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Process Design and Techno-Economic Analysis of Heat Pump-Assisted Distillation for Crude Phenol Separation

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Abstract

In China, crude phenols, mixtures commonly produced in the coal industry, are inexpensive and abundant in supply, but their valorization is hindered by high energy consumption in the separation process. It is of great academic and commercial significance to improve the separation process of crude phenols to achieve energy efficiency and cost reduction. In this study, a heat pump-assisted distillation (HPD) system for crude phenol separation was developed. External vapor recompression was adopted due to the strong corrosiveness, high toxicity, heat sensitivity, and easy polymerization of crude phenols. Compared with conventional distillation (CD), HPD showed clear advantages in lowering operating costs. The effects of design variables including pressure, the number of theoretical plates and temperature differences between the condenser and reboiler on reflux ratios, kettle temperature, equipment costs, operating costs, and total annual cost (TAC) were investigated and optimized in detail. The effect of steam prices on process economic feasibility was also studied. It was found that HPD reduced at least 55% of the operational cost compared to CD when the steam price was higher than 10.8 USD/GJ. Carbon emission evaluation indicated that CO_2 generated by the HPD process was 56.3% lower than CD.

Keywords: crude phenols; heat pump assisted distillation; techno-economic analysis

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Academic Editor: Anastasios Zouboulis

Received: 12 September 2025
Revised: 10 October 2025
Accepted: 20 October 2025
Published: 23 October 2025

Citation: Meng, D.; Qin, L.; Zhao, Y.; Zhao, J.; Yan, C.; Mou, C.; Xiong, J.; Zhang, C. Process Design and Techno-Economic Analysis of Heat Pump-Assisted Distillation for Crude Phenol Separation. *Separations* **2025**, *12*, 290. https://doi.org/10.3390/separations12110290

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1. Introduction

Crude phenol is a mixture primarily composed of phenol and its homologues, which are mainly presented in coal tar from many coal chemical processes and in wastewater from semicoke production. Crude phenols can be extracted from coal tar by alkali washing [1–3] or from wastewater using organic solvent extraction [4–7]. After extraction, the general strategy for crude phenol purification is vacuum distillation with a high column to yield pure compound or isomeric mixtures, such as phenol, cresol or xylenol [8]. These compounds are important raw materials to produce bisphenol A [9], bisphenol F [10], and phenolic epoxy resin [11], etc. However, due to the small difference in boiling points among components in crude phenols and thus the great difficulty in separation, the distillation of crude phenol is an energy-intensive process with large reflux ratios and high steam consumption, resulting in high production costs and low economic value [8]. Processes with

reduced energy consumption and operation costs attract the attention of both academia and industry.

Heat pump-assisted distillation (HPD) as an energy efficient distillation technology has shown promising potential in recent years. Several articles have thoroughly reviewed recent progress [12–14], and the advantages and disadvantages of HPD are briefly summarized in Table 1. By converting low-quality heat from the condenser to high-quality heat via vapor compression, HPD can utilize the heat released from the condenser for heating in the reboiler at the expense of a relatively small amount of electricity in the compressor. For crude phenol separation, where a large amount of heat is required for reboilers, HPD could greatly reduce steam consumption. Therefore, researchers have attempted to use HPD for crude phenol separations [8,15]. The most typical example is the research from Gao et al. [8], conducting a comparative analysis of VRC (vapor recompression distillation column), IMVRC (improved middle vapor recompression distillation column), and other crude phenol separation technologies combined with heat pumps. It was discovered that the utilization of IMVRC in crude phenol processing managed to reduce the total annual cost (TAC) by 41.76–74.92% depending on different payback years [8].

Table 1. The advantages and disadvantages of heat pump-assisted distillation compared to conventional distillation.

Advantages	Disadvantages
Reducing energy consumption by recovering heat	High capital investment and longer payback periods
Lower operation costs	Sensitive to energy prices
Reduce CO_2 emission and beneficial for environment	Difficulty in process integration

Although HPD is undoubtedly energy-saving for crude phenol separation, some severe issues in crude phenol processing are still unsolved. Crude phenols are corrosive, heat-sensitive, and chemically unstable under high temperatures. The industrial distillation of crude phenols often results in asphalt-like phenol residues, which may cause blockages in equipment, pipelines, valves, and instruments. Such characteristics of crude phenols greatly increase the difficulty of distillation design and operation, particularly for HPD using high-temperature vapor. For instance, due to the corrosion and instability of phenolic compounds, it is impractical to compress phenolic vapor or handle phenols at high temperature (typically above 180 °C), while previous literature references did not consider these constraints. The separation of phenolic compounds is also rather challenging, which requires numerous industrial experiences. Therefore, the refining process of crude phenols in combination with the heat pump-assisted distillation should be carried out and optimized in consideration of these features of phenolic compounds, to propose feasible separation strategy, to achieve practical improvement in separation efficiency, and to reduce energy consumption. Another disadvantage of HPD is the high capital costs for compressors. Compared to other equipment, such as columns or heat exchangers, steam compressors are quite expensive, which greatly increases the payback period of the HPD process despite the reduced operation costs. Compressors working with steam at relatively high temperatures may cost a million dollars [16]. For example, HPD might cost more than conventional distillation (CD) in regions where steam is inexpensive and readily obtainable, so that TAC of HPD process becomes higher than CD due to elevated equipment capital costs.

There have been a few in-depth studies on crude phenol separation in the past, as well as a lack of analysis on the effect of crucial parameters such as column pressure or theoretical stages on TAC. Moreover, the application of heat pumps in crude phenol separation in previous research is not only scarce but also fails to consider practical issues that cannot be ignored during the crude phenol separation process, such as thermal sensitivity, coking, and

corrosion. Therefore, it is of great significance to explore the application of HPD technology on crude phenol separation based on the existing production schemes, to achieve reduced energy consumption, and to lower TAC. In this work, separation schemes using CD and HPD were designed and analyzed to achieve maximum productivity using crude phenol from coal tar as the feed. The capital cost and operation cost of each process were carefully estimated to ensure authenticity. A comprehensive techno-economic evaluation was conducted to demonstrate the advantages and disadvantages of each process. The effect of operation parameters on separation and cost was investigated.

