

SELF-OPTIMIZING CONTROL CONFIGURATIONS FOR TWO-PRODUCT DISTILLATION COLUMNS

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The choice of control structures for distillation columns is an important issue for practical industrial operation. There is no single “best” structure for all columns, so some authors feel that each column should be treated independently. Nevertheless, the objective of this work is to find for a structure that is “reasonable” for all columns. In this paper, we consider the steady-state deviations in product composition, assuming that we only have available flows and temperatures for control. By using local methods, including the exact local method and the minimum singular value rule, we search for two “self-optimizing” variables, which when held constant result in small deviations in the presence of disturbances. We find that for most columns, a good choice is to keep a constant reflux to feed ratio L/F and keep a constant temperature in the middle of the bottom section of the column. Especially for multicomponent separations, it does not help to control two temperatures.

KEYWORDS: distillation column, multicomponent distillation, control structure selection.

INTRODUCTION

For a distillation column, the “original” degrees of freedom are $\mathbf{u}_0 = [L \ V \ D \ B]$, where we have assumed that pressure is tightly controlled (Shinskey, 1984). However, levels need to be controlled. This consumes two degrees of freedom and, since the level set point has no steady-state effect, we are left with two steady-state degrees of freedom. For the further analysis it does not matter what these are, so let us choose them as $\mathbf{u} = [L \ V]$. For this study, the main assumptions are:

1. Consider steady state only.
2. Two-product column with given feed and fixed pressure.
3. Two-point product composition control is desired, but the composition measurements are not available (at least not for fast control).
4. Variables available for control: all temperatures and flows (including flow ratios L/D , L/F , etc.) A reasonable cost function for the composition control problem is

$$J = (X_D - X_{Ds})^2 + (X_B - X_{Bs})^2 \quad (1)$$

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The question is: What should we use the two degrees of freedom for, that is, what are the controlled variables \mathbf{c} ? Should L be kept constant or maybe L/D ? Should a temperature, in order to minimize J , be kept constant? To analyze this we consider product composition variations in response to disturbances. Any control structure which controls two intensive variables (e.g. L/D and V/B , or two temperatures) will have perfect disturbance rejection for feed flowrate disturbances. Therefore, as pointed out by Luyben (2005), the key factor to consider is feed composition disturbances.

Two common approaches for identifying controlled variables are (Luyben, 2005a):

1. Look for variables with a small optimal variation in response to disturbances (Luyben, 1975);
2. Look for variables with a large steady-state gain, or more generally, large minimum singular value ($\underline{\sigma}(\mathbf{G})$), from the inputs \mathbf{u} to temperatures \mathbf{c} (Moore, 1992).

These approaches may yield conflicting results, and Skogestad (2000) proposed to combine them by considering the minimum singular value of the scaled gain matrix ($\underline{\sigma}(\mathbf{G}')$). The optimal variation here enters into the scaling factor, together with the implementation error. This approach has a theoretical basis, but there are some assumptions, like assuming a unitary Hessian matrix $\mathbf{J}_{\mathbf{u}\mathbf{u}}$. To improve on this, one may consider $\underline{\sigma}(\mathbf{G}'\mathbf{J}_{\mathbf{u}\mathbf{u}}^{-1/2})$, but also this is not exact. In this paper, we therefore mainly use the exact method of Halvorsen et al. (2003). A local method is numerically much more effective than numerically computing the loss for all possible structures and disturbances. To solve this self-optimizing problem, a scalar cost function J to be minimized must be defined.

SELF OPTIMIZING CONTROL

“Self-optimizing control” is when keeping the selected variables \mathbf{c} constant, indirectly gives optimal operation. Skogestad (2000) derived some desirable properties (requirements) can be derived for the controlled variables \mathbf{c} :

1. We want small optimal variation in the selected variables (as used by Luyben (2005a)).
2. We want to be able to control the selected controlled variables tightly (small “implementation” error).
3. We want flat optimum with respect to the selected controlled variables.

MINIMUM SINGULAR VALUE RULE

Interestingly, it turns out that these desirable properties may be combined into the “maximum gain rule”: *Select controlled variables \mathbf{c} such that we maximize the minimum singular value $\underline{\sigma}$ of the scaled gain matrix \mathbf{G} (from \mathbf{u} to \mathbf{c} ; here \mathbf{u} 's are the “original” degrees of freedom).* This requires that the candidates \mathbf{c} 's have been scaled with respect to their span, where

$$\text{Span} = \text{optimal variation} + \text{implementation error} \quad (2)$$

The derivation of this rule is given by Halvorsen et al. (2003). Although this rule is not exact, especially for plants with an ill-conditioned gain matrix like distillation columns, it is very simple and it works well for most processes (Halvorsen et al., 2003). As the minimum singular value has the monotonic property, we can use the "Branch and Bound" algorithm to obtain the configuration with largest minimum singular value, avoiding the evaluation of all possible configurations (Cao, 1998).

