An Energy-Efficient Cost-Effective Transient Batch Rectifier with Bottom Flashing: Process Dynamics and Control

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Exploring an internal heat source through bottom flashing route, this work introduces a dynamic batch column configuration within the framework of mechanical heat pump system. This batch rectifier with bottom flashing (BRBF) scheme attempts to use the reboiler liquid as a heat exchanging medium in the overhead condenser, thereby avoiding the use of any external coolant stream and reducing the consumption of hot utility in the reboiler. Aiming to operate the proposed transient process unit at an optimal state of energy use, we formulate an online open-loop control policy that estimates the multiple control actions simultaneously. Furthermore, in order to achieve constant product purity, a gain-scheduled closed-loop control system is synthesized with keeping the stability margin constant. Simulating a multicomponent reactive system, the novel BRBF arrangement is evaluated in the aspects of energy savings and cost under both the open-loop and closed-loop control modes. © 2015 American Institute of Chemical Engineers *AIChE J*, 61: 3699–3707, 2015
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Introduction

Exponential growth in energy demand, political uncertainty existed in some part of the oil-rich nations and severe effect of increasing greenhouse gas concentration have strongly motivated the concerned research community to explore the alternative of fossil fuels. It is reported that this hydrocarbon fuel meets about 80% of our primary energy requirement[1] and there is a growing concern on declining rate of its reserve. Keeping these major causes of concerns in mind, the research has been resurrected mainly from 1980s in developing the thermally integrating arrangements to retrofit with the existing and matured process units. In this light, the distillation has emerged as a potential candidate for boosting its energy efficiency performance through heat integration route. This is because of its very low thermodynamic efficiency that is typically 10%[2] and extensive energy use, which is an estimated 10% of the total industrial use in the United States.[3]

There are various heat integration schemes reported in the literature.[4] Most popular ones include the heat pump-assisted distillation,[5,6] internally heat-integrated distillation column[7–10] and dividing wall column.[11–13] Among these energy-efficient continuous flow columns, the direct vapor recompression column (VRC)[6,14,15] of mechanical heat pump system has been proven as a most promising and established technology.

As far as batch distillation is concerned, in recent past, the application of vapor recompression is noticed in open literature.[16] It is a fact that the batch VRC is much more complicated and challenging over its continuous counterpart in design and operation mainly because of the dynamic nature involved in batch processing. This apart, another popular category of the mechanical heat pump family is the bottom flashing arrangement. Although this technology has been developed a long back for continuous distillation,[6,17] there is almost no work reported in exploring the technoeconomic feasibility of bottom flashing in the batch distillation. Very recently, we have started working on the design and development of a novel batch rectifier with bottom flashing (BRBF) scheme.

In this contribution, we develop the BRBF column configuration by synthesizing the control system in both open-loop and closed-loop fashions. Aiming to optimize the use of internal heat source, first we formulate an open-loop control policy, exploring all possible scenarios which may exist in operating the BRBF column during both the startup and production phases. This control scheme devices a simulation tool that leads to properly configure the heat integration arrangement with selecting a couple of manipulated variables and estimating their actions. In order to operate the batch column for obtaining the maximum achievable product purity throughout the entire production period, subsequently a gain-scheduled closed-loop control structure is developed for the top composition loop. Finally, a simulation example of a multicomponent reactive system is adopted to illustrate the advancement made in the novel BRBF technology.

Bottom Flashing in Batch Rectifier

A conventional batch rectifier (CBR) operates at transient state in two phases, namely startup phase and production phase. The former operating phase starts with the introduction of thermal energy to the reboiler (or still pot) and ends as soon

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as the batch column reaches the steady state. Under this total reflux operation, the component composition attained in the reflux drum at steady state is the maximum achievable mole fraction of lightest component. Subsequently, the production phase starts as one begins to take out the distillate stream and lasts until the column reaches a specified mole fraction. With this operating strategy, we calculate the total batch time by combining the startup and production periods.

Referring to Figure 1, in the proposed BRBF configuration, a bottom flashing arrangement can typically be designed to retrofit with a CBR. As shown, the input to the bottom flashing loop is the reboiler liquid and the output is a vapor stream that is called boil-up vapor since the same is produced in the still pot. A fraction of reboiler content first enters a throttling valve to reduce its pressure so that the flashed liquid can act as a heat sink in the overhead condenser against the top vapor behaved as a heat source. Getting the entire flashed liquid evaporated at the exchange of complete condensation of overhead stream, the produced vapor (i.e., cold vapor) is subjected to compression at isentropic condition, and then introduced at the column bottom as a boil-up vapor.

At this point, it should be noted that in the bottom flashing loop, there are mainly two units, namely throttling valve (flash drum) and overhead condenser, where the outgoing vapor and liquid streams can achieve the phase equilibrium, making x_B (liquid-phase composition) different than y_B (vapor-phase composition). This happens in practice with involving the dynamic holdups in those two units. Accordingly, one can call the output vapor from the loop as boil-up vapor. This is what we have followed in this work with neglecting the loop dynamics.

It is obvious that the fraction of reboiler liquid flowed through the bottom flashing loop has served dual purpose. First, it acts as a cooling medium in the overhead condenser, avoiding the use of an external coolant. Furthermore, the same fluid sequentially enters the bottom-most tray as a boil-up vapor, cutting/eliminating the consumption of an external heat source. By this way, the proposed BRBF scheme is likely to have the ability of improving energy efficiency performance over its conventional counterpart.

