Controllability Features of Dividing-Wall Columns

Ariella Janka Tarjani[a], Andras Jozsef Toth[a,*], Tibor Nagy[a], Eniko Haaz[a], Daniel Fozer[a], Anita Andre[a], Peter Mizsey[a,b]

[a]Budapest University of Technology and Economics, Department of Chemical and Environmental Process Engineering
 Budafoki Street 8, H-1111, Budapest, Hungary
[b]University of Miskolc, Department of Fine Chemicals and Environmental Technologies
 Egyetemvaros, H-3515, Miskolc, Hungary
ajtoth@envproceng.eu

The dividing wall columns have they renascence, however, there is lack of comprehensive investigation of column with upper and lower positioned walls. Previous work presented the energy efficiencies of dividing wall columns compared to common and energy integrated column structures.

This paper presents a comprehensive study of controllability features based on frequency dependent controllability indices and their aggregation in the so called "desirability function".

Conventional distillation column sequences and dividing-wall columns are selected for the study. A total of six different distillation arrangements are considered separating three ternary alcohol mixtures with different eases of separation. Rigorous simulations are carried out using Aspen Plus and Aspen Dynamics. Linear state-space representations of the studies systems are obtained using the Control Design Interface. Frequency dependent controllability indices, MRI, CN and RGAno, are calculated by MATLAB. Based on open-loop responses, discrete frequencies are chosen to determine characteristic indices of the systems. Evaluation of the results is supported by the desirability function. The results show that the separated mixtures influence the controllability features. However, from the different results of our work, we select that if indirect separation structure is recommended, DWC with lower partition shows considerable enhancement in controllability properties.

1. Introduction

Dividing-wall columns (DWCs) are todays alternative of sustainable distillation technology. DWCs offer a wide range of new solutions in separation tasks to analyse during process intensification. Using DWCs in a distillation sequence significantly increases the number of possible arrangements (Zhang et al. 2017). These options are worth to be considered as DWCs proved to be attractive in terms of energy consumption. The number of industrial applications is increasing rapidly due to the significant energy and capital cost savings DWCs can offer. Although there are more than 100 equipment in operation (Aurangzeb and Jana, 2016), open literature of DWC control properties provides contradictory results (Dejanovic et al., 2010) though controllability is just as important as energy consumption during the integrated process intensification.

Favourable energy consumption of DWCs is caused by the energy integration technique, thermal coupling. In thermally coupled distillation systems such as DWCs, Petlyuk systems and columns with side-strippers or side-rectifiers the remixing effect is reduced resulting lower heat demand than that of the conventional sequences. Thermal coupling on the other hand generates stronger interactions between the control loops of the columns making the controllability worse than that of any conventional or heat integrated scheme (Mizsey et al., 1998). However, in some cases, thermally coupled distillation sequences can exceed conventional systems in controllability (Hernandez et al., 2005).

In the open literature there are industrial and laboratory applications of DWCs (Egger and Fieg, 2017) proving to have acceptable controllability features. In addition, controllability of DWCs can also be improved by choosing the most suitable control structure and operating condition, which is not necessarily the same as in case of the conventional columns. Operation at nonoptimal conditions, fixing the vapor and liquid splits can enhance controllability properties of DWCs while maintaining low energy efficiency (Serra et al. 2003). Model

predictive controllers have also proved to be a promising tool for making DWCs competitive with conventional column sequences (Dohare et al., 2015). These works do not deal, however, columns with upper and lower positioned dividing wall columns since these columns are new innovations.

In this paper controllability properties of DWCs with partitions in the upper, the lower and in the middle part of the column are compared to that of the alternative conventional column sequences, the conventional direct, indirect sequence and the sloppy system. Results are dedicated to enrich the conflicting literature of DWCs control properties and support industrial application.

2. Case Study

2.1 Mixtures Examined

The mixture of ethanol, n-propanol and n-butanol have already proven to be suitable to investigate controllability of DWCs (Wang and Wong, 2007). The ease of separation index (ESI) of the ethanol, n-propanol, n-butanol mixture is close to 1 thus the separation of A/B and B/C are equally hard. As it is confirmed that the mixture influences the controllability indices (Serra et al., 2003), two other alcohol mixtures are considered with the ESI close to 1.5 and 0.5. Table 1 contains the selected mixtures and their components used in the simulations.