2. Methodology

2.1. Process Design and Simulation

Crude phenols used in this study were from coal tar in Naomaohu, Xinjiang, China. Typically, phenol oil fractions from coal tar with boiling points of 170–220 °C are counter-currently extracted by a binary solvent composed of a polar solvent and a non-polar solvent to remove neutral oils, followed by distillation to recover solvents and obtain crude phenol with minor impurities (pyridines, anilines, alcohols, ketones, thiophenols, etc.) [17]. These impurities were eliminated using chemical methods to produce the crude phenol mixture used in this work. Crude phenols after extraction were free of water and solid residue, and the typical composition and boiling points of components are shown in Table 2. The flow rate of crude phenols was 3125 kg/h.

Table 2. Composition and boiling points of components in crude phenols.

Components	Content (wt%)	Boiling Points (°C) [a]
Phenol	12.76	181.8
o-Cresol	12.19	191.0
m-Cresol	18.02	202.2
p-Cresol	16.98	201.9
2,3-Xylenol	1.44	216.9
2,4-Xylenol	8.71	210.9
2,5-Xylenol	5.17	211.1
2,6-Xylenol	5.03	201.0
3,4-Xylenol	0.44	227.3
3,5-Xylenol	7.58	221.7
o-Ethylphenol	3.37	204.5
m-Ethylphenol	7.50	218.4
p-Ethylphenol	0.82	218.0

[a] Adapted from source [18].

The separation processes of crude phenols were simulated by Aspen Plus simulation (V12) software. Considering that crude phenols were polar systems, the non-random two-liquid (NRTL) model was the thermodynamic model for the simulations. Default binary interaction parameters in the software were used. Missing physical property parameters were estimated by the universal functional activity coefficient (UNIFAC) method. The RadFrac module in the software was used to simulate the distillation column in the process [19,20]. All columns were packed with BX gauze packing of 316 L stainless steel. The theoretical plate number of each column was set to 150 for all columns due to the high difficulty in phenol separation. In the simulation, the pressure drop of all condensers was fixed at 3 kPa and the pressure drop of all reboilers was neglected. The pressure difference in the whole column (excluding condensers and reboilers) was 8 kPa unless otherwise specified. These values were mainly based on industrial experience from crude phenol plants. To ensure sufficient heat transfer rate, the temperature difference for condensers and reboilers were set to be 10 and 15 °C, respectively, unless otherwise specified. The inlet

temperature of cooling water in this study was 32 °C and the outlet temperature was 40 °C. The heat transfer area of heat exchangers was estimated using Aspen Exchangers Design and Rating (V12). The isentropic efficiency of steam compressors or vacuum pumps was set to be 0.72 to estimate their power and electricity usage (based on the actual isentropic efficiency from realistic compressors).

2.2. Economic Analysis and CO_2 Emission Calculations

The financial performance of conventional distillation and heat pump-assisted distillation was assessed with total capital cost (TCC), total operating cost (TOC), and total annual cost (TAC). TCC was composed of capital costs of installed equipment, including columns, heat exchangers, packing materials, vacuum pumps, and compressors. TOC was contributed by the electricity consumption by vacuum pumps and compressors, steam costs for reboilers, and cooling water cost for condensers. The costs of instrumentation, piping, paintings, electrical and others were not considered, as these costs were complicated to estimate and also did not affect the conclusions made in this study. The basis and factors used for calculation were summarized in Table 3. Unit prices were based on market quotes of equipment manufacturers or production plants. TAC was calculated using the following formula:

$$\text{TAC} = \text{TOC} + \frac{\text{TCC}}{\text{payback period}}$$

The capital costs of the distillation column were calculated based on the weight of the shell and the usage of packing material (details are provided in Supplementary Materials). The capital costs of heat exchangers were calculated based on the heat transfer area multiplied by the cost coefficient per unit area from market research.

Table 3. Basis and factors for economic analysis.

Columns (including manufacturing cost)	3733 USD/tonne
Column packing materials (BX gauze)	615 USD/m^3
Capital cost for heat exchanges	267 USD/m^2
Capital cost for steam compressors	2012 USD/kW
Capital cost for vacuum pumps	2051 USD/kW
Payback period	3 years
Electricity	0.1 USD/kWh
Cold water	0.13 USD/tonne
Steam	10.8 USD/GJ
Installation factor	1.3
Running time	8000 h/y
CO_2 emissions for steam	0.0896 kg/MJ
CO_2 emissions for electricity	0.674 kg/kWh (0.187 kg/MJ) [21]

The capital cost for steam compressors was more complicated. Although many researchers used empirical equations combined with price indices to estimate the cost of compressors [19,22,23], actual prices of steam compressors from commercial vendors in 2025 were significantly higher than values calculated from these empirical equations. To account for this discrepancy, compressors in this study used steam as the working medium and work under high temperatures (above 100 °C), leading to their prices being higher than common compressors. Therefore, after careful investigation of the price of steam compressors in the market, it was determined to use the correlation between power and cost of compressors to calculate equipment price [24–27]. The price factor obtained from market research is 2012 USD/kW (not including installation cost). Similar strategies were used to estimate prices of vacuum pumps, using a factor of 2051 USD/kW (not including installation cost).

The CO_2 emissions were calculated based on the amount of energy consumption, namely electricity and steam in this work. For electricity, according to a recent study [21], emission factors for electricity production in Xinjiang are 0.674 kg/kWh. For steam generation, the literature value of 0.0896 kg/MJ was used [21].

3. Process Design

3.1. Conventional Distillation Process

As shown in Table 2, crude phenols contained multiple xylenol and ethylphenol isomers, significantly increasing the complexity in distillation process. The conventional distillation process with four distillation columns is shown in Figure 1. The detailed parameters can be found in Table 4, and stream information (temperature, flow rates, composition, etc.) is provided in Supplementary information as Table S1. Design specifications to determine optimal reflux ratios and recovery rates for each column are provided in the Supplementary Materials. Due to the chemical instability and tendency to polymerization, the industrial practice for processing crude phenols is to avoid heating crude phenols over 170 °C. Therefore, the columns were operated under vacuum at pre-optimized pressure, so that the temperature of the column bottom liquid did not exceed 170 °C. The steam used for CD was saturated steam at 190 °C and 12.5 bar.

