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Fractionation of oleochemical fatty acid using vacuum dividing wall column: A controllability analysis

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Abstract. Dividing wall column (DWC) provides a good alternative for oleochemical fractionation. However, the internal configuration and multiple input multiple output (MIMO) system of DWC leads to complexity in operation and control. This work aims to analyze the controllability of fractionating oleochemical fatty acid using vacuum dividing wall column (VDWC). To achieve this, Aspen Plus and Aspen Dynamics were used to develop a rigorous steady state and dynamic model of the column. Five manipulated variables (MVs) were considered namely reflux flowrate (L), distillate flowrate (D), bottom flow rate (B), side-stream flowrate (S) and vapor boilup (V) while controlled variables (CVs) were the product compositions. Pairing of MV and CV to determine the best 3×3 control configuration was performed using relative gain array (RGA) and singular value analysis (SVA). The selected control structure was tested on PID controllers for several regulatory and servo problem. The results of RGA and SVA shows that DSV was the best control configuration. Performance analysis was found to be successful in rejecting the disturbances as well as obtaining good set point tracking. However, distillate and bottom composition shows poor controllability compare to middle composition.

1. Introduction

Dividing wall column (DWC) provides a good alternative for processes using typical distillation (DC) column due to possible saving in both energy and capital cost. Because of its advantages, extensive research has been done and the first industrial application of DWC's was implemented in 1985 by BASF [1]. So far, about 40 DWCs are in operation worldwide and about 30 of them within the BASF group [2]. The potential of DWC is however restricted and not applied to broad range of the separation processes due to the challenges in design, simulate, operation and control [3-4]. In the oleochemical industry particularly in Malaysia, mostly used typical (DC) for its product fractionation. In our recent study, fractionating oleochemical fatty acids using DWC reduces around 20% of capital and operating cost compared to typical DC [5].

The integration of two columns into one shell leads to changes in the operating mode and controllability thus becoming a potential hurdle for commercial implementation of DWC [6]. Moreover, distillation columns exhibit a multiple-input multiple-output (MIMO) system in which manipulated variables (MVs) affect multiple controlled variable (CVs) [7]. To provide good process control in such system it is crucial to consider the probability of pairing CV and MV and applying an effective feedback controller to each selected pair. A good pairing will ensure effective rejection of process disturbances as



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well as maintaining the product specifications. Despite various research on DWC, study on oleochemical fractionation using vacuum dividing wall column (VDWC) received less attention. Therefore, this study aims to analyze the controllability of VDWC for fractionation of oleochemical fatty acid. Our scopes of work in paper include development of steady state and dynamic model in Aspen Plus and Aspen Dynamics. Determination of suitable 3×3 control configuration using steady state relative gain array (RGA) and singular value analysis (SVA) and test the performance of the selected controller configuration to disturbances in feed flowrate, feed composition as well as set point change.

2. Methodology

The process under study involves fractionation of oleochemical fatty acids which constitute of three carbon chains namely C10, C12 and C14. The boiling point of C10, C12 and C14 are 270 °C, 299 °C and 326 °C respectively. To avoid product degradation, the column temperature was operated below 270 °C at pressure between 0.01 to 0.1 bar. The feed information is listed in Table 1. The feed comprises mostly of C12 and C10 is the most least. C10 will be fractionated at the distillate stream whereas C12 and C14 will be fractionated at side and bottom stream respectively. The product purity for each streams were set to 99 mole%.

The steady state VDWC model was developed in Aspen Plus. NRTL was chosen as the thermodynamic model due to the polarity of the fatty acid as well as low operating pressure [5]. Instead of typical two or three model configuration, this work employs four RADFRAC model blocks to mimic the four internal and hydrodynamic behavior of an actual DWC internal sections. Furthermore, four column configuration was usually applied for dynamic simulation. The product purity for each streams were set to 99 mole%. Design of the VDWC was based on the work by Othman and Rangaiah [5]. The design parameters are shown in Table 1.