Table 1: Mixtures Examined

Mixture	A	B	C	α_{AC}	α_{BC}	α_{AB}	ESI
1	ethanol	n-propanol	n-butanol	8.47	3.00	2.82	0.94
2	ethanol	n-propanol	i-butanol	5.52	1.96	2.82	1.44
3	methanol	t-butanol	n-butanol	17.87	6.07	2.95	0.49

According to Table 1 Mixture 2 has an ESI close to 1.5 meaning the separation of B/C is harder than the separation of A/B. Mixture 3 has an ESI close to 0.5 thus the separation of A/B is harder than the separation of B/C. The hardest separation is between n-propanol and i-butanol as the relative volatility of these component is 1.96. Therefore, the separation of Mixture 2 needs the largest number of trays.

The feeds are equimolar, the flow rate is 100 kmol/h, product purities are 95 mol% in all simulations, the thermodynamic model is UNIQUAC.

2.2 Selected Designs

Rigorous steady-state simulations of the studied systems are carried out with Aspen Plus using RadFrac column models. Conventional columns are modeled as sieve tray columns with one feed, one distillate and one bottom product. Number of trays and feed stages of conventional column sequences (Figure 1) are determined by optimization based on shortcut calculations and an Excel subroutine calculating the Total Annual Cost (TAC) of the systems.
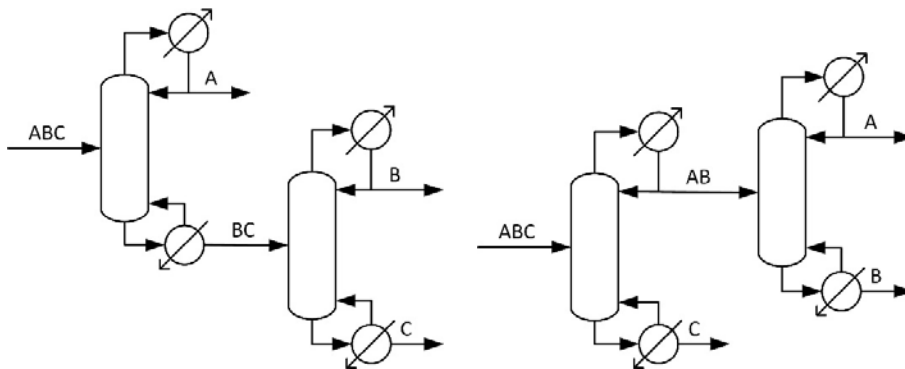

Figure 1: Conventional Direct (left) and Indirect (right) Column Sequences

Number of trays in conventional columns in case of Mixture 1 are: CDS1 = 46, CDS2 = 33, in case of Mixture 2: CDS1 = 46, CDS2 = 85, in case of Mixture 3: CDS1 = 38, CDS2 = 26 where CDS1 is the column with the primary feed and CDS2 is the column with the secondary feed. In case of Mixtures 1 and 2 CDS1 columns are identical for the same components are separated in the first column. Number of trays listed here are used in the indirect column sequences and in the DWCs with upper and lower partitions.

Rigorous simulation of DWCs is a challenging task since there is no commercially available flowsheeting software for this purpose (Asprion and Kaibel, 2010). In this paper DWCs are modelled with thermodynamically equivalent structures of two thermally coupled conventional columns. Figure 2 and 3 show the DWCs with upper and lower partitions with their thermodynamically equivalent models. Design parameters of DWCs are determined by the corresponding conventional column sequence.
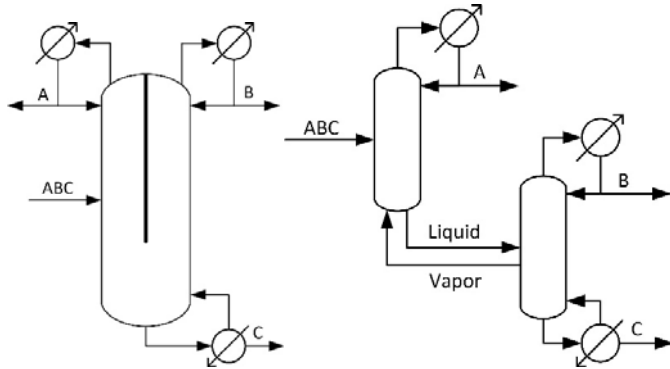