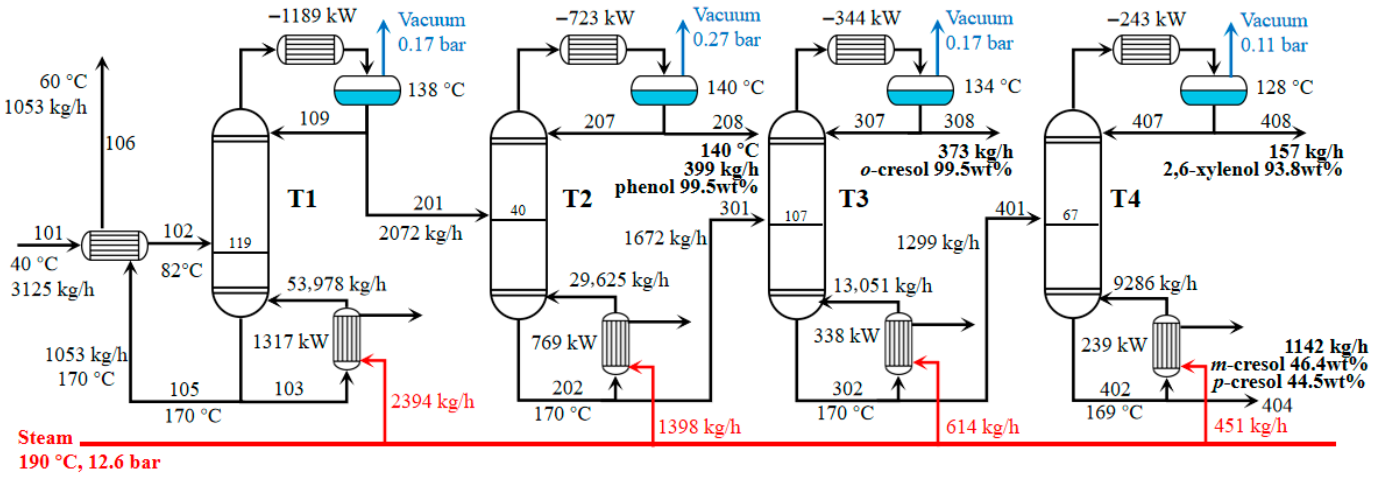


Figure 1. Design variables and parameters of the conventional distillation process for crude phenols.

Table 4. Design parameters of CD process [a].

Parameters	T1	T2	T3	T4
N	150	150	150	150
D/m	1.33	0.98	0.71	0.64
P_{top}/kPa	20	30	20	14
RR	3.13	11.22	5.98	12.16
M_{CW}/tonne·h^{-1}	128.7	78.2	37.2	26.0
A_{cond}/m^2	26.68	16.18	8.08	5.94
A_{reb}/m^2	155.88	95.22	44.08	28.36
P_{vac}/kW	3.37	1.81	1.77	2.01
TCC/10^6 USD	0.26	0.17	0.11	0.08

Table 4. *Cont.*

Parameters	T1	T2	T3	T4
TOC/10^6 USD·y^{-1}	0.65	0.38	0.17	0.13
TAC/10^6 USD·y^{-1}	0.74	0.44	0.21	0.15

[a] abbreviations: N, number of theoretical stages; D, diameter of column; P_{top}, pressure at the top stage of the column; RR, reflux ratio; M_{CW}, mass flow rate of cooling water; A_{cond}, heat transfer area of the condenser; A_{reb}, heat transfer area of the reboiler; P_{vac}, power of the vacuum pump.

Crude phenols were first fed into the first column T1 to remove heavy components, including all xylenols and ethylphenols (except for o-ethylphenol and 2,6-xylenol due to their relatively low boiling points), with the bottom liquid exchanging heat with the feed stream. The top distillate after condensation entered the second column T2 to separate phenol from the mixture, and phenol of 99.5 wt% was obtained from the top distillate. The bottom liquid leaving T2 was subsequently fed into column T3 to obtain o-cresol of 99.5 wt% purity in the distillate. The remaining 2,6-xylenol, m-cresol, *p*-cresol and many other components were separated in the last column T4. A mixture of *m*-cresol and *p*-cresol, as well as 8.1 wt% o-ethylphenol, were discharged from the bottom, while 2,6-xylenol were mainly discharged from the top of the column.

3.2. Heat Pump-Assisted Distillation Process

Due to the small difference in boiling points of components and thus high reflux ratios in each column, the conventional refining process demands significant amounts of energy and steam (Figure 1), leading to a low commercial value of the process. Heat pump-assisted distillation (HPD), which could greatly reduce energy consumption and operation costs, was adopted for crude phenol separation. Typical HPD processes include three schemes: vapor recompression (VRC), bottom flash (BF), and external vapor compression (VC) [13]. Crude phenols are heat-sensitive, highly toxic, and strongly corrosive, and ask high requirements of the heat pump and sealing materials. The polymerization tendency of phenolic substances further limits the use of VRC and BF. The VC scheme uses steam as the cycling medium, which prevents the risk of blockage or corrosion during phenol vapor compression. Moreover, when the released heat from condenser is insufficient for reboilers, the utility system can supply additional heat for the steam, making the heat pump operation convenient and flexible. The stability and durability of steam compressors is also relatively mature at present, making VC the optimal scheme for crude phenol distillation.

The process of crude phenol refining using heat pump-assisted distillation with external vapor compression is shown in Figures 2 and 3, with the same design specifications. Because the heat duty of the condenser and reboiler in each column was not identical, a sink for hot water (90 °C), which can be found in many chemical plants, was used to flexibly withdraw and discharge excess hot water. Similarly, a small amount of makeup steam was also used for columns T1 and T2, as steam from heat pump was not sufficient for reboilers. For each column, hot water at 90 °C from the water sink exchanged heat with the vapor from the top of the column in the condenser, yielding steam and condensed distillate. The steam was then pressurized by steam compressors to increase temperature and pressure, and then mixed with makeup steam (or withdrawn excess steam). The adequate amount of steam entered the reboiler to vaporize liquid in the column kettle and was discharged to the hot water sink. As can be seen in Figures 2 and 3, the electricity input of compressors in each column is significantly lower than the heat duty required for the reboiler, which accounts for the reduced energy consumption in heat pump-assisted distillation compared to conventional distillation. For T1 and T2, a small amount of saturated steam was still necessary, while excess steam was generated for T3 and T4.

