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Optimal Operation and Control of Divided Wall Column

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Abstract

In this paper, possible modes of optimal operations of the three-product divided wall column have been discussed. These modes differ in terms of the given energy price (expensive/cheap) and given product purity constraints. In addition, the control structure scheme for one of these modes has been proposed. In this mode energy is assumed to be cheap and product purity specifications are not fixed. Since, product purity specifications are not fixed, there are three unconstrained degrees of freedom in the column for which the self-optimizing control structure has been proposed.

Keywords: DWC, Petlyuk column, Optimal operation, Minimum energy

1. Introduction

Divided wall columns have gained increasing applications due to their lower energy consumption and investment costs compared with conventional distillation column sequences. A divided wall column (DWC) has a vertical partition that divides the column shell into a pre-fractionator and side draw section. Figure 1 shows the divided wall column with a single reboiler and a single condenser.

Various modes of operation based on operational objective and constraints have been studied by several investigators. Strandberg (2011) considered four different cases of optimal operation of the Kaibel column with feed rate as a degree of freedom. Ghadrdan et al. (2011) extended the investigation of two cases, namely minimizing energy usage for fixed product specifications (Mode- I_{ABC}) and maximizing product purities for fixed boilup (Mode-II₀), Table 1. Dwivedi et al. (2013) mainly focused on the control structure selection for fixed product specifications with minimum energy usage (Mode-I_{ABC}). Further, Khanam et al. (2013) have studied the optimal operation of divided wall (Petlyuk) column for fixed energy and non-optimal vapor split ratio R_v (Mode-II₀). Halvorsen and Skogestad (1999) studied steady-state optimal operation for minimum energy usage (Mode- I_{ABC}) and concluded that energy saving is difficult without a good control strategy. They also discussed candidate feedback variable for self-optimizing control scheme for minimizing the energy usage. In this paper we have investigated all possible modes of operation based on operational objective and constraints as given in Table 1. In addition, we have also studied the self-optimizing control scheme for minimizing the sum of impurities for fixed boilup (Mode-II₀).

2. Modes of Optimal Operation

The column for our study is modeled stage by stage. The column has 6 sections with 12 stages in each of these sections. The study has been conducted with the following assumptions: constant pressure, negligible vapor hold up, a total condenser, equilibrium on all stages, linearized flow dynamics constant relative volatilities and constant molar flows in column's sections.

The feed F is given and it contains three components A (lightest), B and C (heaviest). We have started with investigating all possible modes of optimal operation. The cost function for the three-product divided wall column for this study is:

$$J = p_F F + p_\nu V - p_D D - p_S S - p_R R \tag{1}$$

where *J* is the scalar cost function (\key (\key), F, V, D, S and R are the flow rates (kmol/min) of feed, boilup, distillate, side product and bottom product respectively. Since, B denotes one of the key components therefore R has been used to denote the bottom product flow rate. p_F , p_v , p_D , p_S and p_R are prices (\key) of respective flow streams. The feed is assumed to be a disturbance and thus there are five steady-state degrees of freedom. The steady-state degrees of freedom are V, S, R, R₁ and R_v. R₁ and R_v are liquid split ratio and vapor split ratio respectively. D and R are used to control levels and therefore have no steady-state effects. The plant's economics is mainly dependent on steady-state conditions therefore the effects of dynamics have been neglected in this study, Skogestad (2000). As mentioned earlier, we consider four constraints:

$$x_{D,A} \ge x_{D,A(\min)} ; \quad x_{S,B} \ge x_{S,B(\min)} ; \quad x_{R,C} \ge x_{R,C(\min)} ; \quad V \le V_{\max}$$

$$\tag{2}$$

where A, B and C are key components in distillate D, side stream S and bottom product R respectively. With four possible constraints given in Eq. (2), there are $2^4=16$ different possible combinations of active constraints ("modes of operation") as given in Table 1. We assume that R₁ and R_v are used to control the compositions in the prefractionator for stable operation of the main column. Then, there are three degrees of freedom for the main column, and it is therefore infeasible with four active constraints (Mode-II_{ABC} is infeasible). This leaves 15 modes of operation, the two main modes of operations are:

- (i) Mode-I (V < V_{max}): Minimize energy
- (ii) Mode-II (V=V_{max}): Maximize the value of products

From economic perspective, Mode-I and Mode-II differ in terms of given energy price. Mode-I is suitable when energy is expensive and therefore the objective function turns out to be minimizing the energy. However, Mode-II is suitable when energy is cheap and consequently the objective function turns out to be maximizing the product recovery by using the maximum available energy. Further, these two modes can be subcategorized into various modes for optimal operations based on the objective function and active constraints as given in Table 1.