Figure 2: Dividing-Wall Column with Upper partition (left) and the thermodynamically equivalent model (right)
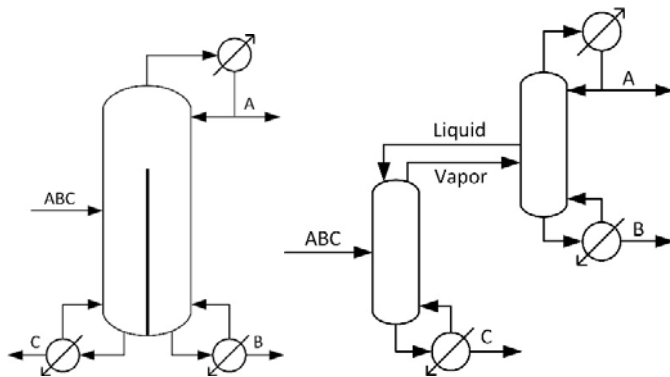

Figure 3. Dividing-Wall Column with Lower partition (left) and the thermodynamically equivalent model (right)

As for the DWC with partition in the middle, generally known as Kaibel column (Figure 4 - left), there is a well-known thermodynamically equivalent structure applicable for simulation, the Petlyuk system (Figure 4 - middle) consisting of two fully thermally coupled columns. Figure 4b shows the additional parameters needed to be determined for the optimal design of the prefractionator in Petlyuk configuration (Annakou and Mizsey, 1996). Number of trays and reflux ratio in the main column are set based on the conventional column properties. In the sloppy system the same number of trays and reflux ratio are applied as those of the Petlyuk system.
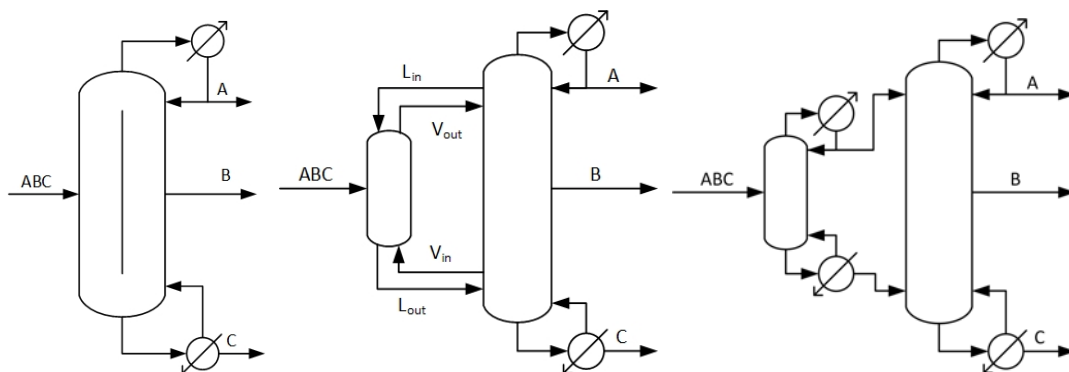

Figure 4. The Kaibel colum (left), the Petlyuk system (middle) and the sloppy system (right)

2.3 Controllability investigation

Rigorous steady-state simulations are exported to Aspen Dynamics and control structures are designed for the columns. Controlling the inventories by the reboiler duty and controlling the level in the reflux drum with the reflux flow of the reflux rate makes the column unstable (Kiss and Rewagad, 2011), therefore these manipulated variables are used to control product compositions. Each examined distillation arrangement is studied with two different control strategies described in Table 2.

Table 2: Composition Control Structures (R: Reflux ratio, L: Reflux stream, Q: Heat duty, S: Side product, 1: Column 1, 2: Column 2)

Controlled variable	Direct Sequence		Indirect Sequence		Petlyuk and Sloppy	
	RQ	LQ	RQ	LQ	RQ	LQ
x_A	R1	L1	R2	L2	R2	L2
x_B	R2	L2	Q1	Q1	S	S
x_C	Q2	Q2	Q2	Q2	Q2	Q2

Dynamic features of the systems are examined through the open-loop responses of 5% step change in the feed flow rate. Frequency dependent controllability indices are determined by MATLAB from the state-space representations obtained by the Control Design Interface (Gabor and Mizsey, 2008). Discrete controllability indices are chosen according to the time constants of the systems determined by the open-loop responses. These three discrete controllability indices (MRI, CN, RGAno) are then aggregated using the desirability functions Eq(1-4) (Haragovics et al., 2012) to make directs comparisons between the studied systems.

