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# Control structure selection for four-product Kaibel column

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# ABSTRACT

Dividing wall column configurations have a large savings potential in terms of capital and energy. This paper uses dynamic simulation to investigate three alternative control structures for one of these configurations, namely the Kaibel column. Four components, here selected as methanol, ethanol, *n*-propanol and *n*-butanol, are separated into pure products within a single column shell. Control structure 1 (CS1) uses only temperature controllers and is therefore particularly interesting from an industrial point of view. Since the control objective is to control the four product compositions, the two other control structures use also composition controllers. Surprisingly, for composition control, the simple temperature control scheme (CS1) is almost as good at steady-state and much better from a dynamic point of view than the two other more complex control structures.

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# 1. Introduction

Distillation is an important and widely used separation process in the chemical industries. However, distillation is generally an energy- and capital- intensive process. Process intensification technologies are able to reduce both energy and costs (Chu et al., 2011; Dejanovic et al., 2010; Emtir et al., 2001; Hernandez et al., 2003; Kiss, 2014; Staak et al., 2014; Yildirim et al., 2011). Dividing wall columns (DWC), which have been successfully introduced into the process industries, provide a promising trend for process intensifications. It is a single shell, direct material coupling distillation column which needs less energy, capital and space than a conventional column (Triantafyllou and Smith, 1992). Compared with conventional distillation configurations, the energy saving amount of DWCs is up to 30% (Triantafyllou and Smith, 1992). Furthermore, DWCs can be applied to azeotropic, extractive, and reactive distillations, which lead to azeotropic dividing wall columns (ADWC) (Kiss and Suszwalak, 2012; Le et al., 2015; Sun et al., 2011; Wu et al., 2014), extractive dividing wall columns (EDWC) (Kiss and

http://dx.doi.org/10.1016/j.compchemeng.2016.07.019 0098-1354/© 2016 Elsevier Ltd. All rights reserved. Ignat, 2012; Kiss and Suszwalak, 2012; Tavan et al., 2014; Xia et al., 2012) and reactive dividing wall columns (RDWC) (Delgado-Delgado et al., 2012; Ignat and Kiss, 2013; Kiss et al., 2009; Lee et al., 2012; Qian et al., 2015; Wang et al., 2014).

The main obstruction for DWC industrialization is the fear of operability problems because of its complex structure and interactions among different control loops. Researchers have investigated controllability and operability of Petlyuk column, ADWC, EDWC and RDWC. Mutalib and Smith (Mutalib and Smith, 1998) investigated degrees of freedom in the three-product Petlyuk (dividing wall) column. Halvorsen and Skogestad (Halvorsen and Skogestad, 1999) studied optimal operation and control of the three-product Petlyuk (dividing wall) column. Serra et al. (Serra et al., 2000) studied the influence of design and operating conditions on the dividing wall column by comparing optimal and non-optimal operations. Skogestad et al. (Dwivedi et al., 2013a, 2013b) studied the control of three-product Petlyuk (dividing wall) column and four-product extended Petlyuk (dividing wall) column. Chien et al. (Wu et al., 2013a; Wu et al., 2013b; Wu et al., 2014) investigated the design and control of azeotropic dividing wall columns (ADWC), extractive dividing wall columns (EDWC) and reactive dividing wall columns (RDWC). Xu et al. (Xia et al., 2013; Xia et al., 2012) studied the different control structures for extractive dividing wall columns (EDWC). Yuan et al. (Qian et al., 2015) proposed a reactive dividing wall columns (RDWC) for selective hydrogenation and separation of C3 stream. Buck (Buck et al., 2011) applied model predictive control





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Fig. 1. The four-product dividing wall column (Kaibel column).

(MPC) of three-product dividing wall column. Kiss and Rewagad (Kiss and Rewagad, 2011; Rewagad and Kiss, 2012) investigated traditional PID control and advanced MPC of three-product dividing wall column.

