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Novel use of dividing wall columns for intensification multicomponent batch distillations

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ABSTRACT

While the dividing wall columns for continuous distillations have become quite popular, we present the first detailed analysis of a dividing wall column for batch distillation. For a dividing wall side stripper batch distillation column, we present an operating sequence and its associated mathematical model. Since there are many operating parameter combinations possible for this column, selecting the right operating parameters according to product specifications is presented as an optimization problem. This new configuration's performance is compared with the conventional batch rectifier and the middle vessel columns using two case studies related to the separation of a ternary mixture. The new batch dividing wall column performance is significantly better than the rectifier or the middle vessel column. As the purity specifications increase, the percentage improvement in profit due to the batch dividing wall column compared to the rectifier and the middle vessel columns increases.

1. Introduction

Batch distillation is a commonly used unit operation in specialty chemicals and pharmaceutical industries. The transient nature of batch distillation allows us to configure the column in several different ways. Fig. 1 [6] shows the important configurations of batch distillation currently in practice or proposed. The column in Fig. 1a is the conventional batch distillation column with the reboiler at the bottom and the condenser at the top, which essentially performs the rectifying operation. A single column can be used to separate several products using the multi-fraction operation of batch distillation presented in Fig. 1b. Some cuts may be desired, and others may be intermediate products. These intermediate fractions can be recycled to maximize profits and/or minimize wastes. Fig. 1c shows a periodic operation in which each charge consists of a fresh feedstock mixed with the recycled off-specification material from the previous charge. Fig. 1d represents a stripping column separating the heavy product as the bottom product where the liquid feed is initially charged into the top. In 1994, Devidyan et al. [10] presented a batch distillation column with stripping and rectifying sections embedded in it (Fig. 1e), namely, the middle vessel column. Recent studies demonstrated that it provides added flexibility for the batch distillation operation, especially for separating three-component mixtures [15]. In 1997, Skogestad et al. [22] described a multivessel column (Fig. 1f), which is similar to the MEBDS (multi-effect batch distillation system) of Hasebe et al. [12]. They showed that the column could obtain purer products at the end of a total reflux operation. These various configurations (1d, 1e, 1f) play an important role in separating complex systems like azeotropic, extractive, and reactive batch distillation systems, and where the batch rectifier configuration for such separations may be very restrictive and expensive.

In continuous distillation, a sequence of distillation columns is often used for the separation of multicomponent mixtures. Thermal coupling with the mass exchange between the columns is used to eliminate a reboiler or a condenser and often reduce heat duty [11, 19]. In this type of thermal coupling, a liquid stream is transferred from the first column to the second, and a vapor stream is returned from the second column to the first column. Agrawal proposed the use of such thermally coupled schemes for batch and extractive distillations [1]. The use of ternary schemes was especially illustrated in detail [3]. An advantage of the thermally coupled schemes is that two or more columns can be combined in one column shell by using one or more dividing walls, thereby leading to potential cost savings. [21] The first dividing wall column (DWC) to separate a feed mixture into three product streams was suggested by Wright [16, 23]. Wright's DWC is thermodynamically equivalent to the fully thermally coupled configuration or Petlyuk

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configuration for a ternary mixture [19]. Kaibel not only used this DWC to distill a mixture into three product streams but also brilliantly modified Wright's DWC to distill a mixture into four products and provided the initial momentum towards the implementation of these DWCs [13]. Later Agrawal introduced DWCs for side rectifier and side stripper configurations [2]. A fundamental advantage of these side stripper and side rectifier DWCs is that vapor flow on each side of the dividing wall can be easily controlled through an external reboiler or a condenser. Due to this feature, their use for batch distillation was first identified by Agrawal [1], and Fig. 2 shows the proposed batch distillation DWCs for side stripper and side rectifier cases. In the last two decades, several new DWCs have appeared for ternary distillations. In addition, we now have a theory to draw DWCs for any n-component distillation configuration [4, 20]. This provides us with an array of DWCs that could be attractive for batch distillations. Another attractive feature of the batch distillation DWCs is that they can be modified to use a middle vessel to increase further the versatility of the configuration (Figs. 2c and d).

While there has been a drastic increase in the number of industrial implementations of DWCs for continuous distillations [9, 18, 24], the performance of DWCs for batch distillation vis-a-vis conventional batch distillations has been completely missing. Recently, Lopez-Saucedo et al. [25] analyzed the conventional dividing wall column version of the fully thermally coupled configuration for batch distillation with optimal

