Performance Investigation of a Variable Speed Vapor Recompression Reactive Batch Rectifier

Kshitiz Johri, G. Uday Bhaskar Babu, and Amiya K. Jana
Dept. of Chemical Engineering, Indian Institute of Technology–Kharagpur, West Bengal-721 302, India

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Introduction

The distillation accounts for an estimated 3% of the world energy consumption.[1] In the US, about 10% of the industrial energy consumption accounts for distillation alone.[2] It is surprising that the overall thermodynamic efficiency of a conventional distillation is only around 5–20%.[3] Apart from the energy and cost savings, the proper utilization of energy also leads to a cleaner environment by minimizing flue gas emissions usually associated with energy consumption. To improve the energy efficiency of the distillation processes, several energy integration techniques have been proposed.

Mah and his team members[4] were devoted in evaluating the heat integrated distillation operations. Since 1980, Takamatsu, Nakaiwa and coworkers[5] have actively been involved in improving heat integration technology. Importantly, a number of research groups[6–9] are also working in this area.

Batch distillation is known to be less energy efficient compared to its continuous counterpart. However, due to its greater flexibility, the batch distillation is widely used in pharmaceutical, fine and specialty chemicals industry where the demand and lifetime of the products may vary significantly with time and may also be uncertain.[10] Keeping the demand of the batch operation in mind, research attention must be paid for improving the energy efficiency.

Almost all published studies have been concentrated mainly on the thermal integration of continuous flow distillation columns with no chemical reaction. In this article, an energy integration technique is explored for a batch distillation, in which the esterification reaction occurs. The proposed energy efficient reactive batch distillation is developed by introducing the compression of top vapor with a variable speed. Along with the manipulation of compression ratio (CR), the external heat input to the still pot and the flow rate of the top vapor leaving for compression have also been adjusted. It is examined that the two variables, among the three, are needed to adjust simultaneously. In this thermally coupled structure, the compressed vapor releases heat in the reboiler through phase change. It is expected that this novel heat integration provides positive energy savings and better economic figures compared to the conventional scheme.

Conventional Reactive Batch Distillation (CRBD) Column

The sample batch reactive distillation column[11] used here for thermal coupling has a total of 8 trays, excluding the reboiler and total condenser. The trays are counted from bottom to top; bottom tray is the 1st tray, and the top tray is the 8th tray. The model is constructed based on the following assumptions: negligible tray vapor holdup, variable liquid holdup, perfect mixing and equilibrium on all trays, reactions occurred on the trays, and in the condenser and reboiler, fast energy dynamics, constant operating pressure (atmospheric), and tray efficiency (Murphree vapor-phase efficiency = 90%), Raoult's law for the vapor–liquid equilibrium, and constant liquid holdup in the reflux drum.

The concerned process produces ethyl acetate and water by the esterification of ethanol with acetic acid

$$\begin{array}{lcccc} \text{acetic acid} & + \text{ethanal} & \rightleftharpoons \text{ethyl acetate} & + \text{ water} & \\ \text{Boiling point (K)} & 391.1 & 351.5 & 350.3 & 373.2 \end{array}$$

The reaction is slightly endothermic and takes place in the liquid phase. The model and system characteristics are reported in Table 1. In the startup phase of batch operation, the sample column operates under total reflux condition. At the end of the startup period, the reactive batch rectifier attains a steady state with the ethyl acetate composition of 0.9213. This composition data imposes an upper limit in the

Correspondence concerning this article should be addressed to A. K. Jana at akjana@che.iitkgp.ernet.in.

Table 1. Column Specifications and Reaction Kinetic Data

Column specifications	
System	acetic acid/ethanol/ethyl acetate/water
Total feed charge, kmol	30.0
Feed composition (startup), mol fraction	0.45/0.45/0.0/0.1
Tray holdup (startup), kmol	0.075
Reflux drum holdup, kmol	0.6
Heat input to the still pot, kJ/min	3200
Reflux ratio, mol/mol	0.955
Distillate composition (steady state), mol fraction	0.9213

Kinetic data

Rate of reaction (kmol/(L min)): $r = k_1c_1c_2 - k_2c_3c_4$
Rate constants: $k_1 = 4.76 \times 10^{-4}$; $k_2 = 1.63 \times 10^{-4}$
Where c_i= concentration (kmol/L) for the ith component

achievable product purity under batch operation. In the subsequent part of the operation, the production phase starts from time = 1,400 min with a reflux ratio, RR (= R/V_8) of 0.955. Figure 1 illustrates the product profile in both the startup and production phase.