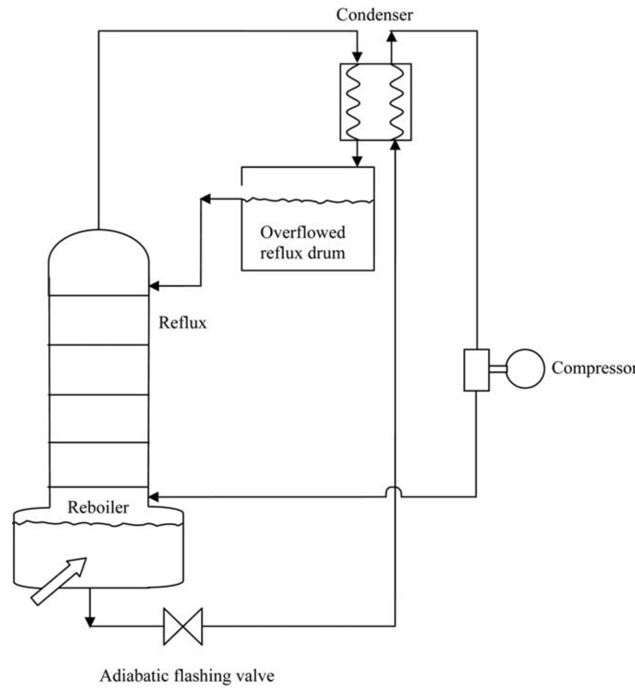

Figure 1. Basic structure of the proposed BRBF configuration.

Mathematical Modeling: The BRBF Column

For developing the model of a tray-type BRBF column, we consider the following assumptions:

A1. Perfect mixing and equilibrium on each stage
A2. Fast energy dynamics
A3. Inefficient trays
A4. No heat loss to the surroundings
A5. Nonideality in liquid phase
A6. Isentropic compression system
A7. Minimum thermal driving force of 20 K[18] required for complete phase change in a heat exchanger
A8. No subcooling/superheating occurred in the compressor
A9. Adiabatic flashing occurred in the throttling valve
A10. No flashed vapor participated in heat exchange with top vapor in the overhead condenser

In the following, we derive the model of all constituent components of the BRBF configuration, namely tray tower, compressor, and adiabatic flash valve.

Tray Tower

The mathematical model of a tray tower consists of mass and energy balance equations coupled with supporting algebraic equations/correlations. The algebraic forms of equations represent the tray hydraulics, phase equilibrium, physical properties, Murphree vapor-phase tray efficiency, and so forth. The resulting differential algebraic equation system includes a number of nonlinear and interactive equations. The complete model of a tray column, consisting of a tray tower, a condenser, and a reboiler, and its computer-assisted simulation algorithm are provided in details in Jana.[19]

Compressor

The following form of correlation is used to find the compressor duty (Q_{Comp})[18]

$$Q_{\text{Comp}} = 3.03\times10^{-5}\,\frac{\mu}{\mu-1}VP_{\text{in}}\left[(\text{CR})^{\frac{\mu-1}{\mu}}-1\right] \tag{1}$$

where the compression ratio (CR) is expressed as

$$\text{CR} = \frac{P_{\text{out}}}{P_{\text{in}}} = \left(\frac{T_{\text{out}}}{T_{\text{in}}}\right)^{\mu/(\mu-1)} \tag{2}$$

Here T_{in} and T_{out} are the inlet and outlet temperatures, respectively, with reference to the compressor. It should be noted that in the above equations, the pressure (inlet pressure, P_{in} and outlet pressure, P_{out}) is in lb_f/ft^2, and the cold vapor stream subjected to compression (V) is in ft^3/min.

For finding the polytropic coefficient (μ), we can use the following form

$$\frac{1}{\mu-1} = \sum_{j=1}^{C}\frac{y_j}{\mu_j-1} \tag{3}$$

in which, C denotes the total number of components and y_j the vapor composition of species j. Note that here the polytropic coefficient for any species j, μ_j ($=C_{Pj}/C_{Vj}$) is temperature dependent and it is calculated based on the heat capacities (C_P) given as temperature polynomials in Perry's handbook.[20]

Adiabatic Flash Valve

The two-phase equilibrium can be expressed as

$$y_{TVj}=k_{TVj}x_{TVj} \tag{4}$$

with

$$\sum_{j=1}^{C} y_{TVj}=1 \tag{5a}$$

$$\sum_{j=1}^{C} x_{TVj}=1 \tag{5b}$$

in which, k_{TVj} denotes the equilibrium coefficient of component j, and y_{TVj} and x_{TVj} are the mole fraction of component j in the flashed vapor and liquid streams, respectively.

The material balance around the throttling valve yields

$$L_B=V_{TV}+L_{TV} \tag{6}$$

$$L_B x_{Bj}=V_{TV}y_{TVj}+L_{TV}x_{TVj} \tag{7}$$

Here, x_{Bj} is the mole fraction of reboiler liquid for species j, and L_{TV} and V_{TV} are the flow rates of the flashed liquid and vapor streams, respectively.

It is now straightforward to have the following form based on Eq. 7

$$x_{TVj}=\frac{x_{Bj}}{1-\Psi(1-k_{TVj})} \tag{8}$$

where Ψ $(=V_{TV}/L_B)$ is the fraction vaporized in the flash operation.

An Open-Loop Multivariable Control Strategy

Why open-loop control strategy?

