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Heat Pump Assisted Reactive Distillation: Wide Boiling Mixture

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Introduction

Distillation is one of the most important and widely used separation techniques both in chemical and petrochemical industries. It is used for about 95% of all fluid separation in the chemical industry.[1] Diez et al.[2] reported that 60% of energy used by the chemical industry was for distillation. It is surprising that the overall thermal efficiency of a conventional distillation is around 5–20%.[3] Because of the improper utilization of heat, the operating cost is not only increased, the environment could also be severely affected. During the transformation of energy in the industrial processes, the thermal effluents are generated in the form of flue gas, condensate, hot water, boiler blow down, etc. They cause thermal pollution and depletion of fossil fuel at a rapid rate.

Therefore, the development of distillation technology aiming to improve the thermodynamic efficiency has captured the attention of many researchers. Most popular techniques of thermal coupling are internal energy integration[4] and heat pumping.[2] In industrial practice, mechanical and absorption heat pumps are frequently used. In the former, the overhead vapor is compressed to a higher pressure and used to heat the bottom liquid in the reboiler, or the bottom liquid is flashed in a valve and used to condense the overhead vapor. In absorption heat pumps, a separate closed-loop fluid system is employed to transfer the heat up the temperature scale by means of heat of mixing.

Heat pumping is an economic way to conserve energy if the temperature difference between the overhead and bottom of the distillation column is small and the heat load is high. To use this technique for wide boiling mixtures, the heat pump can be employed between the intercondenser and interreboiler.[5] This work introduces a novel heat pumping scheme for a reactive multicomponent distillation column, in which the components being separated have widely different boiling points. Based on our knowledge, no work has reported the heat pump assisted distillation with chemical reaction that fractionates a wide boiling mixture.

Representative Reactive Distillation (RD): Ethylene Glycol System

This work considers a reactive distillation column[6] shown in Figure 1 for the production of ethylene glycol (EG) from ethylene oxide (EO) and water (W). The representative process, which is referred to as the conventional reactive distillation column (CRDC), has a total of 10 stages (excluding the bottom reboiler and total condenser). The trays are counted from the bottom up; bottom tray is the first stage, and the top one is the 10th stage. The example column has two sections, namely the reactive section (5th to the 10th stage), and the nonreactive section (1st to the 4th stage). Of course, the separation occurs in both sections. In the top six stages, the following exothermic liquid-phase reaction takes place

$$\underset{C_2H_4O}{\text{Ethylene oxide}} + \underset{H_2O}{\text{Water}} \rightarrow \underset{C_2H_6O_2}{\text{Ethylene glycol}}$$

Boiling point (K) 283.5 373.2 470.4

The following assumptions have been made to derive the mathematical model of the CRDC: negligible tray vapor holdup compared to liquid holdup, variable tray liquid holdup, perfect mixing and equilibrium on all trays, fast energy dynamics, top stage/condenser pressure of 1 atm (=101.33 kPa), with a stage pressure drop of 0.3 kPa, constant tray efficiency (Murphree vapor-phase efficiency = 70%), no side reaction, and ideal vapor–liquid equilibrium.

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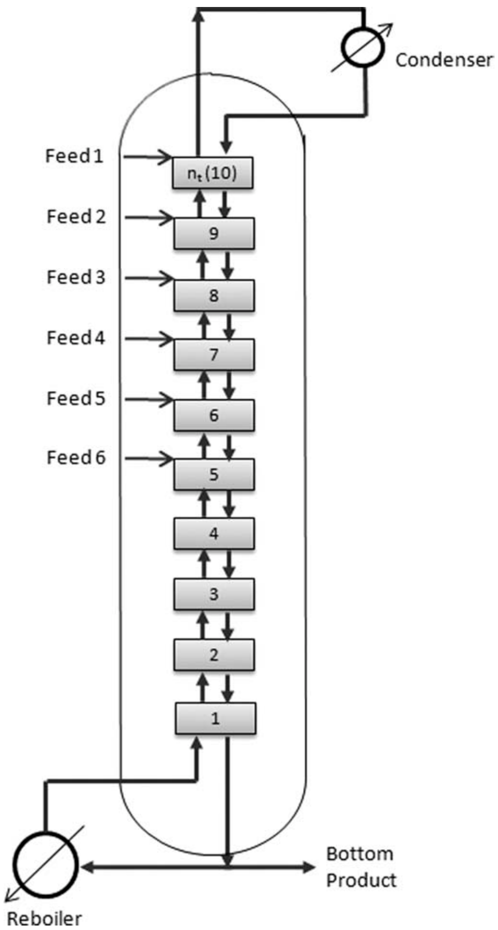

