A Novel Multistage Vapor Recompression Reactive Distillation System with Intermediate Reboilers

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Most of the published studies have focused on the thermal integration of nonreactive distillation columns. The key limitation of reactive distillation (RD) technology is that the necessary conditions (such as pressure and temperature) for the reaction must match those of distillation. Owing to this constraint, the reaction conversion may be adversely affected at the elevated pressure in the reactive section of an internally heat integrated distillation column (HIDiC). This fact forces us to adopt an external heat integration approach for an industrial heterogeneously catalyzed ethyl tert-butyl ether (ETBE) RD column. The direct vapor recompression column (VRC) is an external heat integration scheme that is successfully used as an energy efficient scheme for separating a close-boiling mixture. Interestingly, there exists a large temperature difference between the two ends of the representative ETBE column, and it makes the external heat integration more challenging. Aiming to improve the thermal efficiency of the ETBE column under the VRC framework, various heat pump arrangements with intermediate reboiler(s) (IR(s)) are explored and analyzed with performing a comparative study in terms of energy consumption and economics. To improve further the thermal efficiency, in this contribution, a novel multistage vapor recompression RD column with IRs is introduced addressing a number of practical concerns. An algorithm for the proposed column is formulated showing the sequential steps involved in heat integration. It is inspected that the proposed multistage vapor recompression RD system appears overwhelmingly superior to the classical vapor recompression RD and its conventional stand alone column providing a significant savings in energy as well as cost. © 2012 American Institute of Chemical Engineers *AIChE J,* 59: 761–771, 2013
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Introduction

Environment pollution has become one of the major global problems of the century. As global warming continues to pose more and more serious problems, the demand to suppress the exhaust of the greenhouse gas has increased and technology development to reduce energy consumption in industries has been promoted.[1] Both the energy integration in distillation and the addition of ethyl *tert*-butyl ether (ETBE) in gasoline used in vehicles have a common objective of reducing the greenhouse gas emission to the atmosphere.

Distillation is one of the most energy-intensive units in chemical process industries, and it accounts for an estimated 3% of the world energy consumption.[2] It is reported[3] that 60% of energy used by the chemical industry is for distillation. There is no doubt that energy consumption in distillation and CO_2 gases produced in the atmosphere are strongly related; with the increase of energy demands, the CO_2 emissions to the atmosphere increase. This is because the energy is mostly generated through the combustion of fossil fuel.

Although potentially a reversible process requiring no more work than the net energy difference between the products and the feed, in practice the fractionation by distillation is irreversible and consumes many times the theoretical minimum energy requirement. It is reported[4] that the overall thermodynamic efficiency of a conventional distillation is around 5–20%. A number of research groups[1,5–16] are actively involved in developing the different energy efficient distillation technology. The heat integration techniques can be broadly classified into two groups[17]: internal heat integration (e.g., heat integrated distillation column, HIDiC) and external heat integration (e.g., vapor recompression column, VRC), and it is with this latter group that this work is concerned.

Recall that the VRC 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.[18] For separating the wide-boiling mixtures, the vapor recompression scheme with intermediate exchanger(s) has been explored for nonreactive distillation column in the literature.[19–21] Recently, Shenvi et al.[22] have developed the multistage vapor recompression scheme with intermediate exchangers for a binary distillation column that can offer significant energy efficiency benefits as compared to other heat integration schemes, such as the HIDiC.

In this communication, an industrial heterogeneously catalyzed reactive distillation (RD) column is simulated for the production of ETBE. It is interesting to note that in ETBE RD column, there is a large temperature difference between the two ends of the column. For separating a wide-boiling mixture using the heat-pumping technique, a thermally

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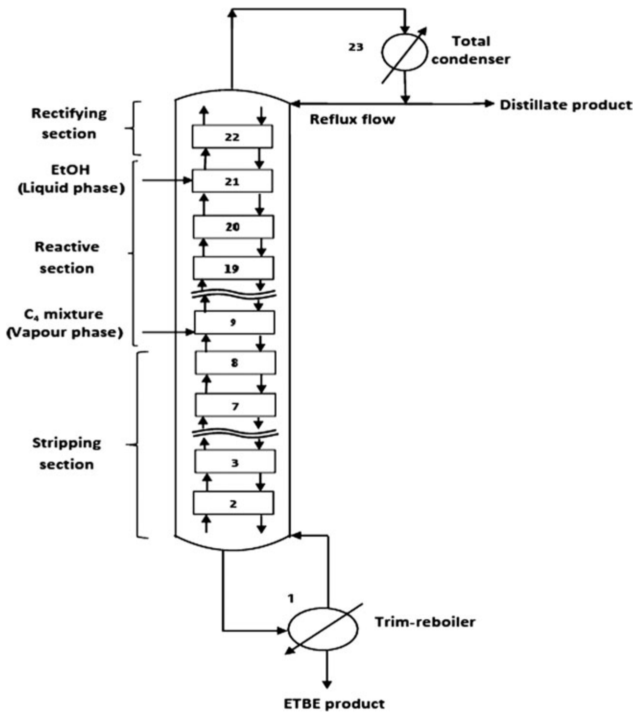

Figure 1. Schematic representation of the ETBE RD column.

integrated RD structure having one intermediate reboiler (IR) is recently proposed in the literature.[21] We have extended their approach and developed various VRC schemes for the ETBE column with a single as well as double IR. However, a number of practical concerns, including the tendency of vapor superheating in the adiabatic compressor, the flashing of condensate in the throttling valve (TV), the reverse flow of vapor from the reflux drum to the overhead vapor line, and so forth are not addressed so far.

In this contribution, we introduce a novel multistage VRC with IRs taking into consideration all the important issues mentioned above. The proposed heat integration scheme is successfully applied on a sample ETBE column. By performing a detailed analysis, it is observed that this novel configuration provides a significant energy savings and better economic figures compared to the classical VRC and its conventional stand alone column. Based on our knowledge, so far no such VRC scheme has been explored for RD.

Motivation

Both internal and external heat integration methods use the compressor and they require electricity, which is several times more expensive than the thermal utility. The amount of vapor flowing through the compressor and the pressure ratio/compression ratio (CR) are two significant factors that can affect the power requirement in the compressor. Note that both these factors also influence the capital investment of compressor. In the HIDiC scheme, the vapor flow rate varies significantly along the both stripping and rectifying sections. Actually, the vapor flow increases from the bottom to the top of the stripper and decreases as it flows up toward the top of the rectifier. For HIDiC, the flow of overhead vapor from the stripping section is usually larger than the average vapor flow in a typical VRC structure.[23] Although the low CR can provide benefits for the HIDiC over the VRC, relatively large vapor flow through the compressor has a negative impact on the compressor power requirement.