The principle objective of the proposed mechanical heat pump system is to explore an internal heat source that can minimize the consumption of thermal utility supplied from external sources. With this, we aim to formulate an open-loop control policy that targets to run the BRBF column over the entire batch period at the same dynamics with the CBR, so that the performance improvement likely to achieve through the bottom flashing arrangement is estimated in a meaningful manner. Therefore, the primary goal is set to maintain the heat duty of both the condenser and reboiler (or their equivalence, e.g., condensation rate and vapor boil-up rate) same between the BRBF and its conventional analogous.

Accordingly, like the CBR, the BRBF should operate its top condenser with complete phase change of overhead vapor. With this, the heat released by the condensing vapor is proposed to utilize for vaporizing the flashed liquid left the throttling valve. Now to accomplish the total phase change in both sides of the heat exchanger, a fraction of reboiler liquid (L_B) needs to be flashed at a throttling valve pressure (P_{TV}) before entering the condenser to maintain a thermal driving force (ΔT) of 20 K. Accordingly, it is proposed to manipulate the L_B and P_{TV} that meet the criteria concerning complete phase change at ΔT of 20 K. It should be noted that these two control variables would lead to run the condenser of BRBF at the same heat duty (or condensation rate) with that of conventional standalone column.

Next we turn our attention to maintain the vapor boil-up rate same between the heat integrated column and its conventional counterpart. Accordingly, first we fix our target to convert the cold vapor to boil-up vapor in the bottom flashing loop itself. For this, a compressor is used, and it needs to run at the variable CR to recover the pressure lost at the time of throttling. It should be pointed out that the supply of boil-up vapor to the column bottom is traditionally made through liquid reboiling in the still pot. Since the same vapor stream is likely to obtain from the bottom flashing loop, the reboiler may consequently reduce its boiling rate by adjusting the external heat supply (Q_E). In fact, the Q_E becomes zero when there is no need of boil-up vapor through liquid reboiling in the still and the resulting configuration is referred to as the ideal BRBF scheme. It is now obvious that the attempt of maintaining the same boil-up rate in BRBF and its conventional analogous leads to adjust the CR and Q_E. So overall, the proposed open-loop control policy needs to simultaneously control (or manipulate) the four variables (L_B, P_{TV}, CR, and Q_E) at every time step to operate the proposed BRBF configuration at the same dynamics with the conventional standalone column. It should be noted that this open-loop control scheme is merely specific to the bottom flashing loop, and hence, it does not lead to affect the actual process, that is, the any part of the conventional configuration.

Computation of Open-Loop Control Actions

Among the four control variables mentioned above, it is straightforward to compute the CR by solving Eq. 2 throughout the transient path of the batch processing. Conversely, the L_B and P_{TV} can be estimated by performing the adiabatic flash calculation based on the following known and unknown terms:

Known Terms: Overhead vapor specifications (i.e., flow rate, mole fraction, and temperature), and reboiler liquid specifications (i.e., mole fraction, temperature, and pressure)

Unknown Terms: Pressure (P_{TV}) and temperature (T_{TV}) in throttling valve, flow rate, and mole fraction of flashed liquid (L_{TV} and x_{TVj}) and vapor stream (V_{TV} and y_{TVj}), and reboiler liquid rate (L_B) subjected to flashing

It is worth noticing that the computation of both the L_B and P_{TV} is carried out by developing an online simulation algorithm consisted of two iterative loops. In the outer loop, iterations are made to determine P_{TV} at every time step with satisfying the following convergence condition

$$F(P_{TV})=\left|\sum_{j=1}^{C}\left(\frac{P^0_{TVj}\gamma_{TVj}}{P_{TV}}x_{TVj}\right)-1\right|\le \text{tol}\,1 \tag{9}$$

in which, P^0_{TV} refers to the vapor pressure of flashed liquid, γ_{TV} the activity coefficient and tol the tolerance limit.

Conversely, the inner loop iterates to calculate L_B by satisfying the following convergence criterion

$$F(\Psi)=\left|\sum_{j=1}^{C}\frac{x_{Bj}}{1-\Psi(1-k_{TVj})}-1\right|\le \text{tol}\,2 \tag{10}$$

In both the stated loops, one needs to use an iterative convergence method with defining the tolerance limit (tol) as around 10^{-5} or so.

Subsequently, the fourth control variable, Q_E is proposed to compute from

$$Q_E = Q_R - L_B\lambda_B = Q_R - Q_{BF} \quad (11)$$

with

$$Q_{BF} = L_B\lambda_B \quad (12)$$

where the newly appeared λ_B denotes the latent heat of reboiler liquid and Q_R the reboiler duty of the CBR.

We know that the condenser and reboiler in a CBR operate with using a separate cooling and heating medium, respectively, both of which are supplied from external sources. However, in case of the proposed BRBF configuration, among those two heat exchangers, only the reboiler may require an external medium, whereas the condenser involves the process fluid (i.e., reboiler liquid) flowed through the bottom flashing loop. With this configuration, maintaining the same condensation and vapor boil-up rates in the BRBF with those in the CBR is, therefore, not a trivial task. In fact, it is hardly possible to meet the above stated condition unless the same is not forced to achieve at the dynamic state. Motivated by this fact, now we aim to device a simulation tool that can properly configure the BRBF column with selecting the suitable control variables and estimating their actions.

Possible scenarios in implementing the open-loop control policy

Based on Eq. 11, there may exist two possibilities in the BRBF system as: $Q_{BF} < Q_R$ (Scenario 1) and $Q_{BF} > Q_R$ (Scenario 2). Considering these two possible scenarios at transient state, we can remodel the open-loop control policy introduced above with making some form of modifications.