Although researchers have investigated control structures for different DWC configurations, relatively few studies have been done on the four-product Kaibel column in Fig. 1. The fourproduct Kaibel column is less energy efficient than the four-product extended Petlyuk (dividing wall) column, but it can still save up to 30% energy cost compared to conventional distillation because it performs a sharp split in the prefractionator (Halvorsen and Skogestad, 2003). More importantly, the capital savings can be up to 50% because three conventional distillation columns can be replaced by a single dividing wall column. This paper considers three alternative single-loop PI control structures for a fourproduct Kaibel column which separates a mixture of methanol, ethanol, *n*-propanol and *n*-butanol. In CS1, only temperature controllers are used. Dwivedi et al. (Dwivedi et al., 2012b) experimentally verified a similar control structure in the lab-scale experiment with good results. Temperature control is faster, more applicable and less expensive than composition control. In CS2, composition controllers are added on top of CS1. The impurity compositions in the outlet streams of distillation columns are controlled in order to retain the main product purity in the product streams. In CS3, the maximum value of light impurity compositions in side product streams and the impurity composition in the bottom stream is controlled by manipulating the reboiler duty. Feedforward controllers are added to accelerate the response and reduce the deviations in the product streams. In addition, control structures CS2 and CS3 use the vapor split as a manipulated variable. The vapor split has so far not been reported as a manipulated variable in industrial scale DWC. However, Dwivedi et al. (Dwivedi et al., 2012a) used the vapor split in the lab-scale experiment with good results, and this may be applied to commercial DWC in the future.

# 2. Process description

The separation of methanol (A), ethanol (B), n-propanol (C) and n-butanol (D) is used as the case study for the Kaibel column. The feed of 1 kmol/h is equimolar saturated liquid. The approximate relative volatilities for methanol (A), ethanol (B), n-propanol (C) and n-butanol (D) are 7.1, 4.43, 2.15 and 1, respectively.

The simulations use the two-shell configuration in Fig. 2, which is thermodynamically equivalent to the four-product Kaibel column in Fig. 1. The steady state design was performed with Aspen Plus, and the dynamic simulations were done with Aspen Plus Dynamics. The thermodynamic model uses the NRTL liquid activity equation.



**Fig. 2.** Prefractionator (P) and main section (M) of Kaibel configuration showing theoretical stages in each section (Thermodynamically equivalent to Fig. 1).



Fig. 3. Vmin diagram for sharp separation of equimolar M-E-P-B feed.

The Vmin diagram in Fig. 3 shows the minimum vapor flows in various sections required for sharp separation of an equimolar A-B-C-D feed. The y-axis shows the minimum boilup (V/F) and the x-axis shows the net product withdrawal (D/F) in a conventional two-product column. The peak  $P_{AB}$  gives the minimum vapor flow (V/F) required for separating A and B. Similarly, the point  $P_{AD}$  denotes the minimum vapor flow required to separate A and D.

In the two-shell Kaibel configuration in Fig. 2, the prefractionator performs a sharp AB/CD split while the main section completes the A/B and C/D separations. The composition profiles of the prefractionator and the main section are shown in Fig. 4. The specifications for the main component in the four products (D, S1, S2, B) are all 99%. The nominal data for the case study Kaibel column are shown in Table 1.

# 3. Control structures

Before the Aspen Plus steady state simulation results are exported to Aspen Plus Dynamics, the tray sizing feature in Aspen Plus is used to size the column. The reflux drum and the sump of the column are sized to provide 10 min holdup with 50% liquid level space (Luyben, 2013; Luyben and Chien, 2011).

The pressure of the column is controlled with the condenser duty (Qc). The two level controllers use the product streams (D and B) as manipulated variables, which corresponds to a standard "LV-configuration". PI controllers are used in this paper, except P controllers for levels. The gains and integral times of the pressure controller and the two level controllers are from Luyben's book (Luyben, 2013). The pressure and level controllers are not shown in the illustrations of the control structures. With these three control loops closed, there are six remaining dynamic (and steady state)



Fig. 4. Composition profiles of the prefractionator and main section.