Table 1. VDWC design parameters

Reflux ratio	46.8
Stages (A/B/C/D) ^a	10 / 11 / 11 / 18
Feed stage	5 (at B)
Pressure, mbar	40
Feed flowrate, kg/h	6000
Mass fraction (C10/C12/C14)	0.05 / 0.71 / 0.24
Feed temperature, °C	30

^a A = Rectifying section, B = Pre-fractionation section, C = Middle section D = Stripping section.

2.1. Analysis tool

DWC implies a multi-input-multi-output (MIMO) control scheme. According to Koko and Barakat [8] there are seven degree of freedom (DOF) of DWC corresponding to seven MVs namely reflux flowrate (L), vapor boilup flowrate (V), side stream flowrate (S), distillate flowrate (D), bottom flowrate (B), liquid split ratio (Rl) and vapour split ratio (Rv). However, Rl and Rv are not suggested to be the MV because it could cause a serious operation and control problem [9-10]. In addition, perfect level control in reboiler and condenser were assumed. This reduces the DOF to three. The controlled variables (CVs) were x_{C10} , x_{C12} and x_{C14} represent mole fraction of distillate, side and bottom stream, respectively. For a 3×3 configuration there are nine possible pairings.

In order to screen suitable pairing of MV-CV, relative gain array (RGA) was applied. RGA has been widely used among the researcher [9-12] to examine the proposed control system in the distillation column and DWC. In RGA, the best control loop pairing was determined by the steady-state gain (K). For a 3×3 system, the steady-state gain matrix is denoted by:

$$K_{ij} = \begin{pmatrix} K_{11} = \frac{\Delta y_1}{\Delta u_1} \Big|_{u_{2,3}} & K_{12} = \frac{\Delta y_1}{\Delta u_2} \Big|_{u_{1,3}} & K_{13} = \frac{\Delta y_1}{\Delta u_3} \Big|_{u_{1,2}} \\ K_{21} = \frac{\Delta y_2}{\Delta u_1} \Big|_{u_{2,3}} & K_{22} = \frac{\Delta y_2}{\Delta u_2} \Big|_{u_{1,3}} & K_{23} = \frac{\Delta y_2}{\Delta u_3} \Big|_{u_{1,2}} \\ K_{31} = \frac{\Delta y_3}{\Delta u_1} \Big|_{u_{2,3}} & K_{32} = \frac{\Delta y_3}{\Delta u_2} \Big|_{u_{1,3}} & K_{33} = \frac{\Delta y_3}{\Delta u_3} \Big|_{u_{1,2}} \end{pmatrix} \quad (1)$$

where y indicates the output and u indicates the input. K_{11} in the matrix indicates the changes on y_1 when u_1 is altered while u_2 and u_3 are constant. K_{12} denotes the changes on y_1 when u_2 is altered but u_1 and u_3 are kept constant and so on. From the steady-state matrix, RGA (Λ) can be calculated using the following relationship:

$$\Lambda = K \otimes (K^{-1}) \quad (2)$$

where \otimes denoted as the element by element multiplication. T denotes the transpose of the steady-state gain matrix. If $\Lambda_{ij} = 0$, it means that y_i does not respond to m_j thus m_j could not be used to control y_i . While $\Lambda_{ij} = 1$ means that y_i only responds to m_j and not interact with other manipulated variables. If $0 < \Lambda_{ij} < 1$ or $\Lambda_{ij} > 1$, then an interaction occurs because more than one y_i react to m_j . Last but not least, if $\Lambda_{ij} < 0$, it means that the interaction exists between the related manipulated and controlled variables is in opposite direction and cause instability. The least interaction, where the arrangement which gives a RGA with diagonal element values close to unity will be selected as the best pairing. For RGA, four possible control configuration schemes were studied namely DB/LSV, LB/DSV, DV/LSB and LV/DSB.