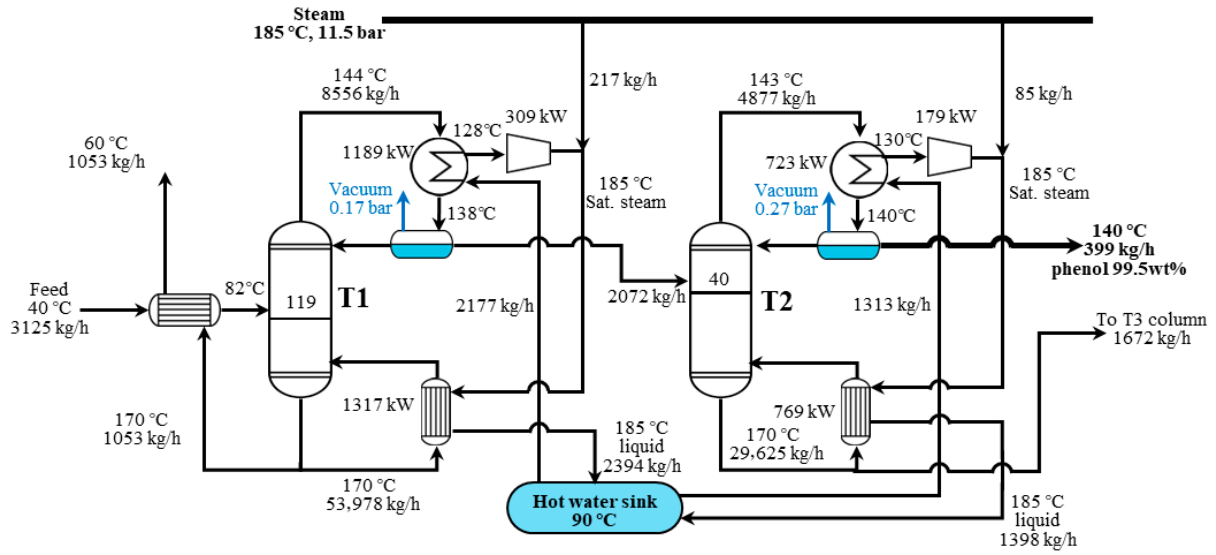


Figure 2. Design variables and parameters of HPD for crude phenol distillation (columns T1 and T2).

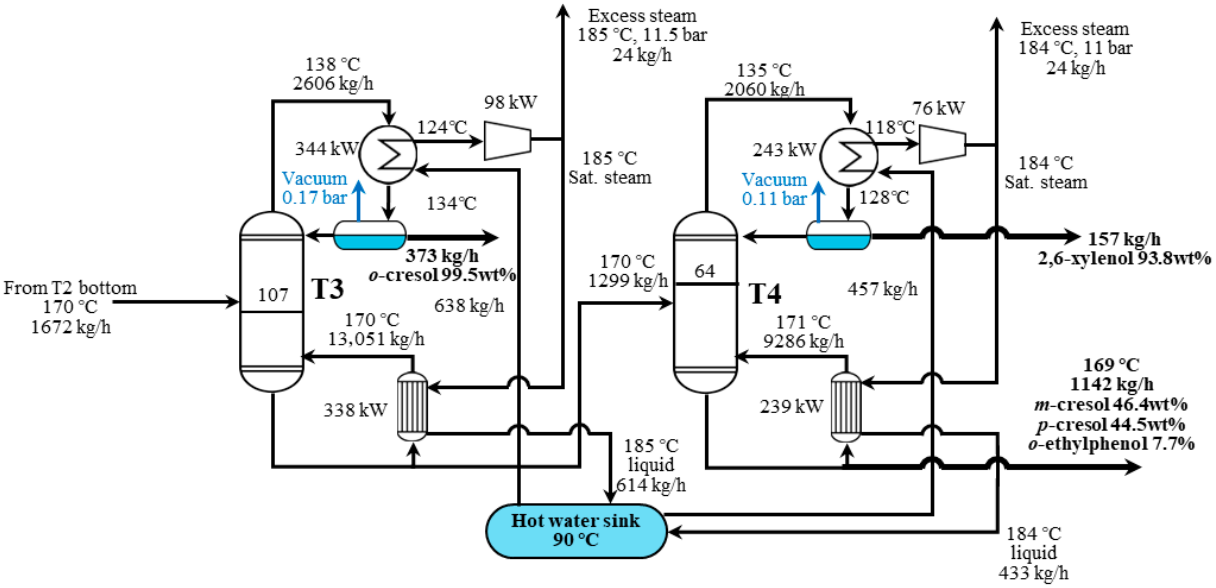


Figure 3. Design variables and parameters of heat pump-assisted distillation for crude phenol distillation (columns T3 and T4).

Compared to CD, HPD showed obvious advantages in terms of TAC, as shown in Table 5. For CD (Table 4), TAC was mainly contributed by operating cost, namely a large amount of pressurized steam for the reboilers, while capital costs for equipment such as columns or heat exchangers were low. For HPD, although capital costs (TCC) were increased due to expensive compressors, the much lower operating cost (TOC) still led to slightly lower TAC. It should also be noted that the cost calculations were based on the steam price of 10.8 USD/GJ and a payback period of three years. Other research has suggested higher steam prices and longer payback periods, and HPD would show larger advantages over CD in these cases. Another advantage of HPD over CD is the reduced consumption of cooling water. As seen in Table 4, CD used several hundred tonnes of cooling water per hour to cool down the top distillates. Although cooling water is readily obtained in most regions, some chemical plants located in arid areas may not have access to such a large amount of inexpensive cooling water. In this respect, HPD may be a desirable alternative over CD for separation processes.

Table 5. Design parameters of HPD process [a].