# Table 1

Nominal data of the Kaibel column.

	Prefractionator	Main section
Total number of theoretical stages	40	70
Feed stage (from top)	20	21/60
Product stage (from top)	1/40	30/50
Top mole flow rate (D) (kmol/h)	0.501	0.251
The upper side product flow rate (S1) (kmol/h)	-	0.248
The lower side product flow rate (S2) (kmol/h)	-	0.249
Bottom mole flow rate (B) (kmol/h)	1.629	0.252
Molar reflux ratio (L/D)	0.600	9.604
Vapor split ratio (R <sub>V</sub> ) <sup>a</sup>	-	0.515
Liquid split ratio (R <sub>L</sub> ) <sup>a</sup>	-	0.352
Liquid rate in the top (Lp and L) (kmol/h)	0.750	2.407
Vapor rate in the bottom (Vp and V) (kmol/h)	1.130	2.162
Operating pressure (atm)	1.136	1
Tray pressure drop (atm)	0.0068	0.0068
Condenser duty QC (kW)	-	26.007
Reboiler duty QR (kW)	-	25.107
Mole fraction of A in top product	0.302	0.99
Mole fraction of B in top product	0.695	0.01
Mole fraction of C in top product	0.003	0
Mole fraction of A in the upper side product	-	0.0076
Mole fraction of B in the upper side product	-	0.99
Mole fraction of C in the upper side product	-	0.0024
Mole fraction of B in the lower side product	-	0.0071
Mole fraction of C in the lower side product	-	0.99
Mole fraction of D in the lower side product	-	0.0029
Mole fraction of B in bottom product	0.001	0
Mole fraction of C in bottom product	0.729	0.01
Mole fraction of D in bottom product	0.270	0.99

<sup>a</sup> The vapor split ratio ( $R_V$ ) is defined as the fraction of vapor that is send to the prefractionator, i.e.,  $R_V = Vp/V$  (where V is the vapor flow below the vapor split and Vp is the vapor flow into the prefractionator). The liquid split ratio ( $R_L$ ) is defined as the fraction of liquid that is send to the prefractionator, i.e.,  $R_L = Lp/L$  (where L is the liquid flow above of the liquid split and Lp is the liquid reflux flow into the prefractionator).

degrees of freedom, which from a control point of view correspond to the following manipulated variables (u):

1 Reflux flow rate (L)

2 Reboiler duty (Qr)

- 3 Upper side product flow rate (S1)
- 4 Lower side product flow rate (S2)
- 5 Liquid reflux from the main section to the prefractionator (Lp)
- 6 Vapor stream from the main section to the prefractionator (Vp).

Note that Vp (or rather the vapor split  $R_V = Vp/V$ ) is not used as a degree of freedom in control structure CS1. The primary (economic) controlled variables (CV<sub>1</sub>) are the four product compositions. In addition, the two prefractionator "products" may be controlled in order to avoid breakthrough of C in the top (Dp) and breakthrough of B in the bottom (Bp). For distillation, the secondary controlled variables (CV<sub>2</sub>) are usually temperatures. According to the plantwide control procedure of Skogestad (Skogestad, 2003),

the control system is divided into a supervisory layer, which controls the primary variables ( $CV_1$ ), and a stabilizing layer which controls drifting or sensitive variables that are easy to measure and control.

The temperature profiles of the prefractionator and the main section are shown in Fig. 5. In order to find the steady-state sensitivities (gains, dT/du) for the tray temperatures (T), small increases (+0.1%) have been made in each of the six independent variables (u). The changes were made one at a time with the other flows constant. The results are shown graphically in Fig. 6 for the prefractionator (left) and main section (right). For stabilizing control, the first issue is to decide which temperatures to control. In general, we need one stabilizing temperature or composition loop for each split (Skogestad, 2007). The prefractionator performs one split, and needs one temperature controller. The main section performs three splits and needs three temperature controllers. We see from Fig. 6 that there are four sensitive trays (stages) which display clear temperature peaks, and fortunately there is one in the prefractionator



Fig. 5. Temperature profiles of the prefractionator and the main section.