Alternatively, singular value analysis (SVA) was also applied. Singular value analysis (SVA) is an alternative to RGA for design of multivariable control systems. Singular values arise from the decomposition of K :

$$K = W \Sigma V^T \quad (3)$$

where Σ is the diagonal matrix of singular values. W and V are unitary matrices. The columns of W are referred to as the input singular vectors whereas the columns of V are the output singular vectors. The final matrix property of interest in the condition number (CN). If K is non-singular, the CN number of K is a positive number defined as the ratio of the largest and smallest nonzero singular values:

$$CN = \frac{\sigma_1}{\sigma_r} \quad (4)$$

If the CN value is small, then the multivariable effects of uncertainties are not likely to be serious. For SVA, three CVs were manipulated by three out of five MVs with total nine possible pairings. In this work, both RGA and SVA were applied to screen possible MV-CV for the VDWC. RGA was conducted first followed by SVA. The steady state gains for these analysis were obtained through the developed Aspen Plus steady state model. The best possible matching from RGA and SVA analysis will be selected for closed loop performance analysis.

2.2. Dynamic model

In dynamic model, modifications were made to the steady state model. Pressure changes along the column were considered by fitting all four column stages were with Mellapak 350Y packing. Reflux

drum and column sump were sized assuming residence time of 5 min and 10 minutes, respectively. Valves, pumps and compressors were added to the dynamic model flowsheet to achieve pressure consistency. Because of the system dependency on pressure, pressure driven mode was selected. The default control loops were reflux drum level control, column sump level control, top column pressure control and bottom column temperature control. Pressure check was made to ensure pressure consistency prior exporting to Aspen Dynamics.

2.3. Closed loop response

The selected controller configuration from the previous step were added to the dynamic model flowsheet. PID controller was adopted in this work. No measurement delay was included. The controller settings were determined using conservative Ziegler-Nichols (ZN) open loop test tuning method. Fastest loop was tuned first and then closed, followed by the second controller tuning while the first controller remains closed. This continues until all control loops were tuned. The controller was tested to several scenarios. First was a regulatory problem in which the process was subjected to feed rate change and change in feed compositions. For the latter three scenarios were considered each with different sets of feed compositions. Second was the servo problem where set point change was introduced to the distillate, side and bottom product composition.

3. Results and discussions

The RGA controllability indices results for all four control configurations is given in Table 2. RGA values with less than 0 were excluded due to caused instability whilst value close to 1 is preferred. The most suitable pairing of MV-CV are D- x_{C10} , S- x_{C12} and V- x_{C14} as their value were close to 1 compared to the other indices. This indicate each MV has a good inner interaction with its correspond CV whilst minimally affect other variables. Table 3 shows the CN results from SVA analysis. Pairing no 7 (D- x_{C10} , S- x_{C12} , V- x_{C14}) and 9 (D- x_{C10} , V- x_{C12} , B- x_{C14}) are having the smallest CN value and therefore are preferred as it shows minimal dependency to other MVs. Pairing 7 is consistent with the 3×3 RGA, but not pairing 9. Therefore, DSV control loop arrangement was selected and the updated controller loop of the VDWC is shown in figure 1(a).