Parameters	T1	T2	T3	T4
N	150	150	150	150
D/m	1.33	0.98	0.71	0.64
P_{top}/kPa	20	30	20	14
RR	3.13	11.22	5.98	12.16
A_{cond}/m^2	204.0	141.3	63.0	42.2
A_{reb}/m^2	208.0	130.5	59.1	40.7
P_{vac}/kW	3.37	1.81	1.77	2.01
TCC/10^6 USD	1.15	0.70	0.39	0.30
TOC/10^6 USD·y^{-1}	0.30	0.16	0.08	0.06
TAC/10^6 USD·y^{-1}	0.68	0.40	0.21	0.16

[a] abbreviations: N, number of theoretical stages; D, diameter of column; P_{top}, pressure at the top stage of the column; RR, reflux ratio; A_{cond}, heat transfer area of the condenser; A_{reb}, heat transfer area of the reboiler; P_{vac}, power of the vacuum pump.

4. Sensitivity Analysis on Process Parameters

As shown above, crude phenol separation using HPD was designed, and preliminary economic performance was evaluated. To further optimize process variables, sensitivity analyses of multiple parameters in the HPD process were conducted in this section.

4.1. The Effect of Column Pressure

The operating pressure of the distillation columns affects the relative volatility of components, thereby affecting the separation difficulty, the required reflux ratio, energy consumption, and costs. The operating pressure also affects TCC, TAC, and TOC, while few studies deal with this topic. For crude phenols, according to industrial practice, vacuum in the columns was often preferred to keep the temperature below 170 °C to avoid decomposition and condensation. The sensitivity analysis of pressure on column costs was conducted to determine the optimum operating pressure. The pressure drop of each column was set constant to 8 kPa, while the pressure drop of condensers was set constant to 3 kPa. The feed stage was fixed and design specifications were satisfied, and the relationship between absolute pressure at the top of the column and reflux ratios is shown in Figure 4. With the increase in the top pressure of the T1 column, the relative volatility decreases, resulting in a gradual decrease in the column temperature difference (between top and bottom) and slightly higher separation difficulty, as the reflux ratio increased slightly from 3.05 to 3.17 with the pressure at the column top which increased from 8 kPa to 30 kPa. From the economic aspect, as shown in Figure 5, the decreased temperature difference between the top and bottom of the column would significantly decrease the required power for compression, leading to lower capital costs for compressors and lower TOC. The increase in column pressure would also lead to a decrease in capital costs of equipment and operation costs. The capital cost of column T1 shell reduced slightly with increasing pressure, as higher pressure implied higher vapor density and slower flow rate, leading to a slightly lower column diameter. The capital costs of heat exchangers and vacuum pumps changed slightly with pressure, as temperature differences were set to be constant. From an economic perspective, higher operating pressure in the column would indicate lower TCC, TAC, and TOC for the distillation process. Therefore, an intermediate pressure of 20 kPa was determined to be optimal so that temperature in the column kettle did not exceed 170 °C and decomposition or polymerization of crude phenols were not significant.

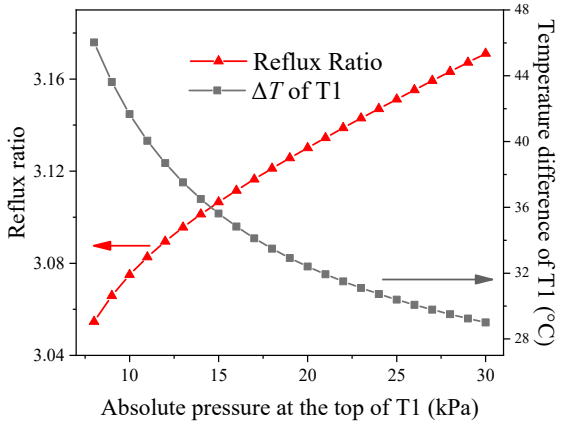


Figure 4. The reflux ratio and temperature difference between the top and bottom of T1 with respect to absolute pressure at the top of T1.

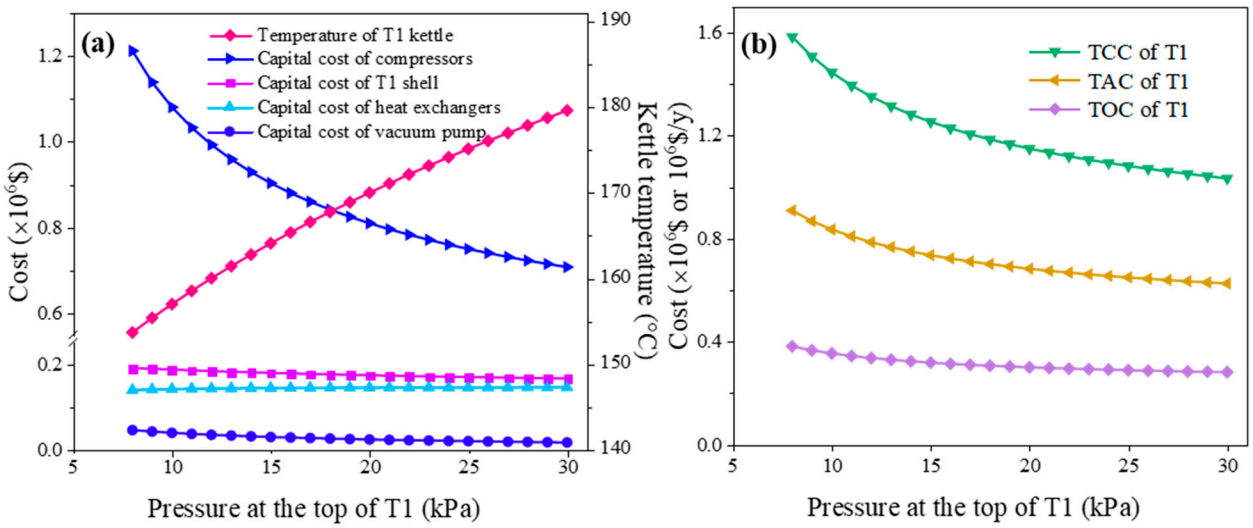


Figure 5. Sensitivity analysis of pressure at the top of T1 column on (**a**) costs of equipment and kettle temperature and (**b**) TCC, TAC, and TOC.