Fig. 6. Process sensitivity profiles (steady state gain, dT/du) for the prefractionator and the main section.

and three in the main section. In the prefractionator it is the 12th tray (above the feed). In the main section it is the 12th tray (above the liquid split), the 43rd tray (between the side products) and the 64th tray (below the vapor split). Thus, we will use for stabilizing control  $CV_2 = [T_{P,12}, T_{M,12}, T_{M,43}, T_{M,64}]$ .

#### 3.1. Control structure 1 (CS1)

Control structure 1 (CS1) with four stabilizing temperature controllers for  $CV_2$  is shown in Fig. 7. The selected controlled variables are the four sensitive temperatures observed in Fig. 6. The pairing also follows from Fig. 6 using the "pair close" rule as explained in the following. Note that we do not control the product composition ( $CV_1$ ) in structure CS1.

There are four temperatures to be controlled, so we only need to use four of the six manipulated inputs (u). In the main section, one of the four manipulated inputs will not be used for stabilizing control, that is, it will be kept constant, at least on a short to intermediate time scale. The vapor split  $(R_V)$  is assumed to be constant in CS1, because it is normally not available as a manipulated variable. The liquid coupling stream to the prefractionator (Lp) is therefor used to control the prefractionator temperature (T<sub>P.12</sub>) because it has a large gain and good dynamics ("pair close rule"). Of the four variables, the side stream flow rates (S1, S2) should not be kept constant, because otherwise it will not be possible to have pure products when there are disturbances in feed rate and feed composition. Essentially, all of component B should go in S1, so we need to have S1 close  $z_BF$  (where  $z_B$  is the mode fraction of B in the feed) and S2 close to z<sub>C</sub>F. One could use feedforward control based on measuring the feed rate and feed composition, but it is unlikely that the accuracy will be sufficient. Thus, S1 and S2 should be used for temperature control. From Fig. 6, we see that S1 mainly affects



Fig. 7. Control structure 1 (CS1).

 $T_{M,43}$ , and this is also a good pairing dynamically according to the "pair close rule". Similarly, S2 mainly effects  $T_{M,43}$  (which is already controlled by S1) and  $T_{M,64}$ , so we choose to control  $T_{M,64}$  with S2, which also is accordance with the "pair close" rule. What remains now is  $T_{M,12}$ , which from Fig. 6 is effected about equally well at steady state by reflux (L) and boilup (Qr). However, the "pair close rule" clearly favors using reflux for controlling  $T_{M,12}$ .

This results in the control structure in Fig. 7 where boilup (Qr) is not used for feedback control. However, we know that the boilup should increase proportionally with the feed rate, and this is the



Fig. 8. Control structure 2 (CS2)

reason for the proposed feedforward (ratio) controller, where Qr/F is kept constant. Next, we need to tune the four temperature controllers. The build-in Tyreus–Luyben tuning procedure in Aspen Plus Dynamics was used to tune the four temperature controllers (with the deadtimes in each loop set to 1 min). The controller tuning parameters for CS1 are shown in Table 2.

# 3.2. Control structure 2 (CS2)

In our case, the primary (economic) objective is to control all four compositions, so we introduce in control structure 2 (CS2) in Fig. 8 six composition controllers on top of structure CS1. Four of the composition controllers adjust temperature setpoints, one adjusts the setpoint for the ratio (Qr/F), and the sixth composition controllers manipulates the vapor split (Rv) which was not used in CS1.

We have assumed that it is optimal, at least close to optimal, to keep the end compositions in the prefractionator constant. Actually, we first tried to use only the four composition controllers in the main section and have a single temperature controller in the prefractionator and Rv constant as in CS1, but we found that it did not work unless we introduced composition control in the prefractionator column.

