CHEMICAL ENGINEERING TRANSACTIONS
VOL. 56, 2017

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet

Guest Editors: Jiří Jaromír Klemeš, Peng Yen Liew, Wai Shin Ho, Jeng Shiun Lim

ISBN 978-88-95608-47-1; **ISSN** 2283-9216
DOI: 10.3303/CET1756190

Modelling and Simulation of Multi-vessel Batch Distillation Column

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Market demand of specialty chemicals, biochemical and pharmaceuticals are increasing. Batch distillation is considered as the most suitable distillation operation to separate all those chemicals due to its flexibility, operability and lower capital cost. Multi-vessel batch distillation is an improvement of less energy efficient batch distillation. This paper focuses on modelling and simulation of multi vessel batch distillation column under total reflux operation for separating a ternary mixture. Total reflux operation leads to production of high purity product. In industry, the modelling and simulation play a very important role. It can help with the description of the system and the choice of the optimal control strategy. The main objective of this paper is to determine the mathematical model of multi-vessel batch distillation which usually precedes the design of the controller. Mathematical model is firstly developed based on the first principles and ordinary differential equations (ODE). MATLAB Simulink is employed to perform the simulation. The vessel holdup is set based on product purity. The model is expected to produce stable response with the changing inputs variables and produce high purity product. The control strategy is determined.

1. Introduction

Nowadays, modelling and simulation plays an important roles for investigating the system's behavior in the industry. Today’s personal computers computational ability is very high, the price is relatively low and the usability of the simulation grows. The application studied in this paper is multi-vessel batch distillation. Multi-vessel batch distillation is a further generalisation of middle vessel and inverted distillation configuration. Multi-vessel has been found to be more profitable, more energy efficient, more flexible and require lower batch time compared to the other unconventional batch distillation (Mahmud et al., 2008). This batch distillation is mainly used in specialised chemical, biochemical and pharmaceutical industries (Fanaei et al., 2012). This paper covers the constructional details of multi-vessel batch distillation, mathematical modeling, and simulation study and control strategy of multi vessel batch distillation.

2. Multi-vessel batch distillation column

Multi-vessel Batch Distillation is the integration of a reboiler, two vessels, two columns and a reboiler as shown in Figure 1 (Skogestad et al., 1997). It is developed from the combination of batch stripper and rectifier column to separate ternary mixture (Fanaei et al., 2012). The operation of multi-vessel batch distillation starts with reboiler being charged with feed. Energy used for the plant is supplied through reboiler. Three desired product fractions are collected in two product vessels and reboiler. The product vessels are mounted along the column. The product is withdrawn from the system when steady state is achieved. All the vapour entering the condenser will condense into liquid. The liquid stream entering each product vessel is returned to the distillation column. This corresponds to operation with total reflux mode (Gruetzmann et al., 2006).

Please cite this article as: Hazwani S.N., Hisyam A., Aziz B.A., 2017, Modelling and simulation of multi-vessel batch distillation column, Chemical Engineering Transactions, 56, 1135-1140 DOI:10.3303/CET1756190

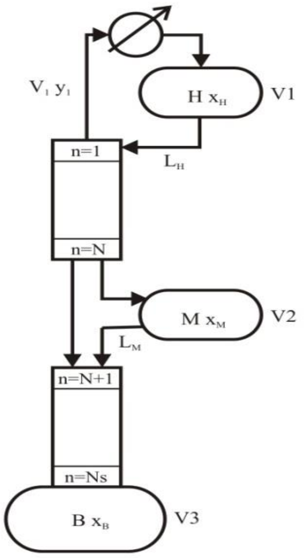

Figure 1: Multi-vessel batch distillation column configuration (Hisyam, 2011)

There are two important advantages of multi-vessel batch distillation identified. The operation with the highest possible separation performance is the first advantage. The second advantage is no reflux strategy is required, the same case as cyclic operation of conventional batch distillation studied by Wittgens et al. (1996). The off-cut characteristic of batch distillation with sequential product withdrawal does not rise when the system is operated under total reflux mode, if the separation efficiency is high enough. Both of these facts lead to significant advantages in terms of the batch time and product yield, and improve the economics of the process (Gruetzmann et al., 2006).

3. Mathematical modeling

The mathematical equations of the separation process in a multi-vessel batch distillation can be presented in Eq(1) - (16) (Tang et al., 2014). The equations include mass balance and energy balance equations at each point, equilibrium equation, equation of unity, and Antoine equation for predicting the component boiling point (Edreder et al., 2009). The model is developed based on the following assumptions. (1) Total condenser (condenser is not considered as stage). The entire vapour from stage 1 is totally condensed in the condenser and then recycled back to the column. (2) Constant vapour rate. (3) Molar vapour rate is always equal to the liquid rate. (4) Constant molar over flow. (5) Total reflux operation. The entire liquid from the condenser is recycled back to the column. (6) Each stage is in equilibrium condition. There is no accumulation in the stage (Hisyam, 2011).