Figure 1. Conventional reactive distillation column (CRDC).

Heat transfer is computed by $UA\Delta T$, where U denotes the overall heat-transfer coefficient (W/m^2·K), A the heat-transfer area (m^2), and ΔT the temperature difference (K). For brevity, the modeling equations are not included in this article and the complete model is available elsewhere.[6]

Column and system specifications are reported in Table 1. Reaction volumes are distributed unevenly between stages 5–10. Pure water with a flow rate of 26.3 kmol/h, is introduced onto the top stage, and a total feed of 27.56 kmol/h of pure EO is distributed among stages 5–10. Among the three species, EO is the lightest; water is the intermediate and EG is the heaviest one. Accordingly, the product EG is taken out from the bottom. The overhead vapor, a highly pure EO (99.7 mol %) stream with a temperature of 16.76°C, is totally converted to liquid state in a condenser by the use of refrigerant ammonia[7] (available at ~1°C). The only product, which is withdrawn at the bottom with a temperature of 113.87°C, contains 94 mol % EG. By simulating the CRDC, the condenser duty, Q_C and reboiler duty, Q_R are obtained as 697.07 kW and 307.21 kW, respectively.

We should note that to perform a meaningful comparison, the input and output specifications of all distillation configurations devised in this study are kept the same with that of CRDC.

Heat Pump Assisted Distillation Column (HPADC): A Conventional Scheme

In this study, the direct vapor recompression technique is applied on the example system. The resulting conventional heat pump assisted reactive distillation column (CHPARDC) is shown in Figure 2. Note that to calculate the energy consumption and cost, we use the following approach.

Energy consumption

The energy consumption involved in operating a thermally integrated column, Q_{cons} is estimated by the sum of the reboiler duty, Q_R plus three times the compressor duty, Q_{comp} as

$$Q_{\text{comp}} = Q_R + 3Q_{\text{comp}} \tag{1}$$

The factor of three for the compression duty is supposed to convert the compressor work into the thermal energy needed to produce an equivalent amount of electrical power. The compressor duty (kW) is calculated from

$$Q_{\text{comp}} = \frac{\mu}{\mu - 1} R_{V_{10}T_{10}} \left[\left(\frac{P_o}{P_i} \right)^{(\mu-1)/\mu} - 1 \right] \tag{2}$$

In the aforementioned equation, R represents the gas constant (= 8.314 J/(mol.K)), V_{10} the flow rate of a vapor stream (kmol/s) leaving the10$^{\text{th}}$ stage, T_{10} the overhead vapor temperature (K), P_0 the pressure (atm) of compressed vapor, and P_i the pressure (atm) of overhead vapor. The polytropic coefficient (μ) is calculated from

$$1/(\mu - 1) = \sum [y_j/(\mu_j - 1)] \tag{3}$$

Table 1. Column and System Specifications

Pure EO feed rates (kmol/hr) [from stages 5-10]	4.89/4.76/4.69/4.97/0.2/8.05
Pure water feed rates (kmol/hr) [from stages 5-10]	0.0/0.0/0.0/0.0/0.0/26.3
Reaction volume (m^3) [from stages 5-10]	0.551/0.481/0.447/0.371/1.447/0.011
Bottoms composition (EO/W/EG)	0.053/0.007/0.94
Bottoms rate (kmol/hr) (EO/W/EG)	1.4604/0.2011/26.099
Column diameter (m)	1.3
Reaction kinetics[5]	
Reaction rate (kmol/m^3.hr): $r = \exp\left[37.0 - \frac{9547.7}{T}\right] x_{EO}\, x_W$, where temperature ($T$) in K	
Heat of reaction = –80 kJ/mol	
Heat of vaporization = 40 kJ/mol	

