

- [11] W. L. Luyben; B. D. Tyreus; M. L. Luyben, *Plantwide Process Control*, McGraw-Hill, New York, 1999.
- [12] T. R. Elliott; W. L. Luyben, *Ind. Eng. Chem. Res.*, 34, (1995) 3907.
- [13] T. R. Elliott; W. L. Luyben, *Ind. Eng. Chem. Res.*, 35, (1996) 3470.
- [14] J. M. Douglas, *Conceptual Design of Chemical Processes*, McGraw-Hill, New York, 1988.
- [15] A. J. Groenendijk; A. C. Dimian; P. D. Iedema, *AIChE J.*, 46 (2000) 133.
- [16] Y. H. Chen and C. C. Yu, *Comput. Chem. Eng.*, 23 (2000) 1077.
- [17] Y. H. Chen and C. C. Yu, *Ind. Eng. Chem. Res.* 2003 (in press).
- [18] A. Papadourakis; M. F. Doherty; J. M. Douglas, *Ind. Eng. Chem. Res.*, 26 (1987) 1259.
- [19] K. L. Wu and C. C. Yu, *Comput. Chem. Eng.*, 20 (1996) 1291.
- [20] K. L. Wu; C. C. Yu; W. L. Luyben; S. Skogestad, *Comput. Chem. Eng.*, 27 (2003) 421.
- [21] T. Larsson, M. S. Govatsmark, S. Skogestad, and C. C. Yu, *Ind. Eng. Chem. Res.* 42 (2003), 1225.
- [22] T. Larsson and S. Skogestad, *Plantwide Control: A Review and A New Design Procedure, Modeling Ident. Cont.*, 21 (2000) 209.
- [23] C. S. Bildea; A. C. Dimian; P. D. Iedema, *Comput. Chem. Eng.* 23 (2000) 209.
- [24] Y. C. Cheng; K. L. Wu; C. C. Yu, *J. Chin. Inst. Chem. Eng.*, 33 (2002) 283.
- [25] Y. C. Cheng and C. C. Yu, *AIChE J.*, 49 (2003) 682.
- [26] M. F. Malone; K. Glinos; F. E. Marquez; J. M. Douglas, *AIChE J.*, 31 (1985) 683.

Chapter D1

Integration of optimal operation and control

Sigurd Skogestad

Department of Chemical Engineering, Norwegian University of Science and Technology,
 N-7491 Trondheim, Norway

1. INTRODUCTION

The focus of this book is on the integration of design and control. The objective is to design a process which, in addition to being economically attractive from a steady-state point of view, is "easy" to control and operate.

The focus in this chapter is different. The issue here is operation of a given plant where the design decisions have already been made. Here it is too late with "integration of design and control", but on the other hand "integration of design people and control people" may give large benefits. When it comes to operation, the "design people" usually focus their attention on optimal economic steady-state operation. The "control people" on the other hand are focused on dynamic operation, and on keeping selected variables at constant setpoints. The "missing link" where the interaction between the two groups is most needed, is the issue of *selecting which variables to control*. For most plants, as illustrated in this chapter, this choice can be made based on steady-state economics, so here the design people are in charge. One needs information about expected disturbances and implementation/measurement errors ("uncertainty"), and both the control and design people can here contribute with their process insight. However, the dynamic behavior (controllability) of the proposed choice must also be considered, and this is the domain of the control people.

It should also be noted that many plants are not operated at the conditions they were designed for. The reason is that the economic conditions are often such that it is optimal to operate the plant at higher capacity than what it was designed for. This usually involves operating one or more units at capacity constraints, and the active constraints may change on a daily basis, or as various units are "debottlenecked". In any case, this means that one needs to rethink the control strategy, so in most plants there will be an ongoing need for interactions between the design and control people.

As mentioned, the focus of this chapter is on selecting controlled variables. More generally, the issue of selecting controlled variables is the first subtask in the **plantwide control** or **control structure design** problem (Foss 1973); (Morari 1982); (Skogestad and Postlethwaite 1996) :

1. *Selection of controlled variables c*
2. *Selection of manipulated variables*
3. *Selection of measurements* (for control purposes including stabilization)
4. *Selection of a control configuration* (structure of the controller that interconnects measurements/setpoints and manipulated variables)
5. *Selection of controller type* (control law specification, e.g., PID, decoupler, LQG, etc.).

Even though control engineering is well developed in terms of providing optimal control algorithms, it is clear that most of the existing theories provide little help when it comes to making the above structural decisions.

The method presented in this paper for selecting controlled variables (task 1) follows the ideas of Morari *et al.* (1980) and Skogestad and Postlethwaite (1996) and is very simple. The basis is to define mathematically the quality of operation in terms of a scalar cost function J to be minimized. To achieve truly optimal operation we would need a perfect model, we would need to measure all disturbances, and we would need to solve the resulting dynamic optimization problem on-line. This is unrealistic, and the question is if it is possible to find a simpler implementation which still operates satisfactorily (with an acceptable loss). The simplest operation would result if we could select controlled variables such that we obtained acceptable operation with constant setpoints, thus effectively turning the complex optimization problem into a simple feedback problem and achieve what we call "self-optimizing control".

