long running period, heat pumps can provide huge economic potential. To improve the economic viability of heat pump, technological innovation such as the decrease in the electricity price from renewable energy resources and policy such as CO₂ tax are explored using sensitivity analysis. The result shows that CO₂ tax is mainly driving force for electrification in distillation. This work can provide insights for the decarbonization of distillation processes via electrification.

1. Introduction

Currently, the industry development is mainly driven by the fossil fuel energy (power and heat). Compared with renewable energy sources, the life cycle of fossil-fuel (i.e., from mining to use for producing energy) can contribute to much more environmental pollution (such as air and water pollution), public health damage, ecological damage, and global warming emissions.

The fossil fuel energy accounts for most CO₂ emission [1]. One main approach to reduce CO₂ emission is to reduce the consumption intensity of fossil-fuel directly [2] via efficiency improvement. The electrification based on renewable energy sources is another important method to

reduce the CO₂ emission [2]. The thermal power can be replaced by green electricity produced by the renewable energy sources (RES) such as solar energy, wind energy. The potential of electrification to achieve carbon neutrality mainly lies in a future scenario where there is a pathway leading to zero-carbon electricity [3,4]. Actually, global renewable energy capacity additions in 2020 reflect unprecedented momentum for the energy transition [5,6].

According to IRENA [2], 37% and 32% carbon emissions reduction can be achieved by efficiency improvement, and electrification using RES, respectively. In the process of net-zero emissions by 2050, contribution of the electrification using renewable energy sources is predicted to be backbone force while contribution of efficiency improvement

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<https://doi.org/10.1016/j.seppur.2022.121065>

Received 3 March 2022; Received in revised form 10 April 2022; Accepted 11 April 2022

Available online 13 April 2022

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reduces from 37% to 21% [4]. By 2050, almost 90% of electricity will be produced by RES [7].

The distillation is the most important and commonly used in the chemical industry due to its simplicity and effectiveness [8], which accounts for more than 90% of separation process. In the foreseeable future, distillation processes still play a predominant role in the chemical process. However, the overall thermal efficiency of a conventional distillation is low, around 5–20% [9]. The distillation is estimated to be responsible for about 3% of global energy use and takes up over 40% of the energy used in the chemical industry [10]. Therefore, much energy consumed in distillation process undoubtedly contributes to large CO₂ emission. Efficiency improvement and electrification of distillation are two main methods to achieve cleaner production of distillation process.

The efficiency improvement of distillation has been investigated extensively in the Chemical Engineering subject. These methods mainly include dividing-wall columns (DWCs) [11–13], heat integration [14–16], heat pump (HP) [17]. Heat integration and heat pump can be used to recover rejected heat from condenser. The operating pressure can be adjusted to achieve enough drive force in heat integration [15,16]. If there is no enough driven force, heat pump improves the quality of heat from condenser and provide enough driven force through adding work of compressor.

Recently, many researchers [18–21] have investigated the application of heat pump in narrow-boiling system extensively and the results prove the attractive performances in energy saving. However, heat pumps also mainly suffer from long payback times due to the additional expensive compressors. Especially for wide-boiling mixtures, heat pump is economically unfeasible for commercialization. The integration of intermediate heating methods (i.e., intermediate reboiler and feed evaporator) is used to address this problem considering intermediate reboiler and feed evaporator need lower quality of steam. Several researches [22–26] have investigated the integration of intermediate heating methods and heat pump, and prove the effectiveness of this method in the wide-boiling mixtures system. Their computation results show that the payback period can be reduced significantly.

The electrification of chemical process is drawing much attention in the industry and academia, which can provide huge potential benefits for CO₂ reduction in the chemical industry [3,27–32]. The methods of the electrification in the chemical process can be roughly divided into two types: direct electrification and indirect electrification [3]. The direct electrification transfers power to heat or use mechanical work directly in chemical process [27]. The indirect electrification produces the alternative feedstock and fuels via electricity [30]. However, indirect electrification is hindered by economically unfeasible for commercialization and the availability of proven technology. In addition, indirect electrification cannot be used for new construction and renovation distillation since in general, reaction and synthesis are not involved in the distillation.

The main function of direct electrification is to convert power to heat since heat is widely used in the chemical process and used almost entirely in the distillation. However, the direct electrification for heating process by simply replacing the heat with electricity is inefficient [3]. The heat source used in distillation via direct electric heat method is unlikely, but may be steam from electric heat method instead of combustion of fossil fuel [8]. However, the steam system used for distillation need be redesigned and make huge change while the heat pump requires minimum modification to match current industrial processes. In addition, the required energy consumption of electrode boilers is more than that of heat pumps if the temperature lifts provided by heat pump don't exceed critical value [27]. Therefore, heat pump is a promising method for the electrification of distillation based on RES, especially suitable for already built distillation column.

Heat pumps have been popular for decades and widely used in many sectors such as chemical process, heating sector. The integration of heat pump with distillation is proved to be an effective method to improve energy efficiency, which have been discussed and reviewed previously.

In recent years, heat pumps become very important and draw much attention due to their significant potential to reduce emissions as the share of renewables in the energy mix increases [33]. An insightful review about heat pump and its key role in the decarbonization of the heating sector is provided by Gaur et al. [33]. In summary, integration of heat pump with renewable energy sources can achieve significant potential in decarbonization of energy-intensive sectors.

From the analysis of previous literature, the importance of the electrification based on renewable energy sources in chemical industry have been demonstrated. Heat pumps play a dual role to achieve carbon neutrality of chemical process, that is, energy saving and electrification, which can accelerate its application to achieve decarbonization in chemical industry. However, very few studies investigate the role of heat pump in the emission reduction from efficiency improvement and electrification perspective simultaneously. Considering ongoing energy transition and foreseeable future for zero-carbon electricity, distillation as end-use sectors should look for opportunity in electrification as end-use sectors. Therefore, the main purpose of this paper is to investigate the dual role of heat pump to achieve carbon neutrality of distillation process from electrification based on renewable energy sources and energy efficient perspective. The extractive dividing-wall column (EDWC) with medium boiling solvent features medium temperature differences with representative characteristics in the wide-boiling system and combination of this EDWC configuration and heat pump hasn't been reported in the open literature, therefore, this EDWC configuration is explored.

To fill these gaps, first we propose several ensemble configurations of extractive distillation for the separation of acetone and methanol as case study. Heat pump is used to recover the latent heat from condenser. Intermediate reboiler and feed evaporator are used to reduce the quality of heat resource. Heat exchanger network is used to achieve the optimal heat matching in the ensemble configurations of extractive distillation. Key performance indicators (KPIs) (i.e., TAC, CO₂ emissions and exergy loss) are used to assess the proposed ensemble configurations of extractive distillation. Then, from electrification perspective, we use the sensitivity analysis to investigate the price of RES and carbon price (carbon tax) on the economic performance of electrification in distillation based on credible prediction report from the world's leading energy authority (i.e., IRENA and IEA). We consider the different levels of economic development of economics since there is no one-size-fits-all approach for electrification in distillation. This work can provide insights for electrification in distillation and roadmaps to achieve clean production of distillation process.

2. Key performance indicators (KPIs)

In this article, economic assessment, thermodynamic efficiency evaluation and environmental impact are used to assess and compare the proposed configurations. TAC, CO₂ emissions and exergy loss are the corresponding key performance indicators (KPIs), respectively.

2.1. Economic assessment

The economic assessment methods [34–36] are widely used in the chemical process design. We use total annual cost to account for the economic performance. The total annual cost consists of two parts: operating cost (steam, cooling water and electricity) and capital cost. The parameters for capital cost are from Douglas's work [34]. To evaluate the effect of electrification based on RES, the electricity from fossil fuel and RES are considered. The prices of steam and electricity based on fossil fuel and water are from Turton et al. work [35]. The detailed information of method to estimate total annual cost is given in the [Supporting information](#).

2.2. Thermodynamic efficiency evaluation

Entropy generation and exergy analysis, based on the second law of thermodynamics, are the fundamental tools to analyze and improve the thermodynamic efficiency of a chemical process [37].