This study deals with an ETBE RD column. To enhance the energy efficiency, an internally HIDiC technique[24] is applied first to the representative fractionator. Dividing the distillation tower into two separate columns, namely rectifier and stripper, the reaction is carried out in the rectifier alone. In HIDiCs, the rectifying and stripping trays are thermally coupled through internal heat exchangers. A compressor and a TV are installed to manipulate the pressure difference between the two diabatic sections. It is noticed for the sample ETBE system that the reaction conversion in the HIDiC rectifier has decreased at the elevated pressure compared to the conversion obtained in the conventional RD (CRD) column. This happens because of the mismatch of necessary conditions between the reaction and separation. As stated, the key limitation involved in RD technology is that the necessary conditions (e.g., pressure and temperature) for the reaction must match those of distillation. Consequently, we fail to achieve the desired ETBE purity in the bottoms.

Table 1. Feed Conditions and Column Specifications

No. of stages including reboiler and condenser			23		
Rectification/reactive/stripping stages			22/9–21/2–8		
Reflux ratio			5		
Reboiler duty (kW)			114.22		
Catalyst loading per stage (kg)			2		
Volume of reboiler drum (m^3)			0.3 (70% filled with liquid at steady state)		
Volume of reflux drum (m^3)			0.1 (70% filled with liquid at steady state)		
Feed 2 (EtOH) stage			21		
Feed 2 flow rate (mol/s)			0.312		
Feed 2 temperature (°C) (bubble point)			50		
Feed 2 composition (mol %)			100% EtOH		
Feed 1 stage			9		
Feed 1 flow rate (mol/s)			1		
Feed 1 temperature (°C) (gas phase)			84		
Feed 1 composition (mol %)			30% IB/35% 1-butene/35% *cis*-2-butene		
Overhead pressure (kPa)			700		
Stage pressure drop (kPa)			4.8		
Reflux drum pressure drop (kPa)			10.13		
	IB	1-Butene	*cis*-2-Butene	EtOH	ETBE
Steady state composition (mol fraction)					
Distillate	0.04183	0.46776	0.46646	0.02391	5×10^{-5}
Bottoms	1×10^{-6}	2×10^{-6}	4.5×10^{-5}	0.08853	0.9114

Table 2. Thermodynamic and Physical Properties and their Sources

Property	Method (Source)
Vapor pressure	Extended Antoine equation (Aspen simulator)
Activity	UNIFAC model[28]
Liquid activity coefficient	UNIFAC model[28]
Vapor fugacity coefficient	Ideal vapor phase
Enthalpy	SRK equation of state[29]
Density	SRK equation of state[29]
Heat capacity (C_p and C_v) coefficients	Polynomial expression (Aspen simulator)

For the fair comparison between the CRD and its heat integrated scheme, we attempt to keep the input and output conditions same. To meet this objective, in this work, we adopt an external heat integration approach, namely the VRC that is well established and most suitable scheme for separating close-boiling components. As the example RD considers the separation of a wide-boiling mixture, it becomes more challenging to improve energy efficiency by the classical vapor recompression RD (CVRRD) column. This motivates us to explore a novel multistage direct compression system that addresses a number of practical concerns and appears as an economically attractive scheme with high energy savings potential.

CRD: ETBE System

Figure 1 shows a CRD column used for the production of ETBE.[25,26] It is well known that ETBE is widely used as an oxygenate additive to the gasoline to reduce the emission of mainly carbon monoxide and unburned hydrocarbons. The representative column integrates reaction and separation in the single unit. Here, the trays are counted from the bottom up; trim-reboiler is the first tray, and trim-condenser is the 23rd tray. Actually, the column consists of 23 theoretical stages: one rectifying (excluding a total condenser), 13 reactive and seven stripping trays (excluding a partial reboiler). The feed conditions and column specifications for the ETBE column under study in this article are given in Table 1.

ETBE reaction kinetics and process model

The ETBE synthesis reaction is the reversible etherification of ethanol (EtOH) and isobutylene (IB) over an acid–base catalyst, such as an acidic ion-exchange resin (e.g., Amberlyst 15).

$$\underset{\text{IB}}{(CH_3)_2C{=}CH_2} + \underset{\text{EtOH}}{C_2H_5OH} \leftrightarrow \underset{\text{ETBE}}{(CH_3)_3COC_2H_5}$$

The reaction kinetics is based on the Langmuir–Hinshelwood–Hougen–Watson model,[27] which involves two adsorbed ethanol sites for reaction in the rate limiting step, and the type of catalyst is Amberlyst 15. The reaction rate (r_{ETBE} in mol/s) expression is given below as

$$r_{\mathrm{ETBE}} = \frac{m_c k_r a_{\mathrm{EtOH}}^2 \left(a_{\mathrm{IB}} - \frac{a_{\mathrm{ETBE}}}{K_{\mathrm{ETBE}} a_{\mathrm{EtOH}}} \right)}{\left(1 + K_A a_{\mathrm{EtOH}}\right)^3} \tag{1}$$

where m_c is the catalyst loading per stage (kg). The activity of any component i (a_i) correlates the activity coefficient (γ_i) and liquid-phase composition (x_i) as

$$a_i = \gamma_i x_i \tag{2}$$

Reaction equilibrium constant

$$K_{\mathrm{ETBE}} = 10.387 + \frac{4060.59}{T} - 2.89055 \ln T - 0.0191544T + 5.28586 \times 10^{-5}T^2 - 5.32977 \times 10^{-8}T^3 \tag{3}$$

Adsorption equilibrium constant

$$\ln K_A = -1.0707 + \frac{1323.1}{T} \tag{4}$$

Reaction rate constant (mol/h/g of catalyst)

$$k_r = 7.418 \times 10^{12} \exp\left(-\frac{60.4 \times 10^3}{RT} \right) \tag{5}$$

The following assumptions have been adopted to derive the mathematical model of the CRD: negligible tray vapor holdup compared to liquid holdup, variable tray liquid holdup, perfect mixing and equilibrium on all trays, fast energy dynamics, no side reaction, and nonideal liquid phase. For brevity, the modeling equations are not included in this article and the complete model along with the optimal column setup is available elsewhere.[25] Table 2 summarizes the methods used to estimate the thermodynamic and physical properties for the representative ETBE RD column.

The CRD model consists of a set of ordinary differential equations (ODEs) coupled with algebraic equations/correlations. The ODEs are obtained from mass and energy balances around each plate of the distillation column. The algebraic equations/correlations are used to predict the thermodynamic and physical properties, reaction kinetics, plate hydraulics, and actual vapor-phase compositions. To simulate these modeling equations, computer codes are developed in MatLab environment, and these codes are available upon request.