Scenario 1 ($Q_{BF} < Q_R$): In this scheme, the amount of heat involved with boil-up vapor (Q_R) is more than the heat available through bottom flashing (Q_{BF}). It clearly indicates that $Q_E \neq 0$ and Scenario 1 involves the manipulation of all four variables, namely L_B, P_{TV}, CR, and Q_E, as discussed earlier. So, there is no need of further elaboration of this scheme.

Scenario 2 ($Q_{BF} > Q_R$): This scheme reveals that the heat generated by an internal source through bottom flashing (Q_{BF}) is more than the constant amount of heat consumed in the reboiler (Q_R). Now, one may think that the use of this excess quantity ($= Q_{BF} - Q_R$) in liquid reboiling may decrease the batch processing time with an improvement in separation efficiency. But this is indeed not true, particularly when the column runs with its optimum setup.

As stated, to maintain the same dynamics between the BRBF and its conventional analogous, in this scenario, the top vapor (V_T) leaving the distillation tower is proposed to split into two fractions: one fraction (V_{TBF}) is thermally coupled with flashed stream in the trim-condenser, which was equipped with the CBR. Conversely, the second fraction (V_{TCM}) is recommended to condense by the use of a separate cooling medium supplied from an external source to a second condenser.

Now these two divided fractions of overhead vapor are calculated as

$$V_{TBF} = \frac{Q_R}{\lambda_T(\text{at} \quad T_T)} \quad (13)$$

in which, λ_T is the latent heat of overhead vapor at temperature T_T. Note that all terms in the right-hand side of Eq. 13 are known. Again, with known V_T, we have

$$V_{TCM} = V_T - V_{TBF} \quad (14)$$

Clearly, the BRBF configuration under Scenario 2 manipulates the overhead vapor splitting, along with L_B, P_{TV}, and CR.

It should be highlighted that both the scenarios of BRBF configuration are proposed to manipulate three common variables, namely L_B, P_{TV}, and CR. Moreover, Scenario 1 adjusts the external heat input to the reboiler (Q_E), while Scenario 2 controls the overhead vapor splitting prior to phase change in two condensers.

It becomes obvious that Scenario 1 of the proposed thermally integrated column requires no second condenser and thus, no external cooling medium at all, and a reduced amount of external heat for the reboiler (Q_E). As far as Scenario 2 is concerned, the BRBF configuration requires no external energy for liquid reboiling (i.e., $Q_E = 0$) but involves an additional condenser and associated cooling medium. At this point, it should be stressed that one can select either of these two extreme scenarios or any point of operation lying in between them, whichever provides the minimum total annual cost (TAC).

Gain-Scheduled Closed-Loop Control Strategy

Like the CBR, the BRBF column in conjunction with the multivariable open-loop control scheme operates at transient state with a varying process gain (K_P). Aiming to keep the stability margin constant, it is suitable to use a closed-loop control system that features a variable gain (K_C). With this objective, a gain-scheduled proportional integral (GSPI) controller is attempted to design for regulating the distillate composition (x_{Dj}) by the manipulation of reflux rate (R). Actually, our target is to maintain the product composition (x_{Dj}) at its steady-state value, which is basically the maximum achievable distillate purity obtained in batch processing.

The nonlinear GSPI has the following form[21]

$$R = R_S + K_C(x_{Dj})\left(e + \frac{1}{\tau_I}\int_0^t e\,dt\right) \quad (15)$$

in which, e represents the error and R_S the bias signal. Note that the controller gain, K_C is varied aiming to keep $K_C K_P$ constant, which then keeps the stability margin unchanged, as

$$K_C(x_{Dj}) = \frac{K_C(x_{D0j})K_P(x_{D0j})}{K_P(x_{Dj})} \quad (16)$$

For a distillation column, the gain of the GSPI controller is computed as given below:

1. When $x_{Dj} > x_{D0j}$

$$K_C(x_{Dj}) = K_{C0}\frac{1 - x_{D0j}}{1 - x_{Dj}} \quad (17)$$

where $K_P(x_{Dj}) = 1 - x_{Dj}$ and $K_C(x_{D0j}) = K_{C0}$.

2. When $x_{Dj} < x_{D0j}$

$$K_C(x_{Dj}) = K_{C0} \quad (18)$$

Obviously, K_{C0} and τ_I are the two tuning parameters involved in the GSPI scheme. At this point, it should be noted that as discussed in Jana and Radha Krishna Adari,[22] batch

Table 1. Cost Estimating Formula and Parameter Value

Column shell (MOC: SS)
Installed cost (\$) $=\left(\frac{M\&S}{280}\right)\ 101.9D_c^{1.066}L_c^{0.802}(c_{in}+c_m c_p)$
where D_c is the column diameter (ft), L_c the column height (ft), $M\&S$=1569, and the coefficients c_{in}=2.18, c_m=3.67, and c_p=1.0.
Column tray (Type: bubble-cap, MOC: SS)
Installed cost (\$) $=\left(\frac{M\&S}{280}\right)4.7D_c^{1.55}L_c(c_s+c_t+c_m)$
where the coefficients c_s=1, c_t= 1.8, and c_m=1.7.
Heat exchanger (MOC: SS)
Installed cost (\$) $=\left(\frac{M\&S}{280}\right)101.3A^{0.65}(c_{in}+c_m(c_t+c_p))$
where A is the heat transfer area (ft^2), and the coefficients c_{in}=2.29, c_m=3.75, c_t=1.35, and c_p=0.
Compressor (centrifugal machine, motor drive, base plate, and coupling)
Installed cost (\$) $=\left(\frac{M\&S}{280}\right)517.5(\text{bhp})^{0.82}(2.11+F_d)$
where F_d = 1.0.

distillation does involve a mild nonlinearity and thus, the GSPI is adequate to provide a constant composition control.