The work of separation minimum (W_{min}) is given.

$$W_{min} = n_D b_D + n_B b_B - n_F b_F \quad (1)$$

Where n_D , n_B and n_F are molar flowrates of distillate stream, bottom stream, and feed stream, respectively.

while b_D , b_B and b_F are corresponding molar availability also named molar exergy.

The loss work (LW) is given.

$$LW = n_F b_F + Q_R \left(1 - \frac{T_0}{T_R}\right) - (n_D b_D + n_B b_B) - Q_C \left(1 - \frac{T_0}{T_C}\right) \quad (2)$$

Where Q_R and Q_C are heat duty of heat and cold source, respectively while T_R and T_C are corresponding temperatures. T_0 is the surrounding temperature. In this article, the surrounding temperature and pressure are assumed as 25 °C and 1 atm, respectively.

Combine Eq. (1) and Eq. (2), the loss work can be expressed by the following equation.

$$LW = Q_R \left(1 - \frac{T_0}{T_R}\right) - Q_C \left(1 - \frac{T_0}{T_C}\right) - W_{min} \quad (3)$$

2.3. CO₂ emission

In this article, the effects of different energy resources (i.e., fossil fuel

and renewable energy sources) on global warmings are evaluated. The CO₂ emission based on fossil fuel is calculated in the Aspen Plus using Carbon Tracking [38]. Utility can be produced from the different ultimate fuel sources (such as natural gas or coal) with different CO₂ emission factor. In this article, the natural gas is used as ultimate fuel source for electricity and steam. The US-EPA-Rule-E9-5711 [39] is selected to be CO₂ emission factor data source. The CO₂ emission factor based on RES is assumed to be zero [3] since RES can be regarded as carbon-free energy source.

3. Process description

The design of the process studied in this paper from Wu et.al [40]. The selection of an appropriate thermodynamic model is important for accurate simulation. Three commonly used thermodynamic methods, i.e., UNIQUAC, NRTL, Wilson, are selected and their binary parameters are from built-in Aspen Plus databanks (V11). The comparison between vapor-liquid equilibrium data and simulation results are conducted to select proper thermodynamic model and the results are given in the Supporting Information. The comparison results demonstrate that UNIQUAC has the best performance, therefore, UNIQUAC chosen in the paper can predict reliable results.

This flowsheet is reproduced in Fig. 1 with minor modifications. The process design parameters are the same with that in the original flow-sheet except for the feed stage and vapor split. The operation pressure of EDWC is 1.0 atm and the tray pressure drop is 0.0068 bar. The feed composition is 50 mol% acetone 50 mol% methanol with 540 kmol/h feed flowrate. The solvent-to-feed ratio is 2.04 with water as entrainer. The purity specifications of acetone, methanol and water are 99.4 mol%

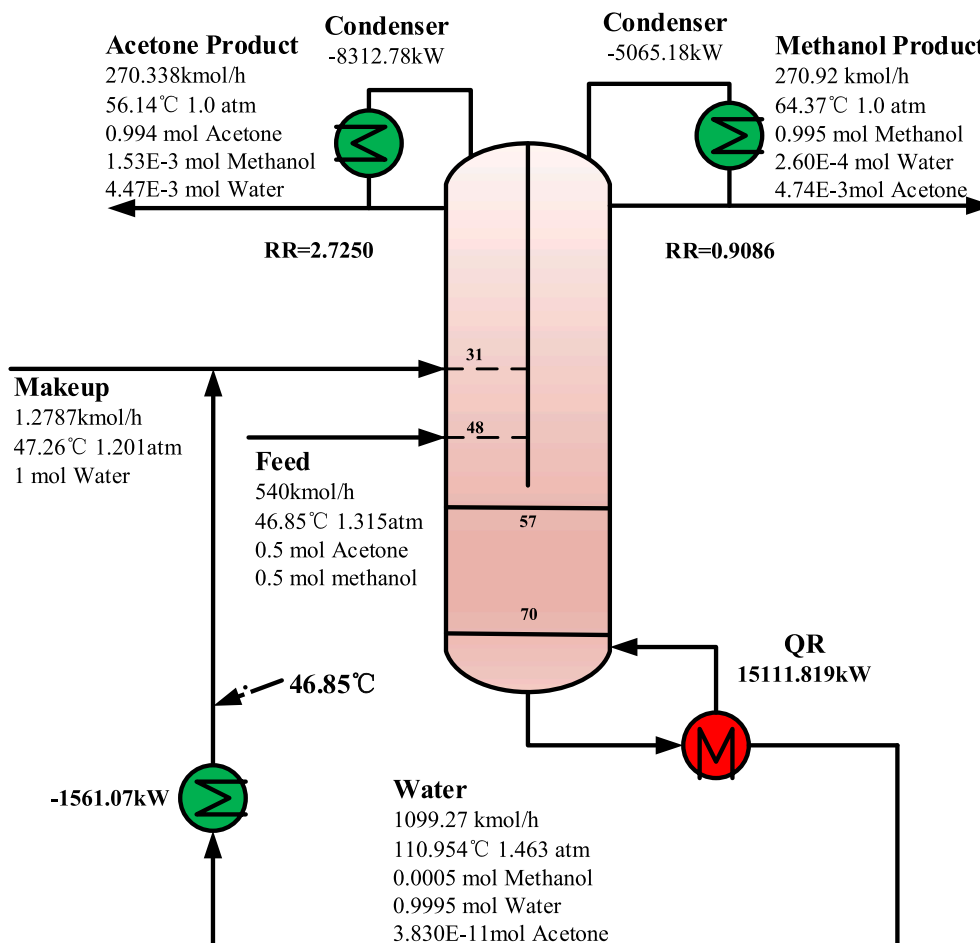


Fig. 1. The existing EDWC configuration for the separation of acetone and methanol.

and 99.5 mol%, 99.95 mol% respectively. The feed stage and vapor split are optimized to achieve the minimum reboiler duty using sensitivity analysis in the Aspen plus. The optimal vapor split ratio (feed section) is 0.654 and the corresponding reboiler duty is 15111.598 kW.

4. Heat pump assisted extractive dividing wall column configurations proposed

In this section, we propose several ensemble configurations of extractive distillation. The minimum heat transfer temperature difference is 5–20 K. The minimum heat transfer temperature difference for heat pump is selected to be 5 K, which reduces the compression ratio as much as possible. A gas preheater before the compressor is installed to avoid the liquefaction during the compression process and the superheat temperature is 3 K.

Pleşu et al. [41] proposed a simple criterion depending on coefficient of performance (denoted as COP) to effectively evaluate the feasibility of an HP system.

$$\text{COP} = \frac{Q}{W} = \frac{1}{\eta_c} = \frac{T_C}{T_R - T_C} \quad (4)$$

Where Q is the thermal duty, W is the required work of the compressor. η_c is the Carnot efficiency. The temperatures of reboiler and condenser are T_R (K) and T_C (K). According to COP, we can divide the distillation system into narrow-boiling system, medium wide-boiling system, and too wide-boiling system. In too wide-boiling system, the COP is lower than 5 and the application of HP is not considered. In medium wide-boiling system, the COP is between 5 and 10 and the detailed analysis should be conducted. In the narrow-boiling system, the COP is larger than 10 and the application of HP is much attractive.

The temperatures of acetone/methanol product and bottom product

are 56.14, 64.37 and 110.95°C, respectively. The temperature differences between distillate and reboiler are 54.81°C and 46.58°C, respectively. The corresponding COPs [41] are 6.008 and 7.246, respectively, which indicate its economic performance should further be investigated.