MODIFIED MINIMUM SINGULAR VALUE RULE

According to Halvorsen et al. (2003), the worst-case loss can be estimated as:

$$\max_{\|e_c\|_2 \leq 1} L = \frac{1}{2} [\bar{\sigma}(\mathbf{J}_{uu}^{1/2} \mathbf{G}'^{-1})]^2 = \frac{1}{2} \frac{1}{[\underline{\sigma}(\mathbf{G}' \mathbf{J}_{uu}^{-1/2})]^2} \quad (3)$$

where \mathbf{G}' and \mathbf{J}_{uu} are scaled matrices. So, we want to select the combinations that gives the largest value of $\underline{\sigma}(\mathbf{G}' \mathbf{J}_{uu}^{-1/2})$. This method has the advantage of not been limited to systems where \mathbf{J}_{uu} is a unitary matrix. As we have the monotonic property, we can apply Branch and Bound algorithm. Using the modified minimum singular value rule, we can select a set of possible best solutions. Afterwards, we can calculate the exact loss to obtain the real optimum solution.

EXACT LOCAL METHOD

The exact local method was presented by Halvorsen et al. (2003). This method utilizes a Taylor series expansion of the loss function. The steady-state model used is:

$$\begin{aligned} \mathbf{y}_1 &= \mathbf{G}_1 \mathbf{u} + \mathbf{G}_{d1} \mathbf{d} \\ \mathbf{y}_2 &= \mathbf{G} \mathbf{u} + \mathbf{G}_d \mathbf{d} \end{aligned} \quad (4)$$

where \mathbf{y}_1 and \mathbf{y}_2 are the primary variables and the measurements, respectively.

The exact value of the worst-case local loss is:

$$\max_{\|[\mathbf{d}^n]^T\|_2 \leq 1} L = \bar{\sigma}(\mathbf{M})^2 / 2 \quad \text{where } \mathbf{M} = [\mathbf{M}_d \ \mathbf{M}_n] \quad (5)$$

$$\mathbf{M}_d = \mathbf{J}_{uu}^{1/2} (\mathbf{J}_{uu}^{-1} \mathbf{J}_{ud} - \mathbf{G}^{-1} \mathbf{G}_d) \mathbf{W}_d \quad (6)$$

$$\mathbf{M}_n = \mathbf{J}_{uu}^{1/2} \mathbf{G}_n^{-1} \mathbf{W}_n \quad (7)$$

The gains \mathbf{G} and \mathbf{G}_d and the derivatives \mathbf{J}_{uu} and \mathbf{J}_{ud} were obtained numerically applying small variations in the inputs. Consider the special case where the cost function can be represented by:

$$J = \mathbf{y}^T \mathbf{Q} \mathbf{y} + \mathbf{u}^T \mathbf{R} \mathbf{u} \quad (8)$$

where \mathbf{Q} and \mathbf{R} are symmetric positive-definite matrices. We can easily show that the derivatives \mathbf{J}_{uu} and \mathbf{J}_{ud} are:

$$\mathbf{J}_{uu} = 2(\mathbf{G}_1^T \mathbf{Q} \mathbf{G}_1 + \mathbf{R}) \quad \text{and} \quad \mathbf{J}_{ud} = 2\mathbf{G}_1^T \mathbf{Q} \mathbf{G}_{d1} \quad (9)$$

DISTILLATION COLUMN

The variable selection methods were applied to a distillation column separating an ideal 4-component mixture (A, B, C, D). The column has 41 stages (including reboiler and condenser) and the feed in middle of the column (stage 21). The stages are numbered from the bottom, with stage 1 as the reboiler and stage 41 as condenser (see Figure 1). All relative volatilities are equal to 1.5 ($\alpha_{AB} = \alpha_{BC} = \alpha_{CD} = 1.5$). The disturbances are the feed flow rate (F), fraction of liquid in the feed (q_F) and feed compositions (z_F).