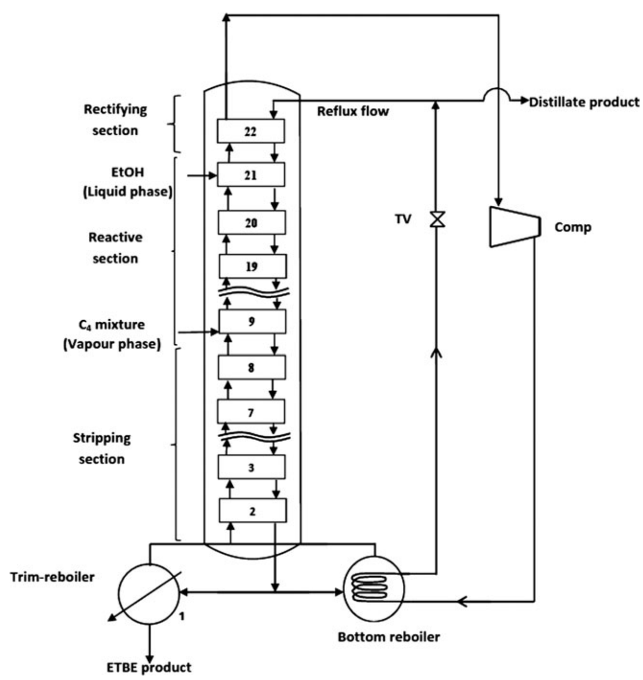

Figure 2. Schematic representation of the CVRRD column [Comp = compressor].

Table 3. Comparison of Estimated Capital (Main Equipment) and Operating (Utilities Per Year) Costs for the CRD and the CVRRD (T_i 335.30 K and $T_o = T_B + 20 = 438.85$ K)

Item	CRD	CVRRD μ 1.10	CVRRD μ 1.18	CVRRD μ 1.30
Condenser				
Duty (kW)	103.34	0.00	0.00	0.00
Area (m^2)	3.86	0.00	0.00	0.00
CW required (ton/yr)	39,241.62	0.00	0.00	0.00
Cost of CW ($/yr)	2354.50	0.00	0.00	0.00
Trim-reboiler (steam-heated)				
Duty (kW)	114.22	2.84	2.84	2.84
Area (m^2)	7.24	0.18	0.18	0.18
Steam required (ton/yr)	1758.16	43.77	43.77	43.77
Cost of steam ($/yr)	38,911.61	968.76	968.76	968.76
Bottom reboiler (compressed vapor-heated)				
Area (m^2)	0.00	7.06	7.06	7.06
Duty (kW)	0.00*	0.00*	0.00*	
Compressor				
CR	0.00	19.31	5.84	3.21
Duty (kW)	0.00	36.62	21.82	14.43
bhp (hp)	0.00	61.38	36.58	24.18
Cost of electricity ($/yr)	0.00	51,266.20	30,552.70	20,195.59
Energy saving (%)	–	1.33	40.20	59.62
Utility cost ($/yr)	41,266.11	52,234.96	31,521.46	21,164.35
Utility cost savings (%)	–	Negative savings	23.61	48.71
Capital cost				
Condenser ($)	29,950.73	0.00	0.00	0.00
Trim-reboiler ($)	45,069.97	4087.24	4087.24	4087.24
Bottom reboiler ($)	0.00	44,336.88	44,336.88	44,336.88
Column ($)	157,949.39	157,949.39	157,949.39	157,949.39
Trays ($)	233,645.88	233,645.88	233,645.88	233,645.88
Compressors ($)	0.00	201,868.21	132,052.85	94,041.03
Total capital cost ($)	466,615.97	641,887.60	572,072.24	534,060.42
TAC ($\theta = 3$) ($)	196,804.77	266,197.49	222,212.21	199,184.49
Payback period, θ (yr)	–	Not feasible	10.82	3.36

*Bottom reboiler receives heat through condensation of compressed overhead vapor.

Classical Vapor Recompression RD (CVRRD) Scheme

It is true that the heat is removed in the condenser at the top and introduced to the reboiler at the bottom of a distillation column. To reuse the heat rejected in the condenser, the temperature of overhead vapor should be raised before thermally coupling the vapor with the reboiler liquid. This can simply be done by some form of heat pump.

Figure 2 represents the CVRRD column, the base case of VRC scheme. The overhead vapor is compressed to such a pressure that its condensation temperature exceeds the boiling temperature of the column bottoms stream. The heat given off by condensation of the compressed overhead vapor is actually used in the bottom reboiler. Note that the condensate leaving the reboiler is flashed across a TV to column top (reflux drum) pressure to provide reflux and distillate stream. By utilizing the internal heat sources, the trim-reboiler duty may be reduced substantially.

In the CVRRD system, the whole overhead vapor is compressed and then condensed in the bottom reboiler supplying heat at the base of the column. The balance of the column heat requirements is then adjusted by steam (an external heating medium) in the trim-reboiler. To judge the operating and economic performance of the CVRRD, in the following, we compute the energy consumption and cost.

Energy consumption

In the thermally integrated schemes, we compute the heat transfer 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). In this work, the energy consumption of a thermally integrated column, Q_{cons} is calculated by the sum of the reboiler duty, Q_R plus three times the compressor duty, Q_{comp} as

$$Q_{\text{cons}} = Q_R + 3Q_{\text{comp}} \tag{6}$$

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.[13] The following equation has been used to estimate the theoretical horsepower (hp) for a centrifugal gas compressor[30]

$$\text{hp} = \frac{(3.03 \times 10^{-5})\mu}{\mu - 1} V_{22} P_i \left[\left(\frac{P_o}{P_i} \right)^{(\mu-1)/\mu} - 1 \right] \tag{7}$$

The polytropic coefficient, μ ($= C_p/C_v$) can be calculated from:

$$1/(\mu - 1) = \sum [y_i/(\mu_i - 1)] \tag{8}$$

In the above equations, the pressure (inlet pressure, P_i and outlet pressure, P_o) is in lb$_f$/ft^2, the overhead vapor flow rate (V_{22}) is in ft^3/min, and y_i denotes the mole fraction of any vapor component i. As reported in Table 2, the values of heat capacity coefficients are taken from the Aspen flowsheet simulator. Using Eq. 8, we obtain the polytropic coefficient at steady-state condition as 1.18.

It is observed that the latent heat released by the compressed overhead vapor (=111.38 kW) is slightly lower than the heat required in the reboiler (=114.22 kW). Therefore, in the CVRRD, as shown in Figure 2, there is no need of

Table 4. Cost Estimating Formula and Parameter Value[30,31]

- *Column shell*: $\left(\frac{M\&S}{280}\right)$ $101.9\, D_c^{1.066} L_c^{0.802}(c_{in} + c_m c_p)$, where D_c is the column diameter, L_c the column height, M & $S = 950$, and the coefficients $c_{in} = 2.18$, $c_m = 3.67$, and $c_p = 1.15$
- *Column tray*: $\left(\frac{M\&S}{280}\right) 4.7 D_c^{1.55} L_c(c_s + c_t + c_m)$, where the coefficients $c_s = 1$, $c_t = 0$, and $c_m = 1.7$
- *Heat exchanger*: $\left(\frac{M\&S}{280}\right) 101.3 A^{0.65}(c_{in} + c_m(c_t + c_p))$, where the coefficients $c_{in} = 2.29$, $c_m = 3.75$, $c_t = 0.1$, and $c_p = 1.35$
- *Compressor*: $\left(\frac{M\&S}{280}\right)$ $2047.24\, Q_{comp}^{0.82}$

any overhead condenser and complete overhead vapor, V_{22} ($=4.487 \times 10^{-3}$ kmol/s) is compressed to supply heat in the bottom reboiler. The rest amount of heat ($=114.22–111.38 = 2.84$ kW) is obtained from external heat source (i.e., steam) in the trim-reboiler. Note that the CR of 5.84 is selected to maintain a reasonable temperature difference ($=20°$C) between two heat exchanging streams in the bottom reboiler. Table 3 reports the percent energy savings ($=[(Q_{CRD} - Q_{CVRRD})/Q_{CRD}] \times 100$) of 40.20% and utility cost savings of 23.61% provided by the CVRRD scheme.