Also, it can be noticed in Figure 5a that the capital costs for compressors were much higher than for other equipment, such as column shells (including packing materials) or heat exchangers, which accounted for the majority of TCC and thus TAC. Although the application of HPD could reduce steam consumption, the capital costs for compressors still pose additional burdens on the profit outlook of the process. As shown later in this work, the profitability of HPD depends heavily on steam prices.

The sensitivity analysis of pressure on reflux ratios and TAC was also carried out on three other columns, and the results are shown in Figure 6. Regarding column T2 and T3, the increase in operating pressure led to slightly decreased reflux ratios and decreased TAC. Therefore, the optimum operating pressures for T2 and T3 were determined to be 30 kPa and 20 kPa, respectively, so that the temperature of the column kettle did not exceed 170 °C. For column T4, the reflux ratio increased more significantly with pressure, likely due to the similar boiling points of 2,6-xylenol and *m*-cresol/*p*-cresol, leading to smaller relative volatility between compounds and higher reflux ratios at increasing pressure. As a result of balancing the costs of heat exchangers and compressors, TAC of T4 column showed a concave curve at intermediate pressure. Accordingly, the pressure at the top of the T4 column was set to 14 kPa to achieve minimum TAC without exceeding 170 °C at the kettle.

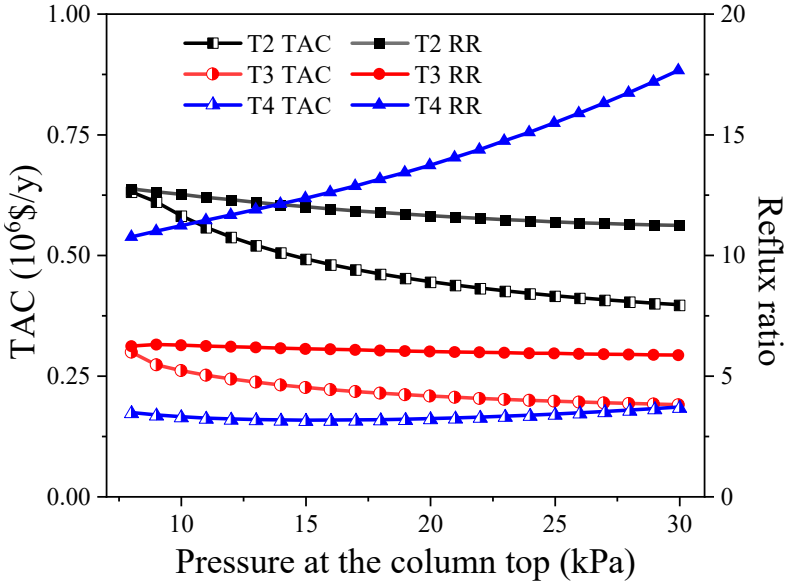


Figure 6. Sensitivity analysis of pressure at the top of column T2, T3, and T4 on TAC and reflux ratio (RR).

4.2. The Effect of Temperature Difference

The mechanism of a heat pump is to compress the vapor from the condenser and supply heat to the reboiler. In order to reduce the energy consumption of heat pumps, it is important to decrease the temperature gap between the condenser and reboiler to reduce the compression ratio and compression power. In general, for condensers, it is appropriate to set the temperature difference between cooling water and distillate to 10 °C. For reboilers, the temperature difference between heating steam and tower condensate is more crucial because an insufficient temperature difference may affect the stable operation of the distillation column. Therefore, it is necessary to analyze the effect of temperature difference between the heating steam and tower condensate on operation costs. Column T1 was used as an example, and the results are shown in Figure 7. The increased temperature difference would significantly lower the capital cost for heat exchangers because less heat transfer area would be required. The increase in temperature difference also leads to higher compression ratio and lower coefficient of performance (COP, defined by the ratio of useful process heat to the amount of primary energy supplied) [22], suggesting that a larger temperature difference would decrease compressor energy efficiency, which is in good agreement with the previous literature [27]. The capital cost for compressors increased as higher power was needed to lift the temperature of the steam, and operation cost for compressors would also increase. As a result, the total cost for equipment and TOC would also increase, suggesting that lower temperature difference would benefit the economic aspects of the HPD process. For reboilers, setting the temperature difference to 10 °C is relatively risky, as the simulation on the heavy components may be less accurate and incomplete vaporization may lead to poor separation. Therefore, it was determined to use 10 and 15 °C for the temperature difference in the condenser and reboiler, respectively.

4.3. The Effect of Theoretical Stages

The number of theoretical stages directly affects reflux ratios, thus affecting the equipment investment cost, operating cost, and TAC. Through sensitivity analysis, the changes in capital costs and operating costs were investigated when the number of theoretical plates varied from 100 to 150, while the feed stage was optimized to the optimal position simultaneously. Although the packed column height may also affect the pressure drop, due to the relatively low resistance of packing materials, the impact of the packing height

on column pressure drop could be neglected. The results are shown in Figure 8. The increase in the theoretical stages of each column resulted in lower reflux ratios (Figure 8a) and higher capital costs of columns (Figure 8b), as expected. Lower reflux ratios further lead to lower operating costs and lower requirements for heat pump power (Figure 8c). Because the capital costs of compressors were much higher than column shells (including packing materials) and heat exchangers combined, the total annual costs (TAC) would tend to decrease with the increase in total number of stages (Figure 8d). Notably, although it is likely that increasing stage number would reduce the capital costs of equipment further, excessively high columns imply additional trouble in safety or construction. Therefore, it is appropriate to use 150 as the optimal value for the number of theoretical stages for four columns in this process to ensure the lowest TAC.