Different sub-modes of operation with a defined objective function are based on the fact that for a given column design, the active constraints region may change depending on the product, feed and energy price as well as the disturbances (feed rate and feed compositions). For example, in Mode- I_{ABC} , all three constraints on product compositions are active.

| Mode | No. of active composition constraints, $x_{D,A}$ in distillate D , $x_{S,B}$ in | | | | |
|------------------|---|--|--|-----------------------|--|
| | side stream S and $x_{R,C}$ in bottom product R | | | | |
| | 0 | 1 | 2 | 3 | |
| Mode-I | Mode-I ₀ | Mode-I _A /Mode- | Mode-I _{AB} /Mode- | Mode-I _{ABC} | |
| Expensive | (1 case) | I _B / Mode-I _C , | I _{BC} /Mode-I _{CA,} | (1 case) | |
| Energy | | (3 cases) | (3 cases) | | |
| $V \leq V_{max}$ | | | | | |
| Mode-II | Mode-II ₀ | Mode-II _A /Mode- | Mode-II _{AB} /Mode- | Infeasible | |
| Cheap Energy | (1 case) | $II_{B}/Mode-II_{C},$ | $II_{BC/}$ Mode- II_{CA} | | |
| $V = V_{max}$ | | (3 cases) | (3 cases) | | |

Table1. Possible modes of operation for the three-product DWC based on active constraints

In Mode-I, we minimize the energy for different sets of constraints on the main component fraction in the product. This mode of operation is optimal when energy is expensive and constraints on all three product purity compositions are active to avoid product give away (e.g., Mode-I_{ABC}). However when constraints on all three products are not active and the energy is expensive then optimal operation is a trade-off between minimizing impurities and minimizing energy. This is because the profit is dependent on both energy saving and the purity of the product (e.g., Mode-I₀).

Mode-II is generally optimal when the energy is cheap and thus we set the column to operate at maximum $V=V_{max}$. This mode of operation is also suitable when the price of product is dependent on its purity. In this case column can be operated for maximizing the sum of product purities or maximizing the profit for even and uneven pricing respectively. However when none of the constraints are active on the products (Mode-II₀) then the optimal operation is only justified for even pricing. While in case of uneven pricing for subcategories of Mode-II, we can minimize the sum of impurities or maximize the profit. According to Skogestad (2000) plantwide control procedure active constraints are controlled first followed by self-optimizing controlled variables for the remaining unconstrained degrees of freedom. As the number of active constraints and unconstrained degree of freedom vary in various modes of operation therefore the control strategy will also vary for various modes given in Table 1.

3. Self-Optimizing Control Structure for Mode-II₀

In Mode-II₀, the constraints on product purity specifications are not active and the boilup is only an active constraint. Also if we assume that the price of each of the three products distillate (D), side stream (S) and bottom product (R) is dependent on the key component present in it.

$$p_D = p_A^0 x_{D,A}; \ p_S = p_B^0 x_{S,B}; \ p_R = p_C^0 x_{R,C}$$
⁽³⁾

It is also assumed that the unit price of each component is same as given below:

$$p_A^0 = p_B^0 = p_C^0 = 1 \tag{4}$$

The cost function given by Eq. (1) can be rewritten as:

$$J = x_{DB}D + (x_{SA} + x_{SC})S + x_{BB}R$$
(5)