Proposed Heat Integration

Vapor recompression reactive batch distillation (VRRBD) scheme

This study aims to evaluate the performance of energy integration in the representative reactive batch rectifier. In order to carry out a meaningful comparison between the CRBD and VRRBD configurations in terms of both energy and cost savings, the input conditions and product specifications are attempted to keep the same. As stated, the target purity level in the top product is set at 92.13 mol %.

Comparing with a conventional column, a typical overhead vapor recompression scheme additionally includes a compressor, a throttling valve and a condenser. The overhead vapor is compressed up to the necessary pressure for its condensation in the still giving the latent heat. Then the pressure is reduced up to the top stage pressure by the employment of a throttling valve. This fact clearly indicates the necessity of a cooler/condenser next to the throttling valve.

The following equation has been used to estimate the theoretical horsepower (hp) for a centrifugal gas compressor[12]

$$\text{hp} = \frac{(3.03 \times 10^{-5})\mu}{\mu - 1} V_8 P_i \left[\left(\frac{P_o}{P_i} \right)^{(\mu-1)/\mu} - 1 \right] \quad (1)$$

The polytropic coefficient (μ) is calculated from

$$1/(\mu - 1) = \sum [y_j/(\mu_j - 1)] \quad (2)$$

In the aforementioned equations, the pressure (inlet pressure, P_i and P_o outlet pressure,) is in lb$_f$/ft,^{2} overhead vapor flow rate (V_8) is in ft^3/min, and denotes the mole fraction of any vapor component j.

As stated, the energy of the cold top stream at temperature T_8 is employed as the energy supply for boiling the hot bottom liquid at temperature T_B. It is apparent that we need to maintain the maximum compression ratio (CR) when the temperature difference $T_B - T_8$ (= ΔT_T) is maximum. As shown in Figure 2 (ΔT_T vs. time), is largest at the end point. However, it will be seen later (see Figure 5) that the largest CR is required at steady state (say at time $t_{,1}$ (= 1,400 min)) because of the highest ethyl acetate composition.

We assume for the example system that the complete condensation of compressed vapor can occur only when the temperature difference, ΔT_o (= $T_{8o} - T_B$) is at least 20°C. Here, T_{8o} refers to the temperature of compressed vapor leaving the compressor. Table 2 reports the affect of CR at t_1th time step on ΔT_o, and heat released by the compressed vapor Q_{cv} (= $V_8\lambda$). Note that the latent heat of any species j, λ_j (kJ/kmol) is considered as a function of temperature, and V_8 is in kmol/min. It is a well-known fact that the Q_{cv} has strong dependence on composition and obviously (see Table 2), weak dependence on temperature (i.e., CR). From Table 2, we observe that the CR of 5 provides the ΔT_o of nearly 20°C at t_1th time step. It implies that to keep the minimum temperature difference of 20°C, at least the CR of 5 (originally 5.23) must be maintained.

Figure 3 displays the amount of heat released by the compressed vapor (CR = 5) with respect to time. As reported earlier, the startup phase takes 1,400 min to reach the steady state. Figure 2 includes the startup profile, in which, the ethyl acetate composition at the top increases with time and then gradually reaches the final state. Virtually there is no acetic