In this chapter we first give an introduction to self-optimizing control (Skogestad 2000), including a distillation column case study. In Skogestad (2000) the focus is selecting single measurements as controlled variables, but more generally variable combinations may be used, and we present briefly the method of Alstad and Skogestad (2002) for finding the optimal variable combination for the case where implementation errors are not important. The final part of this chapter is the application of this method to optimal operation of a gasoline blending process.

2. SELECTION OF CONTROLLED VARIABLES FOR SELF-OPTIMIZING CONTROL

In this chapter, we focus on optimal steady-state operation, because the plant economics are primarily determined by the steady-state operation. Although not widely acknowledged, controlling the right variable is a key element in overcoming uncertainty in operation.

In order to select controlled variables in a systematic way, the first step is to identify the degrees of freedom.

The second step is to quantify what we mean by "desired operation". We do this by defining a scalar cost function J_o which is to be minimized with respect to the available degrees of freedom u_o ,

$$\min_{u_o} J_o(x, u_o, d) \quad (1)$$

subject to the constraints

$$g_1(x, u_o, d) = 0; \quad g_2(x, u_o, d) \leq 0 \quad (2)$$

Here d represents the exogenous disturbances that affect the system, including changes in the model (typically represented by changes in the function g_1), changes in the specifications (constraints), and changes in the parameters (prices) that enter in the cost function (and possibly in the constraints). x represents the internal states. The cost function J_o is in many cases a simple linear function of extensive variables multiplied by their respective prices.

The third step is the definition of uncertainty, including expected disturbances (d) and implementation errors (n). The latter are at steady state mainly due to measurement error.

The fourth step is to find the optimal operating point for the various disturbances by minimizing J_o with respect to the available degrees of freedom u_o . In most cases some of the inequality constraints are active ($g_2^i = 0$) at the optimal solution.

The final steps, the most important in our view (but not considered to be an important issue by many people) is the actual implementation of the optimal policy in the control system. We assume that we have available measurements $y = f_o(x, u_o, d)$ that give information about the actual system behavior during operation (y also includes the cost function parameters (prices), measured values of other disturbances d , and measured values of the independent variables u_o).

Obviously, from a purely mathematical point of view, it would be optimal to use a centralized on-line optimizing controller with continuous update of its model parameters and continuous reoptimization of all variables. However, for a number of reasons, we almost always decompose the control system into several layers, which in a chemical plant typically include scheduling (weeks), site-wide optimization (day), local optimization (hour), supervisory/predictive control (minutes) and regulatory control (seconds). Therefore, we instead consider the implementation shown in Figure 1 with separate optimization and control layers. The two layers interact through the *controlled variables* c , whereby the optimizer computes their optimal setpoints c_s (typically, updating them about every hour), and the control layer attempts to implement them in practice, i.e. to get $c \approx c_s$. The main issue considered in this chapter is then: What variables c should we control?

As mentioned, in most cases some of inequality constraints are active (i.e. $g_2^i = 0$) at the optimal solution). Implementation to achieve this is usually simple: We adjust the corresponding number of degrees of freedom u_o such that these active constraints are satisfied (the possible errors in enforcing the constraints should be included as disturbances). In some cases this

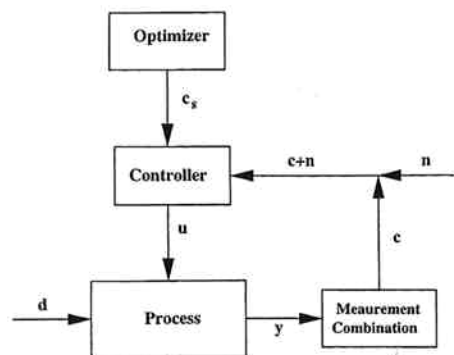


Fig. 1. Implementation with separate optimization and control layers. Self-optimizing control is when near-optimal operation is achieved with c_s constant.

consumes all the available degrees of freedom. For example, if the original problem is linear (linear cost function with linear constraints g_1 and g_2), then it is well known that from Linear Programming theory that there will be no remaining unconstrained variables.