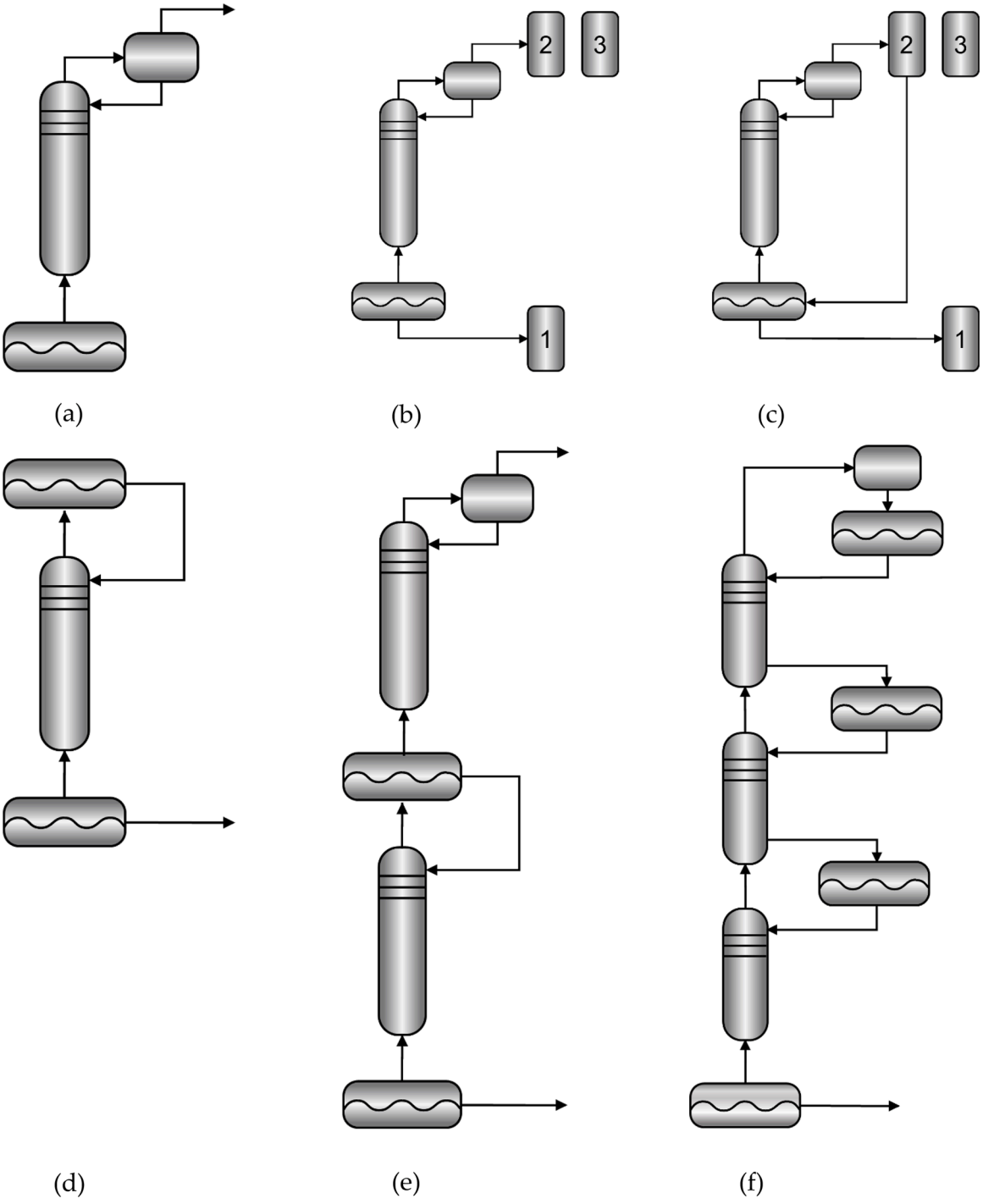

Fig. 1. Currently available configurations of the batch column (reproduced from [6]).