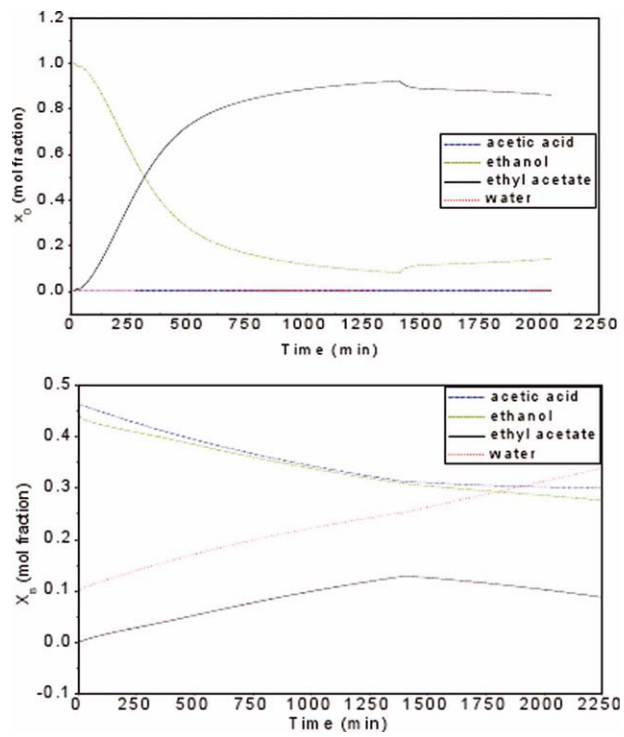

Figure 1. Composition profile throughout the batch operation (*RR* = 0.955 in the production phase).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

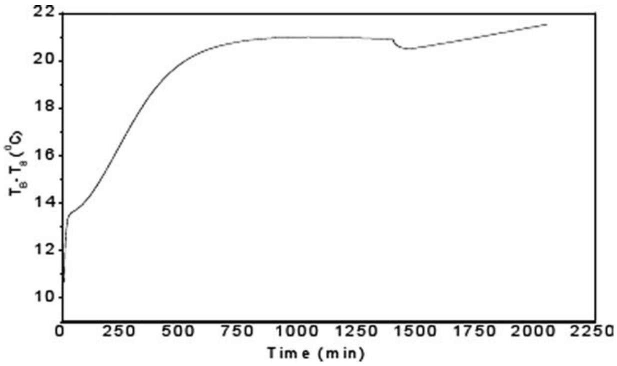

Figure 2. The ΔT_T profile throughout the batch operation.

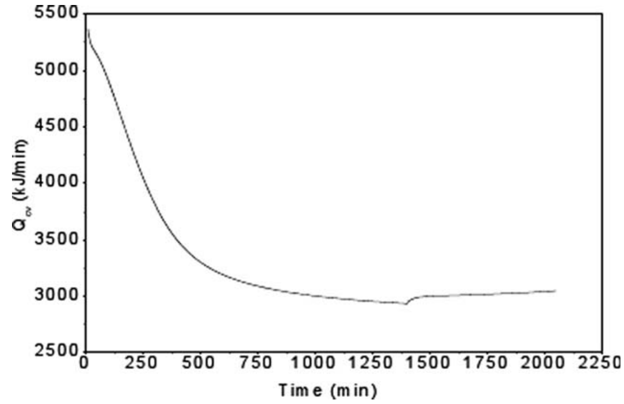

Figure 3. Variation of Q_{cv} with time at CR = 5.

acid in the overhead vapor. So, among the rest of the three components, the latent heat of ethyl acetate is least. As time progresses, the ethyl acetate composition increases and the ethanol concentration decreases (see Figure 1). It is, therefore, logical to obtain the decrease trend of Q_{cv}, and finally a constant value (steady state) in Figure 3. In the production phase Q_{cv} slightly increases due to the same reason stated as earlier.

For the conventional batch rectifier, the constant heat input from external source to the reboiler (i.e., $Q_R = 3{,}200$ kJ/min) is considered. It is evident from Figure 3 that up to 575th min, the heat released by the compressed vapor through phase change is more than the required heat (Q_R). However, in the subsequent time period, the requirement is more (i.e., $Q_R < Q_R$). Therefore, it is suggested to use steam as an external heat source in the reboiler to provide the makeup energy = ($Q_R - Q_R$) beyond 575 th min.

