Self-optimizing control configurations for two-product distillation columns

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Abstract

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.

1. Introduction

For a distillation column, the “original” degrees of freedom are $\mathbf{u}_0 = [L \quad V \quad D \quad B]$, 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 $\mathbf{u} = [L \quad V]$.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.)

The question is: What should we use the two degrees of freedom for, that is, what are the controlled variables c? Could L be kept constant or maybe L/D? Should a temperature 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 approaches for identifying controlled variables are (Luyben, 2005):

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 to temperatures (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 $\mathbf{J}_{uu}$. To improve on this, one may considers $\underline{\sigma}\left(\mathbf{G}'\mathbf{J}'^{-1/2}_{uu}\right)$, 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 defined. A reasonable cost function for the composition control problem is:

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$$J = \left(x_{D} - x_{Ds}\right)^2 + \left(x_{B} - x_{Bs}\right)^2 \tag{1}$$

2. Self optimizing control

"Self-optimizing control" is when keeping the selected variables **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 (2005)).
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.

2.1. Minimum Singular Value Rule

Interestingly, it turns out that these desirable properties may be combined into the "maximum gain rule": *Select controlled variables* **c** *such that we maximize the minimum singular value _ of the scaled gain matrix* **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

$$\text{Span} = \text{optimal variation} + \text{implementation error} \tag{2}$$

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).

2.2. Modified Minimum Singular Value Rule

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

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

where **G'** and **J'$_{uu}$** are scaled matrices. So, we want to select the combinations that gives the largest value of $\underline{\sigma}\left(\mathbf{G}'\mathbf{J}_{uu}'^{-1/2}\right)$. This method has the advantage of not been limited to systems where Juu 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.

2.3. 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:

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

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:

$$\max_{\left\|\left[\mathbf{d}' \;\; \mathbf{n}^{y'}\right]^T\right\|_2 \le 1} L = \bar{\sigma}\left(\mathbf{M}\right)^2 / 2 \qquad \text{where} \quad \mathbf{M} = \left[\mathbf{M}_d \quad \mathbf{M}_n\right] \tag{5}$$

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

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

The gains **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:

$$J = \mathbf{y}^T\mathbf{Q}\mathbf{y} + \mathbf{u}^T\mathbf{R}\mathbf{u} \tag{8}$$

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

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

3. 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 40 stages and the feed in middle of the column. 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 are calculated as:

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

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

3.1. 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.

We use the exact local method. According to Table 1, the best configuration is to control temperatures 10 and 32 (Loss = 2.0238 x 10^{-5}). In summary, we find that it is best to control two temperatures (one above and the other below the feed stage), but it is also good to control one temperature and keep one flow ratio constant (preferably L/F). Several possible configurations were compared by simulation (see Figure 1). During the simulations, we applied the following disturbances:

1. F changes from 1 to 1.1 at t = 0
2. zF changes from 0.5 to 0.55 at t = 50
3. qF changes from 1 to 0.9 at t = 100

Figure 1 confirms that the configuration T_{10}-T_{32} is the best choice. Besides T_{10}-T_{32} configuration, other configurations, like T_{17}-L/F and V/F-T_{32}, also present reasonable control in the presence of these disturbances.

Table 1: Losses and minimum singular values of several possible configurations for binary mixture.

Configuration	Exact loss	Configuration	Exact loss
$T_{10} - T_{32}$	20.238 x 10^{-6}	T_{17} – L/D	359.29 x 10^{-6}
$T_{13} - T_{29}$	30.349 x 10^{-6}	T_8 – L/D	460.71 x 10^{-6}
T_{10} – L/F	34.810 x 10^{-6}	T_4 –L/D	547.94 x 10^{-6}
$T_5 - T_{35}$	62.627 x 10^{-6}	$T_1 - T_{41}$	625 x 10^{-6}
$T_{15} - T_{25}$	85.933 x 10^{-6}	T_{17} – V/B	0.0010
T_{32} - V/F	86.126 x 10^{-6}	L – B	0.0398
T_{17} – L/F	91.287 x 10^{-6}	D – V	0.0405
T_{15} – L	162.93 x 10^{-6}	L/D – V/B	0.0466
T_{10} – L	184.94 x 10^{-6}	L/F – V/B	0.0757
T_{25} – L	226.01 x 10^{-6}	L/D – V	0.0788
T_5 – L	241.81 x 10^{-6}	V/F – L/F	0.2855
T_{15} – V	265.28 x 10^{-6}	L – V	0.4128