Quantitative Performance Indexes

As the qualitative evaluation made before, it becomes apparent that the proposed BRBF configuration has the ability to improve the energetic potential over the conventional standalone column. However, the bottom flashing loop additionally includes a compressor, which again requires electricity for its operation. Moreover, this novel scheme also involves a second condenser under Scenario 2 and thus, additionally requiring a coolant stream for its operation. Therefore, it is logical to perform a quantitative evaluation in the aspects of both energy savings and TAC. In the following, these two performance indexes are briefly highlighted.

Energy Consumption

To evaluate the performance improvement of a thermally intensified unit over its conventional analogous, it is a common practice to estimate the energy savings. For this purpose, here we need to compute the consumption of energy in terms of thermal utility for both the CBR and its heat-integrated counterpart.

For a CBR, the thermal energy is consumed in the reboiler at a fixed rate of Q_R during both the startup and production phases. So the total heat consumption can be calculated from

$$Q_T^{CBR} = Q_R\ (t_{sp}+t_{pp}) \tag{19}$$

in which, t_{sp} denotes the startup period and t_{pp} the production period.

As far as BRBF is concerned, there are two energy components, namely the reboiler having a heat duty of Q_E and the compressor with its duty of Q_{Comp}. Converting the compressor duty to heat duty with a multiplication factor of 3,[23] the total heat consumed by the BRBF (Q_T^{BRBF}) is obtained from

$$Q_T^{BRBF} = \sum_{i=1}^{n}\left[Q_E(i.\Delta t)+3Q_{Comp}(i.\Delta t)\right]\ \Delta t \tag{20}$$

where Δt denotes the sampling instant and n times Δt the last operating point. It should be pointed out that the Q_E and Q_{Comp} in Eq. 20 involved with BRBF scheme are the variable quantity, while as stated above, the Q_R in Eq. 19 involved with CBR is a fixed rate. Anyway, knowing Q_T^{CBR} and Q_T^{BRBF}, one can easily estimate the energy saved through the proposed heat integration route.

Economics

It is a fact that a heat integration arrangement can provide a performance improvement in the aspect of energy efficiency but at the expense of capital cost. Therefore, it is a common practice to further quantify the economic potential of a developed scheme. In fact, attempt should be made to device a configuration through process intensification route that is capable of providing a better energy efficiency as well as economic benefit compared to a conventional standalone column. In this light, we would like to assess the economic potential of the BRBF column in the aspect of TAC.

As we know, the TAC combines the operating and capital costs, both in yearly basis. For this purpose, we consider a payback period of 3 years with 8000 operating hours in each year. The capital investment (CI) includes the cost of all equipments, namely column shell and trays, heat exchanger, and compressor, as reported in Table 1.[18] As far as operating cost (OC) is concerned, there are three utility systems, namely electricity used to drive the compressor, steam used in the reboiler and cooling water spent in the overhead condenser. Costs of these utilities[24] are, respectively, as: \$0.1/kW h, \$13/t, and \$0.03/t. It should be pointed out that the OC of the compressor is calculated as suggested by Douglas[18] based on the bhp (= hp/0.8).

However, the proposed BRBF configuration additionally includes the auxiliaries,[25] such as piping (e.g., pipe, pipe hangers, fittings, insulation, etc.), and electrical equipment and materials (e.g., switches, conduit, wire, fittings, grounding, lighting panels, and associated labor costs) for the bottom flashing arrangement. In this study, we have considered a 20%[26] additional expenses for these auxiliaries, and for additional offsite and indirect costs involved in the BRBF column over its conventional analogous.

A Case Study: Multicomponent Reactive System

A reactive batch distillation example is simulated to investigate the key features of the proposed BRBF system. At first, the heat integrated column is aimed to examine under open-loop control followed by closed-loop control law. In both cases, the performance improvement is quantified with reference to the conventional reactive batch rectifier (CRBR) in terms of energy savings and TAC.

Process Description: The CRBR

Now we concentrate to briefly present the sample CRBR column that consists of a tray tower with eight stages, a total

Table 2. Batch Rectifier Specifications and Reaction Kinetics

Rectifier specifications	
System	acetic acid/ ethanol/ethyl acetate/water
Fresh feed charge (mol)	5000
Feed composition (startup) (mol %)	45/45/0.0/10
Internal plates holdup (mol)	100
Liquid holdup in reflux drum (mol)	12.5
Reboiler heat duty (kJ/min)	1700
Tray efficiency (%)	85
Column diameter (m)	0.175
Weir length (m)	0.14
Weir height (m)	0.0254
Distillate composition (steady state) (mol %)	96.4
Distillate flow rate (mol/min)	34
Kinetic data	
Rate of reaction (kmol/(L min)): $r=k_1c_1c_2-k_2c_3c_4$	
Rate constants: $k_1=4.76\times10^{-4}$; $k_2=1.63\times10^{-4}$	
where c_j = concentration (kmol/L) for the jth component	

condenser and a reboiler. The trays are numbered from bottom to top with the reboiler counted as Tray 1. The column operates at 1 atm pressure with the following esterification reaction occurred in liquid phase in presence of a homogeneous catalyst on all trays

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

The column specifications and the reaction kinetics are reported in Table 2.[27]

Here, the model is developed based on the following considerations, along with the assumptions stated before: nonlinear Francis weir equation to calculate the tray hydraulics, Raoult's law to represent the phase equilibrium and algebraic form of equations for enthalpy calculations. The complete model and simulation algorithm of this sample process unit are available in Jana,[19] and therefore, the same is not reported here.