For heat pump design, two important variables including vapor split ratio, compression ratio should be determined. First, vapor split strategy in heat pump is determined through checking the energy balance between condenser duty and required input heat. If the condenser duty is larger than required input heat, vapor split strategy is required, otherwise, total vapor from condenser (i.e., vapor split ratio is 1) is compressed. The vapor split ratio and compression ratio can be determined to meet two constraints, respectively. The required input heat is exactly equal to the heat duty provided by heat pump, which is met by adjusted by vapor split ratio. The heat transfer temperature difference for heat pump is met by adjusting the compressor ratio. As for intermediate reboiler, location and the flowrate extracted from EDWC need to be determined. The flowrate of stream extracted from EDWC is limited by liquid flowrate from upper stage of location of intermediate reboiler and a certain margin should be set. In this article, 90% of limited value is set to be the flowrate extracted from EDWC.

4.1. Double heat pump assisted extractive dividing wall column (EDWC-DHP)

The double heat pump assisted extractive dividing wall column configuration (EDWC-DHP) for the separation of acetone and methanol is proposed and shown in the Fig. 2. In the EDWC process, there are two condensers. Therefore, both of two vapor streams are compressed to provide required heat duty for bottom reboiler.

Compression ratios of HP from acetone and methanol vapors are 5.487 and 5.665, respectively. The powers of two compressors are

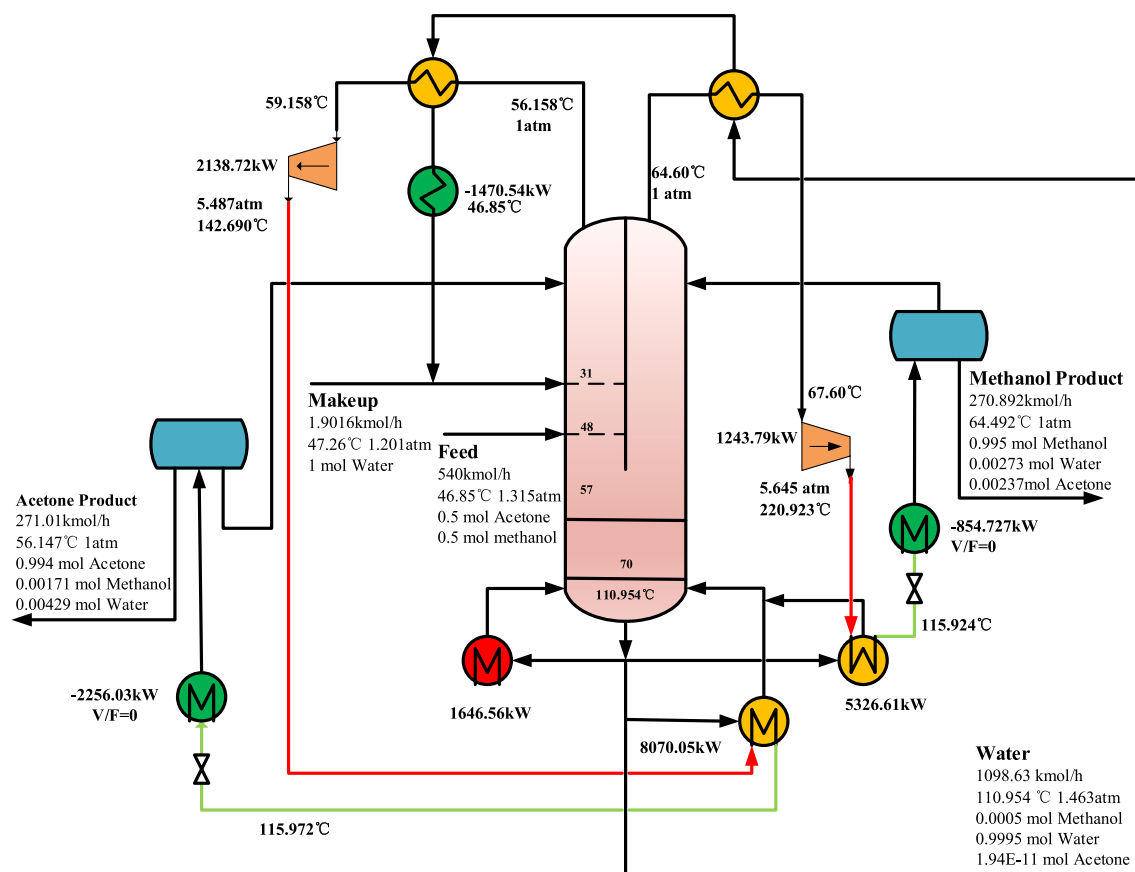


Fig. 2. The EDWC-DHP configuration and corresponding flowsheet for separation of acetone and methanol.

2138.72 kW and 1243.79 kW, which provide 8070.05 kW and 5326.61 kW heat duties, respectively. The ratios between heat duty provided via HP and electricity are 3.77 and 4.28, respectively. The additional heat duties (1646.65 kW) are supplied by the external low-pressure (LP) steam in a steam-driven auxiliary reboiler.

4.2. EDWC-HP coupling intermediate reboiler (EDWC-HP-IR)

The heat pump assisted extractive dividing wall column configuration integrating intermediate reboiler is given in the Fig. 3. Intermediate reboiler can reduce the heat quality of heat source since the tray temperature in the middle location is lower than that of bottom reboiler. Therefore, the required compression ratio can be reduced. Since each of two vapor streams can be compressed to provide heat duty for intermediate reboiler, two configurations of heat pump assisted E-DWC integrating intermediate reboiler (called EDWC-HP-IR and EDWC-HP-IR1) are proposed and shown in the Fig. 3.

Compression ratios of heat pumps in the right and left section of Fig. 3, are 3.364 and 2.739, respectively. The powers of two compressors are 1524.24 kW and 687.944 kW, which provide 8440.08 kW and 5277.31 kW heat duties, respectively. The ratios between heat duty provided via HP and electricity are 5.537 and 7.705, respectively. Since heat duties provided the compressor cannot provide enough heat duties required for reboiler. The additional heat duties supplied by the external low-pressure (LP) steam in a steam-driven auxiliary reboiler are 6808.69 kW and 9854.45 kW, respectively.

4.3. EDWC-HP coupling feed evaporator (EDWC-HP-FPH)

In this section, feed evaporator is used to reduce required compression ratio since feed evaporator requires lower quality of heat source than intermediate reboiler. The EDWC-HP-FPH configuration and flowsheet for separation of acetone and methanol are given in the Fig. 4.

The compression ratio is 1.579 and powers of compressor is 225.892 kW, which provide 3862.28 kW heat duties. The ratio between heat duty provided via HP and electricity is 15.093. The additional heat duties supplied by the external low-pressure (LP) steam in a steam-driven auxiliary reboiler are 10937.932 kW.

4.4. EDWC-HP coupling intermediate reboiler and feed evaporator (EDWC-HP-FPH-IR)

In this section, feed evaporator and intermediate reboiler are used simultaneously to improve the thermal efficiency of the process. The reduction of reboiler duty via heat pump assisted feed evaporator is limited by the flowrate of flowrate and the intermediate reboiler is further used to reduce the reboiler duty. The EDWC-HP-FPH-IR configuration and flowsheet for the separation of acetone and methanol are given in the Fig. 5.

The compression ratios between condenser and feed evaporator and intermediate reboiler are 1.579 and 3.360. The corresponding powers of compressors are 257.878 kW and 910.595 kW, respectively, which provide 3862.27 kW and 5641.55 kW heat duties, respectively. The ratios between heat duty provided via HP and electricity are 14.977 and 6.195. The additional heat duties supplied by the external low-pressure (LP) steam in a steam-driven auxiliary reboiler are 5536.80 kW.

4.5. Multistage heat pump assisted EDWC coupling intermediate reboiler/feed evaporator via heat exchanger network (EDWC-MHP-FPH-IR-HEN)

In this configuration, multistage-heat pump and heat exchanger network are applied to EDWC-HP-FPH-IR to achieve self-heat recuperation and the flowsheet is shown in the Fig. 6. The compression ratios in term of feed reboiler, intermediate reboiler and bottom reboiler are 1.579, 3.360 and 3.458, respectively while corresponding powers of compressors are 530.29 kW, 910.577 kW and 1171.27 kW, respectively. As for multistage HP and HP for intermediate reboiler, the ratios between heat duty provided via HP and electricity are 4.477 and 6.195, respectively. The heat exchanger network is shown in the Fig. 7. The heating demand in the HEN is not needed while the cooling duty of 2283.679 kW is needed.