However, for nonlinear problems (e.g. g_1 is a nonlinear function), the optimal solution may be unconstrained in the remaining variables, and such problems are the focus of this paper. The reason is that it is for the remaining unconstrained degrees of freedom (which we henceforth call u) that the selection of controlled variables is an issue. For simplicity, let us write the remaining unconstrained problem in reduced space in the form

$$\min_u J(u, d) \quad (3)$$

where u represents the remaining unconstrained degrees of freedom, and where we have eliminated the states $x = x(u, d)$ by making use of the model equations. These remaining degrees of freedom u need to be specified during operation, and we use the feedback policy shown in Figure 1 where the u 's are adjusted dynamically to keep the controlled variables c at their setpoints c_s . However, this constant setpoint policy will, for example due to disturbances d (which change the optimal value of c_s) and implementation errors n (which mean that we do not actually achieve $c = c_s$), result in a loss, $L = J - J_{\text{opt}}$, when compared to the truly optimal operation. If this loss is acceptable, then we have a "self-optimizing" control system:

Self-optimizing control (Skogestad 2000) is when we can achieve acceptable loss with constant setpoint values for the controlled variables (without the need to reoptimize when disturbances occur).

1. A subset of the degrees of freedom u_o are adjusted in order to satisfy the active constraints (as given by the optimization).
2. The remaining unconstrained degrees of freedom (u) are adjusted in order to keep selected controlled variables c at constant desired values (setpoints) c_s . These variables should be selected to minimize the loss.

Ideally, this results in "self-optimizing control" where no further optimization is required, but in practice some infrequent update of the setpoints c_s may be required. If the set of active constraints changes, then one may have to change the set of controlled variables c , or at least change their setpoints, since the optimal values are expected to change in a discontinuous manner when the set of active constraints change.

Example. Cake baking. Let us consider the final process in cake baking, which is to bake it in an oven. Here there are two independent variables, the heat input ($u_1 \stackrel{\text{def}}{=} Q$) and the baking time ($u_2 \stackrel{\text{def}}{=} T$). It is a bit more difficult to define exactly what J is, but it could be quantified as the average rating of a test panel (where 1 is the best and 10 the worst). One disturbance will be the room temperature. A more important disturbance is probably uncertainty with respect to the actual heat input, for example, due to varying gas pressure for a gas stove, or difficulty in maintaining a constant firing rate for a wooden stove. In practice, this seemingly complex optimization problem, is solved by using a thermostat to keep a constant oven temperature (e.g., keep $c_1 = T_{\text{oven}}$ at 200°C). and keeping the cake in the oven for a given time (e.g., choose $c_2 = u_2 = 20$ min). The feedback strategy, based on measuring the oven temperature c_1 , gives a self-optimizing solution where the heat input (u_1) is adjusted to correct for disturbances and uncertainty. The optimal value for the controlled variables (c_1 and c_2) are obtained from a cook book, or from experience. An improved strategy may be to measure also the temperature inside the cake, and take out the cake when a given temperature is reached (i.e., u_2 is adjusted to get a given value of $c_2 = T_{\text{cake}}$).

We next consider a distillation case study where we follow the stepwise procedure of Skogestad (2000) for selecting controlled variables. The example also illustrates how to include the implementation error n in the analysis.

3. DISTILLATION CASE STUDY

We consider a binary mixture with constant relative volatility $\alpha = 1.12$ to be separated in a distillation column with 110 theoretical stages and the feed entering at stage 39 (counted from the bottom with the reboiler as stage 1). Nominally, the feed contains 65 mole% of light component ($z_F = 0.65$) and is saturated liquid ($q_F = 1.0$). This represents a propylene-propane splitter where propylene (light component) is taken overhead as a final product with at least 99.5% purity ($x_D \geq 0.995$), whereas unreacted propane (heavy component) is recycled to the

reactor for reprocessing. We assume the feed rate is given and that there is no capacity limit in the column.

Step 1: Degree of freedom analysis

For a given feed rate and given pressure the column has two degrees of freedom at steady state. These may for instance be selected as the vapor and distillate flows,

$$u = \begin{pmatrix} V \\ D \end{pmatrix}$$

Step 2: Cost function and constraints

Ideally, the optimal operation of the column should follow from considering the overall plant economics. However, to be able to analyze the column separately, we introduce prices for all streams entering and exiting the column and consider the following profit function P which should be maximized (i.e. $J = -P$)

$$P = p_D D + p_B B - p_F F - p_V V \quad (4)$$

We use the following prices [\$/kmol]

$$p_D = 20, \quad p_B = 10 - 20x_B, \quad p_F = 10, \quad p_V = 0.1$$

The price $p_V = 0.1$ [\$/kmol] on boilup includes the costs for heating and cooling which both increase proportionally with the boilup V . The price for the feed is $p_F = 10$ [\$/kmol], but its value has no significance on the optimal operation for the case with a given feed rate. The price for the distillate product is 20 [\$/kmol], and its purity specification is

$$x_D \geq 0.995$$

There is no purity specification on the bottoms product, but we note that its price is reduced in proportion to the amount of light component (because the unnecessary reprocessing of light component reduces the overall capacity of the plant; this dependency is not really important but it is realistic).

With a nominal feed rate $F = 1$ kmol/min the profit value P of the column is of the order 4 [\$/min], and we would like to find a controlled variable which results in a loss L less than 0.04 [\$/min] for each disturbance (corresponding to a yearly loss of less than about \$20000).