The four temperature controllers are the same as those in CS1. The controlled variables of the four composition controllers CCD, CCS1, CCS2 and CCP1 are the impurity composition of B in the dis-

#### Table 2

Controller tuning parameters of control structure 1 (CS1).

tillate (D), the heavy impurity composition of C in the upper side product (S1), the heavy impurity composition of D in the second product (S2) and the impurity composition of C in the top overhead vapor stream of the prefractionator (Dp), respectively. The manipulated variables of CCD, CCS1, CCS2 and CCP1 are set points of TC1, TC2, TC3 and TCP, respectively. For controller CCB, the impurity composition of C in the bottom stream (B) is controlled by manipulating the reboiler duty to feed flow ratio setpoint. Finally, for controller CCP2, the impurity composition of B in the bottom liquid stream (Bp) is controlled by manipulating the vapor (Vp) to the prefractionator. As the purity specification of the side products are very high (99%), composition controllers are needed at both ends of the prefractionator to prevent the impurity components entering the main section. The build-in Tyreus-Luyben tuning procedure in Aspen Plus Dynamics did not perform well in terms of dynamic responses. Therefore, the values for the controller gains and integral times for the six composition controllers are obtained from step responses using the SIMC tuning rules (Skogestad, 2003). Deadtimes in the composition control loops are set to be 3 min and  $\tau_c$  in the SIMC tuning are set to be 20 min. The controller tuning parameters of CS2 are shown in Table 3.

# 3.3. Control structure 3 (CS3)

The light impurity compositions in the two side product streams are not controlled in CS2, which sometimes leads to large dynamic deviations in component B in the lower side product (S2B). In control structure 3 (CS3) in Fig. 9, a selector is introduced to avoid this. Also, in CS3, the lower layer stabilizing temperature controllers are removed. The impurity composition of B in the top product stream is controlled by manipulating the ratio of the reflux flow rate to the feed flow rate. The heavy impurity composition of C in the upper side product stream is controlled by manipulating the upper side product flow rate. The heavy impurity composition of D in the lower side product stream is controlled by manipulating the second product flow rate. Because of a max-selector, the maximum value of the light impurity composition of A in the upper side product stream, the light impurity composition of B in the lower side product stream and the impurity composition of C in the bottom product stream is controlled by manipulating the ratio of the reboiler duty to the feed flow rate. The set point of this controller is set to be 0.01. In the prefractionator, the impurity composition of C in the overhead vapor is controlled by manipulating the liquid to the prefractionator, while the impurity composition of B in the bottom liquid stream is controlled by manipulating the vapor to the prefractionator. The build-in Tyreus-Luyben tuning procedure in Aspen Plus Dynam-

Control loop	Controlled variable	Manipulated variable	Controller gain	Controller integral time (min)
TC1	T <sub>M,12</sub>	L	2.46	10.56
TC2	T <sub>M,43</sub>	S1	6.32	14.52
TC3	T <sub>M,64</sub>	S2	6.20	15.84
TCP	T <sub>P,12</sub>	Lp	4.33	17.16

#### Table 3

Tuning parameters for composition controllers for CS2 (on top of CS1 controllers).

Control loop	Controlled variable	Manipulated variable	Controller gain	Controller integral time (min)
CCD	$\chi_{D,B}$	Set point of TC1	0.034	18.08
CCS1	x <sub>S1,C</sub>	Set point of TC2	0.548	7.06
CCS2	x <sub>S2,D</sub>	Set point of TC3	0.051	4.24
CCB	x <sub>B,C</sub>	Setpoint of Qr/F	0.021	6.93
CCP1	x <sub>Dp,C</sub>	Set point of TCP	0.014	3.72
CCP2	$\chi_{Bp,B}$	Vp	0.142	18.40



Fig. 9. Control structure 3 (CS3).

ics was used with the deadtimes in each loop set to 3 min. The controller tuning parameters of CS3 are shown in Table 4.