Note that the energy savings of 40.20% is obtained when $\mu = 1.18$. Now, we arbitrarily choose another two cases with $\mu = 1.1$ and 1.3. We know for the isentropic pressure change that

$$\mathrm{CR} = \frac{P_o}{P_i} = \left(\frac{T_o}{T_i}\right)^{\mu/(\mu-1)} \tag{9}$$

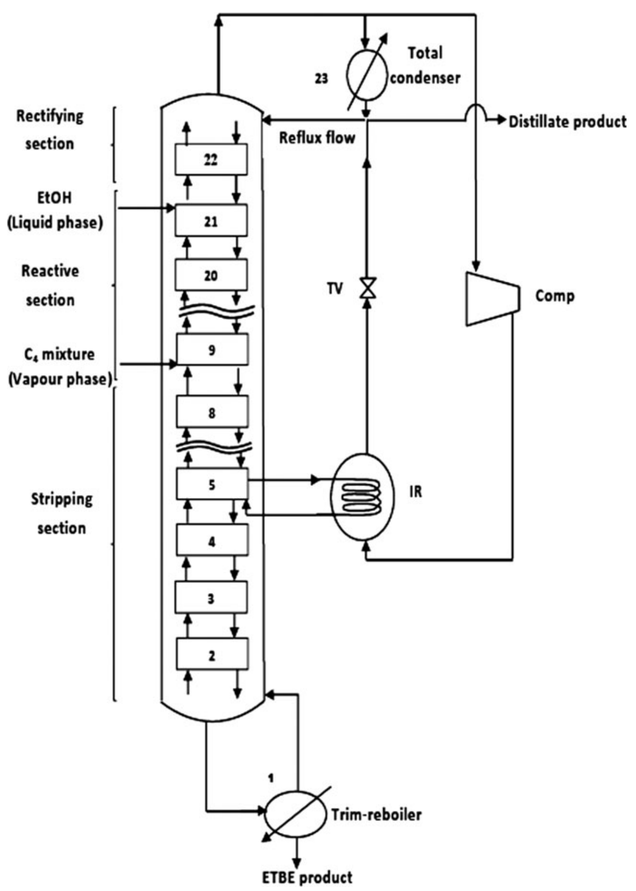

Figure 3. Schematic representation of the VRRDSIR with single compressor column.

It can be seen from Eq. 9 that with the decrease of μ (>1), there is a need to increase the CR for achieving a desired outlet temperature (T_o) with respect to fixed T_i. This may lead to the increase of Q_{comp}, which in turn, decreases the energy savings. This observation is reflected in Table 3. Therefore, we can say that the polytropic coefficient is an important factor that greatly influences the energy consumption.

Cost analysis

Of course, when assessing the relative economics of different arrangements, one must take the capital cost of the system into account as well as the operating costs. In this work, an economic comparison is made in terms of total annual cost (TAC) that is expressed as

$$\mathrm{TAC}(\$/\mathrm{year}) = \text{operating cost (OC)} + \frac{\text{capital investment (CI)}}{\text{payback period}(\theta)} \tag{10}$$

The capital investment is estimated by summing up the cost of equipments (distillation column, heat exchanger, and compressor). The cost estimating formulae are documented in Table 4. For the sake of simplicity, operating costs are taken to be identical to utility [heating steam, cooling water (CW), and electricity] costs, that is, the number resulting from the summation of electricity (0.084 \$/kW h), steam (17 \$/ton), and CW (0.06 \$/ton) costs[12] for a year containing 8000 operating hours. The operating cost of the compressor is calculated as suggested by Douglas[30] based on the bhp (=hp/0.8) and a motor efficiency of 0.6. Here, we assume the compressor efficiency of 0.8.

Like energy efficiency performance study, the cost analysis is also conducted typically considering three cases with polytropic coefficient values of 1.10, 1.18, and 1.3, although the actual value is 1.18. It is evident in Table 3 that increasing the μ value decreases the energy consumption as well as

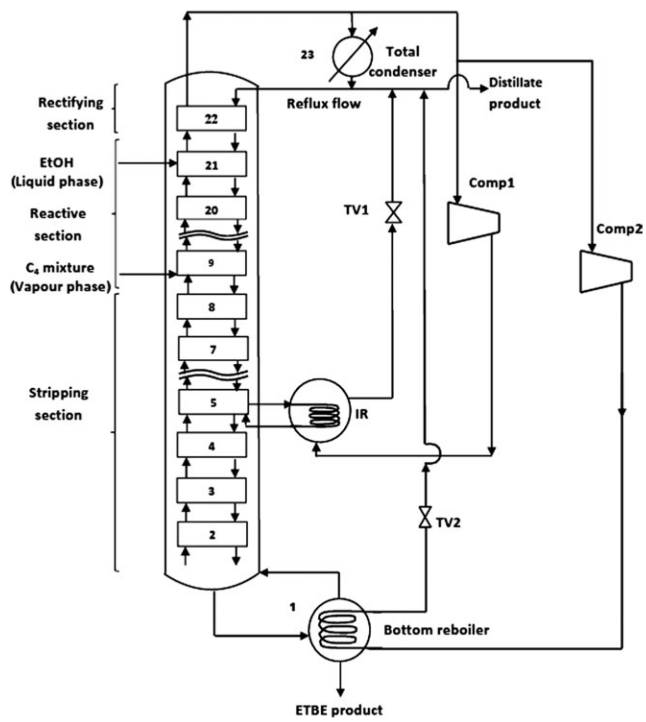

Figure 4. Schematic representation of the VRRDSIR with double compressor column.