Balance at condenser including mass balance, Eq(1) and component balance, Eq(2).

$$\frac{dH_c}{dt} = V_1 - L_H \tag{1}$$

$$\frac{d(H_c.x_c)}{dt} = V_1 y_1 - L_H x_H \tag{2}$$

Balance at top vessel including mass balance, Eq(3) and component balance, Eq(4).

$$\frac{dH_1}{dt} = L_H \tag{3}$$

$$\frac{d(H_1.x_h)}{dt} = L_H x_c - L_H x_H \tag{4}$$

Balance at middle vessel including mass balance, Eq(5) and component balance, Eq(6).

$$\frac{dH_m}{dt} = L_m \tag{5}$$

$$\frac{d(H_m.x_m)}{dt} = L_m(x_n - x_m) \tag{6}$$

Balance at reboiler including mass balance, Eq(7) and component balance, Eq(8).

$$\frac{dH_B}{dt} = L_{n-1} - V_B \tag{7}$$

$$\frac{d(H_b.x_b)}{dt} = L_{n-1}x_{n-1} - V_B y_B \tag{8}$$

Balance at Stage Column 1 including mass balance, Eq(9) - (10) and component balance, Eq(11) - (12).
Stage n=1

$$\frac{dH_n}{dt} = V_{n+1} + L_H - V_1 - L_n \tag{9}$$

$$\frac{d(H_n.x_n)}{dt} = V_{n+1}y_{n+1} + L_H x_H - V_1 y_1 - L_n x_n \tag{10}$$

Stage n=2 to 7

$$\frac{dH_n}{dt} = V_{n+1} + L_{n-1} - V_n - L_n \tag{11}$$

$$\frac{d(H_n.x_n)}{dt} = V_{n+1}y_{n+1} + L_{n-1}x_{n-1} - V_n y_n - L_n x_n \tag{12}$$

Balance at Stage Column 2 including mass balance, Eq(13) - (14) and component balance, Eq(15) - (16).
Stage n=8

$$\frac{dH_n}{dt} = V_{n+1} + L_m - V_8 - L_n \tag{13}$$

$$\frac{d(H_n.x_8)}{dt} = V_{n+1}y_{n+1} + L_m x_m - V_8 y_8 - L_n x_n \tag{14}$$

Stage n=9 to 14

$$\frac{dH_n}{dt} = V_{n+1} + L_{n-1} - V_n - L_n \tag{15}$$

$$\frac{d(H_n.x_n)}{dt} = V_{n+1}y_{n+1} + L_{n-1}x_{n-1} - V_n y_n - L_n x_n \tag{16}$$

4. Mathematical modelling for control

From the process control perspective, the mathematical model can be used to determine the choice of input and output variables and the control strategy. Based on the degree of freedom, there are 28 process variables, 16 mathematical equations, 6 specified variables, and 3 constants. There are two manipulated variables (L_H, L_m) and one disturbance variable (V_1) obtained. All the variables are used to choose the control strategy. Two level control loop can be chosen.

5. Simulation

The multi-vessel batch distillation column is simulated using MATLAB Simulink. Simulink provides a graphical editor, customisable block libraries, and solvers for modelling and simulating dynamic systems. It is integrated with MATLAB where MATLAB algorithms can be incorporated into models and the simulation results are exported to MATLAB for further analysis. A simulation model in Simulink is presented in Figure 2.
The model consists of s-function block named multivess3comp.m and subsystem of temperature for each stage. In the simulation, three components are charged initially in the reboiler (B), top vessel (H) and middle vessel (M). The product will be collected at the reboiler denoted as xB, top vessel denoted as xH and middle vessel denoted as xM after the composition of the product reach steady state or constant.

6. Result and discussion

A case study of a non-zeotropic mixture consisting of ethanol, 1-propanol, and n-butanol is considered. Their physical properties are shown in Table 1. The product is collected when the entire vessels are already filled up with liquid feed and composition of all the vessels satisfy the product specifications (Hasebe et al., 1999).

