

The Investigation of Purity Improvement for the Production of Methyl Propionate in Different Types of Batch Distillation Systems

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ABSTRACT

Methyl propionate, also known as methyl propanoate is a clear colourless liquid with a characteristic odour (fruity smell and taste). In this study, the formation of methyl propionate through the esterification of propionic acid and methanol was investigated in a reactive distillation system using a conventional (CBC) single feed (SF-SBD), and double feed semi-batch distillation (DF-SBD) columns for the first time. The performances measured of these distillation systems were evaluated in terms of minimum batch time for a given separation task. The optimization results clearly showed that the DF-SBD system is a more attractive operation in terms of reaction conversion, at maximum achievable purity as compared to the SF-SBD, and CBD processes.

1. Introduction

Methyl propionate is a very important component which has useful applications in a variety of areas in the chemical industry such as solvents for cellulose nitrate, lacquers, plasticizers, chemical intermediates, fragrances, flavors, a raw material in organic synthesis for the production of varnishes, paints, and other chemical compounds such as methyl methacrylate [1]. Methyl propionate can be synthesized from propionic acid and methanol by a catalytic esterification over Amberlyst-36. The research studies on the esterification operation of propionic acid (PrA) with ethanol to yield ethyl propionate have been reported in the literature [2]. The production of n-butyl propionate via the catalytic esterification of propionic acid and n-butanol has been studied by some researchers [3,4]. In fact, few studies have discussed the esterification reaction of propionic acid and methanol to form methyl propionate (MePr) in the past [1,5]. For example, Lilja et al., (2002) studied experimentally the same reaction system in a laboratory-scale batch reactor over the fiber catalyst (Smopex-101) [1]. Tsai et al. (2010) [5] also developed several kinetic models such as the ideal-quasi-homogeneous (IQH), the non-ideal-quasi-homogeneous (NIQH), Eley-Rideal (ER), and Langmuir-Hinshelwood-Hougen-Watson (LHHW) to study experimentally the kinetic behavior of the synthesis of methyl propionate (MePr) over Amberlyst-36 using a fixed-bed reactor. They found out that the LHHW model yields the best representation for the methyl propionate production which can be further used for the synthesis of MePr or recovering waste propionic acid in the reactive distillation technique. However, they achieved a conversion of PrA into MePr of 94.50% with MeOH to PrA feed molar ratio of 5. More recently, Shi et al., (2017) [6] and Wang et al., (2014) [7] explored the feasibility and effectiveness of reactive dividing-wall distillation (RDWD) for the optimal design of mixed acid esterification (acetic acid and propionic acid) with methanol to form methyl acetate, and methyl propionate.

In this work, different batch reactive configurations were performed to see if an increased conversion level of PrA, and maximum achievable quality of MePr were possible. For this purpose, the application of a conventional batch distillation column (CBD), and both semi-batch with single feed charge (SF-SBD) and semi-batch with double feed charge (DF-SBD) distillation configurations for the synthesis of methyl propionate was used in this study.

The performances of CBD, SF-SBD, and DF-SBD processes were measured in terms of minimum operating batch time. The reflux ratios, pure propionic acid fed rate (in case of SF-SBD), and pure propionic acid and methanol fed rates (for DF-SBD) were utilized in the optimization study which had been already discretized using Control Vector Parameterization (CVP) method [8,9]. A detailed dynamic model for each of these column operations was incorporated within the optimization framework. Next, the dynamic optimization problem was converted into the non-linear programming problem (NLP) and next was solved using a SQP based technique within gPROMS Software (2017) as shown in Figure 1 [10].

2. Process models

With reference to the three column configurations (CBD, SF-SBD, and DF-SBD) displayed in Figure 2, the detailed dynamic model contains unsteady mass

and energy balance equations, rigorous phase equilibrium and reaction kinetics. The process model assumes no vapour holdup, molar holdup on the trays and in the reflux drum, adiabatic operation, perfect mixing of liquid on the stages, fast energy dynamics, and total condensation without sub-cooling. It should be noted that more details about these batch distillation configurations can be found in Edreder et al. (2009) [11] and Aqar et al. [12-15]. Also, the rigorous models for both CBD, SF-SBD, and DF-SBD column schemes have been illustrated in Appendix A.