Table 5. Comparison of Estimated Capital (Main Equipment) and Operating (Utilities Per Year) Costs for the Various Alternatives of VRRDSIR ($\mu = 1.18$)

Items	Single compressor (compressed vapor for IR and steam for trim-reboiler)			Double compressor (compressed vapor for IR and bottom reboiler)		
	L5	L6	L7	L5	L6	L7
Trim-reboiler (steam-heated)						
Area (m^2)	3.33	3.38	3.49	–	–	–
Duty (kW)	52.50	53.25	54.98	–	–	–
Steam required (ton/yr)	808.08	819.63	846.25	–	–	–
Bottom reboiler (compressed vapor-heated)						
Area (m^2)	–	–	–	3.33	3.38	3.49
Duty (kW)	–	–	–	0.0*	0.0*	0.0*
IR						
Area (m^2)	3.48	3.41	3.22	3.48	3.41	3.22
Duty (kW)	0.0*	0.0*	0.0*	0.0*	0.0*	0.0*
Condenser						
Area (m^2)	1.92	1.93	1.99	0.09	0.08	0.07
Duty (kW)	51.15	51.43	52.95	2.44	2.02	1.94
CW required (ton/yr)	19,418.36	19,523.28	20,100.32	926.25	766.99	734.67
Compressors						
Comp1						
CR1	4.77	4.19	2.81	4.77	4.19	2.81
Duty (kW)	9.62	8.68	5.88	9.62	8.68	5.88
Comp2						
CR2	–	–	–	5.84	5.84	5.84
Duty (kW)	–	–	–	10.29	10.44	10.78
Total energy						
Consumption (kW)	81.36	79.29	72.62	59.73	57.36	49.98
% Energy saving	28.77	30.58	36.42	47.71	49.78	56.24
Utility cost						
Steam ($)	17,884.52	18,140.00	18,729.35	–	–	–
CW ($)	1165.10	1171.40	1206.02	55.57	46.02	44.08
Electricity for Comp1 ($)	13,456.33	12,145.41	8227.26	13,456.33	12,145.41	8227.26
Electricity for Comp2 ($)	–	–	–	14,390.98	14,596.57	15,070.79
Total utility cost ($)	32,505.95	31,456.81	28,162.63	27,902.88	26,788.00	23,342.13
Utility cost savings (%)	21.23	23.77	31.75	32.38	35.08	43.43
Capital cost						
Column ($)	157,949.39	157,949.39	157,949.39	157,949.39	157,949.39	157,949.39
Trays ($)	233,645.88	233,645.88	233,645.88	233,645.88	233,645.88	233,645.88
Trim-reboiler ($)	27,192.91	27,444.79	28,021.10	0.00	0.00	0.00
Bottom reboiler ($)	–	–	–	27,192.91	27,444.79	28,021.10
Condenser ($)	19,022.18	19,088.92	19,453.78	2632.05	2328.28	2264.04
IR ($)	27,966.06	27,618.26	26,595.82	27,966.06	27,618.26	26,595.82
Comp1 ($)	67,462.35	62,023.99	45,066.21	67,462.35	62,023.99	45,066.21
Comp2 ($)	–	–	–	71,281.32	72,115.27	74,030.90
Total capital investment ($)	533,238.77	527,771.23	510,732.18	588,129.96	583,125.86	567,573.34
TAC ($\theta = 3$) ($)	210,252.21	207,380.55	198,406.69	223,946.20	221,163.29	212,533.24
Payback period (θ) (yr)	7.61	6.23	3.37	9.09	8.05	5.63

*Bottom reboiler receives heat through condensation of compressed overhead vapor.

the payback period. Note that the total cost increases with increasing CR (i.e., decreasing μ) mainly due to the increased electricity and compressor costs. Actually, the cost of the compressor increases nearly proportionally to the break power. It confirms that μ plays a vital role in heat integration.

Although we have achieved 40.20% reduction in energy consumption, the results given in Table 3 show that the CVRRD column ($\mu = 1.18$) provides a payback period of 10.82 years, which is reasonably high. In this external heat integration scheme, it happens mainly because of the (see Table 3): (1) low polytropic coefficient value and (2) large temperature difference between the two ends of the column (=83.55 K). The first reason is related to the physical property (i.e., heat capacity) of the concerned system and therefore, this work is devoted to propose a VRRD structure that can efficiently handle the case with wide-boiling mixture separation. In the following, several heat pump arrangements are explored and analyzed.

Vapor Recompression RD with IR

In a conventional distillation column, heat is supplied from an external source only to the reboiler where the temperature is the highest, and heat is removed using a cooling medium only from the condenser where the temperature is the lowest. There is no doubt that the heating costs increase with increasing temperature and the cooling costs increase with decreasing temperature. We have observed for the example ETBE system that the CVRRD scheme is not economically so attractive. Therefore, it is suggested[21,32] to use intermediate/side heat exchanger(s) to treat a large-boiling range mixture in a VRC structure.

In this work, we propose a vapor recompression RD with IR (VRRDIR) for the ETBE RD. Here, we develop two configurations of this VRRDIR scheme on the basis of the number of IR used. They are named as the vapor recompression RD with single IR (VRRDSIR) and vapor recompression RD with double IR (VRRDDIR). Both the mechanisms are detailed in the following subsections.

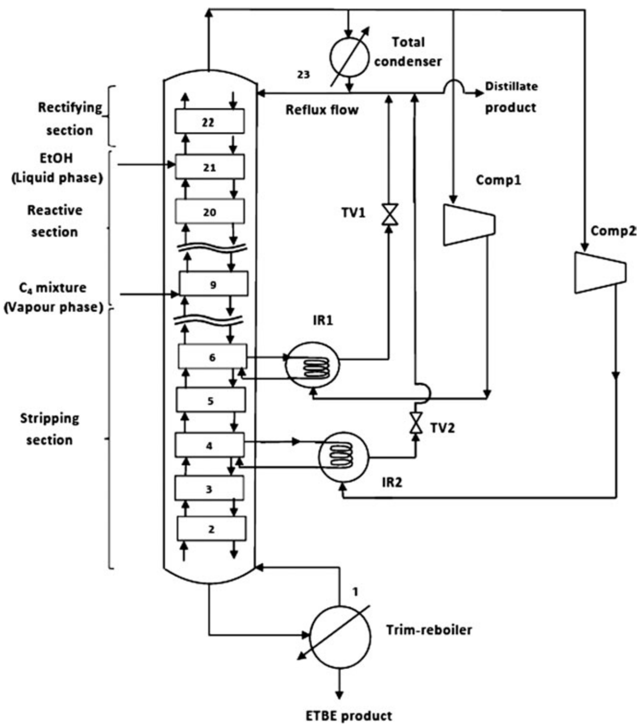

Figure 5. Schematic representation of the VRRDDIR column.

The VRRDSIR scheme

The VRRDSIR scheme consists of a trim-reboiler (steam-heated), a bottom reboiler (compressed vapor-heated), and an IR (compressed vapor-heated). Previously, it is inspected for the CVRRD column that the complete condensation of compressed overhead vapor provides heat which is lower than the required reboiler heat duty for normal steady-state operation. Therefore, at this stage, it is logical to utilize the whole overhead vapor as a heat source. Of course, we can split this overhead vapor and compress the vapor fractions in separate compressors to use in both bottom reboiler and IR. Alternatively, we can use the whole or a part of compressed overhead vapor in only the IR and use a heating medium (i.e., steam) from external source in the trim-reboiler. For a wide-boiling mixture separation, earlier it is investigated for the CVRRD that the use of compressed overhead vapor in the bottom reboiler is not economically advantageous.