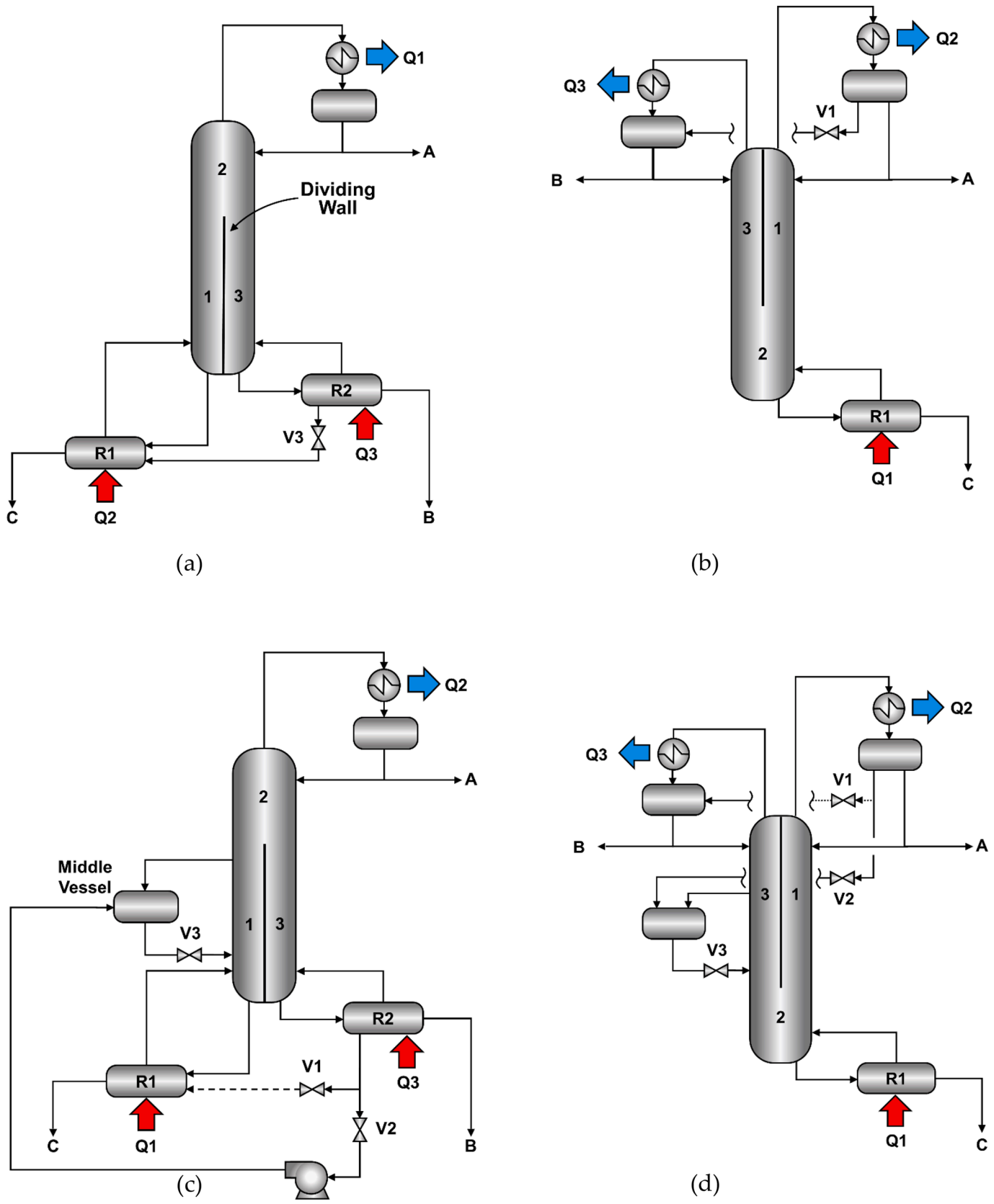

Fig. 2. Batch distillation columns with dividing wall (a) Side stripper DWC, (b) Side rectifier DWC, (c) Side stripper DWC with a middle vessel, (d) Side rectifier DWC with a middle vessel. A is the most volatile, and C is the least volatile component in the mixture. (Source: [1]).

reflux operation and compared the heat duties of this dividing wall column with that of the batch rectifier for a single product with purity specification. Since they only considered single component product separation from the multicomponent mixture, no significant benefit was observed from the dividing wall version used in their work. Here we develop a model and analyze a dividing wall side stripper batch distillation column. We will show that this configuration can separate multiple components more effectively and profitability than the conventional rectifier or the emerging columns like the middle vessel column.

The paper is divided into the following sections. The next section presents the dividing wall side stripper batch distillation column along with the dynamics of this column. Section 2 presents the dynamic model and operating modes. Section 3 is devoted to results and discussions involving two case studies, and the last section is conclusions.

2. Modeling of the dividing wall side stripper batch distillation column

Fig. 2a shows the dividing wall side stripper batch distillation column configuration. As shown in Fig. 2a, the distillation zones 1 and 3 can be built within one column shell. A dividing wall partitions the bottom section into two distillation zones 1 and 3. Each side of the wall has adequate separation stages. Distillation zones 1 and 2 constitute the main column of Fig. 1a, and distillation zone 3 is equivalent to the side stripping column. Liquid descending in distillation zone 2 is distributed between zones 1 and 3. Similarly, vapor ascending in zones 1 and 3 provides the needed vapor stream for the distillation zone 2. The boilup at the bottom of zone 1 is provided through the first reboiler R1, while the boilup at the bottom of zone 3 is provided through the second reboiler R2. A transfer line through valve V3 connects the two reboilers and as explained below this connection allows the transfer of liquid from the second reboiler R_2 to the first reboiler R_1.

The basic operating steps of the side stripper DWC (Fig. 2a) are: (1) Charge the feed containing components A, B, and C in both reboilers R_1, R_2, and holdups on plates. The primary reboiler is R_1, where the majority of the feed is charged. (2). The column is operated at total reflux to establish liquid-vapor inventory throughout the column height. (3) The reflux at the top of the column and the liquid split at the top of the dividing wall are adjusted to ensure the concentration of the heaviest impurity (C in this case) is below the desired level in the vapor and the liquid at the top of the dividing wall (or bottom of Zone 2). (4) The vapor boil-up in reboiler R_2 is adjusted to accumulate intermediate volatility component B while rejecting the volatile component A from Zone 3 to Zone 2 up the column. (5) The presence of the heavy impurity (component) C due to the initial charging of the feed in the reboiler R_2 must be removed by some other means as there is no outlet for this component through Zone 3 under the various liquid-vapor flowrates in various zones. We propose that heavy impurity containing liquid be withdrawn from the reboiler R_2 via valve V3 and fed to the main reboiler R_1. This should be continued till the concentration of C in the intermediate volatility product B has dropped below the acceptable value. Various other versions of this five-step process can be developed for the operation of the side stripper batch DWC, and some of them are described elsewhere [1]. For example, reboiler R_2 may not be charged with a liquid containing heavy component C but with a liquid, which is either a mixture of A and B or just B or even A. In such a case, care must be taken during step 2, while developing liquid-vapor inventory in the column, not to allow passage of the heavy component C from Zone 1 to either Zone 2 or 3. While we have described the operating steps for a ternary mixture, the side stripper DWC can be used to fractionate mixtures containing more than three components into fractions, each enriched in one of the components. Additional operating methods for the DWCs shown in Fig. 2 are described by Agrawal [1].

2.1. Column Dynamics

The number of design parameters for a batch DWC can be substantially larger than the corresponding continuous distillation column. Additionally, the dividing wall side stripper batch distillation column's dynamics involve further integration because of the addition of different dynamics of the column's dividing wall section. To simplify the dynamics, we are assuming a constant molar overflow assumption to eliminate heat balance equations. Therefore, the modeling assumptions for analysis are given below.

- Negligible vapor holdup
- Adiabatic operation
- Theoretical plates
- Constant molar holdup
- Constant molal overflow

To study the dynamics of the column presented in Fig. 2a and its operation for a ternary system, A the start of the operation, we charge the feed from the top so that compositions of both the reboiler and on the plates is equal to the feed composition. We start the column with a total reflux condition. The liquid fraction x is split at the top of the dividing wall to allow flow to the dividing wall side stripper Zone 3. Although not essential, in our simulations, this split is kept constant for the total reflux operation and for each cut. After reaching equilibration, we start withdrawing the products. Fig. 3 illustrates the configuration of the products with important operating variables. In this column, the three products (products 1, 2, and 3) are separated, as shown in Fig. 3. Product 1 will be the first top product (first cut), Product 2 will be accumulated in the dividing wall reboiler R_2, and product 3 in the main column reboiler R_1. There will be a small waste cut after the first cut. For each cut, we change the reflux ratio, R, and the liquid fraction split x. We can change R and x more often (optimal reflux operation) to increase the yield and purity. However, for simplicity of operation, we are keeping R and x constant for each cut. The flow from the dividing wall stripper reboiler to the main reboiler is calculated such that the holdup (H_{div}) in the dividing wall stripper reboiler is kept constant. This is another variable that can be changed to optimize the column performance.