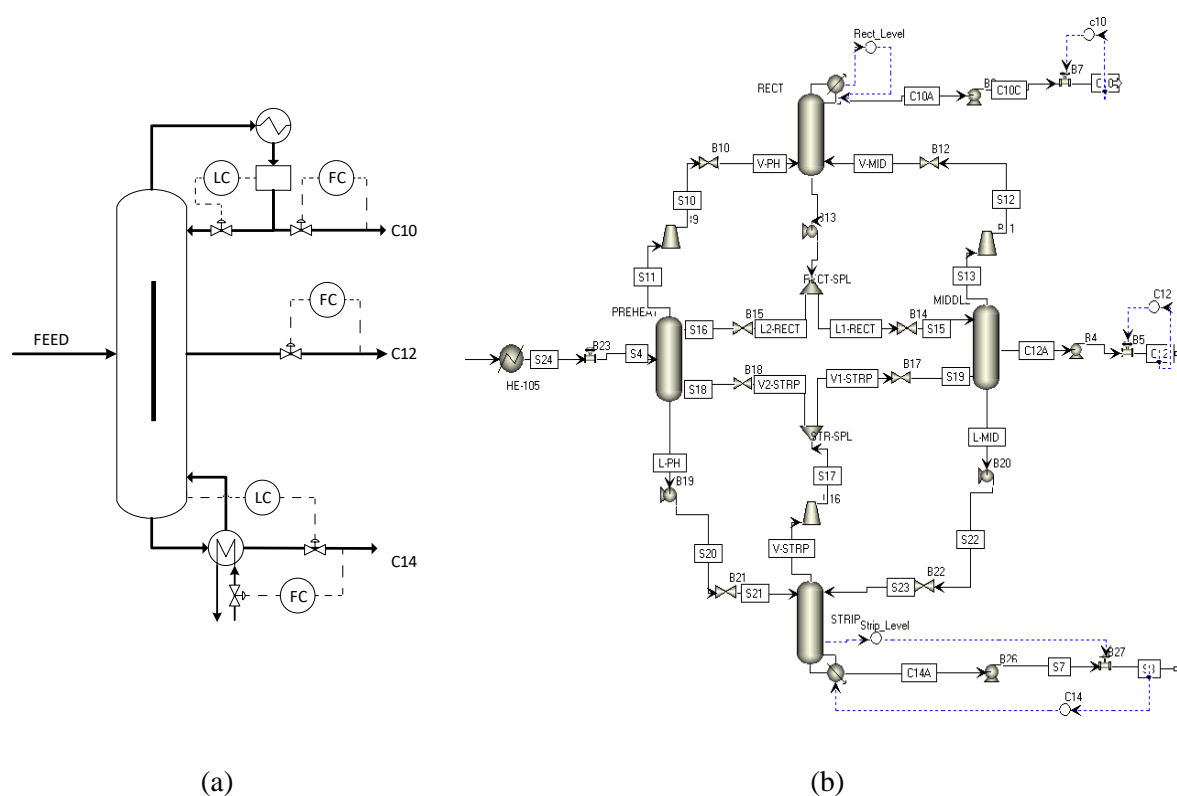
Table 2. RGA steady state controllability indices for 3×3 control problem. The CVs are x_{C10} , x_{C12} and x_{C14} .

Controlled variables, x_i	Manipulated variables, m_j		
	L	S	V
x_{C10}	-3.3070	4.3080	-0.0010
x_{C12}	4.2978	-3.4826	0.1848
x_{C14}	0.0092	0.1746	0.8162
	L	S	B
x_{C10}	-3.0273	4.0208	0.0065
x_{C12}	0.6892	-0.4059	0.7166
x_{C14}	3.3381	-2.6149	0.2768
	D	S	V
x_{C10}	0.9916	-0.0949	0.1033
x_{C12}	-0.1153	1.1151	0.0002
x_{C14}	0.1237	-0.0202	0.8965
	D	S	B
x_{C10}	-13.2389	-3.4140	17.6529
x_{C12}	0.7780	-0.2493	0.4713
x_{C14}	13.4609	4.6632	-17.1242

Table 3. CN values for steady state controllability analysis for 3×3 control problem. The controlled variables are x_{C10} , x_{C12} and x_{C14} .

Pairing	Controlled variables	Manipulated variables ^a	CN
1	x_{C10} , x_{C12} , x_{C14}	LDS	2765.00
2	x_{C10} , x_{C12} , x_{C14}	LSV	147.84
3	x_{C10} , x_{C12} , x_{C14}	LSB	222.00
4	x_{C10} , x_{C12} , x_{C14}	LDV	139.46
5	x_{C10} , x_{C12} , x_{C14}	LDB	18.81
6	x_{C10} , x_{C12} , x_{C14}	LVB	1004.33
7	x_{C10}, x_{C12}, x_{C14}	DSV	3.83
8	x_{C10} , x_{C12} , x_{C14}	DSB	33.03
9	x_{C10} , x_{C12} , x_{C14}	DVB	4.22

^a In each pairing, the first controlled variables is paired with the first manipulated variable, and so on i.e. in pair 1, x_{C10} is paired with L, x_{C12} is paired with D and x_{C14} is paired with S.