5. Results and discussion

In this section, the economic performance and thermodynamic efficiency are obtained and analyzed. In general, the expected payback time is less than 2–3 years and payback time up to 5 years can also be accepted by some companies when it comes to investments into their

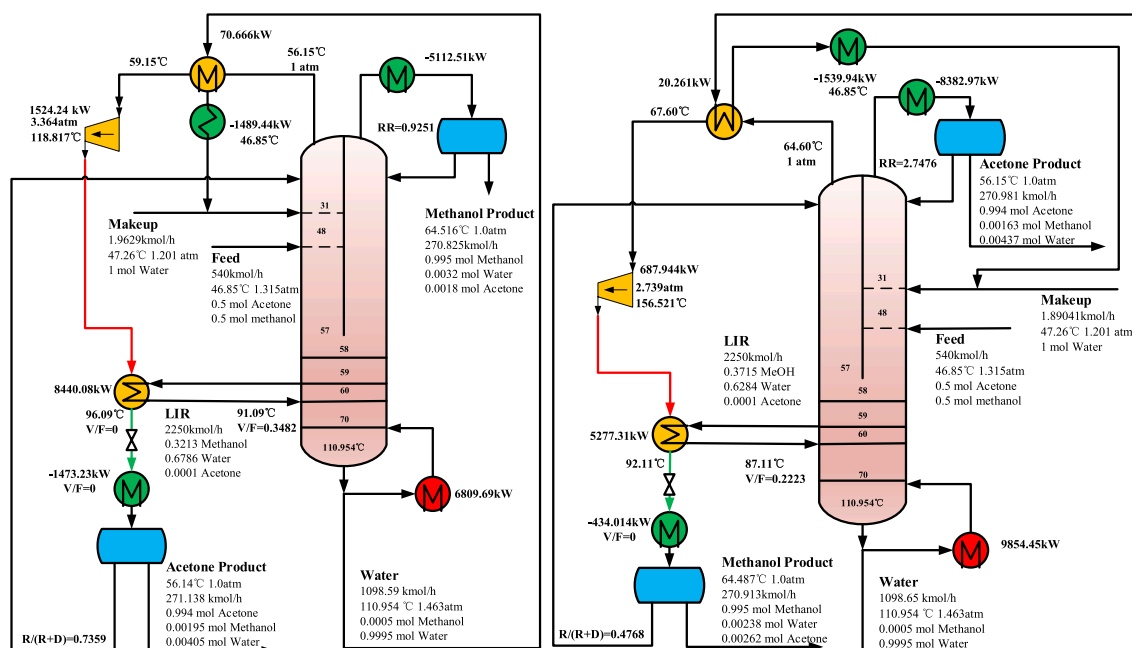


Fig. 3. The EDWC-HP-IR configuration and corresponding flowsheet for separation of acetone and methanol.

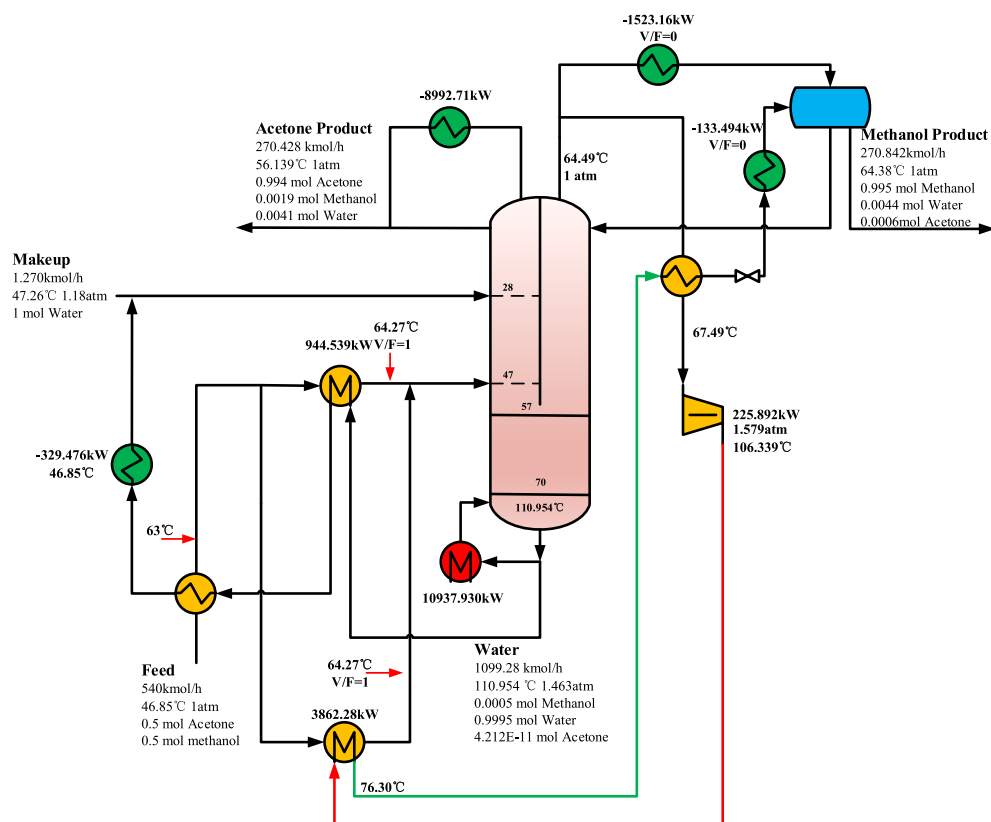


Fig. 4. The EDWC-HP-FPH configuration and flowsheet for the separation of acetone and methanol.

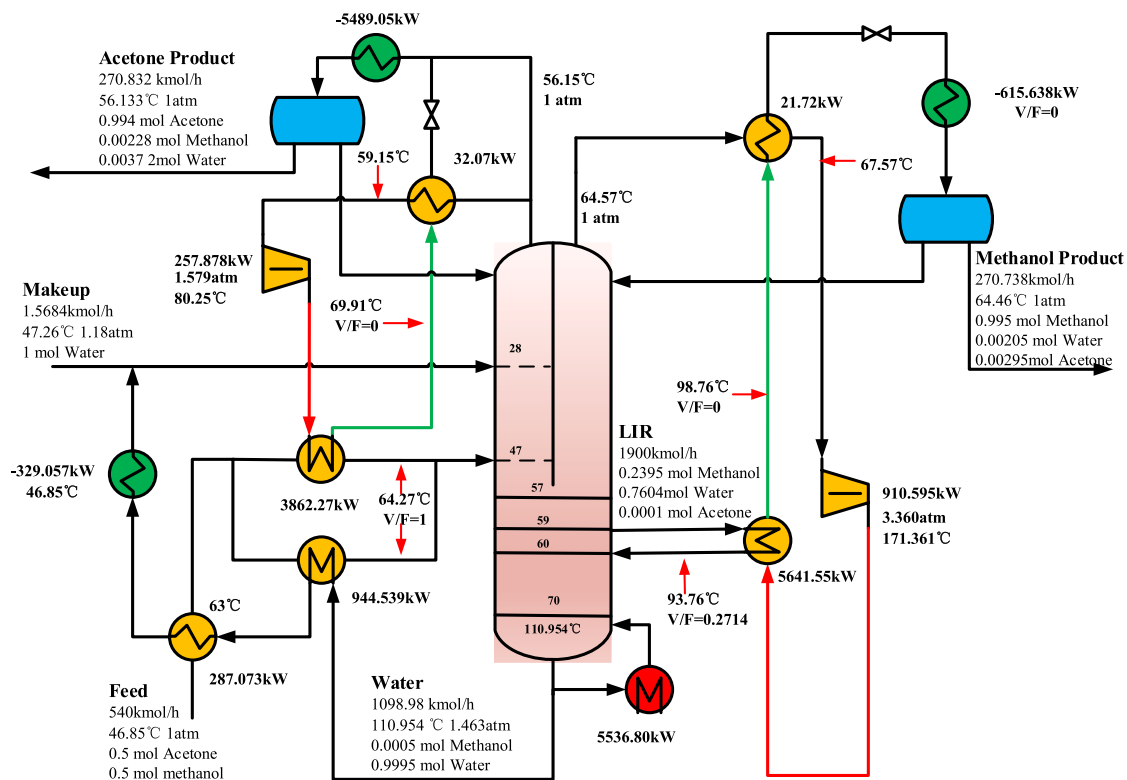


Fig. 5. The EDWC-HP-FPH-IR configuration for the separation of acetone and methanol.