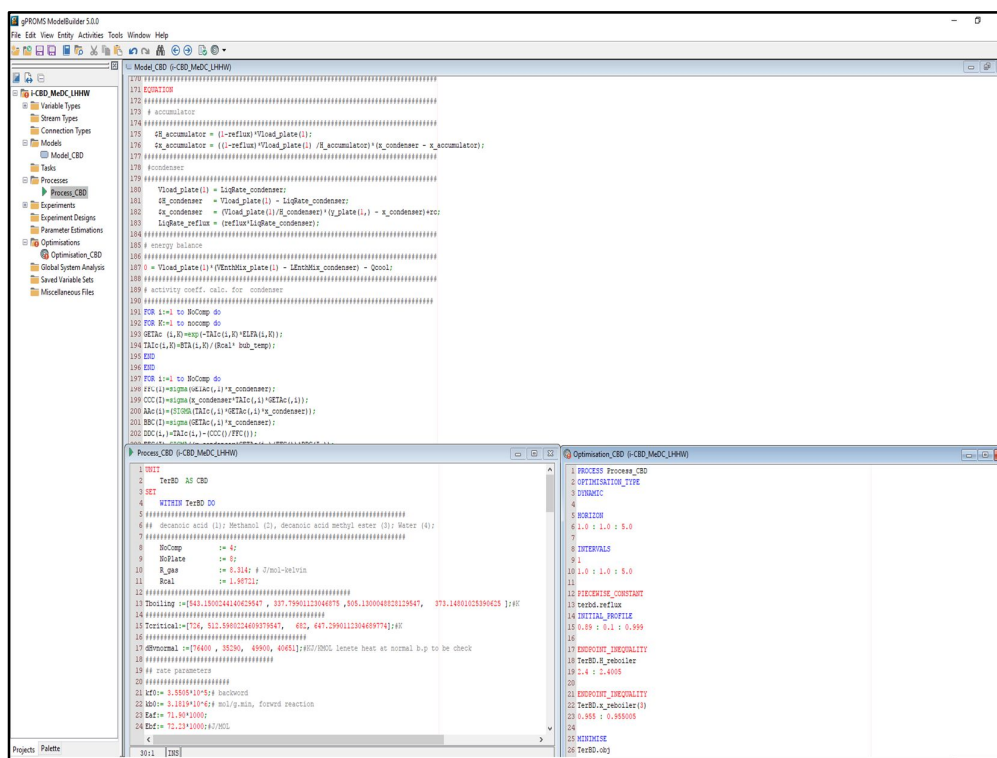


Figure 1. gPROMS platform for the batch process model

3. Dynamic optimization problem

The optimization problems for CBD, SF-SBD and DF-SBD operations can be stated as follows:

3.1. Minimum Operating Time Problem

The optimization problem can be written as follows:

- Given: The column configurations, the feed concentration, the vapour load to the condenser, the desired product amount and its quality
- Determine: Reflux ratio (R) (for CBD column)
 Or, Reflux ratio, and PrA feed rate (for SF-SBD column)
 Or, Reflux rate, PrA feed rate, and MeOH feed rate (for DF-SBD column)
- So as to: Minimize the operating batch time
- Subject to: Model equations, Process constraints

The optimization problem (OP) for the different batch columns (Figure 1) can be described mathematically as:

$$\begin{array}{lll}
 \text{OP} & \text{Min} & t_p \\
 & R_{\text{CBD}} & \text{(For CBD Column)} \\
 & R_{\text{SF-SBD}}(t), F_{\text{PrA}}(t) & \text{(For SF-SBD Column)} \\
 & R_{\text{DF-SBD}}(t), F_{\text{PrA}}(t), F_{\text{MeOH}}(t) & \text{(For DF-SBD Column)}
 \end{array} \quad (1)$$

Subject to :

$$D_{\text{MePr}} \geq D_{\text{MePr}}^* \quad \text{(Inequality Constraints)}$$

$$x_{\text{MePr}} \geq x_{\text{MePr}}^* \quad \text{(Inequality Constraints)}$$

Where, D_{MePr} , x_{MePr} are the amount of distillate product (2.5 kmol for all columns), and concentration of methyl propionate at the end batch time t_p (denotes that the D_{MePr}^* , x_{MePr}^* are specified). Note that the model mathematical equations for those column configurations are described by the set of highly coupled nonlinear differential-algebraic equations (DAEs) acting as equality constraints to the dynamic optimization framework.