**Figure 1.** (a) DSV control configuration (b) Aspen Dynamics VDWC layout for DSV control configuration

The controller loops were added to the dynamic model. Figure 1(b) shows the Aspen Dynamic flowsheet. The dynamic flowsheet layout consists of five control loops corresponding to the DSV configuration as well as level controller for sump and reflux tank. The controller tuning for each controller loop was performed using the Tuning Option. The value is shown in table 4. Time variation of the product composition when subjected to 2% and 4% changes in the feed rate is shown in Figure 2a & 2b, respectively. We see from the simulations that middle composition ($C12$) provides much better control compared to distillate ($C10$) and bottom composition ($C14$). Bottom composition oscillates more than distillate composition. Variation in feed flowrate seems to have minimal effect on the middle

composition. This is due to the large amount of C12 in the feed stream and minimal effect in the internal flows. Overall, the feed rate change disturbance was able to be rejected.

Figure 2c on the other hand, shows the time profile when the process was subjected to several feed composition variation scenarios namely Scenario 1, 2 and 3. From the results, distillate composition has poor controllability compared to the middle and bottom composition with high overshoot and long settling time. Bottom composition incur some oscillation but has a lower overshoot and faster settling time compare to distillate composition. Since large portion of the feed contain C12, variation of C10 and C12 in the feed affect the internal flows and purity which eventually effect the controllability of the distillate and bottom stream. Middle composition is however unaffected by variation in feed composition with good controllability. Overall, variation of feed stream has minimal effect on middle composition.

Table 4. PID tuning results based on ZN tuning method.

Loop	K	τ_I	τ_D
D	107.4	90.2	8.5
S	111.0	5.6	-
V	4.0	23.1	2.1
Reflux level	1	20	-
Sump level	1	20	-