The temperatures, for simplicity, are assumed to depend linearly on liquid composition and calculated as:

$$T_i = 10x_{B,i} + 20x_{C,i} + 30x_{D,i} \quad (10)$$

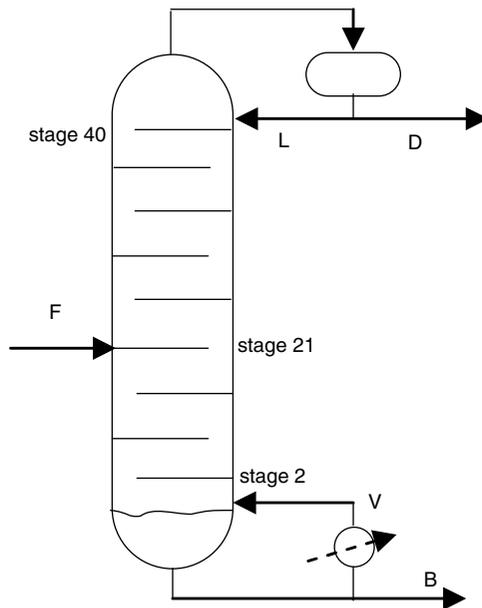


Figure 1. Distillation column

The model used is represented by Eq. 4, where $\mathbf{u} = [L \ V]^T$, $\mathbf{d} = [F \ z_F \ q_F]^T$ and $\mathbf{y}_1 = [x_D \ x_B]^T$. The implementation errors used were: 15% for flow ratios, 10% for flows and 0.5 K for temperatures.

BINARY MIXTURE

The first example is a binary mixture of B and C with feed composition of 50% each. The column operates with 99% of B in top and 99% of C in bottom.

The results using the exact local method are given in Table 1. Only the results with the best temperature are shown. The smallest loss of 28×10^{-6} is obtained when we control temperatures on stages 12 and 30, that is, with one temperature in the middle of the top section and one in the middle of the bottom section. The best choice with a flow and a temperature is to use L/F and T_{15} , which has a loss of 83×10^{-6} , followed by V/F and T_{16} with a loss of 131×10^{-6} . The best combination of two flows is L/D and V/B, with a loss of 25100×10^{-6} . Keeping L and V constant gives a loss of 402200×10^{-6} . Perhaps surprisingly, the loss with L/F and V/F constant is twice as large. The reason is the implementation error, which is larger with ratios than single flows.

Several configurations were compared by simulation (see Figure 2). The controllers were tuned using SIMC rules (Skogestad and Postlethwaite, 2005), with $\tau_c \geq 1$ and we applied the following disturbances:

1. F changes from 1 to 1.1 at $t = 0$.
2. q_F changes from 1 to 0.9 at $t = 40$.
3. z_F changes from 0.5 to 0.55 at $t = 60$.

Figure 2 confirms that the configuration T_{12} – T_{30} is the best choice.

Table 1. Losses of several possible configurations for binary mixture

Configuration	Exact loss ($\times 10^{-6}$)	Configuration	Exact loss ($\times 10^{-6}$)
T_{12} – T_{30}	28	L–B	44300
T_{15} –L/F	83	D–V	45000
T_{16} –V/F	131	L/D–V	53400
T_{19} –L	149	T_{40} –B/F	62800
T_{15} –L/D	174	T_{40} –D/F	62800
T_{22} –V	216	T_{40} –B	89200
T_{24} –V/B	292	T_{40} –D	89200
L/D–V/B	25100	L–V	402200
L/F–V/B	34600	L/F–V/F	810600

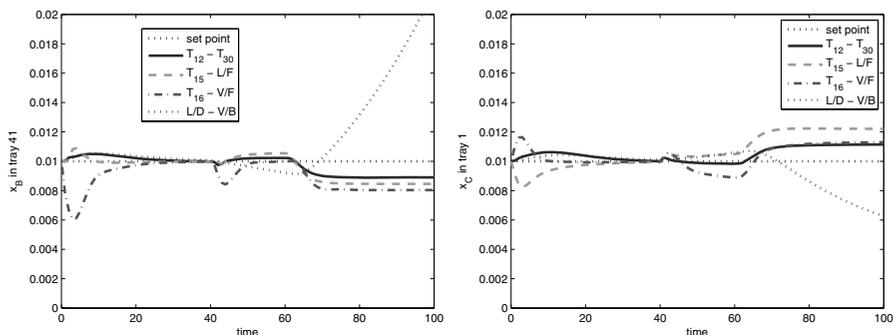


Figure 2. Comparing control structures for binary mixture

MULTICOMPONENT DISTILLATION COLUMN

The feed has 25% of each component (A, B, C, D). First we consider separation between components B and C (key components). As we want 99% recovery of B and C, then the bottom product must have 0.005% of B and the top product 0.005% of C.