Therefore, we attempt to utilize the compressed overhead vapor either only in the IR or both in the IR and bottom reboiler of the example ETBE system. Accordingly, we again classify the VRRDSIR into two structures based on the number of compressors used as: VRRDSIR with single compressor (Figure 3) and VRRDSIR with double compressor (Figure 4). In the former scheme, a part of the overhead vapor is compressed and then used in the IR to vaporize the tray liquid of the ETBE column, and the rest amount of the overhead vapor is fed to the trim-condenser. In the later strategy, the overhead vapor is split into three parts: one goes to the first compressor (Comp1) and is subsequently used to reboil the tray liquid in the IR; another part is fed to the second compressor (Comp2) and then used to reboil the bottoms in the bottom reboiler; and the rest amount is sent to the trim-condenser. Obviously, unlike the CVRRD, both the VRRDSIR schemes require the trim-condenser.

In this work, the CR for all VRC schemes is selected, so that there exists a temperature difference of 20°C between the compressed vapor and the tray/bottom liquid. Throughout this study, we assume that this 20°C temperature difference is sufficient for complete condensation of the overhead vapor in the reboiler.

We now turn our attention to find the optimum position of IR. To avoid any negative impact on the liquid phase reaction, it is decided to supply heat through IR to a point/tray located within the stripping zone. It is true that we require lowest compressor work and highest trim-reboiler duty when the vapor is condensed at as low a temperature as possible. It clearly indicates the necessity of finding the optimum position of IR for both single and double compressor schemes.

Table 5 summarizes a comparative study in terms of energy savings and TAC (or payback period). Three tests are conducted and in each test, one tray [among Trays 5 (i.e., location 5 or L5), 6 (i.e., L6), and 7 (i.e., L7)] is coupled with the IR. It is observed in some earlier studies[19,21] and confirmed here that the overall economic performance is deteriorated when the intermediate exchanger is near the trim-reboiler. Therefore, the trays below fifth one have not been considered here for testing. Again, Tray 8 has not been considered for thermal coupling suspecting its adverse impact on liquid phase reaction. So, for single and double compressor mechanisms, total six options have been analyzed. By conducting sensitivity tests, we determine for all six cases that about 50% of the liquid stream leaving a stripping tray is vaporized in the IR. We fix it at 50% based on two important criteria: matching of input–output conditions between VRRDSIR and CRD, and economic performance in terms of TAC.

It is evident in Table 5 that the all three double compressor schemes provide almost 20% more energy savings compared to their single compressor counterparts. However, the VRRDSIR with single compressor cases show better economic figures. The results indicate that as the IR is shifted upward, the payback period reduces and ultimately the best economic performance is achieved by the VRRDSIR-L7 with single compressor. It confirms that as the position of the intermediate exchanger moves down the column and comes closer to the trim-reboiler, the TAC increases. For identifying the optimal location of IRs, detailed guidelines are provided in the literature.[19,33]

Based on the cost considerations, the VRRDSIR scheme with steam-heated trim-reboiler is preferred to that with compressed vapor-heated bottom reboiler scheme. Therefore, in the subsequent investigations, only the steam-heated reboiler is selected to use with the VRC schemes.

The VRRDDIR scheme

Figure 5 represents the VRRDDIR. This strategy considers two separate compressors for two IRs and a steam-heated trim-reboiler. The percent of tray liquid vaporization is selected for the VRRDDIR, like the VRRDSIR, by performing sensitivity tests based on the criteria mentioned earlier. The detailed analysis of various combinations is presented in Table 6.

Recall that as we move the location of IR toward the column base, more work is required to compress the overhead vapor and less heat duty is involved in the steam-heated trim-reboiler. For the example wide-boiling mixture separation, we observe for the case of VRRDSIR that the use of compressed vapor as a heating medium below location seven (L7) is relatively less cost effective. In the same direction,

Table 6. Comparison of Estimated Capital (Main Equipment) and Operating (Utilities Per Year) Costs for the Various Alternatives of VRRDDIR (μ = 1.18)

Item	L5–L6	L5–L7	L6–L7
% Vaporization	30–50	30–50	30–50
Trim-reboiler			
Area (m^2)	2.19	2.27	2.31
Duty (kW)	34.51	35.78	36.39
Steam required (ton/yr)	531.18	550.73	560.11
Condenser			
Area (m^2)	1.34	1.38	1.41
Duty (kW)	35.72	36.87	37.45
CW required (ton/yr)	13,560.50	13,997.66	14,216.23
Compressor (Comp)			
Comp1			
CR1	4.18	2.75	2.63
Duty (hp)	11.58	7.71	7.28
Duty (kW)	8.64	5.75	5.43
Comp2			
CR2	4.75	4.64	3.52
Duty (hp)	3.89	3.92	3.27
Duty (kW)	2.90	2.92	2.44
IR			
IR1			
Area (m^2)	3.40	3.21	3.18
Duty (kW)	0.0*	0.0*	0.0*
IR2			
Area (m^2)	1.05	1.07	1.03
Duty (kW)	0.0*	0.0*	0.0*
Total energy consumption (kW)	69.13	61.79	60.0
Energy saving (%)	39.48	45.90	47.47
Operating cost			
Steam ($)	11,756.09	12,188.72	12,396.52
CW ($)	813.63	839.86	852.97
Electricity for Comp1 ($)	12,079.11	8041.07	7590.78
Electricity for Comp2 ($)	4058.91	4089.97	3407.35
Total utility cost ($)	28,707.74	25,159.62	24,247.62
Utility cost savings (%)	30.43	39.03	41.24
Capital cost			
Column ($)	157,949.39	157,949.39	157,949.39
Trays ($)	233,645.88	233,645.88	233,645.88
Trim-reboiler ($)	20,702.19	21,194.27	21,428.44
Condenser ($)	15,062.65	15,376.52	15,532.17
IR1 ($)	27,564.22	26,533.42	26,396.31
IR2 ($)	12,858.42	13,041.80	12,725.74
Comp1 ($)	61,746.20	44,228.17	42,186.81
Comp2 ($)	25,248.62	25,406.92	21,873.75
Total capital investment ($)	554,777.57	537,376.37	531,738.49
TAC (θ = 3) ($/yr)	213,633.60	204,285.08	201,493.78
Payback period (θ) (yr)	6.11	4.13	3.67

*Bottom reboiler receives heat through condensation of compressed overhead vapor.

as shown in Table 6, the VRRDDIR with L6–L7 combination provides a least payback period among the double IR schemes. It can be concluded now that the VRRDSIR-L7 with single compressor is still the best performer among the various VRC structures discussed till now in this paper.

A Novel Multistage Vapor Recompression RD Column with IRs

So far we analyzed various advanced VRC schemes for the representative ETBE column. Aiming to improve further the energy efficiency and to make it more realistic by addressing some of the practical concerns, a novel multistage vapor recompression scheme having IRs is proposed. Figure 6 illustrates this structure. Probably, the most common assumption we make for heat integrated columns is that there are no superheating and flashing occurred in the compressor and TV, respectively. As shown in Figure 6, there is a possibility of reverse flow of vapor from the reflux drum to the overhead vapor line and usually we disregard this flow. These assumptions are not so serious when the thermally coupled column is operated under a relatively small CR. Note that in the proposed multistage vapor recompression RD scheme, these specific idealizations have been avoided.