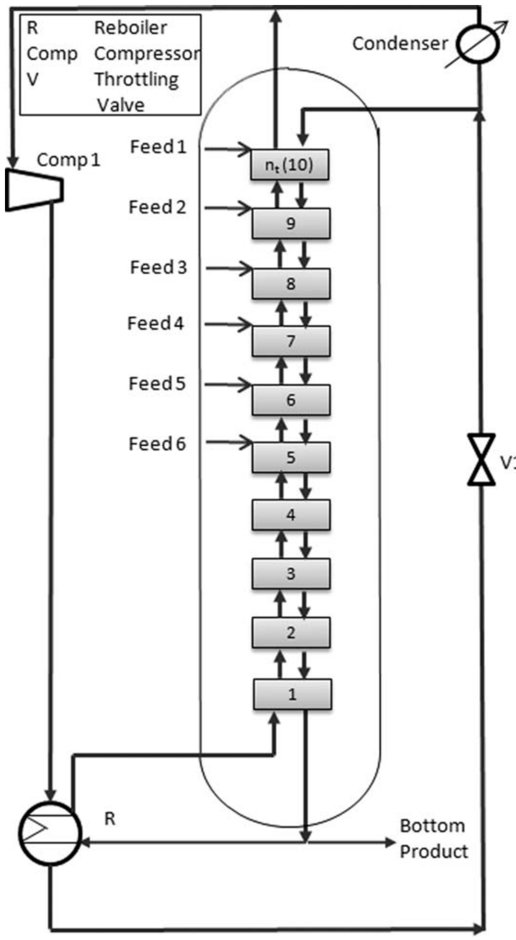

Figure 2. Conventional heat pump assisted RD column (CHPARDC).

as 1.3. Here, y_j denotes the vapor composition of any species j. We suppose 8,000 operating hours in every year.

It is observed that the latent heat released by the compressed overhead vapor (= 639.05 kW) is higher than the heat required in the reboiler (= 307.21 kW). Therefore, in the CHPARDC, as shown in Table 2, a part of the overhead vapor (= 44.43 kmol/h) is compressed for supplying the exact amount of heat required in the bottom reboiler. The remaining amount of V_{10} (= 48.87 kmol/h) is condensed in the overhead condenser. The compression ratio (CR) of 4.9 is selected in order to maintain a reasonable temperature difference (= 30°C) between two heat exchanging streams in the reboiler. It is shown in Table 3 that the CHPARDC provides the percent energy savings (= $[Q_{CRDC} - Q_{CHPARDC})]/Q_{CRDC}] \times 100$) of -4.60%.

Cost calculation

The energy integration in a distillation column generally provides a significant energy savings, but at the cost of an increased capital investment. It is expected that a successful heat integrated structure should provide positive energy savings, as well as better economic figures. In order to perform an economic analysis, we use the following equation to calculate the total annual cost (TAC)

$$\text{TAC(\$/yr)} = \text{operating cost} + \frac{\text{captial investment}}{\text{payback period}} \quad (4)$$

The capital cost is obtained by summing up individual equipment (distillation column, heat exchanger and compressor) costs, and the operating cost includes the cost of utilities (heating steam and electricity) and refrigeration cost. The cost estimating formulas used in this article are those given by Douglas.[8] The operating cost of the compressor is calculated as suggested by Douglas[8] assuming a motor efficiency of 0.75. For computing the heat-transfer areas, the temperature differences of 20 and 30°C are considered between two heat exchanging streams in the condenser (ΔT_c) and reboiler (ΔT_R), respectively. The refrigeration and utility costs are reported in literature[7] as: steam cost of \$4.25/ton, refrigeration (ammonia) cost of \$2.0/ton-day (288,000 Btu removed), and electricity cost of \$0.04/kW.h.