Step 3: Disturbances

We consider five disturbances:

d_1 : An increase in feed rate F from 1 to 1.3 kmol/min.

d_2 : A decrease in feed composition z_F from 0.65 to 0.5

d_3 : An increase in feed composition z_F from 0.65 to 0.75

d_4 : A decrease in feed liquid fraction q_F from 1.0 (pure liquid) to 0.5 (50% vaporized)

d_5 : An increase of the purity of distillate product x_D from 0.995 (its desired value) to 0.996

The latter is a possible safety margin for x_D which may take into account its implementation error. In addition, we include the implementation error n for the other selected controlled variable (see below).

Step 4: Optimization

In Table 1 we give the optimal operating point for the five disturbances; larger feed rate ($F = 1.3$), less and more light component in the feed ($z_F = 0.5$ and $z_F = 0.65$), a partly vaporized feed ($q_F = 0.5$), and a purer distillate product ($x_D = 0.996$).

As expected, the optimal value of all the variables listed in the table ($x_D, x_B, D/F, L/F, V/F, P/F$) are completely insensitive to the feed rate, since the column has no capacity constraints, and the efficiency is assumed independent of the column load.

Step 5: Candidate controlled variables

The top product purity constraint is always active, that is, it is always optimal to have $x_D = 0.995$, so the distillate composition x_D should be selected as a controlled variable (c_1).

We are then left with one unconstrained degree of freedom which we want to specify by keeping the setpoint of a controlled variable at a constant value.

From Table 1 we see that the optimal bottom composition x_B stays fairly constant around 0.04. This indicates that a good strategy for implementation may be to control x_B at a constant value of 0.04. However, there are at least two practical problems associated with this choice. First, on-line composition measurements are often unreliable and expensive. Second, dynamic performance may be poor because it is generally difficult to control both product compositions ("dual or "two-point" control) due to strong interactions. e.g. (Shinskey 1984) (Skogestad and Morari 1987). Thus, if possible, we would like to control some other variable.

The following six alternatives for the second controlled variable (c_2) are considered

$$x_B; D/F; L; L/F; V/F; L/D$$

We consider implementation errors of about 20% in all variables, including x_D (the other controlled variable). From Table 1 we see that the optimal value of D/F varies considerably, so we expect this to be a poor choice for the controlled variable (as it violates requirement 1). For the other alternatives, it is not easy to say from our requirements or from physical insight which variable to prefer. We will therefore evaluate the loss.

Step 6: Evaluation of loss

In Table 2 we show for $F = 1$ [kmol/min] the loss $L = P_{\text{opt}} - P$ [\$/min] when each of the six candidate controlled variables are kept constant at their nominally optimal values. Recall that

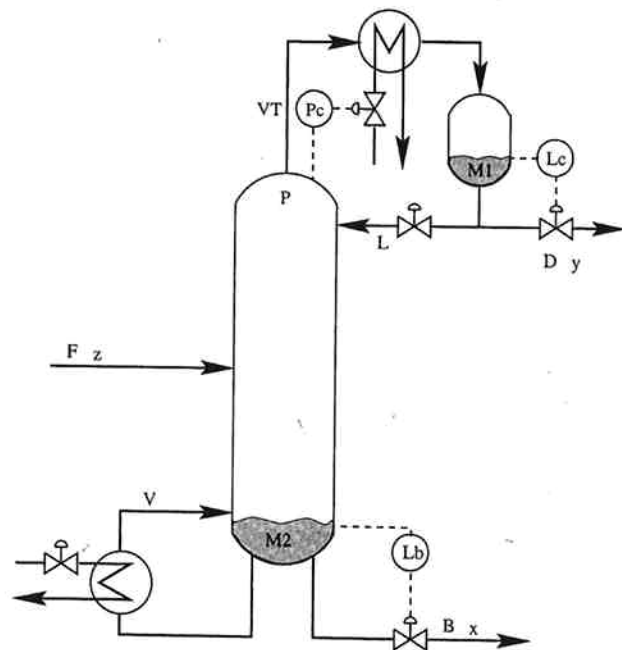


Fig. 2. Typical distillation column controlled with the LV-configuration

	x_D	x_B	D/F	L/F	V/F	L/D	P/F
Nominal	0.995	0.040	0.639	15.065	15.704	23.57	4.528
$F = 1.3$	0.995	0.040	0.639	15.065	15.704	23.57	4.528
$z_F = 0.5$	0.995	0.032	0.486	15.202	15.525	31.28	2.978
$z_F = 0.75$	0.995	0.050	0.741	14.543	15.284	19.62	5.620
$q_F = 0.5$	0.995	0.040	0.639	15.133	15.272	23.68	4.571
$x_D = 0.996$	0.996	0.042	1.274	15.594	16.232	24.47	4.443

Nominal values: $F = 1, z_F = 0.65, q_F = 1.0$

Table 1
Optimal operating point (with maximum profit P/F) for distillation case study

we would like the loss to be less than 0.04 [\$/min] for each disturbance. We have the following comments to the results given in Table 2:

	$x_B = 0.04$	$D/F = 0.639$	$L = 15.065$	$L/F = 15.065$	$V/F = 15.704$	$L/D = 23.57$
Nominal	0	0	0	0	0	0
$F = 1.3$	0	0	0.514	0	0	0
$z_F = 0.5$	0.023	inf.	0.000	0.000	0.001	1.096
$z_F = 0.75$	0.019	2.530	0.006	0.006	0.004	0.129
$q_F = 0.5$	0.000	0.000	0.001	0.001	0.003	0.000
$x_D = 0.996$	0.086	0.089	0.091	0.091	0.091	0.093
20% impl.error	0.012	inf.	0.119	0.119	0.127	0.130

inf. denotes infeasible operation

Nominal values: $x_D = 0.995, z_F = 0.65, q_F = 1.0$

20% impl.error: $x_B = 0.048, D/F = 0.766, L = 18.08, L/F = 18.08, V/F = 18.85, L/D = 28.28$

Unacceptable loss (larger than 0.04) shown in bold face

Table 2

Loss [\$/min] for distillation case study.

1. As expected, we find that the losses are small when we keep x_B constant.
2. Somewhat surprisingly, for disturbances in feed composition z_F it is even better to keep L/F or V/F constant.
3. Not surprisingly, keeping D/F (or D) constant is not an acceptable policy, e.g., operation is infeasible when z_F is reduced from 0.65 to 0.5.
4. All alternatives are insensitive to disturbances in feed enthalpy (q_F).
5. L/D is not a good controlled variable, primarily because its optimal value is rather sensitive to feed composition changes.
6. For a implementation error (overpurification) in x_D where x_D is 0.996 rather than 0.995 all the alternatives give an unacceptable loss of about 0.09. We conclude that we should try to control x_D close to its specification.
7. For reflux L and boilup V one needs to include "feedforward" action from F (i.e. keep L/F and V/F constant).

8. Use of L/F or V/F as controlled variables is very attractive when it comes to disturbances, but these variables are rather sensitive to implementation errors.
9. Other controlled variables have also been considered (not shown in Table). For example, a constant composition (temperature) on stage 19 (towards the bottom), $x_{19} = 0.20$, gives a loss of 0.064 when z_F is reduced to 0.5, but otherwise the losses are similar to those with x_B constant.

Step 7: Further analysis and selection of controlled variables

The previous steps are based on steady-state economics only, and in the final selection other factors must also be considered, including their controllability properties. This may change the order of candidate controlled variables. Hopefully, at least one of the control structures that was acceptable from a steady-state economic point of view, is also acceptable from a dynamic point of view. Otherwise, one may consider design changes in order to improve the controllability, or consider the need for in-line optimizing control.

For our case study, we find from Table 2 that the following three candidate sets of controlled variables yield the lowest losses

$$c^1 = \begin{pmatrix} x_B \\ x_D \end{pmatrix}; \quad c^2 = \begin{pmatrix} L/F \\ x_D \end{pmatrix}; \quad c^3 = \begin{pmatrix} V/F \\ x_D \end{pmatrix}$$

As mentioned, the "two-point" control structure c^1 where both compositions are controlled, results in a difficult control problem. The loss will then be larger than indicated, and it is probably better to keep L/F or V/F constant. Since it is usually simpler to keep a liquid flow L/F rather than a vapor flow V/F constant (less implementation error), we conclude as follows:

Proposed control system.

- V is used¹ to keep $x_D = 0.995$.
- $L/F = 15.07$ is kept constant.

Remark. If it turns out to be difficult to keep L/F (or V/F) constant, then we may consider using L (or V) to keep a temperature towards the bottom of the column constant.

4. OPTIMAL CHOICE OF CONTROLLED VARIABLES

Above we selected the controlled variables c simply as a subset of the measurements y . However, more generally we may allow for variable combinations and write $c = h(y)$ where the

¹There are other possible choices for controlling x_D , e.g. we could use the distillate flow D . However, V has a more direct effect.

function $h(y)$ is free to choose. Here the number of controlled variables (c 's) is equal to the number of degrees of freedom. If we only allow for linear variable combinations then we have

$$\Delta c = H \Delta y \tag{5}$$

where the constant matrix H is free to choose. Does there exist a variable combination with zero loss for all disturbances, that is, for which $c_{\text{opt}}(d)$ is independent of d ? As proved by Alstad and Skogestad (2002) the answer is "yes" for small disturbance changes, provided we have at least as many independent measurements (y 's) as there are independent variables (u 's and d 's). The derivation Alstad and Skogestad (2002) is surprisingly simple: In general, the optimal value of the y 's depend on the disturbances, and we may write this dependency as $y_{\text{opt}}(d)$. Locally, that is for small deviations from the optimal operating point, the value of $y_{\text{opt}}(d)$ depends linearly on d ,