$$d_{MRI} = 1 - exp(-MRI \cdot 10) \tag{1}$$

$$d_{CN} = exp\big(-(a + b \cdot CN)\big) \tag{2}$$

$$d_{RGAno} = exp\left(-\frac{RGAno}{10}\right) \tag{3}$$

$$D = \left(\prod_{i=1}^{k} d_i^{m_j}\right)^{\frac{1}{\sum m_j}} \tag{4}$$

3. Results

D values of the systems with the studied control structures are presented on a -log scale (Figures 5-7). Each Figure shows the results of a single mixture. The smaller the -log(D) value is the better the controllability of the system. Performance of the control structures are not to be compared with this methodology.
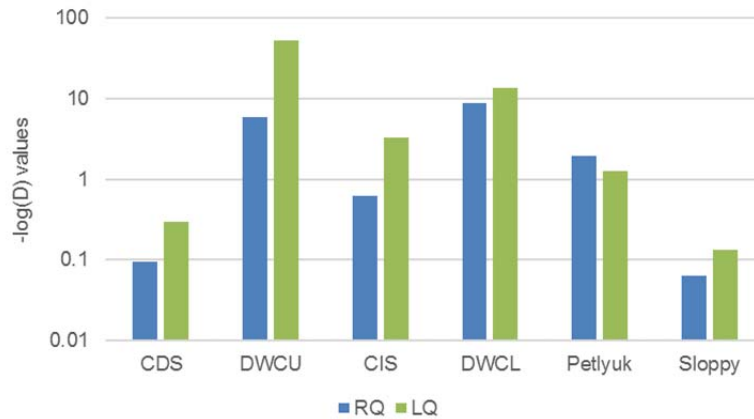

Figure 5. Results of Mixture 1 on -log(D) scale (CDS: Conventional Direct Sequences, DWCU: Dividing-wall columns with Upper partition, CIS: Conventional Indirect Sequences, DWCL: Dividing-wall columns with Lower partition)

In the case of Mixture 1 there is a great difference between the controllability of DWCs and conventional column sequences. Based on the D-values and the single controllability indices, conventional column sequences have favourable controllability properties than those of the DWCs. Considering Mixture 1, the conventional direct sequence and the sloppy system have the best controllability properties of the studied arrangements.
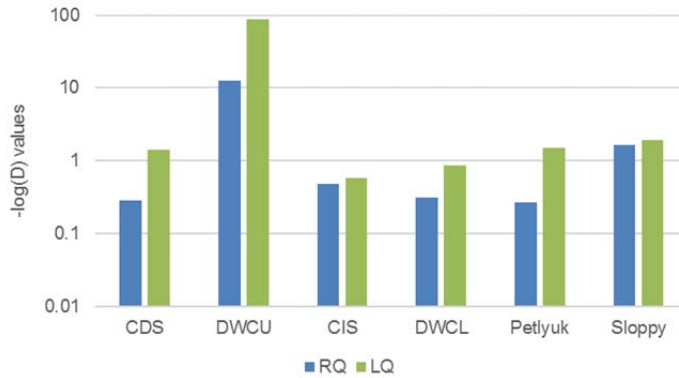

Figure 6. Results of Mixture 2 on -log(D) scale (CDS: Conventional Direct Sequences, DWCU: Dividing-wall columns with Upper partition, CIS: Conventional Indirect Sequences, DWCL: Dividing-wall columns with Lower partition)

Results of Mixture 2 show a slightly different trend. D-values of the DWC with lower partition and the Petlyuk system proved to be competitive with those of the conventional columns. It is known that Petlyuk configuration is more attractive in a controllability point of view with large number of trays (Serra et al. 2003). However, the DWC with upper partition still has poor controllability as it has two condensers and only one reboiler and liquid descends slower in the column than vapor ascends, making the system generally slower than the DWC with lower partition which has two reboilers and one condenser.
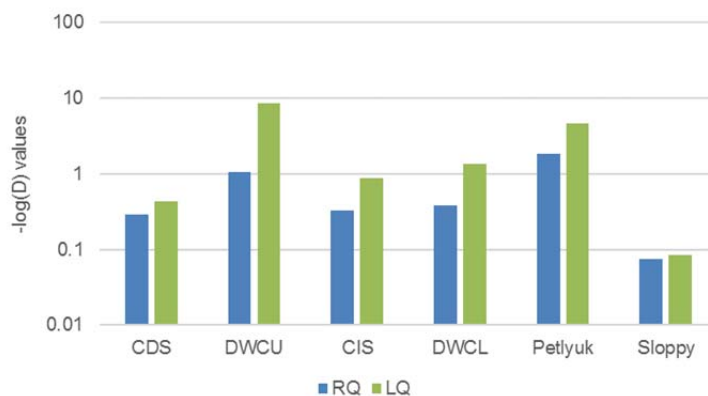

Figure 7. Results of Mixture 3 on -log(D) scale (CDS: Conventional Direct Sequences, DWCU: Dividing-wall columns with Upper partition, CIS: Conventional Indirect Sequences, DWCL: Dividing-wall columns with Lower partition)

In the case of Mixture 3 the trend is quite similar to that of Mixture 1, as these systems have comparable number of trays. Heuristic rules prefer to make the hardest separation at the end of the sequence, therefore components of Mixture 3 are advised to be separated in the indirect sequence. This heuristic rule influences controllability in this case as DWC with lower partition shows significant improvement in controllability compared to the results of the symmetric mixture.