The results given in Table 3 show that the CHPARDC provides a negative (−4.60%) energy savings and a reasonably large payback period of 8.3 years. This happens because of the high-energy consumption (due to large CR) involved in separating a wide boiling range mixture. This study confirms that the heat pumping is not an economic way to conserve energy when a reasonably large temperature difference exists between the two ends of the column.

Proposed Distillation Schemes

In this contribution, various distillation schemes have been proposed aiming to improve the thermodynamic efficiency of the example reactive system. By performing a comparative analysis, finally an energy efficient structure is identified. The details of these proposed schemes are presented systematically in the following.

Double-reboiler RD column (DRRDC)

In Figure 3, the CRDC is modified to a double-reboiler RD column (DRRDC). Along with the trim-reboiler, this configuration includes a side reboiler at the intermediate position and both the reboilers use the external heat-transfer medium (i.e., steam). By conducting sensitivity tests in terms of energy and cost savings, the side heat exchanger is coupled with the second stage. We should remember that as the liquid flow to the side reboiler increases, the heat duty of that reboiler, as well as overhead condenser may increase. Interestingly, when about 40% of outgoing tray liquid is reboiled, it is inspected that the column (above the 2nd stage) runs dry for sometime.

Table 2. Overhead Vapor Splitting for Compression and Condensation

Scheme	Total overhead vapor rate (kmol/hr)	Vapor flow to Comp1 (kmol/hr)	Vapor flow to Comp2 (kmol/hr)	Vapor flow to overhead condenser (kmol/hr)
CHPARDC	93.3	44.43	0.0	48.87
DRRDC	93.3	0.0	0.0	93.3
HPARDC-T1	93.3	12.68	30.29	50.33
HPARDC-T2	93.3	0.0	30.29	63.01

Table 3. Comparison of Estimated Capital and Operating Costs

Item	CRDC	CHPARDC	DRRDC	HPARDC-T1	HPARDC-T2
Condenser duty (kW)	697.07	315.22	697.07	398.36	485.20
Cost of refrigeration ($/yr)	132226.62	59794.74	132226.62	75564.80	92037.84
Bottom reboiler duty (kW)	307.21	0.0*	86.84	0.0*	86.84
Intermediate reboiler duty (kW)	0.0	0.0	211.87	0.0*	0.0*
Steam required (ton/yr)	3618.65	0.0	3518.51	0.0	1022.92
Cost of steam ($/yr)	15379.28	0.0	14953.67	0.0	4347.41
Compressor duty for int_reb (kW)	0.0	0.0	0.0	26.14	26.14
Compressor duty for bot_reb (kW)	0.0	107.12	0.0	16.25	0.0
Cost of electricity ($/yr)	0.0	45642.53	0.0	18063.72	11139.48
% Energy savings	–	−4.60	2.77	58.60	46.20
Total cost of energy ($/yr)	147605.90	105437.27	147180.29	93628.51	107524.73
Capital cost ($)					
Condenser	139101.10	83043.23	139101.21	96689.87	109913.60
Reboiler(s)	50145.24	50145.24	61443.79	61443.79	61443.79
Column	145727.59	145727.59	145727.59	145727.59	145727.59
Column trays	10588.41	10588.41	10588.41	10588.41	10588.41
Compressor(s)	0.0	406137.07	0.0	214282.60	127766.99
Total capital cost ($)	345562.34	695641.54	356861.0	528732.26	455440.38
Payback period (yr)	–	8.30	26.56	3.39	2.74

*Reboiler receives heat through condensation of the compressed overhead vapor.