Model Verification

Performing a simulation experiment under total reflux condition, it is noticed that the batch rectifier reaches steady state with attaining a 96.4 mol % purity in the distillate within a startup period of 591.82 min (i.e., 9.86 h). Table 3 compares the results of the representative CRBR and those produced by Monroy-Loperena and Alvarez-Ramirez[28] at startup phase, verifying our model with a reasonably close accuracy.

Subsequently, the validated model is used to run the simulator in production phase with a fixed distillate rate of 34 mol/min (about 70% of top vapor rate at steady state) until the distillate composition crosses 86 mol % purity, yielding an average composition of about 93 mol % with a production period of 10.75 min. This corresponds to a product yield of 15.11%. It should be noted that this reasonably low yield for the sample esterification reaction is not unusual.

Table 3. Comparison of Simulation Results

	Simulation results	
Item	Present model	Reported model[28]
Number of stages	8	8
Total fresh feed (mol)	5000	5000
Feed composition (mol %) (acetic acid/ethanol/ethyl acetate/water)	45/45/0.0/10	45/45/0.0/10
Column pressure (atm)	1	1
Internal plates holdup (mol)	100	100
Liquid holdup in reflux drum (mol)	12.5	12.5
Distillate composition (mol fract)		
Acetic acid	0.00	0.00
Ethanol	0.0357	0.03
Ethyl acetate	0.964	0.964
Water	2.9×10^{-4}	0.006

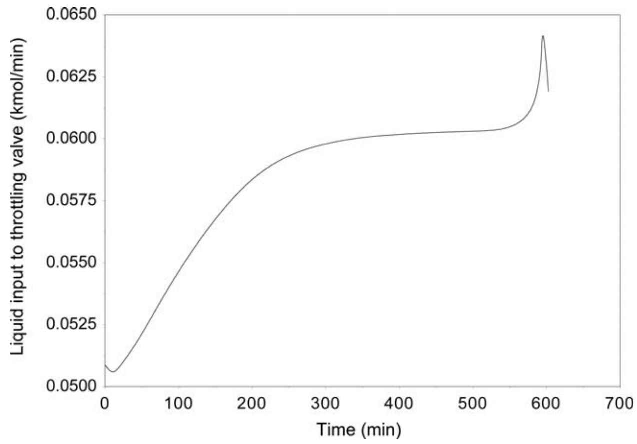

Figure 2. Transient profile of reboiler liquid input to throttling valve (L_B) throughout the entire operation of reactive BRBF column.

Development of the Proposed BRBF Column

As described the mechanical heat pump system before, the bottom flashing loop is accordingly aimed to integrate with the CRBR, yielding a reactive BRBF configuration. The reboiler liquid is first delivered to the adiabatic flashing valve prior to its thermal coupling in the overhead condenser with the top vapor. The produced vapor (i.e., cold vapor) in the condenser is then compressed for pressure adjustment before entering into the column bottom. By this way, the reboiler liquid acts as a heat exchanging medium in the condenser, thereby cutting/avoiding the utility consumption in both the condenser

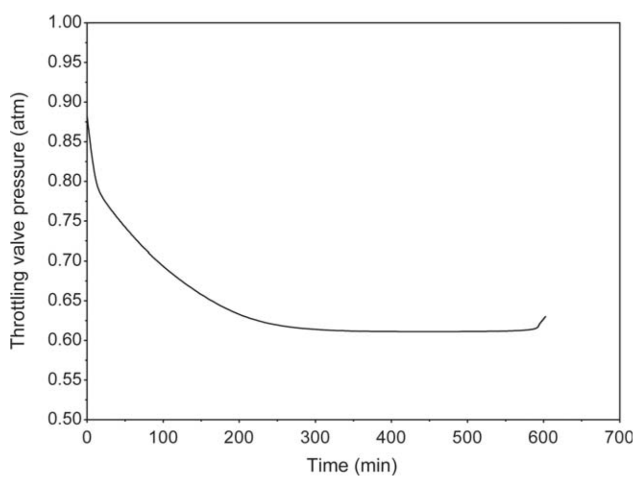

Figure 3. Transient profile of throttling valve pressure (P_{TV}) throughout the entire operation of reactive BRBF column.

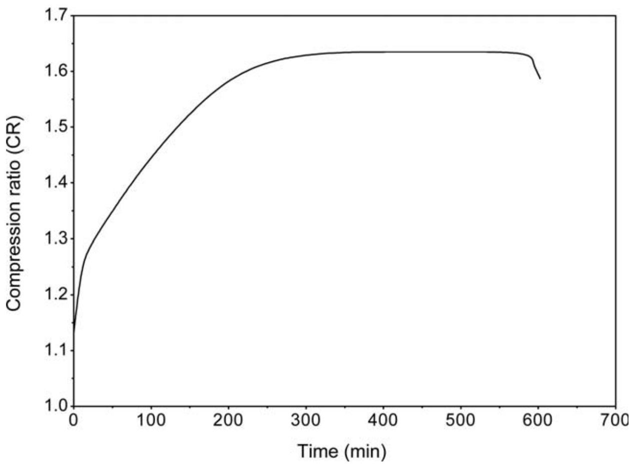

Figure 4. Transient profile of compression ratio (CR) throughout the entire operation of reactive BRBF column.