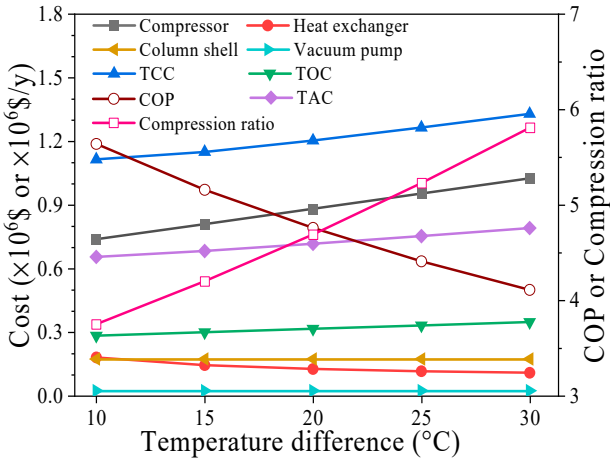


Figure 7. The effect of temperature difference in the reboiler on economic aspects of T1 column.

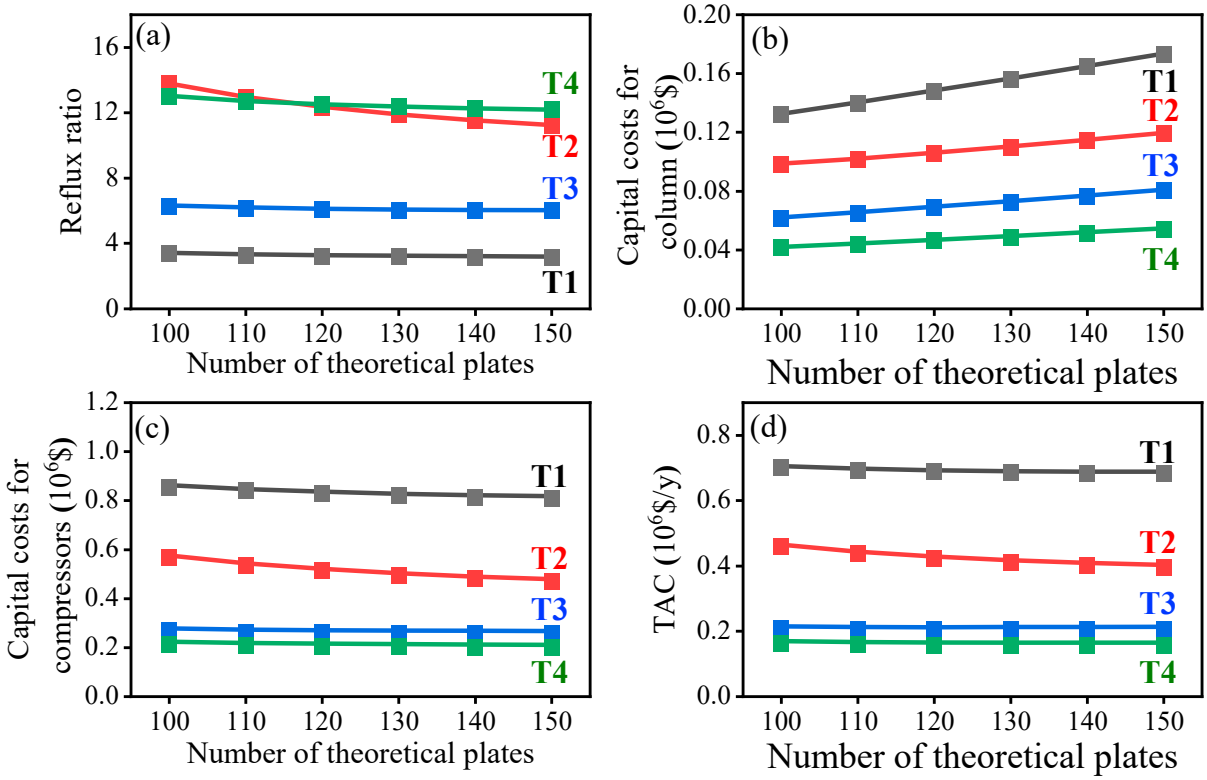


Figure 8. The effect of theoretical plate numbers on (**a**) reflux ratio, (**b**) capital costs of columns, (**c**) capital costs of steam compressors, and (**d**) TAC.

4.4. The Effect of Steam Cost on Process Economics

The major advantage of heat pump-assisted distillation (HPD) is using heat pumps to convert low-quality heat energy to high-quality heat energy to reduce steam consumption. For scenarios where steam generation is inconvenient or relatively expensive, the immense heat required for reboilers can be supplied by vapor condensation at the expense of a relatively small amount of electricity. From the perspective of external energy consumption, HPD is undoubtedly energy efficient compared to conventional distillation (CD). However, HPD requires additional expenditure on compressors, which are more expensive than other equipment in the process, as shown in Figure 5a. If the steam price is relatively low, the reduced cost of steam consumption might not be able to compensate for the additional capital costs in heat pumps. In this respect, a threshold value for the steam price exists so that HPD is not competitive against CD in terms of TAC. To unveil such value, sensitivity analysis of steam price on process economics was conducted as shown in Figure 9, with steam price ranging from 3 to 21 USD/GJ. It can be noted that the operational cost responds strongly to steam price in CD, as CD consumes a large amount of steam in reboilers. For HPD, the energy input was mostly electricity and only a small amount of steam was used to compensate for the energy gap between supply and demand in reboilers, so the steam price barely affected the operation costs of HPD.