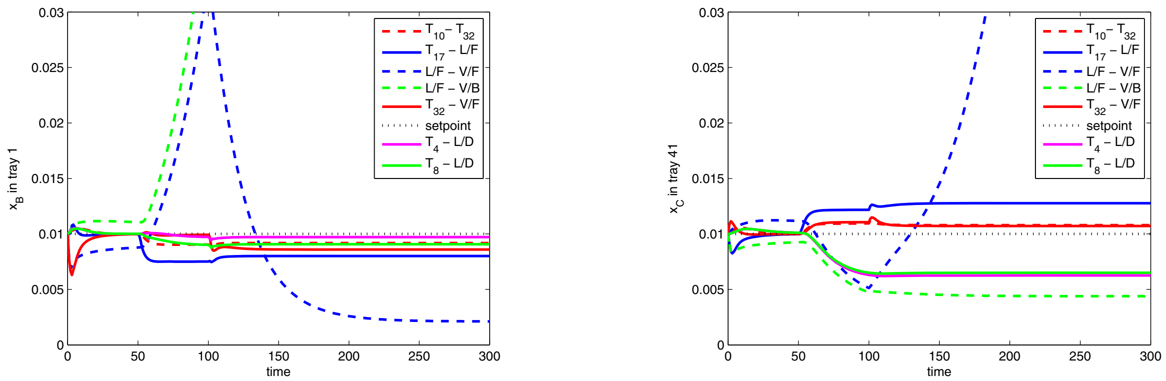

Figure 1: Comparing control structures for binary mixture.

3.2. Multicomponent Distillation Column

The feed has 25% of each component (A, B, C, D). We want to separate 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. The best configuration obtained using exact local method is to T_{17}-L/F (Loss = 9.2755 x 10^{-5}). The results show that, for multicomponent system, it is not so good to control two temperatures as was for the binary. It is better to control just one temperature (preferably below the feed stage (manipulating V) and to keep one flow ratio constant (L/D or L/F). To compare the different control configurations, we applied the following disturbances:

1. F changes from 1 to 1.1 at t = 0
2. zF changes from [0.25 0.25 0.25 0.25] to [0.3 0.2 0.25 0.25] at t = 50
3. qF changes from 1 to 0.9 at t = 100
4. zF changes from [0.3 0.2 0.25 0.25] to [0.3 0.25 0.2 0.25] at t = 250
5. zF3 changes from [0.3 0.25 0.2 0.25] to [0.3 0.25 0.25 0.2] at t = 300

The V/F-L/F configuration gives a good control for feed disturbances but it fails to keep the compositions close to set point when we have disturbance in q_F. Besides T_{17}-L/F configuration, other configurations, like T_{10}-T_{32} and V/F-T_{32}, also present reasonable control in the presence of these disturbances.

Table 2: Losses and minimum singular values of several possible configurations for multicomponent mixture.

Configuration	Exact loss	Configuration	Exact loss
T_{17} – L/F	92.755 x 10^{-6}	T_{17} – V/B	497.43 x 10^{-6}
T_{15} – L	117.67 x 10^{-6}	T_5 – L	0.0017
T_{10} – L/F	144.42 x 10^{-6}	T_4 – L/D	0.0035
T_{13} – T_{29}	158.50 x 10^{-6}	T_5 – T_{35}	0.0046
T_{10} – L	163.34 x 10^{-6}	L – B	0.0411
T_{17} – L/D	169.76 x 10^{-6}	D – V	0.0417
T_{15} – V	169.96 x 10^{-6}	L/D – V/B	0.0572
T_{15} – T_{25}	187.33 x 10^{-6}	T_1 – T_{41}	0.0705
T_{25} – L	219.09 x 10^{-6}	L/D – V	0.0902
T_8 – L/D	299.47 x 10^{-6}	L/F – V/B	0.0950
T_{10} – T_{32}	327.60 x 10^{-6}	L – V	0.3227
T_{32} – V/F	429.46 x 10^{-6}	V/F – L/F	0.3928

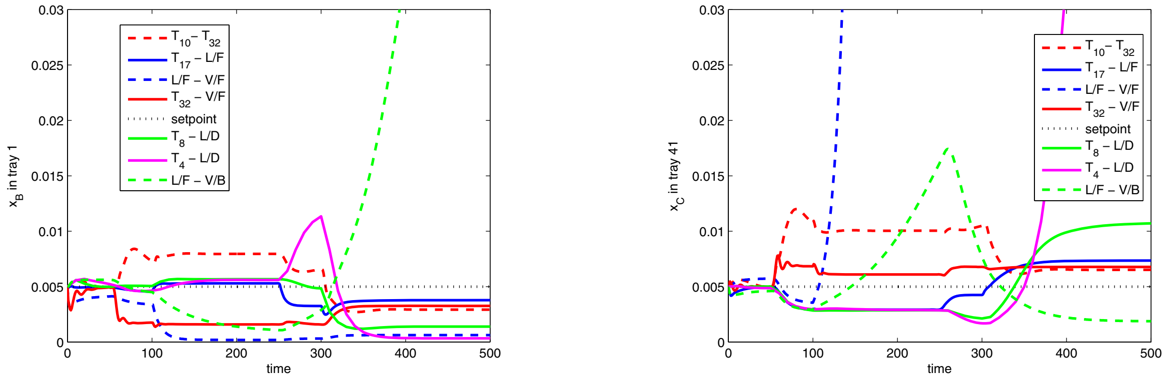

Figure 2: Comparing control structures for multicomponent mixture.