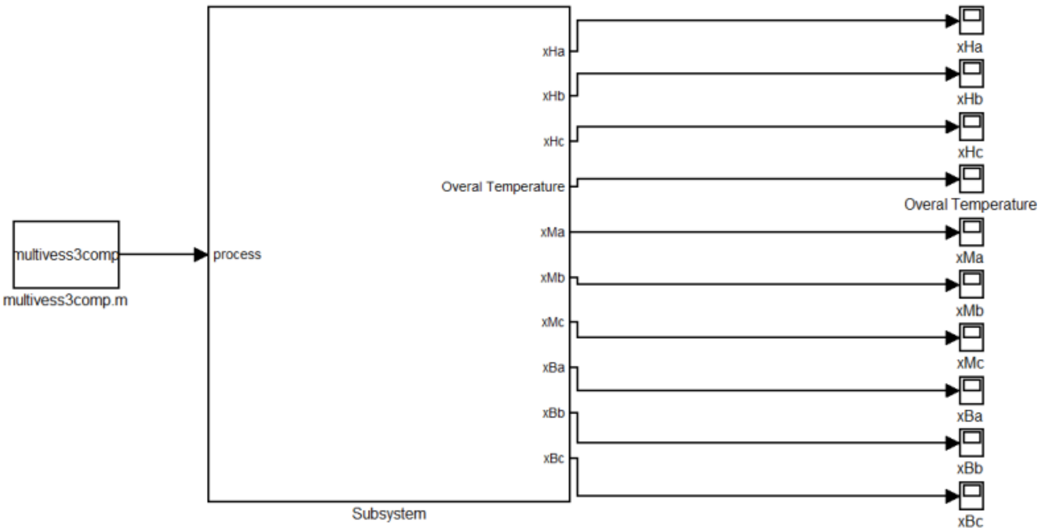

Figure 2: Simulink model of multi vessel batch distillation

Table 1: Physical Properties of Mixtures (Felder and Rousseau, 2000)

Properties	Ethanol (C_2H_5OH)	1-Propanol (C_3H_8O)	N-Butanol ($C_4H_{10}O$)
Molecular weight, g/mol	46.07	60.0950	74.1216
Boiling point, K	351.65	370.3	390.6
Density, kg/m^3	789	804.13	809.70

The simulation model is developed based on mathematical model as shown in section 3 due to fast supply, reliable information regarding feasibility and flexibility for adaption of control system. A stage to stage calculation is performed by using Antoine equation, bubble T equation, equilibrium equation, and unity equation. Relative volatility is assumed to be changing depending on temperature on each stages. In this study, the separation technique is based on ideal mixture. The most volatile component will be the lightest component and will vaporise as soon as the system reach its boiling point. The heaviest component will stay in reboiler even longer compared to the other components. All the components will be vaporised based on their boiling point. In this system, the lightest component (ethanol) will accumulate in top vessel. Second lightest component (1-propanol) will accumulate in middle vessel and the heaviest component (n-butanol) will accumulate in reboiler. The model is operated under total reflux. The vessel holdup must be specified first and keep constant (Wittgens et al., 2000). The vessel holdup is specified by taking into account the initial feed composition and amount of feed to ensure desired product composition achievable (Skogestad et al., 1995). The value of feed composition and the vessel holdup is shown in Table 2.
Figure 2 shows the simulation results of the concentration profile of component on top vessel, middle vessel and reboiler (still pot) respectively based on the data in Table 2.
From Figure 3, ethanol appears to be dominant in top vessel and 1-propanol dominant in middle vessel and in reboiler, dominant by n-butanol. Almost no n-butanol is present in top vessel. Based on the result, ethanol concentration has correlation with 1-propanol only due to their small boiling point difference. The impurity of top vessel is 1-propanol. In the middle vessel the impurity is ethanol and n-butanol. This is because the boiling point of 1-propanol is in between the boiling point of ethanol and n-butanol. In order to see the effect of vessel holdup to the final composition of product, the value of vessel holdup is changed to half of the previous value. The concentration profile for vessel holdup (65 : 200 : 200) is shown in Figure 4. The concentration of 1-propanol in middle vessel increases from 82 % to 87 % and n-butanol in reboiler (still pot) increases from 90 % to 94 %. This can be concluded that to obtain high purity product the vessel holdup must be low until certain value with regard to the mass balance.

Table 2: Vessel Holdup and Initial Composition

Components	Vessel Holdup, molar volume, mL	Initial Composition, mole fraction
Ethanol	100	0.170
1-propanol	400	0.415
n-butanol	400	0.415

The temperature profiles of stages are also presented in this paper as shown in Figure 5. The separation behaviour during the process can be monitored more easily by referring to temperature. The temperature changes as a result of the change of composition during the separation processes. Since the composition of the components always change with time, the temperature also keeps changing from time to time. The temperature tends to get constant as there is no composition change anymore when the system achieves steady state. The temperature profile can be used to identify the process condition during separation process instead of concentration profile.