Table 2 presents the values of the losses for several different possible control configurations, using the same criterion as Table 1. In this case, the loss with two temperatures ($T_{15}-T_{26}$) is 73×10^{-6} , which is significantly larger than in the binary case. This is not surprising, as temperature is generally less reliable as a composition measure in the multi-component case. On the other hand, the configuration with L/F and a single temperature (T_{15}) constant has a loss of only 77×10^{-3} , which is less than for the binary case. Otherwise, the results for the multicomponent case (Table 2) are very similar to the binary case (Table 1). The results are confirmed by the simulations in Figure 3 for the following disturbances:

Table 2. Losses of several possible configurations for multicomponent mixture for B/C separation

Configuration	Exact loss ($\times 10^{-6}$)	Configuration	Exact loss ($\times 10^{-6}$)
$T_{15}-T_{26}$	73	L-B	45800
$T_{19}-L/F$	77	D-V	46400
$T_{20}-L$	88	L/D-V	54300
$T_{16}-L/D$	91	$T_{40}-B/F$	88100
$T_{20}-V/F$	102	$T_{40}-D/F$	88100
$T_{21}-V$	123	$T_{40}-D$	131500
$T_{23}-V/B$	169	$T_{40}-B$	131500
L/D-V/B	25500	L-V	211700
L/F-V/B	33300	L/F-V/F	378800

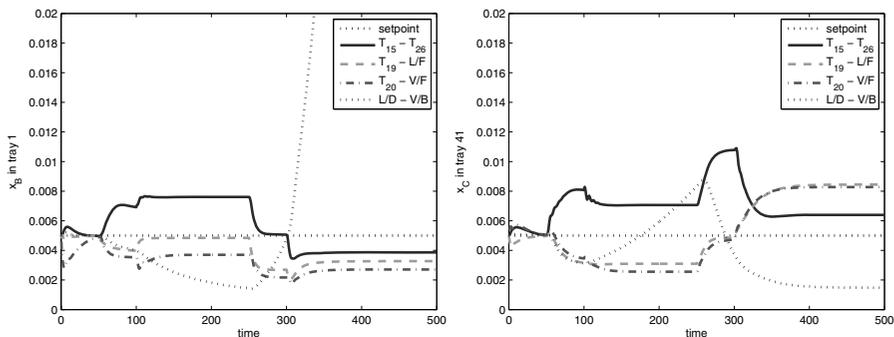


Figure 3. Comparing control structures for multicomponent mixture

1. F changes from 1 to 1.1 at $t = 0$
2. z_F changes from [0.25 0.25 0.25 0.25] to [0.3 0.2 0.25 0.25] at $t = 50$
3. q_F changes from 1 to 0.9 at $t = 100$
4. z_F changes from [0.3 0.2 0.25 0.25] to [0.3 0.25 0.2 0.25] at $t = 250$
5. z_F changes from [0.3 0.25 0.2 0.25] to [0.3 0.25 0.25 0.2] at $t = 300$

In Table 3, we show similar results for the two multicomponent separations (A/B and C/D separation). For these cases, the control of two temperatures is not the best. For the A/B separation, the best is to control V/F and T_{29} (in the middle of the top section) with a loss of 27×10^{-6} . For the C/D separation, the best is to control a temperature in the middle of the bottom section (T_{10}) and L/D or L/F. These structures have a loss of 30 and 35×10^{-6} , respectively.

COMPARING METHODS FOR VARIABLE SELECTION

In this section we compare the three different methods presented for variable selection: exact method, minimum singular value rule and its modified version. The minimum singular value rule can give a completely wrong result, as can be seen by Table 4. The best configuration (for binary mixture) obtained using exact local method is T_{12} – T_{30} , but the minimum singular value rule indicates that the best choice would be L/F–V/B. Figure 2 confirms that the configuration T_{12} – T_{30} is the best choice, while L/F–V/B is not. Halvorsen et al. (2003) had already reported that the minimum singular value rule fails when the matrix \mathbf{G}_1 is ill-conditioned, as it is for this system, where the condition number is 145.6. However, if we compare similar cases, for example, two temperatures, one temperature and one flow, or two flows, then the minimum singular value gives the right order in most cases.