4. Comparing Methods for Variable Selection

In this section we compare the three different methods used for variable selection: exact method, minimum singular value rule and its modified version. The exact method always gives the best solution but, to obtain it, it is necessary to evaluate all possible combinations. For large systems, with several inputs and outputs, this method can be unfeasible. The minimum singular value rule is useful when we have well conditioned systems; otherwise it can give a completely wrong result, as can be seen by Table 3. The best configuration (for binary mixture) obtained using exact local method is T_{10}-T_{32}, but the minimum singular value rule indicates that the best choice would be L/F-V/B. As can be seen in figure 2, the T_{10}-T_{32} is the best configuration while L/F-V/B configuration is not.

Figure 1 confirms that the configuration T_{10}-T_{32} is the best choice, while L/F-V/B is not. This example shows that, the minimum singular value rule does not give necessarily the best configuration. Halvorsen et al. (2003) had already reported that the minimum singular value rule fails when the matrix $\mathbf{G}_1$ is ill-conditioned (has large condition number). In this case, the optimal values of all the variables are strongly correlated, such that the assumption of independent variations in $y_2 - y_{2,\mathrm{opt}}$ does not hold. For this system, the condition number is equal to 145.6 (it is ill-conditioned). So, the minimum singular value rule does not apply, as can be seen by the results presented in Table 1 and Figure 1.

Table 3: Comparing selection methods for a binary mixture.

Configuration	Exact loss	$\underline{\sigma}(\mathbf{G})$	$\mathrm{Loss} = 1/\left(2\underline{\sigma}(\mathbf{G}\mathbf{J}_{uu}^{-1/2})^2\right)$
$T_{10} - T_{32}$	20.238×10^{-6}	1.5768	74.802×10^{-6}
$T_{13} - T_{29}$	30.349×10^{-6}	1.3932	95.443×10^{-6}
T_{10} – L/F	34.810×10^{-6}	1.5324	147.78×10^{-6}
T_{32} - V/F	86.126×10^{-6}	1.1358	358.29×10^{-6}
T_{17} – L/F	91.287×10^{-6}	1.5293	164.97×10^{-6}
T_{17} – V/F	113.56×10^{-6}	1.1254	205.00×10^{-6}
L/F – V/B	0.0757	1.6025	0.0656
L/F – V/F	0.2855	1.5963	1.1825

The modified minimum singular value rule (maximize $\underline{\sigma}(\mathbf{G}\mathbf{J}_{uu}^{-1/2})$) does not necessarily gives the best configuration, but its result is much more accurate than the usual minimum singular value rule when we have ill conditioned systems. Also, 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. According to Table 3, this method produces results very similar to the exact method.

5. Depropanizer case study

The above results are based on idealized mixtures with constant relative volatility, and assuming constant molar flows. We also did the same study for other separation problems (A/B and C/D separation) obtaining very similar results.

Also, 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 find also here that the smallest composition loss is obtained using a constant L/F and temperature in the middle of the bottom selection (the same as obtained for the ideal multicomponent case).

6. Conclusions

We have considered which two variables to keep constant (or control) in order to achieve (indirect composition control at steady-state. We found that we never should keep *D* or *B* constant. We may keep *L* or *V* constant in combination with a temperature.

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. Control of two temperatures does not reduce the loss significantly for binary mixtures, and generally increases the loss for multicomponent mixtures, mainly because of the effect of implementation error (measurement noise). The results 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.

Although the minimum singular value rule is a very simple tool to use, it doesn’t necessarily give the best solution, as was shown in the example above. It fails when the plant is ill-conditioned (has large condition number). The exact local method gives the best control structure but it is still necessary to find a way to obtain it without trying all possible combinations. The computation of minimum singular value of $\mathbf{G}(\mathbf{J}_{uu})^{-1/2}$ gives a good result even if the process is ill-conditioned and it is not necessary to evaluate all possible configurations because, as it has the monotonic property, it is possible to use Branch and Bound algorithm to select the best configuration.

The results show that it is possible to select variables that have a good control for several different operational conditions.

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