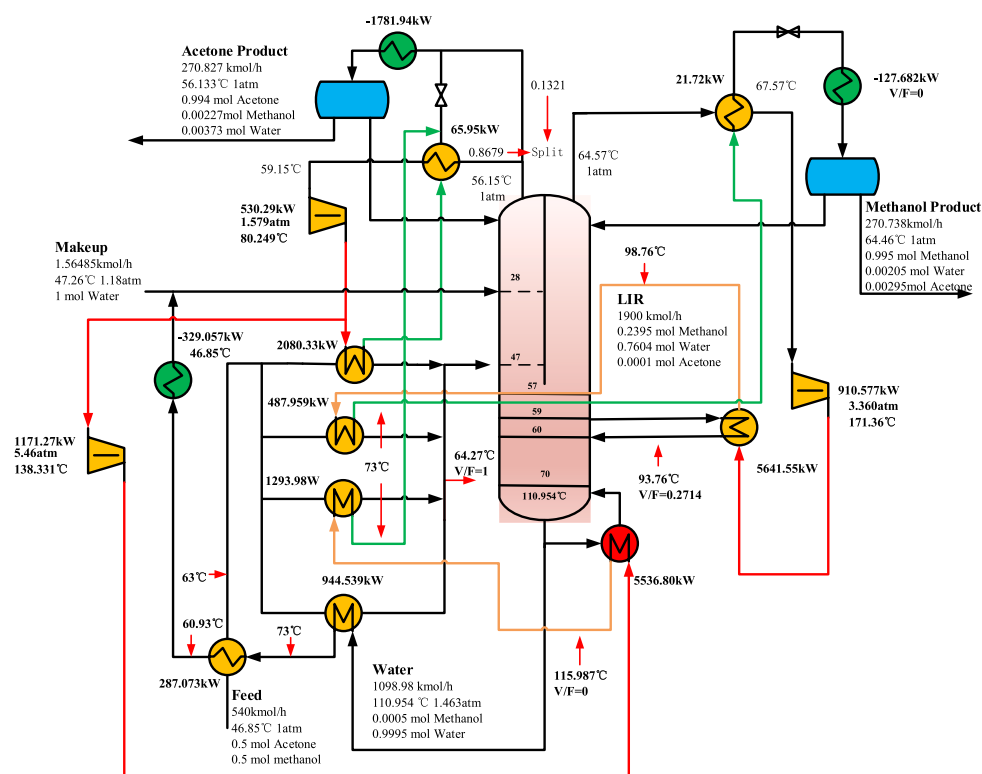


Fig. 6. The EDWC-MHP-FPH-IR-HEN configuration for the separation of acetone and methanol.

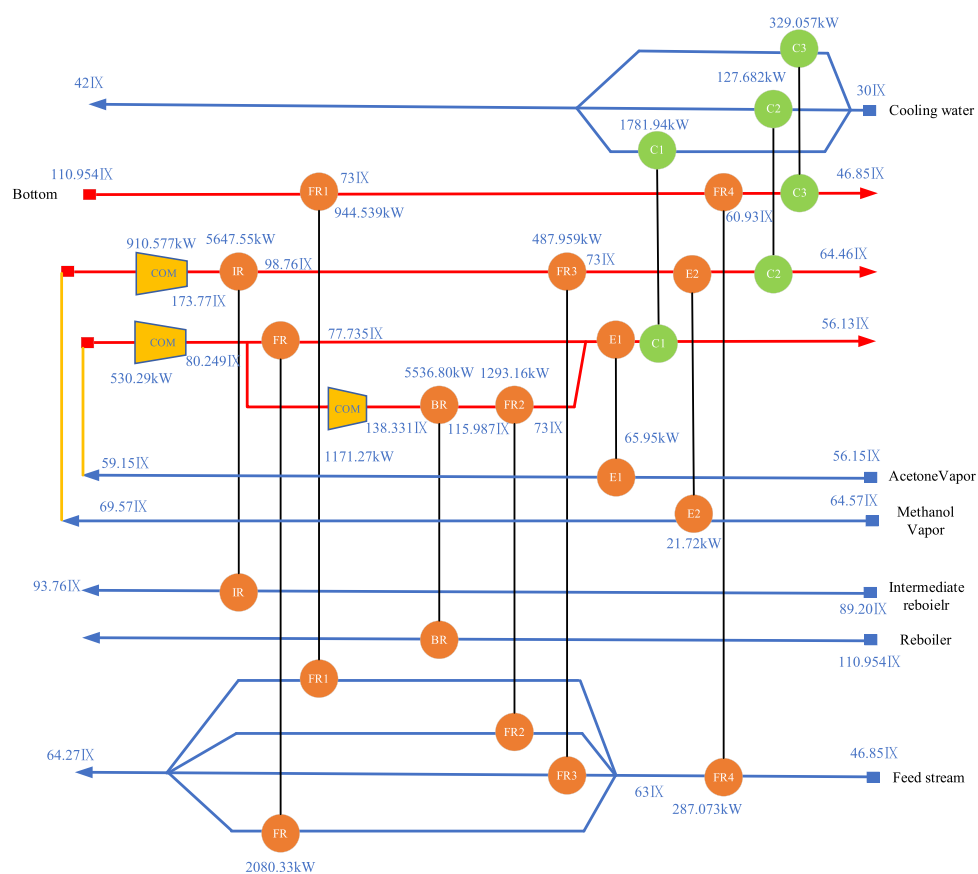


Fig. 7. The heat exchanger network of EDWC-MHP-FPH-IR-HEN.

Table 1

The KPIs of several EDWC configurations proposed for separation of acetone and methanol.

	EDWC	EDWC-DHP	EDWC-HP-IR	EDWC-HP-IR1	EDWC-HP-FPH	EDWC-HP-FPH-IR1	EDWC-MHP-FPH-IR1-HEN
Total reboiler duty (kW)	15111.82	1646.56	6809.69	9854.45	10937.93	5536.80	0
Total electric (kW)	–	3382.51	1524.24	687.944	229.13	1168.47	2612.16
Compressor capital cost 10 ³ \$/y	–	9910.85	4171.01	2172.36	955.99	4063.93	8938.51
Capital cost -10 ³ \$/y	4434.58	16108.30	9366.42	7125.34	5854.07	9463.73	14820.54
Exergy Loss	4111.18	3677.60	3307.46	3337.02	3199.88	2659.12	2493.97
TAC-10 ³ \$/y (5 years)	4491.58	5353.55	4262.88	4121.20	3892.91	3799.36	4274.46
TAC-10 ³ \$/y (10 years)	4048.13	3701.45	3326.24	3408.66	3309.14	2852.98	2792.40
Energy cost-10 ³ \$/y	3604.67	2090.62	2389.60	2696.13	2723.73	1906.61	1310.35
Payback time	0	7.71	4.06	2.96	1.61	2.96	4.53
CO ₂ Emission (kg/h) based on fossil-fuel	3577.12	1563.16	2140.69	2571.30	2667.48	1626.51	906.167
CO ₂ Emission (kg/h) based on RES	3577.12	389.76	1611.93	2332.66	2589.13	1310.62	0.00
Capital saving	–	263.24%	111.21%	60.68%	32.01%	113.41%	234.20%
Energy saving	–	–42.00%	–33.71%	–25.20%	–24.44%	–47.11%	–63.65%
TAC reduction (5 years)	–	19.19%	–5.09%	–8.25%	–13.33%	–15.41%	–4.83%
TAC reduction (10 years)	–	–12.42%	–25.85%	–22.90%	–26.46%	–42.80%	–44.97%
Exergy Loss reduction	–	–10.55%	–19.55%	–18.83%	–22.17%	–35.32%	–39.34%
CO ₂ Emission reduction based on fossil-fuel	–	–56.30%	–39.32%	–28.16%	–25.43%	–54.30%	–73.70%
CO ₂ Emission saving (kg/h) (Fossil-fuel via RES)	0	1173.4	528.76	238.64	78.35	315.89	906.167

energy infrastructure [17]. The detailed information is given in the Table 1.