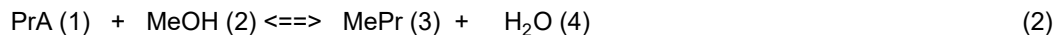
4. The synthesis of methyl propionate system

4.1. Statement of the problem

The synthesis of methyl propionate was carried out in an 8-plates column (excluding a condenser and a reboiler) with condenser vapour load of 2.5 (kmol/h) for the three batch schemes (CBD, SF-SBD, and DF-SBD). The column stages were numbered from the top-down. 4% of the total initial amount was the total column holdup. Fifty percent of this total holdup was taken as the total condenser holdup and the rest was taken as the tray holdup (equally divided). It is noteworthy that the same strategy was used for the catalyst loading distribution for the three batch columns [16-18]. The total initial quantity of feed was five kmol with the feed composition $\langle \text{PrA}, \text{MeOH}, \text{MePr}, \text{H}_2\text{O} \rangle$ is: $\langle 0.5, 0.5, 0.0, 0.0 \rangle$, respectively.

4.2. Reaction kinetics and phase equilibria (VLE) for the propionic acid esterification

Tsai et al. (2010) [5] experimentally explored the kinetic behaviour of the heterogeneous catalytic formation of methyl propionate. The reversible reaction schemes together with the boiling points (K) of the components for the esterification of propionic acid (PrA) and methanol (MeOH) to produce methyl propionate (MePr) and water (H₂O) over an ion-exchange resin (Amberlyst-36) are:



(Propionic Acid) (Methanol) (Methyl Propionate) (Water)

B.P (K) 414.50 337.85 353.00 373.15

For the formation of methyl propionate, a Langmuir-Hinshelwood-Hougen-Watson (LHHW) activity ($a_i = x_i \gamma_i$) based kinetic model is used which can be represented as [5]:

$$-r_{PrA} = m_{cat} \left\{ \frac{9.15 \times 10^{11} \exp\left(\frac{-6966.8}{T}\right) \left[a_{PrA} a_{MeOH} - 7.1 \times 10^{-3} \exp\left(\frac{56.0}{T}\right) a_{MePr} a_{H_2O} \right]}{\left[1 + 1.96 a_{PrA} + 1.71 a_{MeOH} + 6.55 a_{MePr} + 6.94 a_{H_2O} \right]^2} \right\} \quad (3)$$