4. Conclusions

In this paper controllability features of several conventional distillation sequences and dividing-wall columns are compared with different mixtures and control structures. Controllability properties of the studied systems are obtained by rigorous simulations. Frequency dependent controllability indices are calculated by MATLAB based on the state-space representations provided by the Control Design Interface of Aspen Dynamics. Using the desirability function, studied systems are compared directly. Results are shown on -log scale diagrams and discussed.

Distillation arrangements have an impact on the controllability of the systems. Generally, conventional column sequences have favourable controllability features than those of the DWCs, as the interaction in the columns increases with the thermal coupling. The DWC with lower partition can outperform the DWC with upper partition in controllability as it has only one composition controlled by the descending liquid and two compositions controlled by the ascending vapor which gives a more efficient control than contrariwise. Controllability of the Petlyuk system improves significantly when large number of trays is applied. With large number of trays, controlled compositions get far from each other, reducing interaction in the system. Studied mixtures also effect the controllability. When heuristic rules suggest an indirect separation sequence, DWC with lower partition shows considerable enhancement in controllability properties.

References

Annakou O., Mizsey P., 1996, Rigorous Comparative Study of Energy-Integrated Distillation Schemes, Industrial & Engineering Chemistry Research, 35 (6), 1877−1885.

Asprion N., Kaibel G., 2010, Dividing wall columns: Fundamentals and recent advances, Chemical Engineering & Processing, 49 (2), 139−146.

Aurangzeb Md., Jana A.K., 2016, Dividing wall column: Improving thermal efficiency, energy savings and economic performance, Applied Thermal Engineering, 106, 1033-1041.

Dejanovic I., Matijasevic Lj., Olujic Z., 2010, Dividing wall column—A breakthrough towards sustainable distilling, Chemical Engineering and Processing, 49, 559-580.

Dohare R.K., Singh K., Kumar R., 2015, Modeling and model predictive control of dividing wall column for separation of Benzene–Toluene-o-Xylene, Systems Science & Control Engineering, 3:1, 142-153.

Egger L.S., Fieg G., 2017, Decentralized Process Control of Reactive Dividing Wall Columns, Chemical Engineering Transactions, 57, 1693-1698.

Gabor M., Mizsey P., 2008, A Methodology To Determine Controllability Indices in the Frequency Domain, Industrial & Engineering Chemistry Research, 47 (14), 4807−4816.

Haragovics M., Kencse H., Mizsey P., 2012, Applicability of Desirability Function for Control Structure Design in the Frequency Domain, Industrial & Engineering Chemistry Research, 51 (49), 16007−16015.

Hernandez S., Gudino-Mares I.R., Cardenas J.C., Segovia-Hernandez J.G., Rico-Ramirez V., 2005, A Short Note on Control Structures for Thermally Coupled Distillaion Sequences for Four-Component Mixtures, Industrial & Engineering Chemistry Research 44,5857-5863.

Kiss A.A., Rewagad R.R., 2011, Energy efficient control of a BTX dividing-wall column, Computers and Chemical Engineering, 35, 2896– 2904.

Mizsey P., Hau N.T., Benko N., Kalmar I., Fonyo Z., 1998, Process control for energy integrated distillation schemes, Computers & Chemical Engineering, 14, 1213−1236.

Serra M., Espuna A., Puigjaner L., 2003, Controllability of Different Multicomponent Distillation Arrangements, Industrial & Engineering Chemistry Research, 42, 1773-1782.

Tarjani A. J., Toth A. J., Nagy T., Haaz E., Mizsey P., 2016, Dynamic Controllability Comparison of Conventional Distillation Sequences and Dividing-Wall Columns with Upper and Lower Partitions Using the Desirability Function, Industrial & Engineering Chemistry Research, 56, 952-959.

Wang S., Wong D.S.H., 2007, Controllability and energy efficiency of a high-purity dividedwall column, Chemical Engineering Science, 62, 1010–1025.

Zhang Y., Han G., Sun W., 2017, Estimation of the Number of Distillation Sequences with Dividing Wall Column for Multi-component Separation, Chemical Engineering Transactions, 61, 343-348.