5.1. Economic performance analysis

Compared with EDWC-DHP, the payback time of EDWC-HP-IR, EDWC-HP-IR1 and EDWC-HP-FPH are reduced significantly, which is less than 5 years. This result show that intermediate reboiler and feed evaporator are beneficial for electrification in the wide-boiling system in term of economic performance. However, the electrification degree using feed evaporator is limited by the flowrate of feed stream while intermediate reboiler can provide more heat transfer capacity. Therefore, integration of feed evaporator and intermediate reboiler can be used to improve the electrification degree in distillation via heat pump. We also notice that this integration configuration has payback time of less than 3 years.

Although CO₂ emission intensity of steam (0.2367 kg CO₂/kW-h) is lower than that of electricity (0.3469 kg CO₂/kW-h) due to substantial energy losses involved in the electricity generation and transmission, heat pumps can produce severalfold heat energy than consumed electricity. Therefore, higher electrification degree in distillation can achieve more CO₂ emission reduction. If the RES is used as ultimate energy source, the advantages of complete electrification in distillation are more prominent, and CO₂ emission can be reduced to zero.

To achieve complete electrification in distillation, complete ensemble configuration called EDWC-MHP-FPH-IR-HEN is proposed and achieve the most CO₂ emission reduction. This configuration also has the best economic performance in term of energy saving, exergy loss and its payback period is also less than 5 years. Therefore, the complete electrification in distillation may be feasible and has commercial prospects in the wide-boiling system.

However, we can notice that this complete electrification configuration has only 4.83% TAC reduction in case of 5 payback period year. Referred to several open literature [42–44], heat pump can achieve above 10% TAC reduction in case of 5 payback period year compared with existing process in the normal-boiling system. As for complete electrification configuration, temperature lift provided by HP is large, which belongs to medium wide-boiling system, though multistage HP has been used in complete electrification configuration to improve the coefficient of performance (the ratios between heat duty provided via HP and electricity) of HP. Compressor capital cost in this complete electrification configuration significantly contributes to total capital cost. Therefore, only 4.83% TAC reduction can be achieved in this

complete electrification configuration. This complete electrification configuration can achieve significant TAC reduction with 44.97% in case long payback period with 10 years. This result demonstrate that heat pumps have huge economic potential in long running periods. However, in general, the expected payback time is less than 2–3 years and payback time up to 5 years can also be accepted by some companies. If 3 payback period year is used, only EDWC-HP-FPH with the lowest electrification level is economic. Therefore, the economic disadvantage still impedes the electrification process in the wide-boiling system. Fortunately, in case of 5 payback period year, EDWC-HP-FPH-IR1 configuration with the second most electrification level has the lowest TAC. In addition, technological innovation and policy may solve economic problem. Technological innovation can decrease the price of RES subsequently can improve economic performance of electrification process. Policy such as carbon tax can worsen the economy of non-electrification process and thereby highlight the economy of electrification process. This issue is discussed in the next section using sensitivity analysis.

5.2. Sensitivity analysis

The sensitivity analysis is used to investigate the price of RES and carbon price (carbon tax) on the economic performance of electrification in distillation.

According to “Renewable Power Generation Costs In 2020” [45] report by IRENA in 2021.6, the global weighted-average LCOE (the Levelized cost of electricity) and PPA (Power Purchase Agreement) /auction prices for renewable energy resources can be reduced unceasingly in the next few years. Especially for solar photovoltaic and onshore wind, their global weighted-average PPA/auction prices have been lower than that of the cheapest fossil-fuel-based electricity. The data also suggests that there is an increasing number of projects with very low electricity costs, at below USD 0.03/kWh. In summary, the prices of renewable energy resources are no longer a major obstacle to large-scale use of renewable energy.

Taxation has become an effective economic instrument to internalize environmental externalities due to its compulsory and law-based nature [46]. Carbon tax, as a part of current environmental taxation, attracts great attention in policy [46,47], which can boost the energy innovation by means of the tax revenue [47]. According to the report “Net Zero by 2050-A Roadmap for the Global Energy Sector” [48] published by IEA in 2021, the CO₂ price for electricity, industry and energy production are shown in the Table 2.

Table 2CO₂ prices for electricity, industry, and energy production in the NZE.

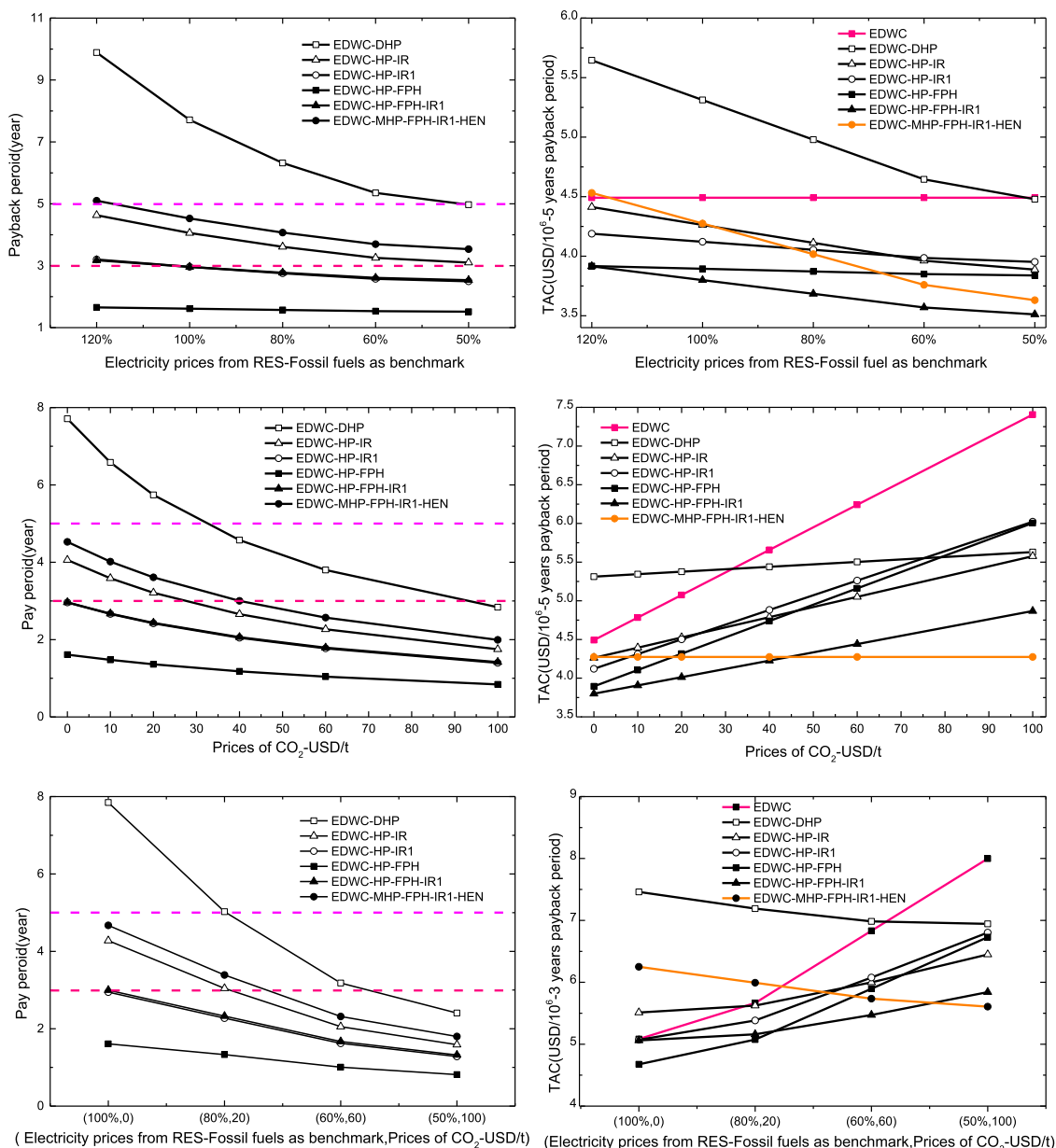
USD (2019) per tonne of CO ₂ price	2025	2030	2040	2050
Advanced economies	75	130	205	250
Selected emerging market and developing economies*	45	90	160	200
Other emerging market and developing economies	3	15	35	55