Based on the observation noticed, we suggest two vapor recompression approaches for thermal coupling in the example CRBD process. Those two typical vapor recompression schemes can be operated under (1) the manipulation of process and operating variables, and (2) no manipulation. Based on the configurations and process conditions described earlier for both the columns, the aim of the former approach is to keep the dynamical performance of VRRBD and CRBD identical. The dynamics of the two schemes should differ for the case of no manipulation. It is true that there will be no dynamical difference if exactly 3,200 kJ/min of heat is provided to the reboiler by compressed vapor condensation and/or the use of steam. In addition to the same input conditions and product specifications, this work deals with the thermal integration with fixed dynamical behavior and the case of distinct dynamics will be studied in the next phase.

Table 2. Variation of Q_{cv} and ΔT_o with CR at t_1th Time Step

CR	Q_{cv} (kJ/min)	ΔT_o (°C)	CR	Q_{cv} (kJ/min)	ΔT_o (°C)
1.5	3080.51	−11.24	4.5	2996.74	16.58
2.0	3057.59	−4.16	5.0	2989.20	19.36
2.5	3040.30	1.43	5.5	2982.45	21.89
3.0	3026.53	6.06	6.0	2976.35	24.22
3.5	3015.05	10.02	6.5	2970.79	26.37
4.0	3005.26	13.49	7.0	2965.68	28.37

Variable speed VRRBD scheme

As previously mentioned, along with the same input and output specifications, a comparative study between the CRBD and VRRBD is aimed to conduct with fixed dynamical performance. In order to keep the heat input to the still pot constant (= Q_R), the two variables are to be manipulated simultaneously. They are (1) CR, and (2) the flow rate of overhead vapor entering the compressor (or reboiler heat input through steam (Qr)). Actually, the CR is considered as an operating variable, whereas the other two manipulated variables are the process variables. Typically, the manipulation of CR is required to meet the condition of equals 20°C. At this point, we justify the necessity of overhead vapor-flow manipulation. As stated, the latent heat is strongly dependent on composition and weakly dependent on temperature. Since a batch distillation is an unsteady-state process, the tray liquid composition varies from time to time. We must determine the rate of

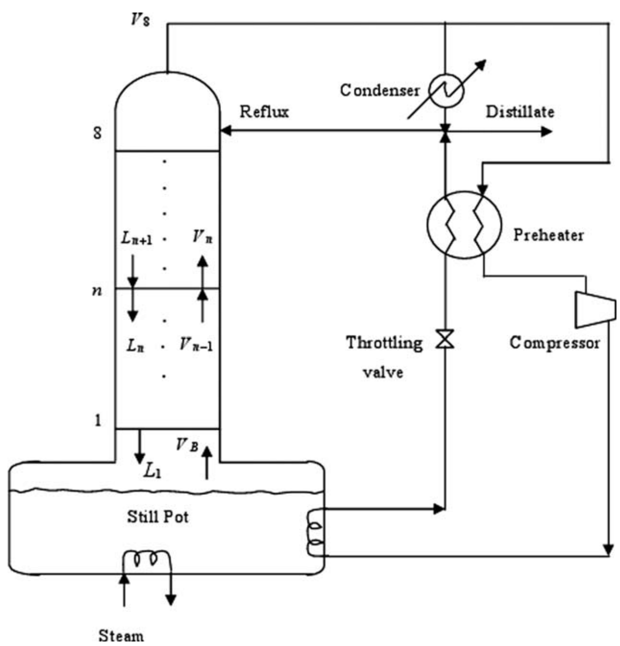

Figure 4. Schematic representation of the proposed variable speed VRRBD scheme.

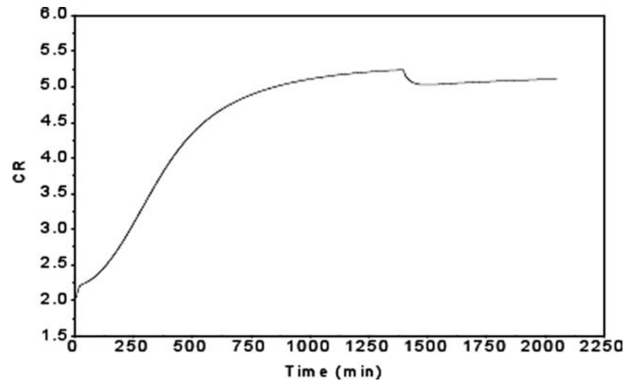

Figure 5. Compression ratio profile throughout the operation.