To avoid this situation, in this simulation, 30% of the liquid stream leaving 2nd stage is chosen to introduce to the intermediate reboiler. This leads to keep the overhead vapor rate unchanged that is evident from Table 2.

As shown in Table 3, the consumption of moderate-pressure (4 bara) steam in the standard configuration (Figure 1) is 307.21 kW. With the intermediate reboiler, the consumption of moderate-pressure steam is reduced to 86.84 kW in the base reboiler, while the consumption of low-pressure (1 bara) steam is 211.87 kW in the intermediate reboiler. However, compared to the CRDC, there is no savings achieved in terms of condenser duty (= 697.07 kW). It is calculated from Table 3 that the annual savings in energy cost is about $425.61 (i.e., 0.29%). This insignificant cost savings cannot compensate the additional installed cost of the intermediate reboiler within a reasonable payback period. Because of the large payback time (i.e., 26.56 years), it can be concluded that the DRRDC is not an attractive alternative to the CHPARDC.

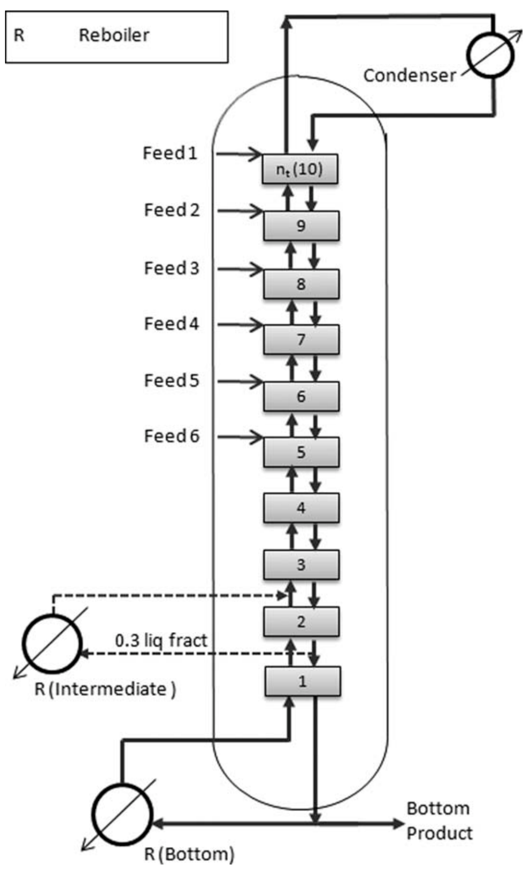

Figure 3. Double-reboiler RD column (DRRDC).

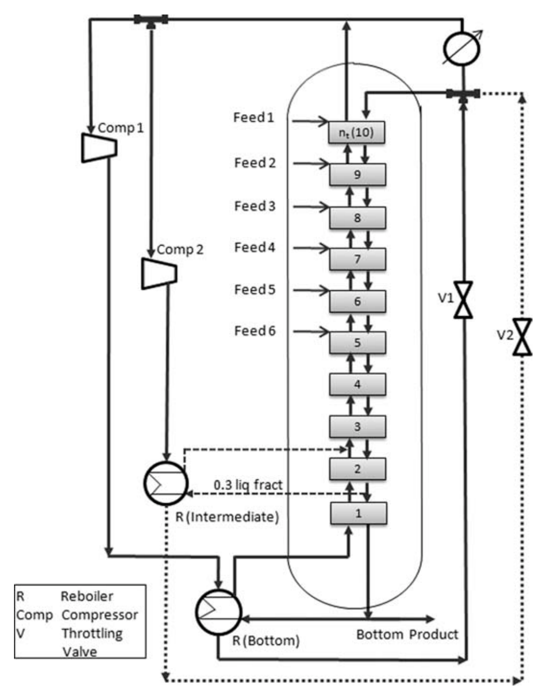

Figure 4. Heat pump assisted RD column–type1 (HPARDC–T1).