$$\Delta y_{\text{opt}}(d) = F \Delta d \tag{6}$$

where the sensitivity $F = dy_{\text{opt}}(d)/dd$ is a constant matrix. We would like to find a variable combination $\Delta c = H \Delta y$ such that $\Delta c_{\text{opt}} = 0$. We get $\Delta c_{\text{opt}} = H \Delta y_{\text{opt}} = H F \Delta d = 0$. This should be satisfied for any value of Δd , so we must require that H is selected such that

$$H F = 0 \tag{7}$$

This is always possible provided we have at least as many (independent) measurements y as we have independent variables (u 's and d 's) (Alstad and Skogestad 2002): First, we need one c (and thus one extra y) for every u , and, second, we need one extra y for every d in order to be able to get $H F = 0$.

Implementation error

One issue which we have not discussed so far is the implementation error n , which is the difference between the actual controlled variable c and its desired value ($n = c - c_s$). In some cases there may be no implementation error, but this is relatively rare.

Figure 1 is a bit misleading as it (i) only includes the contribution to n from the measurement error, and (ii) gives the impression that we directly measure c , whereas we in reality measure y , i.e. n in Figure 1 represents the combined effect on c of the measurement errors for y .

In any case, the implementation error n generally needs to be taken into account, and it will affect the optimal choice for the controlled variables. Specifically, when we have implementation errors, it will no longer be possible to find a set of controlled variables that give zero loss. One way of seeing this is to consider the implementation error n as a special case of a disturbance d . Recall that to achieve zero loss, we need to add one extra measurement y for each disturbance. However, no measurement is perfect, so this measurement will have an associated error ("noise"), which may again be considered as an additional disturbance, and so on.

Unfortunately, the implementation error makes it much more difficult to find the optimal measurement combination, $c = h(y)$, to use as controlled variables. Numerical approaches may be used, at least locally (Halvorsen *et al.* 2003), but these are quite complicated.

5. EXAMPLE: OPTIMAL OPERATION OF BLENDING OF GASOLINE

The following example illustrates clearly the importance of selecting the right controlled variables, and illustrates nicely of the method of Alstad and Skogestad (2002) for selecting optimal measurement combinations, for the case when implementation error is not an important issue.

Problem statement. We want to make 1 kg/s of gasoline with at least 98 octane and not more than 1 weight-% benzene, by mixing the following four streams

- Stream 1: 99 octane, 0% benzene, price $p_1 = (0.1 + m_1)$ \$/kg.
- Stream 2: 105 octane, 0% benzene, price $p_2 = 0.200$ \$/kg.
- Stream 3: 95 octane, 0% benzene, price $p_3 = 0.12$ \$/kg.
- Stream 4: 99 octane, 2% benzene, price $p_4 = 0.185$ \$/kg.

The maximum amount of stream 1 is 0.4 kg/s. The disturbance is the octane contents in stream 3 ($d = O_3$) which may vary from 95 (its nominal value) and up to 96. We want to obtain a self-optimizing strategy that “automatically” corrects for this disturbance.

Solution. For this problem we have

$$u_o = (m_1 \quad m_2 \quad m_3 \quad m_4)^T$$

where m_i [kg/s] represents the mass flows of the individual streams. The optimization problem is to minimize the cost of the raw material

$$J(u_o) = \sum_i p_i m_i = (0.1 + m_1)m_1 + 0.2m_2 + 0.12m_3 + 0.185m_4$$

subject to the 1 equality constraint (given product rate) and 7 inequality constraints.

$$m_1 + m_2 + m_3 + m_4 = 1$$

$$m_1 \geq 0$$

$$m_2 \geq 0$$

$$m_3 \geq 0$$

$$m_4 \geq 0$$

$$m_1 \leq 0.4$$

$$99 m_1 + 105 m_2 + O_3 m_3 + 99 m_4 \geq 98$$

$$2m_4 \leq 1$$

At the nominal operating point (where $O_3 = d^* = 95$) the optimal solution is to have

$$u_{o,\text{opt}}(d^* = 95) = (0.26 \quad 0.196 \quad 0.544 \quad 0)^T$$

which gives $J_{\text{opt}}(d^*) = 0.13724$ \$. We find that three constraints are active (the product rate equality constraint, the non-negative flowrate for m_4 and the octane constraint). The same three constraints remain active when we change O_3 to 97, where the optimal solution is to have

$$u_{o,\text{opt}}(d = 97) = (0.20 \quad 0.075 \quad 0.725 \quad 0)^T$$

which corresponds to $J_{\text{opt}}(d = 97) = 0.126$ \$.