In this thermal integration mechanism, heat is supplied by pressurizing the overhead vapor in the first stage of the compressor (Comp-S1) to an appropriate pressure, then condensing a part of the compressed vapor in thermal contact with a tray liquid in the topmost IR (IR1). The pressure of the condensate from the IR1 is equalized with that of the reflux drum through a TV (TV1). Remaining portion of the vapor leaving Comp-S1 is re-entered to the second stage of the compressor (Comp-S2) before treating it as a heat source in the bottommost IR (IR2). The condensate formed in IR2 at higher pressure is let down through TV (TV2) to IR (IR1) at lower pressure thus recovering work at the same time. For L6–L7 combination, which provides the best economic performance under VRRDDIR as seen in Table 6, the complete multistage VRC algorithm is given in the Appendix. This algorithm actually explains the computations involved in the vapor recompression mechanism starting from the

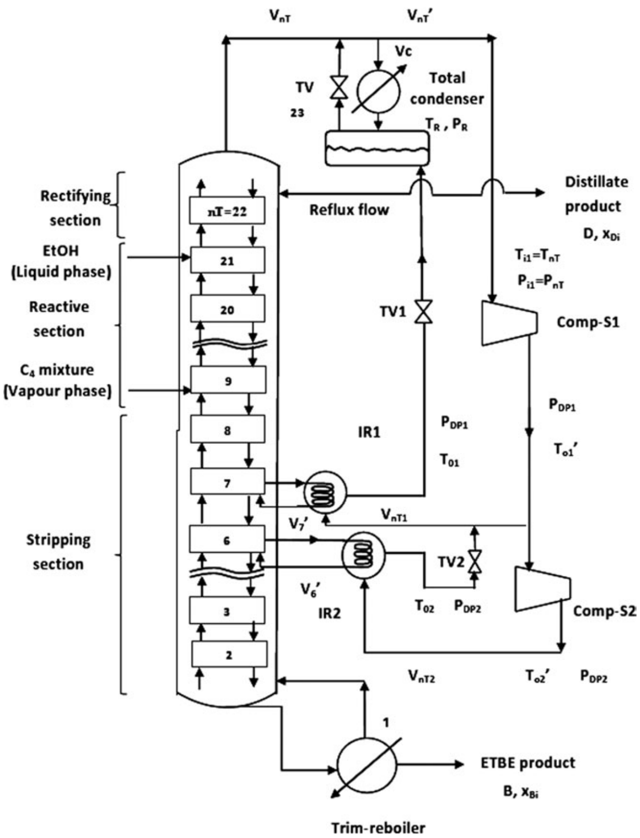

Figure 6. Schematic representation of the double-stage vapor recompression RD column with double IR.

compression of overhead vapor to the reverse vapor flow from the reflux accumulator to the overhead vapor line.

To show the energy efficiency and economic performance of the proposed scheme, we have conducted a detailed analysis in Table 7. It is investigated that the multistage direct compression system with L6–L7 combination requires less overhead vapor for IRs ($=V_{nT1}$) compared to its idealized counterpart (i.e., VRRDDIR with L6–L7 combination) ($= V_{nT1} + V_{nT2}$). For this, the capital investment for condenser and CW cost although increase, at the same time, we should notice for the proposed scheme that the costs of compressor and electricity that have more influence on economic performance decrease. It is observed that the proposed scheme achieves a significant energy savings (=50.60%). Importantly, it also provides a least payback period (=3.23 years) compared to all other schemes discussed so far in this study. So, the proposed multistage VRC structure may be an attractive proposition because of its energy savings potential, low payback period, and practical importance.

Conclusions

This article deals with an industrial heterogeneously catalyzed ETBE RD column that has a large temperature difference between condenser and reboiler. Aiming to improve the thermodynamic efficiency, we first attempt to develop the HIDiC scheme, probably the most popular among the heat integrated schemes. However, it is investigated that the HIDiC method is not suitable for the representative process due to the decrease of reaction conversion in the reactive rectifier operated at elevated pressure. Then, we turn our attention to explore the possibility of external heat integration using the VRC technique, in which, there is no need of any internal pressure elevation that may adversely affect the reaction.

It is well-known fact that the VRC scheme improves energy efficiency for the case of close-boiling mixture separation. However, the sample ETBE column involves a wide-boiling mixture separation and consequently, the classical VRC scheme is unable to improve the thermal efficiency expectedly. In this situation, we explore various advanced VRC configurations that include IR(s) along with a single or double compressor. However, all these VRC configurations are based on a number of simplifications. To avoid the unrealistic assumptions and to improve the energy efficiency further, a novel multistage vapor recompression RD column with IRs is introduced. An algorithm for this proposed scheme is devised showing all computational steps in

Table 7. Comparison of Estimated Capital (Main Equipment) and Operating (Utilities Per Year) Costs for the Proposed Multistage Vapor Recompression RD Column with IRs (μ = 1.18)

Item	L6–L7
% Vaporization	30–50
Trim-reboiler	
Area (m^2)	2.31
Duty (kW)	36.39
Steam required (ton/yr)	560.11
Condenser	
Area (m^2)	2.10
Duty (kW)	55.94
CW required (ton/yr)	21,236.92
Compressors	
Comp1	
CR1	3.09
Duty (hp)	8.16
Duty (kW)	6.09
Comp2	
CR2	1.46
Duty (hp)	0.79
Duty (kW)	0.59
IR	
IR1	
Area (m^2)	3.18
Duty (kW)	0.0*
IR2	
Area (m^2)	1.03
Duty (kW)	0.0*
Total energy consumption (kW)	56.43
Energy saving (%)	50.60
Operating cost	
Steam ($)	12,396.52
CW ($)	1274.21
Electricity for Comp1 ($)	8516.01
Electricity for Comp2 ($)	824.35
Total utility cost ($)	23,011.09
Utility cost savings (%)	44.24
Capital cost	
Column ($)	157,949.39
Trays ($)	233,645.88
Trim-reboiler ($)	21,428.44
Condenser ($)	20,161.91
IR1 ($)	26,396.31
IR2 ($)	12,725.74
Comp1 ($)	46,359.14
Comp2 ($)	6832.07
Total capital investment ($)	52,5498.88
TAC (θ = 3) ($/yr)	198,177.38
Payback period (θ), yr	3.23

*Bottom reboiler receives heat through condensation of compressed overhead vapor.

sequence. It is examined that the proposed multistage direct compression system appears overwhelmingly superior to the classical VRRD and its conventional stand alone column providing a significant savings in energy as well as cost.

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Appendix

An Algorithm for the Proposed Multistage Vapor Recompression RD Column with IRs (See Figure 6)

Step 1: Performing sensitivity tests, determine the amount vaporized (in mol %) of a tray liquid leaving sixth stage (i.e., V'_6) and seventh stage (i.e., V'_7), so that we obtain same output condition and reasonably good economic performance. Vapor boil-up rate in the trim-reboiler is kept unchanged, because it is observed earlier that it is not cost effective to substitute the steam-heated reboiling in the trim-reboiler by compressed vapor-heated reboiling in the trim-reboiler and/or IR(s).