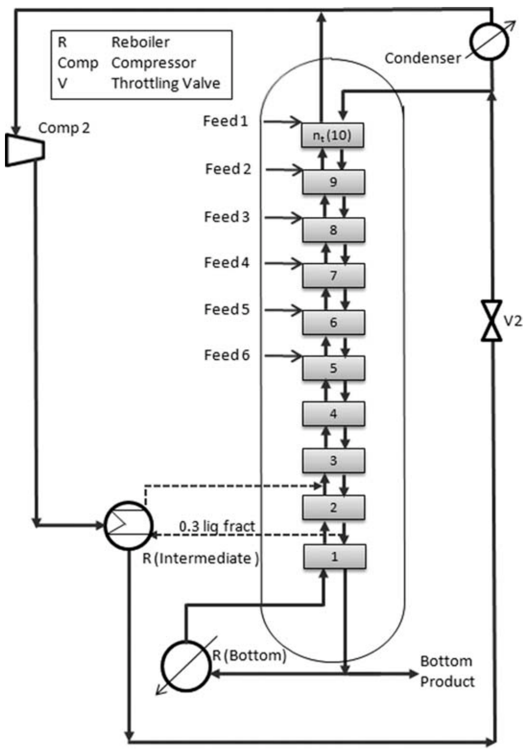

Figure 5. Heat pump assisted RD column–type2 (HPARDC–T2).

Heat pump assisted RD column–type1 (HPARDC-T1)

To improve the thermodynamic performance, we turn our attention to restructure the DRRDC to a distillation scheme, namely heat pump assisted RD column–type 1 (HPARDC–T1). As shown in Figure 4, the compressed overhead vapor, instead of steam, is used as a heating medium in both the intermediate and bottom reboilers. Table 2 provides the amounts of overhead vapor entered the overhead condenser, compressor 1 (Comp1) and compressor 2 (Comp2). For maintaining the ΔT_R of 30°C, the CRs obtained for Comp1 and Comp2 are 4.9 and 3.1, respectively. With reference to the CRDC, the HPARDC–T1 achieves a significant energy savings (58.60%), and a payback period of 3.39 years.

Hear pump assisted RD column–type2 (HPARDC–T2)

It is observed that the HPARDC–T1 provides quite impressive performance in terms of energy and cost savings. However, it requires high CR, particularly for the bottom reboiler. Aiming to reduce the payback period further, we consider the use of steam, instead of compressed overhead vapor, in the bottom reboiler. The resulting configuration is referred to as HPARDC–T2 and presented in Figure 5. It is interesting to note that the CR of 3.1 is kept unchanged for Comp2. Here, the overhead vapor is divided into two streams and they are introduced to the compressor and condenser. As detailed in Table 3, the attractiveness of the HPARDC–T2 system can be measured by the payback time of 2.74 years.

Conclusions

This work introduces a heat pump assisted scheme for a total reflux multiple feed RD column. In this reactive process, the components being separated have widely different boiling points. It leads to a large temperature difference between the two ends of the column. At the beginning, it is scrutinized and confirmed that the heat pumping is not an economic way to conserve energy if the temperature difference is large. To avoid the high-energy consumption, it is suggested to include an additional side reboiler at a suitable position. The resulting double-reboiler RD column uses steam in both the reboilers and provides a large payback period of 26.56 years due to insignificant energy savings and additional capital cost of the second reboiler. In the next phase, it is observed that the thermodynamic efficiency is improved a lot when we use compressed overhead vapor in both the heat exchangers. Aiming to reduce the payback period further, it is investigated that the compressed overhead vapor should be used only in the intermediate reboiler and steam in the bottom reboiler. This proposed heat pump system (HPARDC-T2) appears overwhelmingly superior to the first three investigated schemes. It provides about an energy savings of 46.2%, and a payback period of 2.74 years.

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