Countries with different levels of economic development has different CO₂ price. Advanced economies, other major economic country (i.e., China, Russia, Brazil, and South Africa) and other emerging market and developing economies have the highest, middle, and lowest CO₂ price, respectively. The sensitivity analysis results of price of RES and Prices of CO₂ are shown in the Fig. 8., respectively.

The results in the top figure in the Fig. 8. illustrate that EDWC-DHP, EDWC-IR and EDWC-MHP-FPH-IR1-HEN are more sensitive to the prices of green-electricity from RES than EDWC-IR1, EDWC-FPH and

EDWC-HP-FPH-IR1 in term of payback period and TAC. The reason is the former configurations use more electricity than the latter configurations. In case of 3 years payback period as short time, the complete electrification configuration (i.e., EDWC-MHP-FPH-IR1-HEN) is not uneconomical even though the electricity prices from RES can be reduced to very low price with 0.03\$/kW-h. In case of 5 years payback period as moderately long time, the complete electrification configuration is economic but not preferred among six configurations proposed. The analysis shows that the decrease in electricity prices can be beneficial for economic performance of complete electrification in distillation. However, its beneficial effect is limited.

The results in the middle figure in the Fig. 8. illustrate that the prices of CO₂ have the similar effect on payback period to the electricity prices from RES. However, as for TAC, EDWC-IR1, EDWC-AFPH, EDWC-IR and EDWC-HP-AFPH-IR1 are more sensitive to the prices of CO₂ than EDWC-MHP-FPH-IR1-HEN and EDWC-DHP since the latter configurations have higher electrification levels. The CO₂ tax can increase the costs of non-fully electrified configurations and their increase rates are

**Fig. 8.** The effect of price of RES and prices of CO₂ on economic performance of process using sensitivity analysis.

proportional to the product of the CO₂ price and non-electrical level. In case of 3 years payback period, the complete electrification configuration (i.e., EDWC-MHP-AFPH-IR1-HEN) is economical until the prices of CO₂ are more than 40USD/t. In case of 5 years payback period, the complete electrification configuration is preferred until the prices of CO₂ are more than about 50USD/t. The results in the bottom figure in the Fig. 8 illustrate that in case of 3 years payback period as short time, the complete electrification configuration will be preferred along with decreased electricity prices from RES and increased prices of CO₂.

The analysis show that CO₂ tax is the main driving force for electrification in distillation. This beneficial effect can be seen only in the advanced economies and some middle-income countries in the foreseeable future according to predicted CO₂ prices in the Table 2. Moreover, CO₂ tax will play a more and more important role to achieve complete electrification in distillation in the advanced economies and some middle-income countries by 2050. However, the complete electrification configuration (i.e., EDWC-MHP-AFPH-IR1-HEN) is uneconomical even though by 2040 in the other emerging market and developing economies. In a word, complete electrification in distillation is attractive for advanced economies and some middle-income countries and high electrification in distillation is attractive for other emerging market and developing economies.

6. Conclusion

In this article, we investigate the role of heat pump in the decarbonization distillation process from efficiency improvement and electrification perspective. We design several ensemble configurations for EDWC as wide-boiling system. Heat exchanger network can comprehensively and effectively recovery waste energy to achieve energy efficiency improvement. A novel multistage heat pump is proposed by combination of heat exchange network and intermediate heating methods to achieve complete decarbonization of distillation process. The technological innovation such as decrease in the electricity price from renewable energy resources and policy such as CO₂ tax are explored using sensitivity analysis. Several key findings are given below:

- 1) Although CO₂ emission intensity of electricity is larger than that of steam due to substantial energy losses involved in the electricity generation and transmission. Heat pump itself can reduce the CO₂ emission via efficiency improvement since heat pumps can produce severalfold heat energy than consumed electricity.
- 2) The heat pump between condenser and bottom reboiler in the wide-boiling system is economically infeasible. The intermediate heating methods can reduce the payback period of heat pump can be reduced significantly.
- 3) Economic performance of complete electrification has not enough competitiveness and is only superior to original EDWC process with 4.83% TAC reduction in case of five-years payback period although the payback period of complete electrification configuration can be reduced to 5 years. The complete electrification configuration can achieve significant TAC reduction with 44.97% in case long payback period with 10 years. This result demonstrate that heat pumps have huge economic potential in long running periods.
- 4) Technological innovation such as decrease in the electricity price from renewable energy resources and policy such as CO₂ tax can improves the economic viability of heat pump. CO₂ tax is the main driving force for electrification in distillation since the CO₂ tax increase the unit cost of steam used via policy-making.

CRedit authorship contribution statement

Jiaying Zhu: Conceptualization, Writing – original draft, Software, Visualization, Investigation. **Lijun Chen:** Writing – review & editing, Visualization. **Zixuan Liu:** Writing – review & editing, Visualization. **Lin**

Hao: Supervision, Writing – review & editing. **Hongyuan Wei:** Supervision, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Appendix A. Supplementary material

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.seppur.2022.121065>.