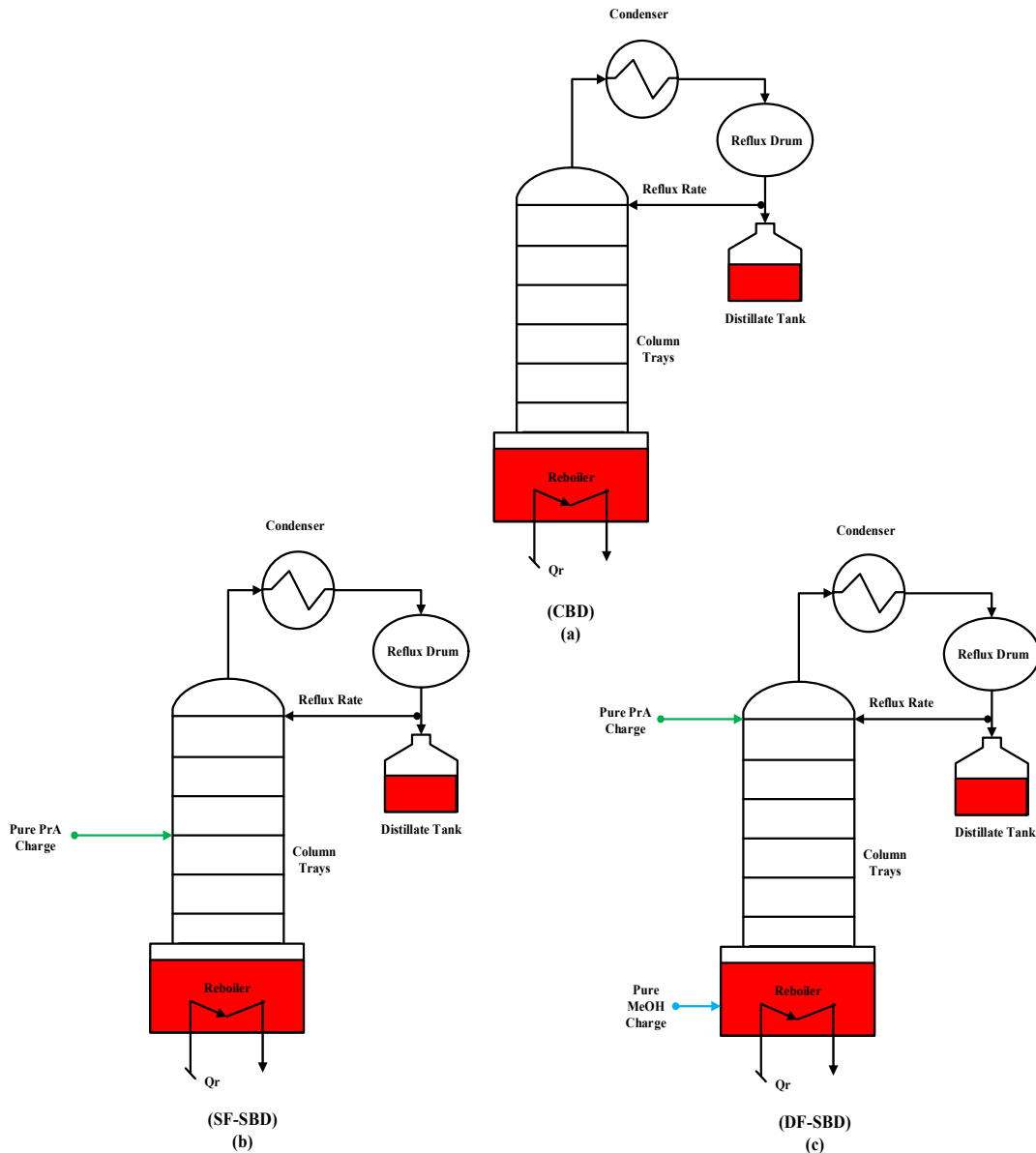


Figure 2. Different types of batch distillation columns for producing methyl propionate: (a) conventional (CBD), (b) single feed (SF-SBD), and (c) double feed semi-batch distillation (DF-SBD)

4.3. Phase equilibria (VLE)

The vapour-liquid equilibrium equation was calculated from (Eq. 4) where (y_i) is calculated using the NRTL model. The saturated pressure (P_i^{sat}) for each pure component is obtained by employing Antoine's equation:

$$\log_{10} P_i^{sat} = A + \frac{B}{T} + C \log_{10} T + DT + ET^2 \quad (4)$$

Where A, B, C, D, E are the regression constants for the Antoine equation and T is the temperature in Kelvin. The NRTL binary interaction constants were taken from Tsai et al. (2010) [5] and the Antoine constants were taken from Yaws (1997) [19]. Also, the enthalpy parameters for all pure components were taken from Aspen Plus.

$$y_i = \frac{P_i^{\text{sat}} x_i \gamma_i}{P} \quad (5)$$

5. Results and discussion

5.1. CBD operation

Table 1 summarizes the optimum operation policy including reflux ratios, the processing-batch time, and the total energy consumption for the CBD operation. As can be seen in Table 1, increasing the concentration of MePr product decreases all the reflux ratios, and the operation batch time, as well as the energy usage rate. However, it was impossible to accomplish methyl propionate > 0.520 mole fraction using a conventional batch system. This is due to the reverse reaction being active and a quick removal of the methanol from the propionic acid reactant in the still tank due to the huge difference in boiling point temperatures of the reaction reactants.