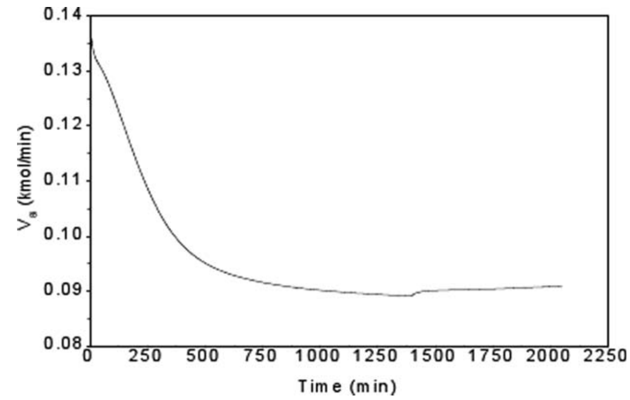

Figure 6. Compressed vapor rate profile throughout the operation.

overhead vapor for compression so that the reboiler receives the heat input of 3,200 kJ/min up to 575th min and in this time period, there is no need of any auxiliary heat input to the still. Beyond this time step, interestingly, the condensation of complete overhead vapor in compressed form can provide lower than Q_R amount of heat. Therefore, 575 min onward, along with the manipulation of CR, the adjustment of steam input, instead of overhead vapor rate, is suggested.

In order to implement the concept of operating/process variable manipulation, we should divide the overhead vapor (V_8) into two streams as: V_{8i} (compressor input) and (overhead condenser input). Of course $V_8 = V_{8i} + \overline{V}_8$. Note that 575 min onward $\overline{V}_8 = 0$. A typical layout of the proposed variable speed VRRBD column is shown in Figure 4. The saturated overhead vapors have been superheated in the preheater above their dew point before being compressed in order to avoid condensation. The preheater in Figure 4 shows the two heat exchanging streams. It is assumed that the hot stream releases heat and finally becomes saturated liquid with regard to top stage pressure.

Calculation of Manipulated Variables

Compression ratio

At a particular time instant, the values of the following variables are obtained from the VRRBD simulator: T_B, T_8 and μ. Accordingly, T_8 ($= T_B + 20$) and λ (T_{8o}) are calculated. Now, we can easily determine the CR for the variable speed VRRBD structure (with P_i equals 1 atm) from

$$CR = \frac{P_o}{P_i} = \left(\frac{T_{8o}}{T_8}\right)^{\mu/(\mu-1)} \tag{3}$$

Overhead vapor fraction (V_{8i})

We have used the following equation to compute time-varying up to 575th min

$$V_{8i}\,\lambda(T_{8o}) = 3200 \tag{4}$$

So the vapor entered the overhead condenser equals $V_8 - V_{8i}$. The manipulations of CR, V_{8i} and reboiler heat input (Q_r) are demonstrated in Figures 5, 6 and 7, respectively.

Energy Savings

As stated, the CRBD provides a distillate composition of 0.9213 at steady state. In this study, we consider the continuous withdrawal of the top product until the distillate composition remains above 0.86. Accordingly, Figure 2 shows the total production period of 651 min.

The heat load involved in operating the thermally integrated column, Q is estimated by the sum of the reboiler duty Q_r, plus three times the compressor duty Q_{comp} (Eq. 1)

$$Q = Q_r + 3Q_{comp} \tag{5}$$

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, and is determined empirically, taking in to account the energy costs of electricity in Japan.[13]

For the example system, Eq. 5 is used for finding the energy consumption in both startup phase (Q_{SP}), as well as production phase (Q_{PP}). The total energy consumption of the variable speed VRRBD (Q_{VRRBD}) is then calculated as

$$Q_{VRRBD} = Q_{SP} + Q_{PP} \tag{6}$$

It is supposed that in every year, 232 batch cycles are operated. Accordingly, we obtain Q_{CRBD} of 6.56×10^6 kJ and