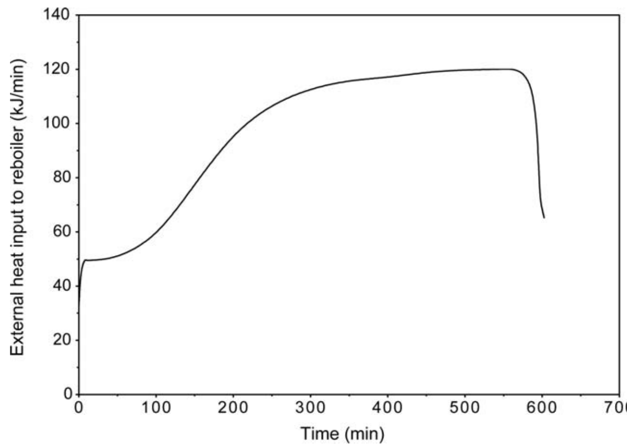

Figure 5. Transient profile of external heat input to the reboiler (Q_E) throughout the entire operation of reactive BRBF column.

and reboiler. However, we should remember that the bottom flashing loop additionally involves a compressor that runs with consuming electrical power. Hence, in the following, a systematic quantitative analysis is performed by comparing them under open-loop followed by closed-loop control system.

Open-Loop Control Policy

As indicated, there would be hardly any point of operation when a certain amount of reboiler liquid flowed through the bottom flashing loop can lead to exactly substitute both the external cooling medium in the condenser and heating medium in the reboiler. We should also note that if the column is chosen to operate beyond Scenario 1 and toward Scenario 2, an additional CI and associated OC for the second condenser are involved, although the OC of the reboiler gets lowered because of the requirement of less external heat utility.

Applying the open-loop control policy developed earlier on the representative reactive system, we observe that it is economic to select Scenario 1 among either of the two extreme cases (i.e., two scenarios) or the control operation at any intermediate point between them. Accordingly, the reactive BRBF adjusts simultaneously the four variables, namely L_B, P_{TV}, CR, and Q_E, based on the proposed variable manipulation algorithm, and their transient profiles are depicted in Figures 2–5.

Closed-Loop Control Policy

The proposed open-loop control policy leads to run the reactive BRBF configuration at the same dynamics with the CRBR, which is required for a fair comparison between them. Accordingly, the heat-integrated column attains the same ethyl acetate composition of 96.4 mol % in the distillate at steady state. Aiming to maintain this maximum achievable product purity throughout the production period, we further use the GSPI controller* ($K_C = 3.53$ and $\tau_I = 0.25$ min) presented earlier. Note that in this closed-loop study, the liquid level in reflux drum is assumed constant. Moreover, as mentioned earlier, the column operates at 1 atm. For maintaining this atmospheric pressure, the column is equipped with an overflowed (i.e., flooded) reflux drum as shown in Figure 1, thus requiring no additional pressure controller.[29]

As shown in Figure 6, the controller regulates the process at a constant composition (96.4 mol %) with gradually increasing its reflux rate as time progresses. The production phase ends when the distillate mole fraction consistently moving away from 0.964 and after a short span of time, it straightway falls vertically. We get exactly same closed-loop responses for the CRBR since its open-loop dynamics is same with its heat-

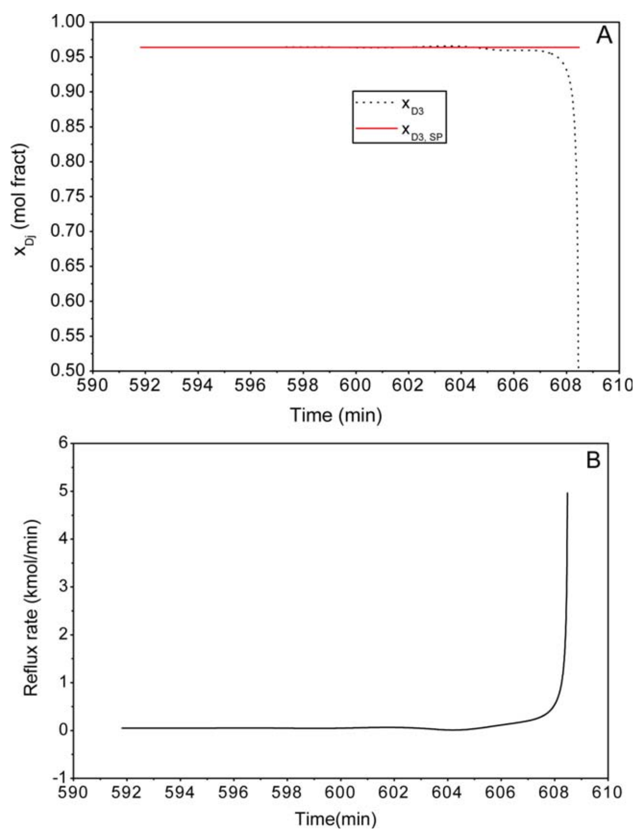

Figure 6. Constant composition control under the GSPI scheme: (A) distillate composition profile and (B) reflux rate profile.

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

*Tuned based on the integral of the square error (ISE) performance criterion.