Table 1. Summary of optimization results for CBD column

Product Puri Of MePr	Optimal Reflux Rati R	Final Batch time, t _p , hr	Energy Usage, Q _{tot} , GJ
0.490	0.604	2.52	0.229
0.500	0.495	1.98	0.179
0.510	0.377	1.61	0.145
0.520	--- ^a	--- ^a	--- ^a

^a Infeasible.

5.2. SF-SBD operation

As mentioned previously, the concentration of methyl propionate product was changed from 0.60 to 0.660 mole fraction in each case, while, the product quantity in the distillate tank was kept constant at 2.5 kmol so that the performance comparison of SF-SBD mode could be made with CBD mode in terms of maximum conversion of acid, and the highest achievable product purity. The optimization results in terms of feed rate and reflux ratio which minimize the operating batch time subject to constraints on the quantity and quality of MePr at the final batch time are presented in Table 2.

It was found that all values of optimal feed rate, reflux ratio, and the operating batch time with the total heat consuming, increased gradually by increasing the MePr purities. A comparison of the results between the MePr concentration using the SF-SBD configuration and the CBD process (Table 1) shows that for the same product amount in the accumulator tank (2.5 kmol), the SF-SBD system produced methyl propionate at a higher composition (0.65

compared to 0.51 mole fraction). However, it was not possible to obtain purity of MePr beyond 0.65 mole fraction.

Table 2. Summary of optimization results for SF-SBD column

Product Purity Of MePr	Optimal Feed Rate, kmol/hr	Optimal Reflux Ratio R	Final Batch time, t_p , hr	Energy Usage, Q_{tot} , GJ
0.600	0.22	0.481	1.93	0.180
0.625	0.28	0.587	2.42	0.228
0.650	0.41	0.774	4.42	0.433
0.660	--- ^a	--- ^a	--- ^a	--- ^a

^a Infeasible.

5.3. DF-SBD operation

Two case studies are examined here: one (Case A) with single-reflux interval strategy and the second one (Case B) with multi-reflux intervals policy of process. The performance of DF-SBD operation is compared to the performance of SF-SBD operation in terms of maximum achievable purity of ester, operation batch time, and the lower energy required.

5.3.1. Optimum operation using one-reflux interval (Case A):

For the four top product concentrations considered, the summary of optimization results containing optimum PrA feed rate, MeOH feed rate, reflux ratios profiles, the operation batch time, and the total energy consumption for the DF-SBD column is presented in Table 3. It is clear from the table that employing DF-SBD operation outperformed the SF-SBD mode in terms of the maximum achievable purity of ester.

Obviously, DF-SBD column produced a higher purity of MePr (0.875 mole fraction) as compared to that obtained by SF-SBD column (Table 2). However, it should be noted that for 0.875 of product concentration, there was a sharp increase in the total energy usage due to the enormous increase in the reflux ratio and the operating batch time (compared to others). This makes even DF-SBD operation utilizing single control process an uncompetitive procedure at higher product quality and therefore the multi-control policy is recommended.

Table 3. Summary of optimization results for DF-SBD column for Case A

Product Purity Of MePr	Optimal Pr Rate, kmol/hr	Optimal MeOH Rate, kmol/hr	Optimal Reflux Ratio, R	Final Batch time, t_p , hr	Energy Usage, Q_{tot} , GJ
0.750	0.68	2.66	0.791	4.79	0.484
0.800	0.69	3.48	0.854	6.87	0.715
0.850	0.63	4.29	0.916	11.94	1.281
0.875	0.70	7.07	0.950	19.87	2.419

5.3.2. Optimum operation using two-reflux intervals (Case B):

For each distillate purity consideration, Table 4 shows the optimum process results in terms of both feed rates, reflux ratios, switching time, total operation batch time, and the total required heat to satisfy the product within the constraints.

It is obvious from Table 4 that the use of multi-control approach resulted in significant saving in the operating batch time, and energy usage rate as compared to the one-reflux DF-SBD operation (Table 3).

For example, at 0.875 mole fraction concentration the reduction in the processing batch time is almost 34.57%, and in the heat expense rate it is about 41.75 %, as compared to one-reflux DF-SBD operation.