The dynamic equations for this column are presented below. We interchangeably refer to Zone 2 in Fig. 2a as the dividing wall section or the side section.

Condenser and accumulator dynamics

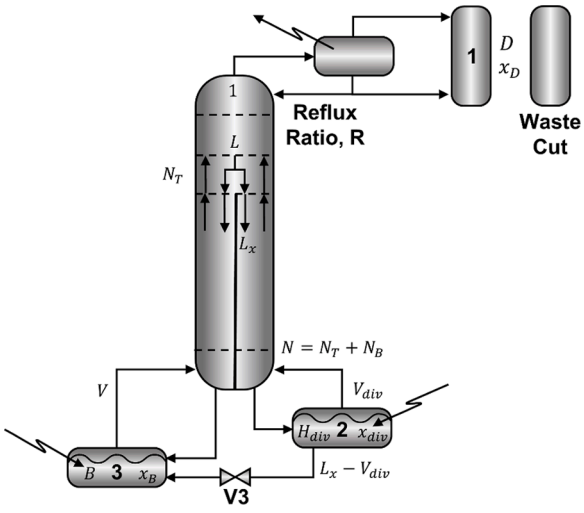

Fig. 3. The Dividing Wall Batch Column Product Configuration (Here the numbers 1, 2, and 3 show products)

$$\frac{dx_D^{(i)}}{dt} = \frac{V_1}{H_D}\left(y_1^{(i)} - x_D^{(i)}\right),\ i = 1,2,\ldots n \tag{1}$$

Plate dynamics (main column)

$$\frac{dx_j^{(i)}}{dt} = \frac{1}{H_j}\left(V_{j+1}\, y_{j+1}^{(i)} + L_{j-1}\, x_{j-1}^{(i)} - V_j\, y_j^{(i)} - L_j\, x_j^{(i)}\right),\ i = 1,2,\ldots n; J = 1\ldots N \tag{2}$$

Reboiler dynamics (main column)

$$for\ \left(LS_{N_B} - V_{div}\right) \geq 0$$

$$\frac{dx_B^{(i)}}{dt} = \frac{1}{B}\left\{L_N\left(x_N^{(i)} - x_B^{(i)}\right) - V\left(y_B^{(i)} - x_B^{(i)}\right) + x_{div}^{(i)}\left(LS_{N_B} - V_{div}\right)\right\},\ i = 1,2,\ldots n$$

$$for\ \left(LS_{N_B} - V_{div}\right) \langle 0$$

$$\frac{dx_B^{(i)}}{dt} = \frac{1}{B}\left\{L_N\left(x_N^{(i)} - x_B^{(i)}\right) - V\left(y_B^{(i)} - x_B^{(i)}\right) + x_B^{(i)}\left(LS_{N_B} - V_{div}\right)\right\},\ i = 1,2,\ldots n \tag{3}$$

Plate dynamics (dividing side}

$$\frac{dxs_j^{(i)}}{dt} = \frac{1}{Hs_j}\left(VS_{j+1}\, ys_{j+1}^{(i)} + LS_{j-1}\, xs_{j-1}^{(i)} - VS_j\, ys_j^{(i)} - LS_j\, xs_j^{(i)}\right),\ i = 1,2,\ldots n; J = 1\ldots N_B \tag{4}$$

Reboiler dynamics (dividing wall)

$$for\ \left(LS_{N_B} - V_{div}\right) \geq 0$$

$$\frac{dx_{div}^{(i)}}{dt} = \frac{1}{H_{div}}\left\{LS_{N_B}\, xs_{N_B}^{(i)} - V_{div}\, y_{div}^{(i)} - x_{div}^{(i)}\left(LS_{N_B} - V_{div}\right)\right\},\ i = 1,2,\ldots n$$

$$for\ \left(LS_{N_B} - V_{div}\right) \langle 0$$

$$\frac{dx_{div}^{(i)}}{dt} = \frac{1}{H_{div}}\left\{LS_{N_B}\, xs_{N_B}^{(i)} - V_{div}\, y_{div}^{(i)} - x_B^{(i)}\left(LS_{N_B} - V_{div}\right)\right\},\ i = 1,2,\ldots n \tag{5}$$

Flowrate calculations:
At the top of column

$$L_0 = R\frac{dD}{dt};\ V_1 = (R+1)\frac{dD}{dt} \tag{6}$$

On the plates (main column)

$$L_j = L_{j-1} = \ldots. = L_0 = L,\ j = N_T \tag{7}$$

$$L_{jj} = L_{jj-1} = \ldots. = L_{N_B+1} = L_{N_T}(1-x),\ jj = N_B + N_T = N \tag{8}$$

$$V_{j+1} = V_j = \ldots. = V_1 = V + V_{div},\ j = N_T \tag{9}$$

$$V_{jj+1} = V_{jj} = \ldots. = V_{N_B+1} = V,\ jj = N_B + N_T = N \tag{10}$$

At the bottom of the main column

$$\frac{dB}{dt} = L_N - V + \left(LS_{N_B} - V_{div}\right) \tag{11}$$

On the plates (dividing wall)