The modified minimum singular value rule (maximize $\underline{\sigma}(\mathbf{G}\mathbf{J}_{uu}^{-1/2})$) is not exact, but according to Table 4, this method produces results very similar to the exact method. Also,

Table 3. Losses of several possible configurations for multicomponent mixture for A/B and C/D separations

Configuration (A/B separation)	Exact loss ($\times 10^{-6}$)	Configuration (C/D separation)	Exact loss ($\times 10^{-6}$)
T ₂₉ -V/F	27	T ₁₀ -L/D	30
T ₃₀ -V/B	28	T ₁₀ -L/F	35
T ₂₈ -V	28	T ₁₁ -L	41
T ₂₉ -L/F	28	T ₁₀ -V/F	50
T ₂₈ -L	29	T ₁₁ -V	70
T ₂₇ -L/D	70	T ₉ -T ₂₇	100
T ₁₉ -L/F	92	T ₁₃ -V/B	309
T ₁₆ -T ₂₁	99	L/D-V/B	84900
L/D-V/B	51200	L/F-V/B	88400
L/F-V/B	111800		

Table 4. Comparing selection methods for a binary mixture

Configuration	Exact loss ($\times 10^6$)	$\underline{\sigma}(\mathbf{G})$	Loss = $\frac{\bar{\sigma}(\mathbf{J}_{uu})}{2\underline{\sigma}(\mathbf{G})^2}$	$\underline{\sigma}(\mathbf{G}\mathbf{J}_{uu}^{1/2})$	Loss = $\frac{1}{2\underline{\sigma}(\mathbf{G}\mathbf{J}_{uu}^{1/2})^2}$ ($\times 10^6$)
T ₁₂ -T ₃₀	28	1.5079	1.7115	78.3172	82
T ₁₂ -T ₂₉	29	1.4418	1.8720	75.1663	88
T ₁₄ -T ₂₈	35	1.2411	2.5263	64.4779	120
T ₉ -T ₃₂	46	1.5478	1.6242	79.1531	80
T ₁₅ -T ₂₆	50	0.9562	4.2559	49.9123	201
T ₁₅ -L/F	84	1.5305	1.6612	60.7430	136
T ₁₆ -V/F	132	1.1249	3.0753	49.8319	201
T ₁₉ -L	150	0.8145	5.8649	40.0200	312
T ₁₅ -L/D	174	0.7267	7.3689	34.2050	427
T ₂₂ -V	216	0.6392	9.5253	30.4771	538
T ₂₄ -V/B	293	0.5714	11.9191	26.0734	735
T ₁ -T ₄₁	2500	0.2709	53.0150	14.1421	2500
L/D-V/B	25100	0.8780	5.0480	3.9703	31700
L/F-V/B	34600	1.6025	1.5152	2.7602	65600
L-B	44300	0.8045	6.0128	2.0097	123800
D-V	45000	0.6344	9.6686	2.0128	123400
L/F-V/F	810600	1.5963	1.5270	0.6503	1182500

it has the advantage of not requiring the evaluation of all possible configurations because, as it has the monotonic property, we can apply Branch and Bound algorithm (Cao, 2005).

DEPROPANIZER CASE STUDY

The above results are based on idealized mixtures with constant relative volatility, and assuming constant molar flows.

However, similar results have been obtained for a depropanizer case study, that has 7 components (C_2 , C_3 , $i-C_4$, $n-C_4$, $i-C_5$, $n-C_5$, $n-C_6$).

We found also here that the smallest composition loss is obtained using two-temperatures or a constant L/F and temperature in the middle of the bottom section (the same as obtained for the ideal multicomponent case).

CONCLUSIONS

Overall, for binary and multicomponent separations, a good control structure for “indirect composition control” is to control a temperature in the middle of the bottom section and keep a constant reflux to feed ratio (L/F). For both binary and multicomponent mixtures, the temperature sensor needs to be located away from the column end. A common heuristic is to select a tray where the change in temperature from tray to tray is the largest (steep temperature profile) (Luyben, 2005b). The heuristic is confirmed for binary mixtures, but not for multicomponent mixtures, which have a steep profile towards the column ends. Control of two temperatures gives better composition control (smaller loss) for binary mixture, but not for multicomponent mixtures, mainly because of the effect of implementation error (measurement noise). Note that the results are for steady state and are independent of how we do the level control. For example, it is possible to use L for condenser level control, and then adjust D at a slower time scale to “reset” L to a desired steady-state value. Also note that with good indirect composition control, we get less variation in levels because we avoid redistribution of components in the columns. So, the configuration of L/F and a temperature in the bottom section is good for all multicomponent cases.

The minimum singular value rule is a very simple tool to use, but it does not necessarily give the best solution, as was shown in the example above. It fails when the plant is ill-conditioned (has large condition number).

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