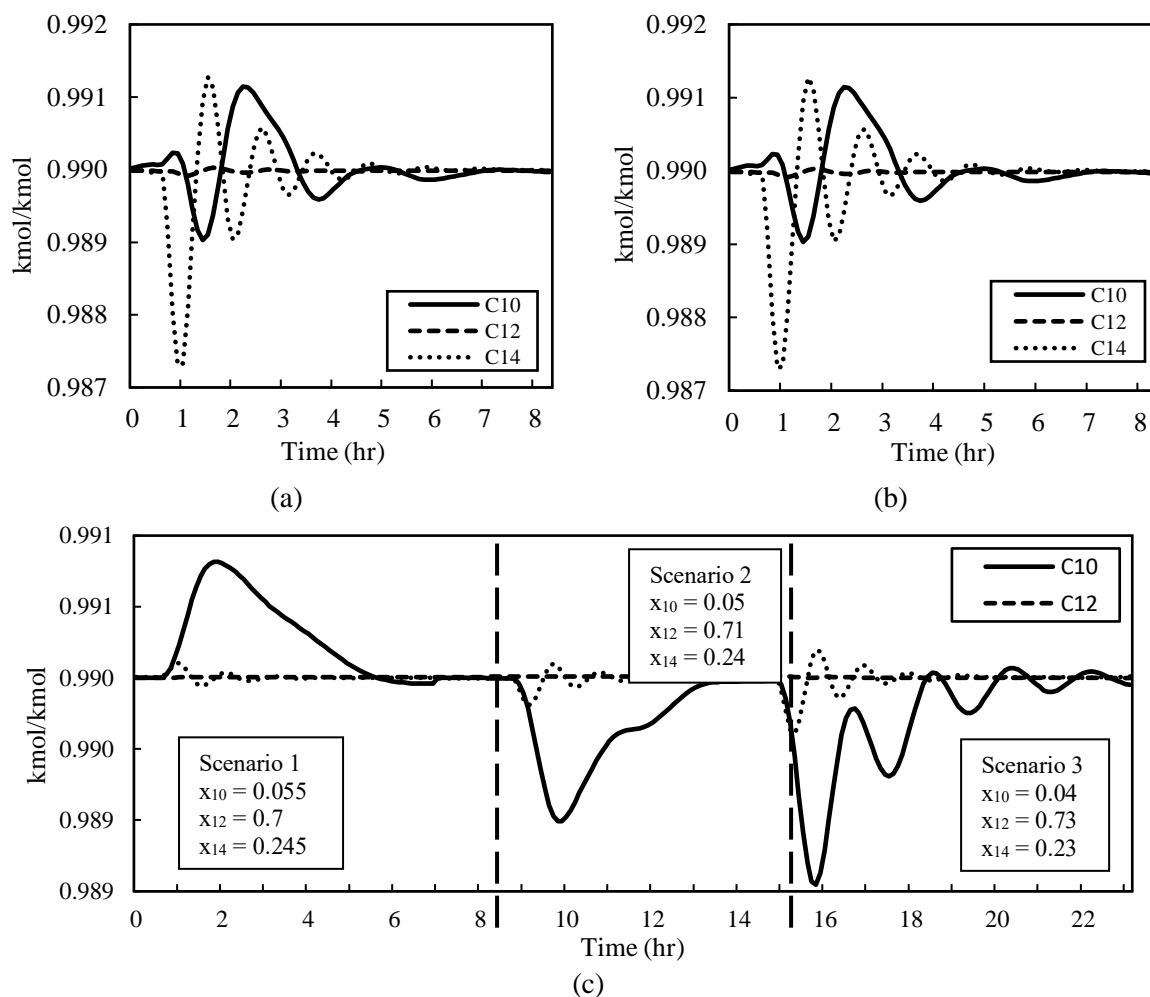


Figure 2. Closed loop response to (a) 2% step change in feed flow (b) 4% step change in feed flow (c) variation in feed composition

Figure 3 shows the result of set point tracking in all product stream with change of 0.001. We can see that distillate and bottom composition control shows some oscillation and settle after almost five hours. Middle composition on the other hand, has very good response with almost no overshoot and fast settling time. This is reasonable and consistent with previous results due to the large amount of C12 in the feed stream and has minimal effect in the internal flows.

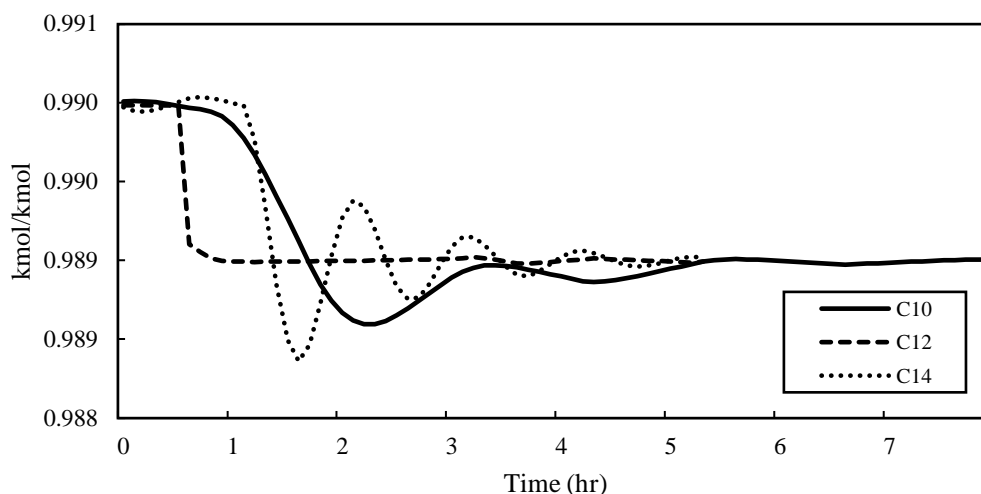


Figure 3. Closed loop response to set point change of 0.001 in distillate, middle and bottom composition.

4. Conclusions

VDWC controllability analysis for fractionating oleochemical fatty acid has been studied in this work. Steady state and dynamic model of the column have been successfully developed using Aspen Plus and Aspen Dynamics. Pairing of 3×3 control configuration was performed using relative gain array (RGA) and singular value analysis (SVA). Both approach resulted in DSV configuration being the most suitable configuration. The configuration was applied to the dynamic model and the controller performance was tested to feed rate and feed composition variations as well as set point change. Performance analysis was found to be successful in rejecting the disturbances as well as obtaining good set point tracking. However, distillate and bottom composition shows poor controllability compare to middle composition mainly due to the composition proportion of the feed.

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