The proposed control strategy is then to use three of the degrees of freedom in u_o to control the following variables (active constraint control)

1. Keep the product rate at 1 kg/s
2. Keep the octane number at 98
3. Keep $m_4 = 0$

This leaves one unconstrained degree of freedom (which we may select, for example, as $u = m_1$, but which variable we select to represent u is not important as any of the three variables m_1 , m_2 or m_3 will do). We now want to evaluate the loss imposed by keeping alternative controlled variables c constant at their nominal optimal values, $c_s = c_{\text{opt}}(d^*)$. The available measurements available are a subset of u_o , namely

$$y = (m_1 \quad m_2 \quad m_3)^T$$

Here we have excluded m_4 since it is kept constant at 0, and thus is independent of d and u . Let us first consider keeping each individual flow constant (and the two others are adjusted to satisfy the active product rate and octane number constraints). We find when $d = O_3$ is changed from 95 to 97:

- $c = m_1$ constant at 0.26: $J = 0.12636$ corresponding to loss $L = 0.12636 - 0.126 = 0.00036$
- $c = m_2$ constant at 0.196: Infeasible (requires a negative m_3 to satisfy constraints)
- $c = m_3$ constant at 0.544: $J = 0.13182$ corresponding to loss $L = 0.13182 - 0.126 = 0.00582$

Let us now obtain the optimal variable combination that gives zero loss. We use a linear variable combination

$$c = Hy = h_1 m_1 + h_2 m_2 + h_3 m_3$$

The relationship between the optimal value of y and the disturbance is indeed linear in this case and we have

$$\Delta y_{\text{opt}} = F\Delta d = \begin{pmatrix} 0.20 & -0.26 \\ 0.075 & -0.196 \\ 0.725 & -0.544 \end{pmatrix} \frac{1}{2} \Delta d = \underbrace{\begin{pmatrix} -0.03 \\ -0.06 \\ 0.09 \end{pmatrix}}_F \Delta d$$

To get a variable combination with zero loss we must have $HF = 0$ or

$$-0.03h_1 - 0.06h_2 + 0.09h_3 = 0$$

In this case we have 1 unconstrained degree of freedom (u) and 1 disturbance (d), so we need to combine at least 2 measurements to get a variable combination with zero loss. This is confirmed by the above equation which may always be satisfied by selecting one element in H equal to zero.

We then find that the following three combinations of two variables give zero loss:

1. $c = m_1 - 0.5m_2$: Zero loss (derived by setting $h_3 = 0$ and choosing $h_1 = 1$)
2. $c = 3m_1 + m_3$: Zero loss (derived by setting $h_2 = 0$ and choosing $h_3 = 1$)
3. $c = 1.5m_2 + m_3$: Zero loss (derived by setting $h_1 = 0$ and choosing $h_3 = 1$)

There are an infinite number of variable combinations of 3 measurements (m_1, m_2, m_3) with zero disturbance loss. However, if we also include the implementation error, then there will be a single optimal combination of 3 measurements.

Change in prices. In the above example, the prices were assumed constant. If the prices change, then we may easily correct for this. It may be done in two different ways:

1. Make the setpoint c_s a function of prices (this is probably the simplest and most obvious approach).
2. Keep constant setpoints, and instead include the prices as extra "measured disturbances".

The latter approach is probably less obvious so let us illustrate how it can be applied to our blending example. We consider the case where the price of stream 2 may vary. Specifically, changing the price p_2 from 0.2 to 0.21 gives the new optimum

$$u_{\text{opt}}(p_2 = 0.21, O_3 = 95) = (0.28 \quad 0.188 \quad 0.532 \quad 0)^T$$

and defining

$$y = (m_1 \quad m_2 \quad m_3 \quad p_2)^T$$

$$d = (O_3 \quad p_2)^T$$

gives

$$\Delta y_{\text{opt}} = \underbrace{\begin{pmatrix} -0.03 & 2.0 \\ -0.06 & -0.8 \\ 0.09 & -1.2 \\ 0 & 1 \end{pmatrix}}_F \Delta d$$

We then have

$$c = Hy = h_1m_1 + h_2m_2 + h_3m_3 + h_4p_2$$

To get a variable combination with zero loss we must have $HF = 0$ or

$$-0.03h_1 - 0.06h_2 + 0.09h_3 = 0$$

$$2h_1 - 0.8h_2 - 1.2h_3 + h_4 = 0$$

The first equation is the same as above (and has the same solutions), and from the last equation the price correction factor is:

$$h_4 = -2h_1 + 0.8h_2 + 1.2h_3$$

This gives the following optimal variable combinations with price correction:

1. $c = m_1 - 0.5m_2 - 2.4p_2$ (since $h_4 = -2 \cdot 1 + 0.8 \cdot (-0.5) + 1.2 \cdot 0 = -2.4$)
2. $c = 3m_1 + m_3 - 4.8p_2$
3. $c = 1.5m_2 + m_3 + 2.4p_2$

It seems here that the sum of the first and third variable combination gives a possible "magic" controlled variable, which is independent of the price p_2 . However, it turns out that this variable is $m_1 + m_2 + m_3$, which indeed is independent of the price, is also identical to one of the equality constraints (the total mass flow is always 1), so this variable is degenerate and fixing its value does not provide any additional information.