$$LS_j = LS_{j-1} = \cdots. = LS_1 = L.x,\ j = N_B \tag{12}$$

$$VS_{j+1} = VS_j = \ldots. = VS_1 = V_{div},\ j = N_B \tag{13}$$

where

- B = amount remaining in the main reboiler, moles
- D = distillate collected in the accumulator at the top of the column, moles
- F = amount of feed, moles
- H_{div} = reboiler holdup for the dividing wall section, moles
- H_j = holdup on plate j in the main section of the column, moles
- HS_j = holdup on plate j in the side section (dividing wall section) of the column, moles
- L_j = liquid flow leaving plate j in the main section of the column, moles/hr
- LS_j = liquid flow leaving plate j in the side section (dividing wall section) of the column, moles/hr
- n = number of components
- N = total number of plates
- N_B = number of plates at the bottom of the column
- N_T = number of plates at the top of the column
- nfr = number of fractions or cuts
- R = reflux ratio
- t = time, hrs
- T = total batch time, hrs
- T_j = batch time for fraction j
- V = vapor rate in the main column, moles/hr
- V_{div} = vapor boilup rate for the dividing wall section, moles/hr
- V_j = vapor flow leaving plate j in the main section of the column, moles/hr
- VS_j = vapor flow leaving plate j in the side section (dividing wall section) of the column, moles/hr
- x = fraction of the liquid flow going to the dividing wall.
- $x_B^{(i)}$ = reboiler composition of component i for the main column
- $x_D^{(i)}$ = instantaneous distillate composition of component i
- $x_F^{(i)}$ = feed composition of component i
- $x_{Davg}^{(i)}$ = average distillate composition of component i
- $x_{div}^{(i)}$ = dividing wall reboiler composition of component i
- $x_j^{(i)}$ – liquid composition of component i leaving plate j in the main column
- $xs_j^{(i)}$ – liquid composition of component i leaving plate j in the dividing wall section
- $y_B^{(i)}$ = vapor composition of component i leaving reboiler for the main column
- $y_{div}^{(i)}$ = vapor composition of component i leaving dividing wall reboiler
- $y_j^{(i)}$ – vapor composition of component i leaving plate j in the main column
- $ys_j^{(i)}$ – vapor composition of component i leaving plate j in the dividing wall section

As stated earlier, the startup operation of this column is the total reflux condition. The main column (Zones 1 and 2) as well as the dividing wall section part (Zone 3) is charged with feed from the top so that initially the reboiler compositions for both reboilers and the plate composition on each plate (both main column and dividing wall section) is same as the feed composition.

$$x_B^{(i)} = x_j^{(i)} = xs_{jj}^{(i)} = x_F^{(i)},\ i = 1,..n; j = 1,..,N; jj = 1,\ldots,N_B \tag{14}$$

We use the same dynamic equations from above (equations 1 to 5, and 7 to 13) with equation 6 is replaced by equation 15 below for the startup operation with total reflux.

$$L_0 = V_1 \tag{15}$$

The startup operation is complete when equilibration is achieved. After that, we start taking out different fractions or cuts.

There are $n\,(N+N_B+2)+3$ differential equations, $(2n+1)(N+N_B+2)+5+N+N_B$ algebraic equations for the novel

batch dividing wall column. There are two degrees of freedom for each cut, namely, the batch time and reflux ratio for each cut. As stated earlier, to separate pure components in this column, there are many possible combinations of these variables. To find the right feasible combination, we use nonlinear optimization [7]. In this paper, we are concentrating on three pure component products with specified purities. The aim of optimization is to maximize the total of all three products per unit batch time. This objective function is the variant of the objective function used in a number of studies in the literature like Kerkhof and Vissers [14], Diwekar and Rivier [8]. The optimization will find the values of R, x, T, *and* V_{div} *for each fraction*.

The optimization problem can be written as follows

$$\max_{R,\ x,T_j,\ and\ V_{div}\ for\ each\ fraction,} E(Profit) = \frac{P_r\ (B+D+H_{div}) - C_0F}{T = \sum_{j=1}^{nfr} T_j} \tag{15}$$

Subject to

$$x_{Davg}^{(1)} \geq x_{D\ specified}$$

$$x_{div}^{(2)} \geq x_{div\ specified}$$

$$x_{B}^{(3)} \geq x_{B\ specified}$$

dynamic equatons $1-13$

where

- Pr = cost of products, $ per mole. We assumed all costs to be $100 per mole.
- C_0 = cost of raw material, $ per mole. Raw material cost is assumed to be negligible.

The dividing wall column model with optimization is implemented in the *MultiBatch*DS^{TM} batch distillation process simulator. *MultiBatch*DS^{TM} is specialized software developed by Dr. Diwekar with the help of Stochastic Research Technologies LLC, USA, and Equinox Software limited, India [6, 17]. *MultiBatch*DS^{TM} can simulate, design, and optimize multiple column configurations shown in Fig. 1.

We compare the performance of the dividing wall column with the same products (with the same specified purity and the same amount of product) from the rectifier product configuration shown in Fig. 4 and the middle vessel product configuration shown in Fig. 5 using *MultiBatch*DS^{TM} (with the new capability of simulating the dividing wall column).

3. Results and Discussions

The case studies are selected to consider a generic mixture (non-azeotropic) where separation of various components can be studied in one column. Our goal has been to compare the separation of a generic mixture in different state of the art batch distillation columns (conventional rectifier, middle vessel) with the side rectifier dividing wall column operated according to our proposed methodology. A mixture such as pentane/hexane/heptane represents a generic mixture which is being separated into three product streams. It is obvious that the batch dividing wall column is suitable when you want to separate multiple components as multiple products. For binary distillation, this column does not show any advantages, therefore, we have considered a ternary mixture here.

For the two case studies, we consider an equimolar ternary feed mixture of Pentane, Hexane, and Heptane. We use thermodynamic models and databank of MultiBatchDS for simulation. Ideal liquid and ideal vapor is assumed to simulate the thermodynamics for this system. We want to obtain three relatively pure products of Pentane, Hexane, and Heptane. The primary input details for the two case studies are presented in Table 1 for all three columns.