 $\langle \alpha \rangle$

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The cost function as given above is the total sum of impurities in product streams coming out of the main column. The unconstrained degrees of freedom for self-optimizing control are reflux flow rate, side stream flow rate and the liquid split ratio as given below:

$$u^T = [L \ S \ R_l] \tag{6}$$

There are five disturbances and they are feed flow rate, composition of A and B in the feed, the boilup which is fixed and set at the maximum and the vapor split ratio:

$$d^T = \begin{bmatrix} F & z_A & z_B & V & R_v \end{bmatrix} \tag{7}$$

Self-optimizing control scheme is the most suitable for $Mode-II_0$ because the product purity specifications are not fixed and there are three unconstrained degrees of freedom, Eq. (6). These unconstrained degrees of freedom can be used to control three controlled variables to run the column at optimal or near optimal conditions. The column data with feed conditions and other process parameters for this study are given in Table 2.

Table 2. Process data for the three-product divided wall column

| Physical data | | | |
|---|---------------------------------------|--|--|
| Component A, B and C | Ethanol, Propanol and n-Butanol | | |
| Boiling points of A, B and C | [78.37 97 117.4] | | |
| Relative volatilities [A (lightest), B, C | [4.2 2.1 1] | | |
| (heaviest)] | [= =] | | |
| Number of stages | 12 in each section | | |
| Nominal feed flow rate, F^* | 1 [kmol/min] | | |
| Nominal feed composition, $[z_A^* z_B^* z_C^*]$ | [0.333 0.333 0.333] | | |
| Nominal liquid feed, q_F^* | 1 | | |
| Disturbances (Deviations) | | | |
| Feed, F | $F^* \pm 10\%$ | | |
| $\begin{bmatrix} z_A & z_B \end{bmatrix}$ | $[z_A^* \pm 10\% \ \ z_B^* \pm 10\%]$ | | |
| V _{max} | $V_{max}^* \pm 10\%$ | | |
| R_{v} | $R_v^* \pm 10\%$ | | |
| Implementation errors | | | |
| Control error (integral action) | 0.0000 | | |
| Measurement error (temperatures) | <u>±0.5 °C</u> | | |

Table 3. The steady state RGA (relative gain array) for the selected controlled variables

| Temperature | L | S | R_l |
|-----------------|----------|-------------------------|-------------------------|
| T_{10} | -0.00026 | 1.05 x 10 ⁻⁵ | 1.000252 |
| T ₃₈ | 0.989655 | 0.010629 | -0.00028 |
| T_{60} | 0.010608 | 0.98936 | 3.17 x 10 ⁻⁵ |



Figure 1. Self-optimizing control configuration (keeping three temperatures at their nominal setpoints using unconstrained degrees of freedom)

Bi-directional branch and bound method for average loss criterion (Kariwala et al. 2008) was used to find three best sets of temperatures. For these sets of measurements, the average loss was calculated by using H and norm of M(H) matrix as given in recent literature by (Yelchuru and Skogstad, 2012). The average loss calculated for first 10 sets of measurements were nearly same in magnitude. For example the loss corresponding to the best temperature sets (T₉, T₃₈ and T₅₈) was 9.31e-4 and the losses corresponding to other next best sets of temperatures were 9.32 x 10⁻⁴, 9.39 x 10⁻⁴, 9.41 x 10⁻⁴, 9.43 x 10⁻⁴, and 9.63 x 10⁻⁴. Also the average loss corresponding to the combination of all 72 measurements was 7.5166 x 10⁻⁴ which was nearly same as the loss corresponding to three temperatures used as measurements. The sets of temperatures with different combinations were tested on the non-linear model for larger disturbance in the feed flow rate. The temperatures to be kept constant for self-optimizing control which gives acceptable loss are: T₁₀, T₃₈, T₆₀ (Figure 1). Based on the value of stead-state RGA as given in Table 3, it is found that these temperatures are also good for stabilizing control as suggested by Khanam (2014).

4. Conclusions

In this paper, it is found that there are 15 possible modes of optimal operation of the three-product divided wall column for given constraints on energy and product purity specifications. The control structure selection for one of these modes with fixed energy

and unconstrained product purity specifications shows that the economic selfoptimizing control layer is same as the regulatory control layer of the column.

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