It can be seen from Table 4 that for each composition specification, the DF-SBD operation operates at higher reflux ratio for the first-time interval to push the water as rapidly as it is produced as the bottom product. Lower reflux ratio is required in the second-time interval to retain both reaction reactants propionic acid and methanol in the reaction region to have further chemical reaction between them.

Table 4. Summary of optimization results for DF-SBD column for Case B

Product Purit Of MePr	Optimal Feed Rates, F_{PrA1}, F_{PrA2}	Optimal Fee Rates, F_{MeOH1}, F_{MeOH}	Optimal Reflux Ratios R_1, R_2	Batch Time Interva t_1, t_2, hr	Final Batch time, t_p, hr	Energy Usage, $Q_{tot},$ GJ
0.750	0.60, 0.82	15.31, 1.63	0.982, 0.70	0.28, 4.22	4.49	0.469
0.800	7.51, 0.59	30.44, 0.89	1, 0.786	0.36, 4.67	5.03	0.547
0.850	0.66, 0.63	12.30, 1.74	1, 0.872	0.73, 7.82	8.55	0.869
0.875	1.11, 0.65	29.87, 2.91	1, 0.920	0.49, 12.50	13.00	1.409

6. Conclusions

In this study, for the first time, the performance of different types of batch distillation arrangements were determined in terms of minimum operation batch time under single and two-control intervals operations for the synthesis of methyl propionate via the esterification reaction of propionic acid and methanol. Control variables (i.e. reflux ratio and/or feed rate) were employed as a piecewise-constant, which were next discretised utilizing CVP algorithm. An optimization problem was formulated including the process model within gPROMS modelling tool. The product quantity and its concentration were used as operational constraints. Observation results employing single-control policy (for DF-SBD) and feed rate (for CBD and SF-SBD) showed that DF-SBD was more appropriate than both CBD and SF-SBD processes in terms of minimum operating time, and maximum product quality. Furthermore, theoretically, the removal of both reactants in DF-SBD operation should increase the composition of methyl propionate and will reduce the operating time. Optimum process of DF-SBD for this reaction scheme should be considered. In addition, the optimization results obviously revealed that the use of multi-reflux strategy is a more promising and interesting option as compared to the one-reflux interval in DF-SBD column in terms of minimum processing batch time and energy usage rate.

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Appendix A

A.1 Process Model for the CBD Mode

A.1.1 Reflux Drum and Distillate Tank: j=1

- Accumulator Tank Mass Balance:

$$\frac{dH_a}{dt} = D \quad (6)$$

- Component Mass Balance:

a) Distillate Receiver:

$$H_a \frac{dx_{ai}}{dt} = D (x_{Di} - x_{ai}) \quad (7)$$

b) Reflux Drum Holdup:

$$H_c \frac{dx_{ci}}{dt} = V_c y_2 - (V_c + \Delta n_1 H_c) x_{Di} + r_{1i} H_c \quad (8)$$

- Energy Balance:

$$0 = V_C H_2^V - (V_C + \Delta n_1 H_C) H_1^L - Q_c \quad (9)$$

- Physical Properties and other equations:

$$H_1^L = H_1^L(x_{D1}, T_1, P) \quad (10)$$

$$T_1 = T_1(x_{D1}, P) \quad (11)$$

$$r_{1j} = r_{1j}(k_e, x_{Di}) \quad (12)$$

$$\Delta n_1 = \sum r_{1j} \quad (13)$$

$$L_1 = R(V_C + \Delta n_1 H_C) \quad (14)$$

$$D = (1 - R)(V_C + \Delta n_1 H_C) \quad (15)$$

A.1.2. Intermediate Stages: $j = 2$ to $N-1$

- Total Mass Balance:

$$0 = L_{j-1} + V_{j+1} - L_j - V_j + \Delta n_j H_j \quad (16)$$

- Component Balance:

$$H_j \frac{dx_j}{dt} = L_{j-1} x_{j-1} + V_{j+1} y_{j+1} - L_j x_j - V_j y_j + H_j r_{ji} \quad (17)$$