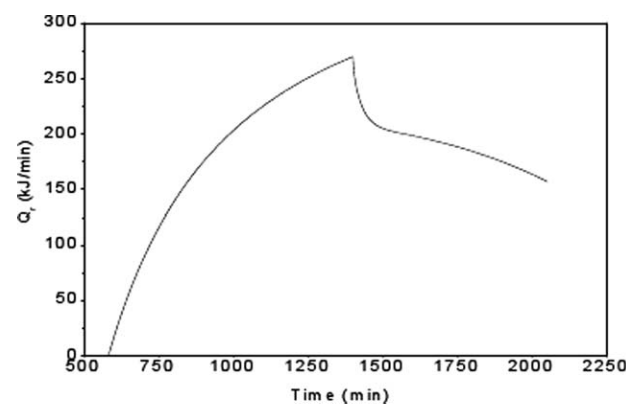

Figure 7. Reboiler heat input profile throughout the operation.

Table 3. Comparison of Estimated Capital (main equipment) and Operating (utilities per year) Costs in $ for the CRBD and the Variable Speed VRRBD Schemes

Cost component	CRBD	Variable Speed VRRBD
Hardware		
Column shell	37510.29	37510.29
Column tray	1549.78	1549.78
Compressor	0.0	24359.55
Reboiler	18748.70	18748.70
Condenser	37130.44	20531.12
Preheater	0.0	16599.32
Total	94939.21	119298.76
Utilities		
Steam	12818.0	528.5
Cooling water	1280.64	87.68
Electricity	0.0	7413.15
Total	14098.64	8029.33
TAC (for 5 years payback time)	33086.48	31889.08 (3.62% savings)
Payback period = 4.01 years		

Q_{VRRBD} of 2.24×10^6 kJ. It corresponds to the maximum energy savings ($[(Q_{CRBD} - Q_{VRRBD})/Q_{CRBD}] \times 100$) of 65.85%.

Economics

The energy integration in a distillation process usually provides a significant energy savings, but at the cost of an increased capital investment. Therefore, for proposing a heat integrated structure, it is a common practice to show positive energy savings along with better economic figures. It is already shown that the proposed variable speed VRRBD scheme provides a significant energy savings (65.85%). The purpose of this discussion is to perform an economic comparison in terms of total annual cost (TAC) between the conventional and the proposed energy integrated reactive batch rectifier. We know that

$$\text{TAC}(\$/\text{yr}) = \text{operating cost} + \frac{\text{capital investment}}{\text{payback period}} \tag{7}$$

The cost of equipment (distillation column, heat exchanger and compressor) is included within the capital investment, and the operating cost combines the cost of utilities (heating steam, cooling water and electricity). The cost estimating formulas used in this article are those given by Douglas.[12] The operating cost of the compressor is calculated as suggested by Douglas[12] based on the bhp (= hp/0.8), and a motor efficiency of 0.6. Here we assume the compressor efficiency of 0.8. The costs of utilities are taken from literature[14] as: 17 $/ton of steam, 0.06 $/ton of cooling water, and electricity at a cost of 0.084 $/kW.h.

The results given in Table 3 show that the proposed VRRBD column provides a 43% reduction in operating cost, but at an expense of 1.26 times more fixed investment than its conventional counterpart. In the cost analysis, a payback time of 4 years is obtained.

Conclusions

This communication introduces a novel variable speed VRRBD column. For proper utilization of internal heat source, in addition to the compression ratio, the auxiliary heat input to the still pot and the flow rate of overhead vapor leaving for compression have been manipulated. It is observed that among the three manipulated variables, two are required to adjust simultaneously. The proposed energy efficient VRRBD scheme has the ability to provide more than 65.85% energy savings and a payback period of 4 years is calculated. Mainly due to the unsteady-state nature of the batch operation, the thermal integration in a batch column involves significant complexity compared to its continuous counterpart.

The proposed energy integration scheme deals with a slightly endothermic reaction system. The extension of this energy efficient scheme to a batch rectifier having exothermic reaction is currently under consideration.

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