The optimization problem associated with the first case study is given below.

$$\max_{R,\ x,\ T_j,\ and\ V_{div}\ for\ each\ fraction,} E(Profit) = \frac{100(B+D+H_{div}) - 0}{T = \sum_{j=1}^{nfr} T_j} \tag{16}$$

Subject to

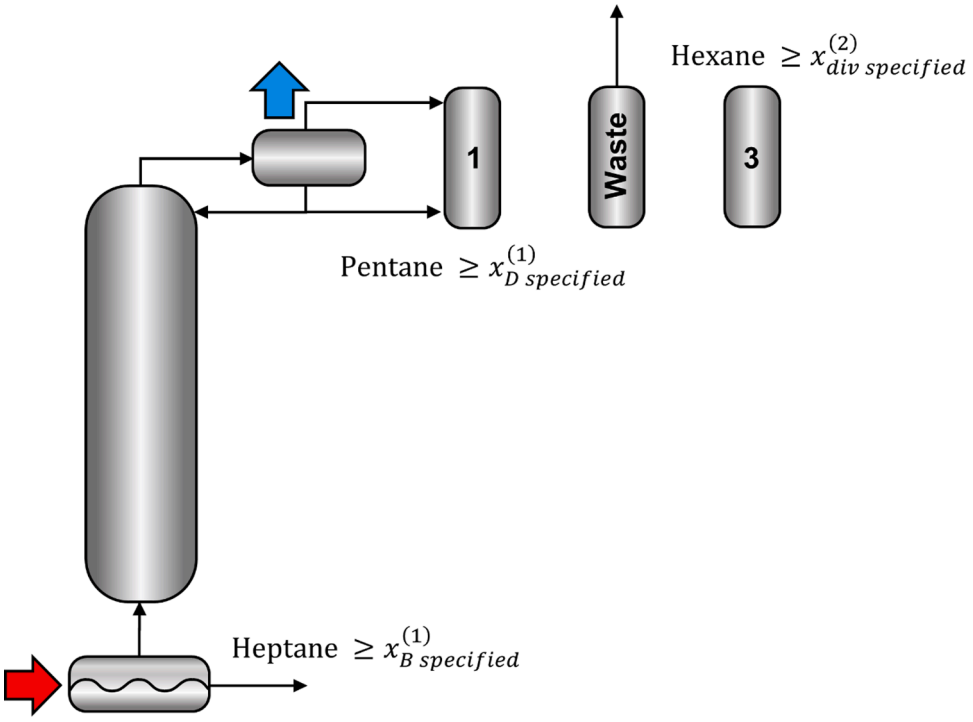

Fig. 4. Batch Rectifier Product Configuration

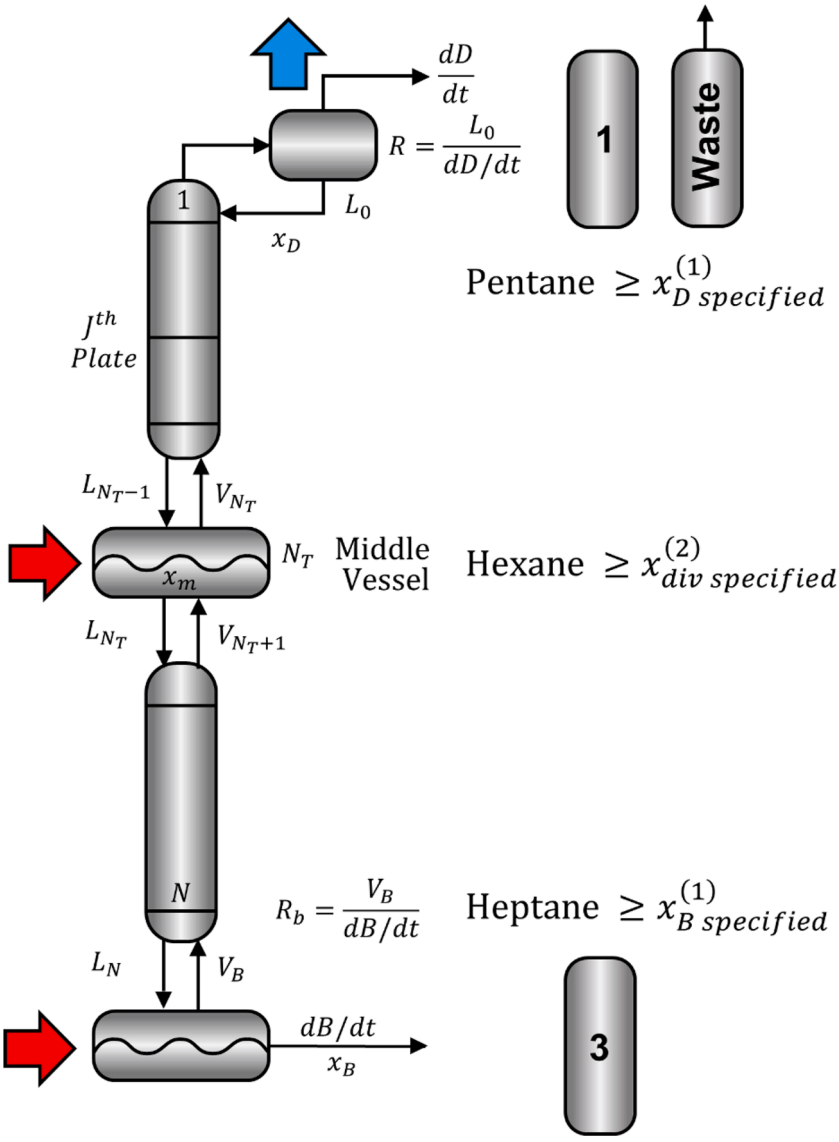

Fig. 5. The Middle Vessel Column Product Configuration

Table 1
The primary input for the case study

Input	Values
Components	Pentane (1), Hexane (2), Heptane(3)
Pressure	1 atm
F(moles)	200
$x_F^{(i)}$ (mol.fra.)	0.333,0.333,0.334
V (moles/hr)	120
N_T	10
N_B	15
$N = N_T + N_B$	25

$x^{(1)}_{Davg} \geq 0.95$

$x^{(2)}_{div} \geq 0.8$

$x^{(3)}_{B} \geq 0.85$

dynamic equations $1 - 13$

Table 2 presents the three products obtained in the dividing wall column after optimization. Table 3 presents the optimal operating conditions. This problem is nonconvex and has multiple solutions. This is one of the solutions. Fig. 6 shows the product trajectories for this

Table 2
Product distribution for the dividing wall column, case study 1. The purities are in mole fraction and total amount in moles.