References

- [1] IEA, Global CO₂ emissions in 2019, in, 2020.
- [2] IRENA, Tracking SDG 7: the Energy Progress Report (2020), in, Paris, France, 2020.
- [3] C. Chen, Y. Lu, R. Banares-Alcantara, Direct and indirect electrification of chemical industry using methanol production as a case study, *Appl. Energy* 243 (2019) 71–90.
- [4] Z. Caineng, B. XIONG, X. Huaqing, D. ZHENG, G. Zhixin, W. Ying, L. JIANG, P. Songqi, W. Songtao, The role of new energy in carbon neutral, *Petroleum Exploration and Development*, 48 (2021) 480–491.
- [5] Irena, Renewable capacity statistics 2021 International Renewable Energy Agency (IRENA), in, Abu Dhabi (2021).
- [6] IEA, Renewables 2021, in, Paris, 2021.
- [7] S. Bouckaert, A.F. Pales, C. McGlade, U. Remme, B. Wanner, L. Varro, D. D'Ambrosio, T. Spencer, Net Zero by 2050: A Roadmap for the Global Energy Sector, (2021).
- [8] A.A. Kiss, R. Smith, Rethinking energy use in distillation processes for a more sustainable chemical industry, in: *Energy*, 203, 2020, p. 117788.
- [9] G. Koeijer, K. Signe, Minimizing Entropy Production Rate in Binary Tray Distillation, *Int. J. Thermodyn.* 3 (2000) 105–110.
- [10] A.A. Kiss, Advanced distillation technologies: design, control and applications, John Wiley & Sons, 2013.
- [11] M.A. Schultz, D.G. Stewart, J.M. Harris, S.P. Rosenblum, M.S. Shakur, Reduce costs with dividing-wall columns, *Chem. Eng. Prog.* 98 (2002) 64–71.
- [12] C. Jing, J. Zhu, L. Dang, H. Wei, Extractive Dividing-Wall Column Distillation with a Novel Control Structure Integrating Pressure Swing and Pressure Compensation, *Ind. Eng. Chem. Res.* 60 (2021) 1274–1289.
- [13] D. An, W. Cai, M. Xia, X. Zhang, F. Wang, Design and control of reactive dividing-wall column for the production of methyl acetate, *Chem. Eng. Process. Process Intensif.* 92 (2015) 45–60.
- [14] L. Xu, Y. Liu, W. Bai, Z. Tan, W. Xue, Design and control of energy-saving double side-stream extractive distillation for the benzene/isopropanol/water separation, in: *Energy*, 239, 2022, p. 121952.
- [15] A. Yang, S. Sun, T. Shi, D. Xu, J. Ren, W. Shen, Energy-efficient extractive pressure-swing distillation for separating binary minimum azeotropic mixture dimethyl carbonate and ethanol, in: *Sep. Purif. Technol.*, 229, 2019, p. 115817.
- [16] Z. Zhu, L. Wang, Y. Ma, W. Wang, Y. Wang, Separating an azeotropic mixture of toluene and ethanol via heat integration pressure swing distillation, *Comput. Chem. Eng.* 76 (2015) 137–149.
- [17] A.A. Kiss, C. Ferreira, Heat Pumps in Chemical Process Industry, *Heat Pumps in Chemical Process Industry* (2016).
- [18] N. Wang, Q. Ye, L. Chen, H. Zhang, J. Zhong, Improving the economy and energy efficiency of separating water/acetonitrile/isopropanol mixture via triple-column pressure-swing distillation with heat-pump technology, in: *Energy*, 215, 2021, p. 119126.
- [19] H. Xia, Q. Ye, S.Y. Feng, R. Li, X.M. Suo, A novel energy-saving pressure swing distillation process based on self-heat recuperation technology, *Energy* 141 (2017) 770–781.
- [20] A. Yang, S. Jin, W. Shen, P. Cui, L.L. Chien, J. Ren, Investigation of energy-saving azeotropic dividing wall column to achieve cleaner production via heat exchanger network and heat pump technique, *J. Cleaner Prod.* 234 (2019) 410–422.
- [21] R. Li, Q. Ye, X. Suo, X. Dai, H. Yu, S. Feng, H. Xia, Improving the Performance of Heat Pump-Assisted Azeotropic Dividing Wall Distillation, *Ind. Eng. Chem. Res.* 55 (2016) 6454–6464.
- [22] L. Xu, M. Li, X. Ge, X. Yuan, Numerical simulation of dividing wall column with vapor recompression located at side product stage, *Chem. Eng. Res. Des.* 120 (2017) 138–149.
- [23] A.K. Jana, A. Mane, Heat pump assisted reactive distillation: Wide boiling mixture, *AIChE J.* 57 (2011) 3233–3237.

- [24] V. Kumar, B. Kiran, A.K. Jana, A.N. Samanta, A novel multistage vapor recompression reactive distillation system with intermediate reboilers, *AIChE J.* 59 (2013) 761–771.
- [25] N.V.D. Long, L.Q. Minh, L.C. Nhen, M. Lee, A novel self-heat recuperative dividing wall column to maximize energy efficiency and column throughput in retrofitting and debottlenecking of a side stream column, *Appl. Energy* 159 (2015) 28–38.
- [26] J. Zhu, C. Jing, L. Hao, H. Wei, Inherent safer, eco-friendly and energy saving vapor recompression assisted extractive dividing-wall column process for the separation of minimum-boiling azeotrope, in: *Sep. Purif. Technol.*, 286, 2022, p. 120368.
- [27] H. Son, M. Kim, J.-K. Kim, Sustainable process integration of electrification technologies with industrial energy systems, in: *Energy*, 239, 2022, p. 122060.
- [28] K. van Kranenburg-Bruinsma, E. Schols, H. Gelevert, R. de Kler, M. Weeda, Empowering the Chemical Industry: opportunities for electrification, in: TNO (2016).
- [29] T. Gerres, J.P. Chaves Ávila, P.L. Llamas, T.G. San Román, A review of cross-sector decarbonisation potentials in the European energy intensive industry, *J. Cleaner Prod.* 210 (2019) 585–601.
- [30] J.L. Barton, Electrification of the chemical industry, *Science* 368 (2020) 1181–1182.
- [31] Iea, Renewable energy for industry, in: International Energy Agency, Paris, 2017.
- [32] C. Chen, Using dispatchable energy price to influence renewable penetration in chemical production, in: *J. Cleaner Prod.*, 307, 2021, p. 127274.
- [33] A.S. Gaur, D.Z. Fitiwi, J. Curtis, Heat pumps and our low-carbon future: A comprehensive review, in: *Energy Res. Social Sci.*, 71, 2021, p. 101764.
- [34] J.M. Douglas, *Conceptual Design of Chemical Processes*, McGraw-Hill, 1988.
- [35] R. Turton, R.C. Bailie, W.B. Whiting, J.A. Shaeiwitz, *Analysis, synthesis and design of chemical processes*, Second, Edition ed., Prentice Hall, Englewood Cliffs, NJ, 2003.
- [36] W. Sieder, J. Seader, D. Lewin, S. Widagdo, *Product and process design principles: Synthesis, Analysis and Evaluation*, Fourth, Edition ed., John Wiley & Sons, 2016.
- [37] J.D. Seader, E.J. Henley, D.K. Roper, *Separation process principles*, Wiley New York, 1998.
- [38] J. Zhu, L. Hao, H. Wei, Sustainable concept design including economic, environment and inherent safety criteria: Process intensification-reactive pressure swing distillation, in: *J. Cleaner Prod.*, 314, 2021, p. 127852.
- [39] U.S.E.P.A. Rule, E9-5711: Federal Register / Vol. 74, No. 68 / Friday, April 10, 2009 / Proposed Rules, pp. 16639-16641 (Table C-1. C-2, C-3). in, 2009.
- [40] Y.C. Wu, P.-H.-C. Hsu, I.L. Chien, Critical Assessment of the Energy-Saving Potential of an Extractive Dividing-Wall Column, *Ind. Eng. Chem. Res.* 52 (2013) 5384–5399.
- [41] V. Pleşu, A.E. Bonet Ruiz, J. Bonet, J. Llorens, Simple Equation for Suitability of Heat Pump Use in Distillation, in: 24th European Symposium on Computer Aided Process Engineering, 2014, pp. 1327–1332.
- [42] M. Ferchichi, L. Hegely, P. Lang, Economic and environmental evaluation of heat pump-assisted pressure-swing distillation of maximum-boiling azeotropic mixture water-ethylenediamine, in: *Energy*, 239, 2022, p. 122608.
- [43] T. Shi, Y. Liu, H. Yu, A. Yang, S. Sun, W. Shen, C.K.M. Lee, J. Ren, Improved design of heat-pump extractive distillation based on the process optimization and multi-criteria sustainability analysis, in: *Comput. Chem. Eng.*, 156, 2022, p. 107552.
- [44] A. Yang, S. Sun, A. Eslamimanesh, S.a. Wei, W. Shen, Energy-saving investigation for diethyl carbonate synthesis through the reactive dividing wall column combining the vapor recompression heat pump or different pressure thermally coupled technique, *Energy*, 172 (2019) 320–332.
- [45] IRENA, *Renewable Power Generation Costs in 2020*, in, 2021.
- [46] Z. Tan, Y. Wu, Y. Gu, T. Liu, W. Wang, X. Liu, An overview on implementation of environmental tax and related economic instruments in typical countries, in: *J. Cleaner Prod.*, 2021, p. 129688.
- [47] Y. Cheng, A. Sinha, V. Ghosh, T. Sengupta, H. Luo, Carbon tax and energy innovation at crossroads of carbon neutrality: Designing a sustainable decarbonization policy, in: *J. Environ. Manage.*, 294, 2021, p. 112957.
- [48] IEA, *Net Zero by 2050*, IEA, Paris. , in, 2021.