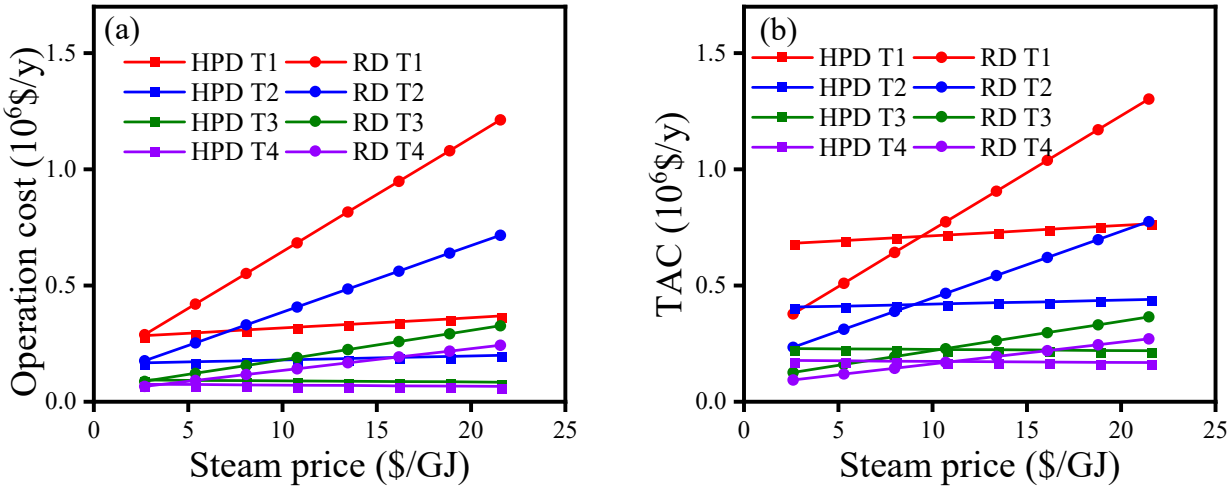


Figure 9. The effect of steam price on (**a**) operation cost and (**b**) TAC of each column in conventional distillation (CD) or heat pump-assisted distillation (HPD).

In terms of TAC, it is anticipated that the line for HPD and the line for CD intersect at an intermediate value. When the steam price was too high, the operation cost would exceed the capital cost for heat pump equipment, making HPD more competitive. Moreover, HPD also greatly reduced cooling water usage compared to CD, which also contributed to the reduced TAC. On the contrary, when steam was inexpensive, the capital costs for compressors could not be offset by reduced steam consumption in the payback period. According to this research, the threshold value lies within the range of 9 to 10.8 USD/GJ. When the steam price on site is higher than 10.8 USD/GJ, HPD is definitely more cost-effective than CD.

5. Environmental Impact

In addition to the reduced cost of energy, HPD shows great advantages over CD in terms of environmental impacts. The CO_2 emissions of HPD or CD can be calculated using factors, as shown in Table 3. According to the literature, the CO_2 emission factor for electricity varies depending on electricity generation or transmission [21]. In this study,

the average emission factor for Xinjiang province (0.675 kg/kWh or 0.187 kg/MJ) was used. The CO_2 emission factor (0.0896 kg/MJ) for steam generation was adopted from the literature [28]. It can be observed from Figure 10 that CO_2 emission of HPD was less than half of that of CD. As shown in Tables 4 and 5, TOC, namely energy consumption (steam and electricity), in HPD was much lower than CD, leading to much lower CO_2 emission. Moreover, because the major energy consumption for HPD was electricity, it is anticipated that the reduction in CO_2 emission of HPD could be further reduced in the future with the development and expansion of renewable electricity.

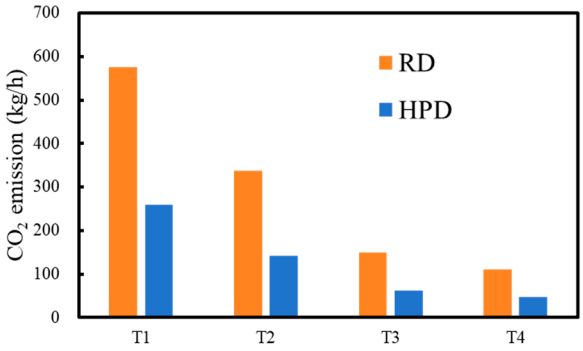


Figure 10. The amount of CO_2 emissions for HPD and CD.

6. Conclusions

Crude phenols are corrosive, heat-sensitive, and chemically unstable under high temperatures, which may cause blockages in equipment, pipelines, valves, and instruments. The application of heat pumps in crude phenol separation in previous research is not only scarce but also fails to consider practical issues that cannot be ignored during the crude phenol separation process. In this study, the practical and feasible separation of crude phenols was simulated using heat pump-assisted distillation (HPD), and a comprehensive techno-economic analysis was conducted. Due to their strong corrosiveness, high toxicity, and tendency to polymerize, crude phenols are only suitable for external vapor compression schemes. The effect of design parameters, such as column pressure, theoretical plate number, or temperature difference in heat exchangers, on process economics was investigated using process simulation software. Compared with conventional distillation (CD), the HPD process required extra expenditure on compressors but a much smaller amount of steam consumption, leading to its higher capital costs and lower operating cost. When the steam price exceeds 10.8 USD/GJ, HPD becomes advantageous over CD in terms of TAC. Moreover, HPD not only reduced steam consumption but also significantly reduced cooling water consumption, which is also important for regions where water was scarce. The carbon emissions generated by HPD are far lower than those of CD, significantly reducing its carbon footprint. With the rapid development and increasing share of renewable electricity, HPD has the potential to further reduce the CO_2 emissions and decrease operating costs. Although this is a simulative study and actual HPD might be less efficient than in the simulation, this work still provides insightful implications on key factors of the HPD process for crude phenol separation.

Supplementary Materials: The following supporting information can be downloaded at https://www.mdpi.com/article/10.3390/separations12110290/s1, Table S1: Design Specifications for distillation column simulation; Table S2: Stream information for conventional distillation process in Figure 1. Reference [29] are cited in the Supplementary Material.

Author Contributions: Conceptualization, Y.Z., J.X. and C.Z.; Methodology, D.M., L.Q. and J.Z.; Software, L.Q. and J.X.; Validation, J.Z. and C.Z.; Formal analysis, C.M.; Investigation, D.M., L.Q. and C.Y.; Resources, D.M. and J.X.; Data curation, C.M.; Writing—original draft, D.M.; Writing—review & editing, C.Z.; Visualization, C.Y.; Supervision, Y.Z. and J.X.; Project administration, Y.Z. and J.X.; Funding acquisition, Y.Z. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Xinjiang Uygur Autonomous Region Key R&D Program Project (2023B01015), Tiandi Co. Lit. Technology Innovation and Entrepreneurship Fund Special Project (2024-TD-QN001) and Technology Development Fund Project of CCTEG China Coal Research Institute (2024ZDI-03).

Data Availability Statement: The original contributions presented in this study are included in the article/Supplementary Materials. Further inquiries can be directed to the corresponding author(s).

Conflicts of Interest: Author D.M., L.Q., Y.Z., J.Z., and C.Y. were employed by the company CCTEG. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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