#### 4. Results and discussion

The dynamic responses of the product compositions and the manipulated variables for structures CS1, CS2 and CS3 to a +10% feed composition disturbance of component A and a +10% feed flow rate disturbance are shown in Figs. 10 and 11, respectively. In addition, the Supplementary material has dynamic responses for other feed composition disturbances and reboiler duty disturbances. A 10% feed composition increase of A means that A is increased from 0.25 to 0.275 with the ratio of the other three components constant. Note that DB, S1A, S1C, S2B, S2D and BC corresponds to, respectively, the impurity component B in the distillate, the light impurity component C in the upper side product, the light impurity component B in the lower side product, the impurity component D in the lower side product and the impurity component C in bottom product.

The dynamic responses of CS1 with only temperature controllers are very smooth. Although the product compositions have some steady state deviations, the deviations are very small (less than 1%). Temperatures (controlled variables) responses of CS1 are shown in Fig. 12. The settling time is very short.

With CS2, the controlled impurity compositions return to their set points. However, the maximum deviations of the light impurity component B in the lower side product (S2B) are relatively large when the feed composition of A increases 10% or the feed composition of C decreases 10%.

CS3 has a selector where the maximum value of the light impurity composition of A in the upper side product stream (S1A), the light impurity composition of B in the lower side product stream (S2B) and the impurity composition of C in the bottom product stream (BC) is controlled by manipulating Qr/F. This reduces some dynamic deviations compared to CS2, but others are larger, so overall this is no significant improvement. The product compositions and the manipulated variables with CS3 settle to the same values as those with CS2.

The changes of the manipulated variable values for CS1 are much smoother and with less oscillations than for CS2 and CS3. Overall, structures CS2 and CS3 have poor performance due to the large interactions. To deal with interactions one could use multivariable control (e.g. model predictive control).

## 5. Conclusions

This paper compares three single-loop control structures for the four-product Kaibel column. Control structure 1 (CS1) has four temperature controllers plus a feed-forward controller to the reboiler duty. This is basically a stabilizing control structure, but we find that it works surprisingly well also in terms of composition control. The cascade control structure 2 (CS2) adds six composition controllers on top of CS1. It also manipulates the vapor split, which is not used in CS1. Control structure 3 (CS3), with only composition controllers, also has a selector to the reboiler duty to control the maximum value of light impurity compositions in side streams and impurity composition in bottom stream. Dynamic simulations for various disturbances show that all three control structures are able to maintain their desired steady state using traditional singleloop PI control. Of course, with only temperature control (CS1) there is some steady-state deviation in the product compositions, but it is surprisingly small. Furthermore, the dynamic performance with only temperature control (CS1) is superior, with much smaller dynamic composition deviations than for CS2 and CS3. This is a surprising result, which is encouraging result for the industrialization of Kaibel columns.

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# Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compchemeng. 2016.07.019.

Table 4	
Controller tuning parameters	of control structure 3 (CS3).

Control loop	Controlled variable	Manipulated variable	Controller gain	Controller integral time (min)
CCD	X <sub>D,B</sub>	L/F	0.186	132
CCS1	x <sub>S1,C</sub>	S1	3.538	47.52
CCS2	x <sub>S2,D</sub>	S2	0.466	39.60
CCB	$max(x_{B,C}, x_{S1,A}, x_{S2,B})$	Qr/F	0.083	42.24
CCP1	x <sub>Dp,C</sub>	Lp	0.175	31.68
CCP2	$\chi_{Bp,B}$	Vp	0.088	54.12



Fig. 10. Compositions and MV responses for a +10% disturbance in feed composition of A. (a) product compositions. (b) manipulated variables.



Fig. 11. Compositions and MV responses for a +10% feed flow rate disturbance. (a) product compositions. (b) manipulated variables.



Fig. 12. Temperatures (controlled variables) responses of CS1. (a) +10% feed composition of A disturbance. (b) +10% feed flow rate disturbance.

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