Component	Top Product	Middle Product	Bottom Product	Waste Cut
Pentane	0.9807	0.0157	0.0008	0.2704
Hexane	0.0193	0.8221	0.147	0.7296
Heptane	0	0.1622	0.8522	0
Total Amount	52.00	50	86	36

Table 3
Optimal operating conditions for the dividing wall column, case study 1.

Variable	Startup	First Cut	Waste Cut
R	Total	3.7655	4.2393
x	0.6729	0.5677	0.4117
T (hrs)	0.366	1.5286	1.3153
Vdiv (moles/hr)	45	45	45
Hdiv (moles)	50	50	50

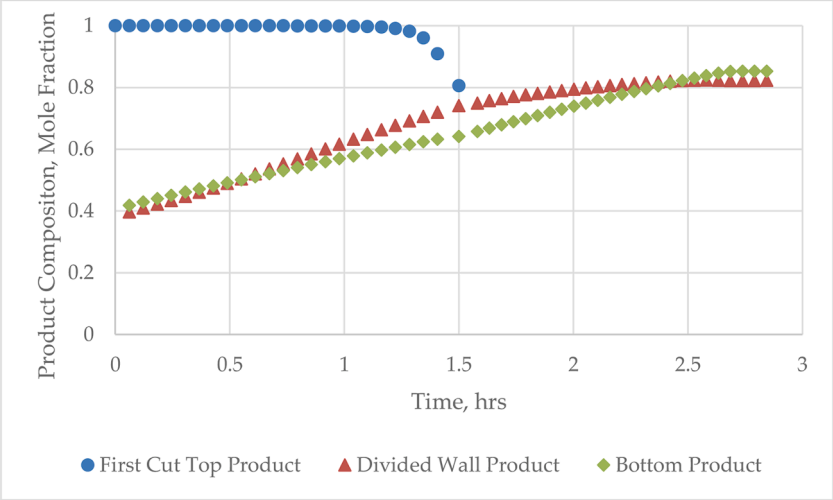

Fig. 6. Product profiles for the dividing wall column, case study 1.

solution. It should be remembered that in this figure, the top composition is the instantaneous distillate composition (top product profile). However, in the specification, we specify the average distillate composition.

To compare other configurations, we kept the products the same and found the rectifier's and the middle vessel's operating conditions, which can give the same products (Table 4). It should be remembered that the equilibration time for all three columns was similar in magnitude. Since both the rectifier and the middle vessel column do not have any decision variable like x (for the DWC), we have not reported the two columns' startup conditions in tables. These conditions are shown in Tables 5 for the rectifier and the middle vessel columns. A comparison of profits and batch times for all the three columns are provided in Table 6. It can be seen that the new configuration outperforms the rectifier by getting 29% more profit and the middle vessel by 12 % more profit.

In the second case study 2, we increased the purity specifications. The second optimization problem we considered is given below.

$$\max_{R,\ x,\ T_j,\ and\ V_{div}\ for\ each\ fraction,} E(Profit) = \frac{100(B + D + H_{div}) - 0}{T = \sum_{j=1}^{nfr} T_j} \tag{16}$$

Subject to

$$x_{Davg}^{(1)} \geq 0.95$$

$$x_{div}^{(2)} \geq 0.9$$

$$x_{B}^{(3)} \geq 0.9$$

dynamic equations $1 - 13$

Table 4
Product distribution for the two columns case study 1.

Rectifier Product Distribution				
Component	First Cut	Third Cut	Bottom Product	Waste Cut1
Pentane	0.9755	0.0404	0.0001	0.0001
Hexane	0.0245	0.8300	0.1437	0.1434
Heptane	0.0000	0.1296	0.8562	0.8565
Total	52.00	50	86	36
Middle Vessel Column Product Distribution				
Component	Top Product	Middle Product	Bottom Product	Waste Cut1
Pentane	0.9686	0.0046	0	0.2709
Hexane	0.0314	0.809	0.14	0.7391
Heptane	0	0.1865	0.86	0
Total	52.00	50	86	36

Table 5
Operating conditions for the two columns, Case study 1.

Rectifier operating conditions			
Variable	First Cut	Waste Cut	Third Cut
R	4.2	1.2	2
T (hrs)	2.2533	0.66	1.25
Middle Vessel operating condition			
Variable	First Cut	Second Cut	No Third Cut
R	3.5	3	
Rb	4	4	
T (hrs)	1.95	1.2	
VB (moles/hr)	100	100	

Table 6
Comparing the three columns configurations, case study 1.

Variable	Dividing Wall	Rectifier	Middle vessel
Profit per batch	$ 6,610.64	$ 5,119.55	$ 5,893.42
Batch time	2.8439	4.1633	3.19
% profit increase for dividing wall		29	12

The product distribution for the dividing wall column is shown in Table 7. It can be seen that as the product purities increase, the waste cut amount increases. Fig. 7 shows the product profiles for the three products.

The optimal operating conditions for the dividing wall column are presented in Table 8. Again, we kept the same products (composition and amount) obtained in the rectifier and the middle vessel configurations (Table 9), as obtained by the dividing wall column shown in Table 7. The corresponding operating conditions for the two columns are presented in Tables 10. Table 11 provides the profit obtained and the total batch time for the three configurations. It can be seen that the

Table 7
Product distribution for the dividing wall column, case study 2. The purities are in mole fraction and total amount in moles.