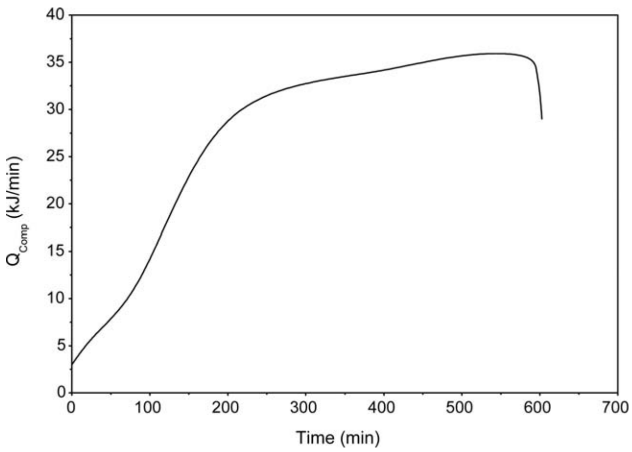

Figure 7. Transient profile of compressor duty (Q_{Comp}) throughout the entire operation of reactive BRBF column.

integrated counterpart. Note that a very close composition profile is shown in Babu and Jana.[16]

Comparative Performance

Energy savings

With the open-loop configuration developed before, it is estimated using Eq. 20 that the total heat consumed throughout the entire batch processing in the thermally integrated column equals 194.56 MJ. In this regard, the transient profiles of external heat input to the reboiler and compressor duty are depicted in Figures 5 and 7, respectively. As far as CRBR is concerned, the total heat requirement, which is calculated based on a batch time of 602.57 min (startup period of 591.82 min + production period of 10.75 min) and a constant reboiler duty of 1700 kJ/min, is obtained as about 1024.37 MJ. Now, one can readily find that the open-loop reactive BRBF column secures a substantial (81%) savings in utility consumption. Conversely, the closed-loop BRBF scheme achieves a close savings of 80.6% with its open-loop analogous.

Economics

In this comparative study, it is evaluated in Table 4 that the proposed open-loop BRBF configuration involves more than about 2% CI with a 78.1% savings in OC compared to the conventional standalone column. Overall, the open-loop arrangement leads to a 24.65% savings in TAC (11% savings with a 20% extra penalty to capital cost), indicating a significant performance improvement achieved through the heat integration route. Conversely, the closed-loop reactive BRBF scheme shows its economic potential in Table 5 with a 25.56% savings in TAC (11.95% savings with a 20% extra penalty), indicating very close economic performance with its open-loop counterpart.

Table 4. Comparison of Estimated Capital and Operating Costs Under Open-Loop Operation

Cost component	CRBR	Reactive BRBF
Capital costs ($)		
Column shell	18,471.50	18,471.50
Column tray	884.65	884.65
Reboiler	17,330.32	9240.12
Condenser	8397.42	8397.42
Compressor	–	9012.75
Total	45,083.89	46,006.44
Operating costs ($/year)		
Electricity	–	1195.32
Cooling water	647.68	–
Steam	6858.02	448.43
Total	7505.70	1643.75
TAC[a] ($/year)	22,533.66	16,979.23
TAC savings (%)	–	24.65
TAC savings (with a penalty of 20% added to the capital cost) (%)	–	11

[a]For a payback time of 3 years.

Table 5. Comparison of Estimated Capital and Operating Costs Under Closed-Loop Operation

Cost component	Closed-loop CRBR	Closed-loop BRBF
Capital costs ($)		
Column shell	18,471.50	18,471.50
Column tray	884.65	884.65
Reboiler	17,330.32	9240.12
Condenser	8596.63	8596.63
Compressor	–	8935.12
Total	45,283.10	46,128.02
Operating costs ($/year)		
Electricity	–	1121.15
Cooling water	645.32	–
Steam	6858.02	325.31
Total	7503.34	1446.46
TAC ($/year)	22,597.71	16,822.47
TAC savings (%)	–	25.56
TAC savings (with a penalty of 20% added to the capital cost) (%)	–	11.95

Applicability of the BRBF Configuration

The feed mixtures are conventionally classified into two classes, namely close-boiling and wide-boiling mixtures. It is well-known that the vapor recompression and bottom flashing mechanisms are best suited for close-boiling mixtures. But this is true only for continuous flow distillation columns because of their purity requirements in both the distillate and bottoms. This leads to a reasonably high pressure (i.e., temperature) change in the heat pump system, which, in turn, requires a large CR for separating a mixture of widely different boiling components. Conversely, in case of batch processing of a wide-boiling mixture, the temperature difference between the two ends (i.e., top and bottom) is not so large, thereby requiring lower CRs. This is because although the batch column produces distillate at the top with a decreasing trend of purity, its bottom (i.e., reboiler) typically includes a mixture of almost all constituent components. Therefore, the proposed BRBF configuration is perhaps suitable for both the close- and wide-boiling systems.

For implementing this BRBF technology in separation industry, a special attention must be taken concerning the plant safety. This remains as a crucial issue since more process units (e.g., compressor and liquid flasher) are getting added in the bottom flashing arrangement.

Conclusions

In this contribution, a bottom flashing loop is proposed to configure with a CBR within the framework of mechanical heat pump system. The unsteady state nature of batch processing makes the design and operation of this heat-integrated column more challenging and complicated compared to its continuous counterpart. Aiming to operate the column with an optimal use of internal heat source, an open-loop control policy is formulated with considering all possible points of operations between two boarder line scenarios. Subsequently, a closed-loop control policy is synthesized to run the batch column with a maximum achievable distillate purity.

Finally, the BRBF arrangement coupled with the open-loop control policy and then the closed-loop control system is illustrated by a multicomponent reactive batch rectifier, showing a promising performance improvement over its conventional counterpart in terms of both energy savings and cost. In our next study, we would like to further verify the performance of the proposed BRBF scheme using some more examples.

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