Step 2: Heat involved for the vaporization of liquid leaving sixth and seventh stage can be calculated, respectively, as

$$Q'_6 = V'_6 \times \lambda_6(T_6)$$
$$Q'_7 = V'_7 \times \lambda_7(T_7)$$

where the corresponding tray temperatures, T_6 and T_7, are known and obtained from the process simulator. Accordingly, we can calculate the latent heat (λ).

Step 3: Amount of compressed vapor $V_{n\mathrm{T1}}$ and $V_{n\mathrm{T2}}$ required for intermediate reboiling can be calculated as

$$V_{n\mathrm{T1}} = \frac{Q'_7}{\lambda_{\mathrm{o1}}(T_{\mathrm{o1}})}$$
$$V_{n\mathrm{T2}} = \frac{Q'_6}{\lambda_{\mathrm{o2}}(T_{\mathrm{o2}})}$$

As assumed, the complete condensation of the overhead vapor in the reboiler occurs when there exists a temperature difference of 20°C between two heat exchanging streams. Accordingly, T_{o1} $(= T_7 + 20)$ and T_{o2} $(= T_6 + 20)$ are known.

Step 4: Let $V'_{n\mathrm{T}} = (V_{n\mathrm{T1}} + V_{n\mathrm{T2}})$. Check whether $V_{n\mathrm{T}} > V'_{n\mathrm{T}}$ or $V_{n\mathrm{T}} < V'_{n\mathrm{T}}$.

1. If $V_{n\mathrm{T}} > V'_{n\mathrm{T}}$, an overhead condenser is needed to condense V_c amount of vapor. Here, $V_{n\mathrm{T}} = V'_{n\mathrm{T}} + V_c$.

2. If $V_{nT} < V'_{nT}$, either it is required to reduce % vaporization of tray liquid or additionally use another external heating medium to keep the vaporization rate unaltered. This case requires a detailed study on operational feasibility and relative cost.

In the proposed vapor recompression RD column, $V_{nT} > V'_{nT}$ and therefore, we need an overhead condenser.

Step 5: For the double-stage compressor, find compression ratio CR1 (for Comp-S1) and CR2 (for Comp-S2) knowing all four temperature values from

$$\mathrm{CR1}\left(=\frac{P_{o1}}{P_{i1}}\right)=\left(\frac{T_{o1}}{T_{i1}}\right)^{\mu/(\mu-1)}$$
$$\mathrm{CR2}\left(=\frac{P_{o2}}{P_{o1}}\right)=\left(\frac{T_{o2}}{T_{o1}}\right)^{\mu/(\mu-1)}$$

At this moment, we consider that P_{o1} and P_{o2} represent the output pressure of Comp-S1 and Comp-S2, respectively. Similar notation (T_{o1} and T_{o2}) is used for temperature.

Step 6: Perform flash calculations for TV, TV1, and TV2. For this, we need input stream information (flow rate, composition, temperature, and pressure) and flash specifications (temperature and pressure). Note that the flash temperature and pressure for TV1 are T_R and P_R, respectively; for TV, they are T_{nT} and P_{nT}, respectively. The flash conditions for TV2 will be explained in Step 7. After flash calculation, update V_c (part of V_{nT} left for condensation). Recall that $V_{nT} = V'_{nT} + V_c$.

We have used the Aspen Plus simulator for flash calculations. It is found that no flashing occurs in TV as well as in TV1, and 100% flashing occurs in TV2. Accordingly,

$$V'_{nT} = V_{nT1} \text{ since } V_{nT1} > V_{nT2}, \text{ and}$$
$$V_C = V_{nT} - V_{nT1}$$

Step 7: Now, we proceed for the calculation related to the double-stage adiabatic compression. First, we discuss the case of first-stage (Comp-S1) and then the same method can be extended to second-stage (Comp-S2). At P_{o1}, the actual temperature of the adiabatically compressed vapor is T_{o1} and the corresponding dew-point temperature is T_{DP1}. In adiabatic compression, $T_{o1} > T_{DP1}$; it means that the compressed vapor leaving Comp-S1 is at superheated state. Now, we propose two vapor recompression mechanisms as detailed in the following.

1. With no update of CR1: When V_{nT1} at P_{o1} and T_{o1} enters the IR1, the heat released by this vapor is estimated as V_{nT1} $(T_{o1} - T_{DP1}) + V_{nT1}\ \lambda_{DP1}\ (T_{DP1})$. It is clear that the temperature difference between T_{DP1} and tray liquid temperature T_7 (denoted by $\Delta T(= T_{DP1} - T_7)$) becomes less than 20°C. Consequently, the partial condensation of V_{nT1} in IR1 should occur, and this (1) leads to the reduction of thermal efficiency of vapor recompression and (2) changes the steady-state condition due to the change in amount of tray liquid vaporization. Note that in this mechanism, the flash occurs (Step 6) in TV2 at P_{o1} and T_{o1}.

2. With an update of CR1: At T_{o1}, the actual pressure of the adiabatically compressed vapor is P_{o1} and the corresponding dew-point pressure is P_{DP1}. In adiabatic compression, $P_{DP1} > P_{o1}$; it implies that the compressed vapor leaving Comp-S1 is a superheated vapor. Now, the new CR is obtained as

$$(\mathrm{CR1})_{\mathrm{new}} = \left(\frac{P_{DP1}}{P_{i1}}\right)$$

At this new/updated CR, the temperature of compressed vapor changes to say, T'_{o1} ($> T_{o1}$) and it is calculated from

$$T'_{o1} = T_{i1} \times \mathrm{CR1}_{\mathrm{new}}^{(\mu-1)/\mu}$$

In addition to the degree of superheat ($= V_{nT1}$ $(T'_{o1} - T_{o1})$), this overhead vapor provides the latent heat ($= V_{nT1}\ \lambda_{o1}\ (T_{o1})$) through complete condensation, as $\Delta T(= T_{o1} - T_7) = 20$°C. Under this second mechanism, V_{nT1} is reduced than the value calculated in Step 3. Therefore, it is required to update the calculations involved in Steps 3 and 4. In addition, CR2 should be updated in Step 5 as

$$\mathrm{CR2}\left(=\frac{P_{o2}}{P_{DP1}}\right)=\left(\frac{T_{o2}}{T'_{o1}}\right)^{\mu/(\mu-1)}$$

Note that the flash occurs (Step 6) in TV2 at P_{DP1} and T'_{o1}.

We can now follow the same mechanism as discussed in Step 7 for Comp-S2.

To achieve better energy efficiency of VRC structures, it is suggested to follow the second mechanism (Step 7). Under this scheme, the degree of superheat can either be utilized for vaporizing the tray liquid (in IR) or be removed using intercooler(s). The former option is favorable for effective heat integration due to the proper utilization of internal source of energy. In the later option, the work requirement is less for a "particular" CR, although it involves additional capital investment and operating cost for the intercooler(s). As we need to maintain ΔT of 20°C, not a fixed CR, for the representative ETBE column, the second mechanism (Step 7) with no intercooler(s) is adopted.

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