Matlab file

```
H = [0.2 0 0 0; 0 0 0 0; 0 0 0 0; 0 0 0 0]
f = [0.1 0.2 0.12 0.185] % prices
A = [-99 -105 -95 -99; 0 0 0 2; -1 0 0 0; 0 -1 0 0;
      0 0 -1 0; 0 0 0 -1; 0 0 0 1]
b = [-98 1 0.4 0 0 0 0]'
Aeq = [1 1 1 1 ]
beq = 1
[X, FVAL]=QUADPROG(H, f, A, b, Aeq, beq)
```

The answer X is the optimal mass fractions of the four streams. The cost ($\$/\text{kg}$) is: $FVAL = 0.5 \cdot X' \cdot H \cdot X + f' \cdot X$

To find active constraints compute: $b-A^*X$.
(The active constraints will correspond to zero values)

Disturbance d: Octane number of stream 3 changed to 97:

```
A = [-99 -105 -97 -99; 0 0 0 2; -1 0 0 0; 0 -1 0 0;
      0 0 -1 0; 0 0 0 -1; 0 0 0 1]
[X, FVAL]=QUADPROG(H, f, A, b, Aeq, beq)
```

Change in price of stream 2 from 0.2 to 0.21

```
f = [0.1 0.21 0.12 0.185] % prices
A = [-99 -105 -95 -99; 0 0 0 2; -1 0 0 0; 0 -1 0 0;
      0 0 -1 0; 0 0 0 -1; 0 0 0 1]
[X, FVAL]=QUADPROG(H, f, A, b, Aeq, beq)
```

6. CONCLUSIONS

The selection of controlled variables for different systems may be unified by making use of the idea of self-optimizing control. The idea is to first define quantitatively the operational objectives through a scalar cost function J to be minimized. The system then needs to be optimized with respect to its degrees of freedom u_o . From this we identify the "active constraints" which are implemented as such. The remaining unconstrained degrees of freedom u are used to controlled selected controlled variables c at constant setpoints. In the paper it is discussed how these variables should be selected. We have in this paper not discussed the implementation error $n = c - c_s$ which may be critical in some applications (Skogestad 2000).

REFERENCES

- V. Alstad and S. Skogestad, Presented in 2002 AIChE Annual Meeting, Indianapolis, USA.
C.S. Foss, AIChE J., 19 (1973) 209.
I.J. Halvorsen, S. Skogestad, J.C. Morud and V. Alstad, Ind. Eng. Chem. Res., 42(2003), 3273.
M. Morari, In: Proc. of Second international conference on chemical process control (CPC-2), Sea Island, Georgia, Jan. 1981. pp. 467-495.
M. Morari, G. Stephanopoulos and Y. Arkun, AIChE J., 26 (1980) 220.
F.G. Shinsky, Distillation Control, McGraw-Hill Book Company, 1984.
S. Skogestad, J. Proc. Control, 10 (2000) 487.
S. Skogestad, and I. Postlethwaite Multivariable Feedback Control, John Wiley & Sons, 1996.
S. Skogestad and M. Morari, AIChE J, 33(1987), 1620.

Chapter D2

Integrated batch control

L. Puigjaner, J.M. Nogués, A. Espuña

Chemical Engineering Department, Universitat Politècnica de ETSEIB, Diagonal 647, E08028 Barcelona, Spain

1. INTRODUCTION

There is an increasing shift in companies towards value-added formulated products such as pharmaceuticals, coatings and speciality products [1]. Such products, which often consist of interrelated items, are mostly produced batch-wise and involve complex processes requiring a high degree of coordination in the materials and manufacturing. To obtain top productivity levels in the industrial facilities where they are produced.

In such instances, batch production is preferred because of the inherent flexibility associated with this mode of operation. It easily accommodates the market fluctuations of the product. Moreover, such products will have to be delivered to the customer in the form of small quantities. The processing [2]. Customer requirements will be more strict and more complex with respect to specification, quality and delivery, requesting more flexible manufacturing processes, a goal that may be more readily achieved in batch rather than continuous production [3].

This has led to an increasing research interest in batch production, essentially addressed to the design, analysis and scheduling of batch plant strategies. The most recent reviews on batch plant design and operation [4,5] reveal spectacular progress in the development of systematic methodologies and optimisation techniques towards improved solutions taking into account equipment availability, material inventories and plant resource constraints.

Surprisingly enough, technology transfer of this progress in the industrial environment is proceeding very slowly. There are some obvious reasons for this. In the first place, modelling batch processes may become very complex when it comes to the level of detail required to adequately represent real-life operations, and very difficult to standardise if it involves a very wide variety of operations, as happens to be the case in batch industries. This reality is reflected in existing commercial packages that offer only partial solutions for individual and local planning/scheduling tasks. However, most significantly, a major limitation of present