Component	Top Product	Middle Product	Bottom Product	Waste Cut
Pentane	0.9675	0.0071	0	0.2326
Hexane	0.0325	0.9078	0.1	0.7674
Heptane	0	0.0851	0.9	0
Total Amount	52.00	25	75	46

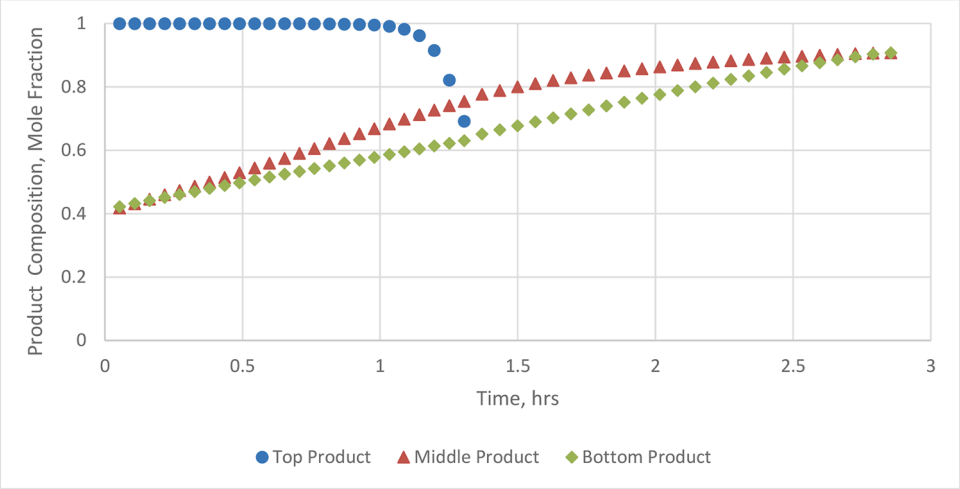

Fig. 7. Product profiles for the dividing wall column, case study 2.

Table 8
Optimal operating conditions for the dividing wall column, case study.

Variable	Startup	First Cut	Waste Cut
R	Total	2.8856	4.0899
x	0.6882	0.4679	0.3
T (hrs)	0.3854	1.3608	1.6143
Vdiv (moles/hr)	30	30	30
Hdiv (moles)	25	25	25

Table 9
Product distribution for the middle vessel, case study 2.

Rectifier product distribution				
Component	First Cut	Third Cut	Bottom Product	Waste Cut
Pentane	0.9653	0.0147	0.0000	0.2418
Hexane	0.0347	0.9072	0.1097	0.7573
Heptane	0.0000	0.0781	0.8902	0.0009
Total	52.00	25	75	46
Middle vessel product distribution				
Component	Top Product	Middle Product	Bottom Product	Waste Cut
Pentane	0.9688	0.0001	0.0000	0.2471
Hexane	0.0312	0.9091	0.0965	0.7627
Heptane	0.0000	0.0909	0.9070	0.0000
Total	52.00	25	75	46

Table 10
Operating conditions for the two columns, case study 2

Rectifier Operating Conditions			
Variable	First Cut	Waste Cut	Third Cut
R	2.8	2	3.5
T (hrs)	1.6467	1.15	0.9375
Middle Vessel Operating Conditions			
Variable	First Cut	Waste Cut	No Third Cut
R	2.6	4.2	
Rb	4	5.5	
T (hrs)	1.56	1.99	
VB (moles/hr)	100	100	

dividing wall column provides 37% more profit than the rectifier and 19% more profit than the middle vessel column. Tables 6 and 11 show that as the purity increased, the profit differential between the dividing wall column and the other two configurations increased. It should also be noted that as the purity of the products increases, in the last waste cut of the DWC, the optimal split fraction x decreased, resulting in closer to no flow between DWC reboiler to main reboiler (Tables 3 and 8). The % of waste cut to feed increased from 16 to 23% (Tables 2 and 7).

Table 11
Comparing the three column configurations, case study 2.

Variable	Dividing Wall	Rectifier	Middle vessel
Profit per batch	$ 5,109.07	$ 3,721.39	$ 4,281.69
Batch time	2.8439	4.1633	3.19
% profit increase for dividing wall		37	19

4. Summary

This paper presented the first analysis of a novel dividing wall side stripper batch distillation column. The new configuration results were compared with the conventional batch rectifier and the middle vessel column for a ternary mixture. The new configuration showed a significant increase in profit due to a reduction in batch time and the number of cuts required. The advantage of this new configuration increases as purity specification increases. Since batch time is reduced significantly, this column is expected to be advantageous in energy requirements.

Even though we have introduced the new configuration and its operating strategies in the context of a ternary mixture, the proposed system is quite versatile. It can easily be extended to higher mixtures. For example, while separating a batch of a four-component mixture ABCD, one could develop operating sequences to either produce B or C or both from the dividing wall column side. Although for batch distillation, we have only considered one of the five types of dividing wall columns proposed for continuous distillation [4], we plan to investigate the other DWC configurations in the future for intensification of multicomponent batch distillations.

The model presented here was based on a constant molal overflow assumption, and hence the model does not carry out heat balance or utility calculations. This can be added in the future for the systems where this assumption was not valid. In the future, we will be considering complex systems like non-ideal or highly polar mixtures. Our experience with the middle vessel column for such systems tells us that

the dividing wall column will also perform well.

Contribution	Author Roles
Conceptualization	Rakesh Agrawal and Urmila Diwekar
Methodology	Urmila Diwekar
Software	Urmila Diwekar
Validation	Urmila Diwekar
Investigation	Urmila Diwekar and Rakesh Agrawal
Writing - Original Draft	Urmila Diwekar
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Supervision	Urmila Diwekar and Rakesh Agrawal
Project administration	Urmila Diwekar
Funding acquisition	None

Declaration of Competing Interest

None.

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