- Energy Balance:

$$0 = L_{j-1} H_{j-1}^L + V_{j+1} H_{j+1}^V - L_j H_j^L - V_j H_j^V \quad (18)$$

- Equilibrium:

$$K_{j,i} = \frac{y_{j,i}}{x_{j,i}} \quad (19)$$

- Summation:

$$\sum y_{j,i} = 1 \quad (20)$$

- Relations Defining Physical Properties and Chemical Reactions:

$$K_{j,i} = K_{j,i}(y_{j,i}, x_{j,i}, T_j, P) \quad (21)$$

$$H_{j,i}^L = H_{j,i}^L(x_{j,i}, T_j, P) \quad (22)$$

$$H_{j,i}^V = H_{j,i}^V(y_{j,i}, T_j, P) \quad (23)$$

$$r_{j,i} = r_{j,i}(k_e, x_{j,i}) \quad (24)$$

$$\Delta n_j = \sum r_{j,i} \quad (25)$$

A.1.3. Still Pot: $j = N$

- Total Mass Balance:

$$\frac{dH_n}{dt} = L_{n-1} - V_n + \Delta n_n H_n \quad (26)$$

- Component Mass Balance:

$$H_n \frac{dx_n}{dt} = L_{n-1}(x_{n-1} - x_n) - V_n (y_n - x_n) + H_n r_n \quad (27)$$

- Energy balance:

$$0 = L_{n-1} (H_{n-1}^L - H_n^L) - V_n (H_n^V - H_n^L) + Q_r \quad (28)$$

A.2 Process Model for the SF-SBD Mode

Note, the model equations for SF-SBD operation will be same as those in the CBD column mathematical model shown above except that the extra charged feed (F_{PrA}) terms to the column plates equations will be added.

2.1 Plate (1)

- Total Mass Balance:

$$0 = L_{j-1} + V_{j+1} - L_j - V_j + F_{PrA} + \Delta n_j H_j \quad (29)$$

- Component Mass Balance:

$$H_j \frac{dx_j}{dt} = L_{j-1} x_{j-1} + V_{j+1} y_{j+1} - L_j x_j - V_j y_j + F_{PrA} x_{PrA} + H_j r_{ji} \quad (30)$$

- Energy balance:

$$0 = L_{j-1} H_{j-1}^L + V_{j+1} H_{j+1}^V - L_j H_j^L - V_j H_j^V + F_{PrA} H_{PrA}^F \quad (31)$$

A.3 Process Model for the DF-SBD Operation

Note, the model equations for DF-SBD operation are exactly similar to those in the SF-SBD column mathematical model shown above except that the extra charged feed (F_{MeOH}) terms to the still pot equations will be added.

2.1 Still Pot: $j=N$

- Total Mass Balance:

$$\frac{dH_n}{dt} = L_{n-1} - V_n + F_{MeOH} + \Delta n_n H_n \quad (32)$$

Component Mass Balance:

$$H_n \frac{dx_n}{dt} = L_{n-1}(x_{n-1} - x_n) - V_n (y_n - x_n) + F_{MeOH} (x_{MeOH} - x_n) + H_n r_n \quad (33)$$

- Energy balance:

$$0 = L_{n-1} (H_{n-1}^L - H_n^L) - V_n (h_n^V - H_n^L) + F_{MeOH} (H_{MeOH}^F - H_n^L) + Q_r \quad (34)$$

مطالعه درجه خلوص متیل پروپیونات حاصله از سیستم های مختلف تقطیر بسته

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چکیده

متیل پروپیونات که معروف به متیل پروپانوات می باشد، یک مایع بی رنگ با بوی میوه ای می باشد. در این مطالعه برای اولین بار، تشکیل متیل پروپانوات را از طریق استریفاسیون اسید پروپونیک و متانول در یک سیستم تقطیر فعال با استفاده از ستونهای تقطیر نیمه بسته معمولی (CBD)، تک خوراکی (SF-SBD) و دو خوراکی (DF-SBD) مورد بررسی قرار گرفته است. عملکرد سیستمهای تقطیر بکار برده شده از نظر زمان جداسازی مورد ارزیابی قرار گرفت. نتایج بهینه سازی نشان داد که سیستم DF-SBD کارکرد بهتری از نظر تبدیل واکنش، و ماکزیمم خلوص در مقایسه به SF-SBD و CBD داشته است.

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