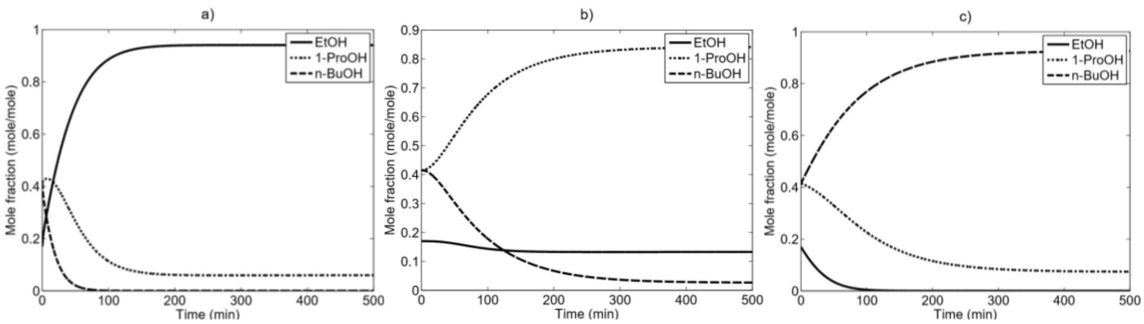

Figure 3: Concentration profile of (a) Top vessel (b) Middle vessel (c) Reboiler

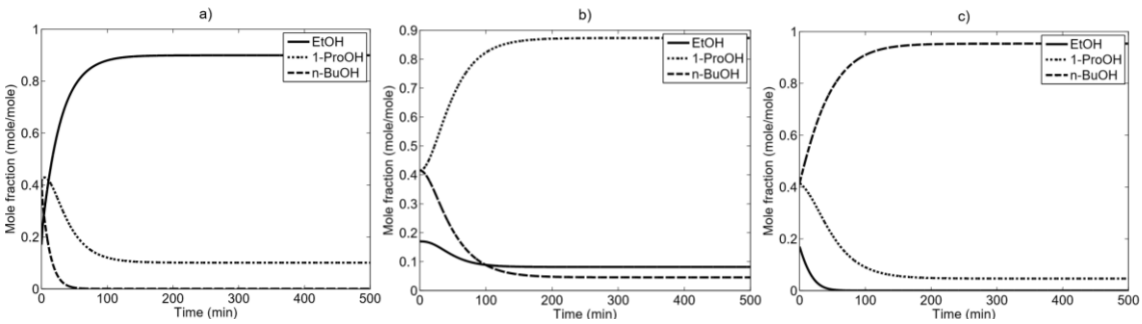

Figure 4: Concentration profile of (a) Top vessel (b) Middle vessel (c) Reboiler with different holdup

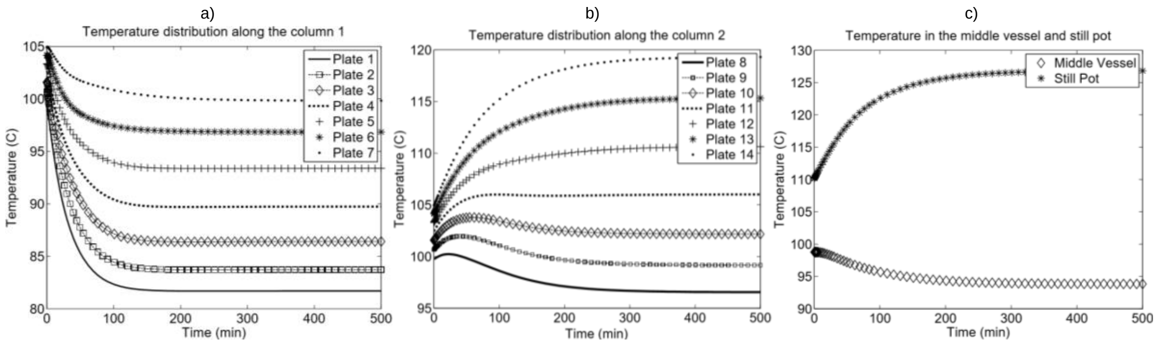

Figure 5: Temperature profile of (a) Column 1 (b) Column 2 (c) Reboiler and Middle vessel

7. Conclusion

In this study, the procedure of modelling and simulation before proceeding to the controller design is shown. From the simulation result, it can be seen that the vessel holdup will affect the concentration of final product. The lower the amount of vessel holdup the higher the product purity. In order to maintain the product purity at higher specification, the system must be operated under total reflux. To maintain the total reflux operation, the holdup in each vessel must be kept constant. This situation can only be realised if only controller is implemented. It is found that the simulation result shows stable response with changing variables. The simulation model is considerably acceptable, safe and preferable for feasibility study. The control strategy is determined based on the basic assumption. Its shows that the system has multi input multi output (MIMO). Further study on interaction analysis can be done to choose the optimum control strategy in order to give better performance for multi-vessel batch distillation.

Acknowledgement

The authors acknowledge academic staff from UiTM, Dr. Nor Azni Binti Shahari and the associate editor and reviewers for their valuable comments and suggestion that helped to improve the paper.

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