Plantwide control: The search for the self-optimizing control structure

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Abstract

Plantwide control is concerned with the structural decisions involved in the control system design of a chemical plant (Foss 1973); "Which variables should be controlled, which variables should be measured, which inputs should be manipulated, and which links should be made between them?" In particular, the first issue about which variables to control has received little attention. It is argued that the answer is related to finding a simple and robust way of implementing the economically optimal operating policy. The goal is to find a set of controlled variables which, when kept at constant setpoints, indirectly lead to near-optimal operation with acceptable loss. This is denoted "self-optimizing" control. Since the economics are determined by the overall plant behavior, it is necessary to take a plantwide perspective. A systematic procedure for finding suitable controlled variables based on only steady-state information is presented. Important steps are degree of freedom analysis, definition of optimal operation (cost and constraints), and evaluation of the loss when the controlled variables are kept constant rather than optimally adjusted. A case study yields very interesting insights into the control and maximum throughput of distillation columns,

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1 Introduction

If we consider the control system in a chemical plant, then we find that it is structured hierarchically into several layers, each operating on a different time scale. Typically, layers include include scheduling (weeks), site-wide (real-time) optimization (day), local optimization (hour), supervisory/predictive control (minutes) and stabilizing and regulatory control (seconds); see Figure 1. The layers are interconnected through the controlled variables. More precisely,

> The setpoints c_s of the **controlled variables** are the (internal) variables that link two layers in a control hierarchy, whereby the upper layer computes the value of c_s to be implemented by the lower layer.

We usually assume time-scale separation which for our purposes implies that the setpoints c_s can be assumed to be immediately implemented by the layers below. Which should these internal controlled variables c be? That is, what should we control? Or to phrase the question in another way: Why do we in a chemical plant select to control a lot of internal variables (e.g. compositions, pressures, temperatures, etc.) for which there are no explicit control requirements? This paper attempts to answer this question.

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* m
3. *Selection of measurements* v (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 in most cases, and the question is if it is possible to find a simpler implementation which still operates satisfactorily (with an acceptable loss). More precisely, the **loss** L is defined as the difference between the actual value of the cost function obtained with a specific control strategy, and the truly optimal value of the cost function, i.e. $L = J - J_{\text{opt}}$. 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 here call "self-optimizing control":

> **Self-optimizing control** is when we can achieve an acceptable loss with constant setpoint values for the controlled variables

(The reader is probably familiar with the term self-regulation, which is when acceptable dynamic control performance can be obtained with constant manipulated inputs. Self-optimizing control is a direct generalization to the case where we can achieve acceptable (economic) performance with constant controlled variables.) The term "self-optimizing control" is short and descriptive, but also other terms have been used to describe the same idea, such as "feedback optimizing control" (Morari *et al.* 1980), and "indirect optimizing control (through setpoint control)"(Halvorsen and Skogestad 1998). A simple example of self-optimizing control is the process of baking a cake, where the operation is indirectly kept

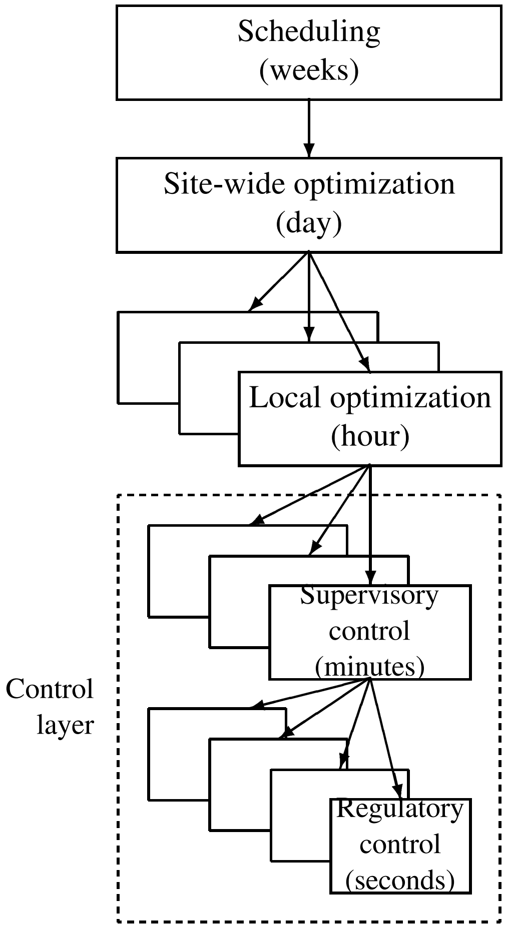


Figure 1: Typical control hierarchy in a chemical plant.

close to its optimum ("a well-baked cake") by controlling the oven temperature and baking time at the setpoints given in the cook book (which in this case is the "optimizer").

The idea is further illustrated in Figure 2, where we see that there is a loss if we keep constant setpoints rather than reoptimizing when a disturbance moves the process away from its nominally optimal operating point (denoted $*$). For the case illustrated in the figure it is better (with a smaller loss) to keep the setpoint c_{1s} constant than to keep c_{2s} constant.

An additional concern with the constant setpoint policy is that there will always be an implementation error $d_c = c - c_s$, e.g. caused by measurement error. The implementation error may cause a large additional loss if the optimum surface is "sharp". To be more specific, we may as illustrated in Figure 3, distinguish between three classes of problems when it comes to the actual implementation:

(a) *Constrained optimum.* In the figure is shown the case where the minimum value of the cost J is obtained for $c = c_{min}$. In this case there is no loss imposed by keeping a constant $c_s = c_{min}$. In addition, implementation of an "active" constraint is usually easy, e.g., it is easy to keep a valve closed.

(b) *Unconstrained flat optimum.* In this case the cost is insensitive to value of the controlled variable c, and implementation is again easy.

(c) *Unconstrained sharp optimum.* The more difficult problems for implementation is when the cost (operation) is sensitive to value of the controlled variable c. In this case, we want to find another controlled variable c in which the optimum is flatter.

The latter unconstrained problems are the focus of this paper.

Important notation

c - controlled variables (selected from the sets of y and m to replace u as degrees of freedom for optimization)

$c_{\text{opt}}(d)$ - optimal value of c for given d (which minimizes J).

c_s - setpoint value for c; in this paper, $c_s = c_{\text{opt}}(d^*)$

d - disturbance variables

d^* - nominal value of disturbances

$d_c = c - c_s$ - implementation error

$e_{cs} = c_s - c_{\text{opt}}(d)$ - setpoint error

$e_c = c - c_{\text{opt}}(d)$ - overall error

$J = J_u(u, d) = J_c(c, d)$ - scalar cost function to be minimized

$J_{\text{opt}}(d)$ - minimum value of J (minimized with respect to u or c)

$L = J_c(c, d) - J_{\text{opt}}(d)$ - loss

m - manipulated variables (control degrees of freedom)

m (as subscript) - measured

n - noise on measurements of y

u - "base set" for the optimization degrees of freedom

v - all available measurements (including c_m, d_m, y_m)

y - dependent "output" variables; usually measured

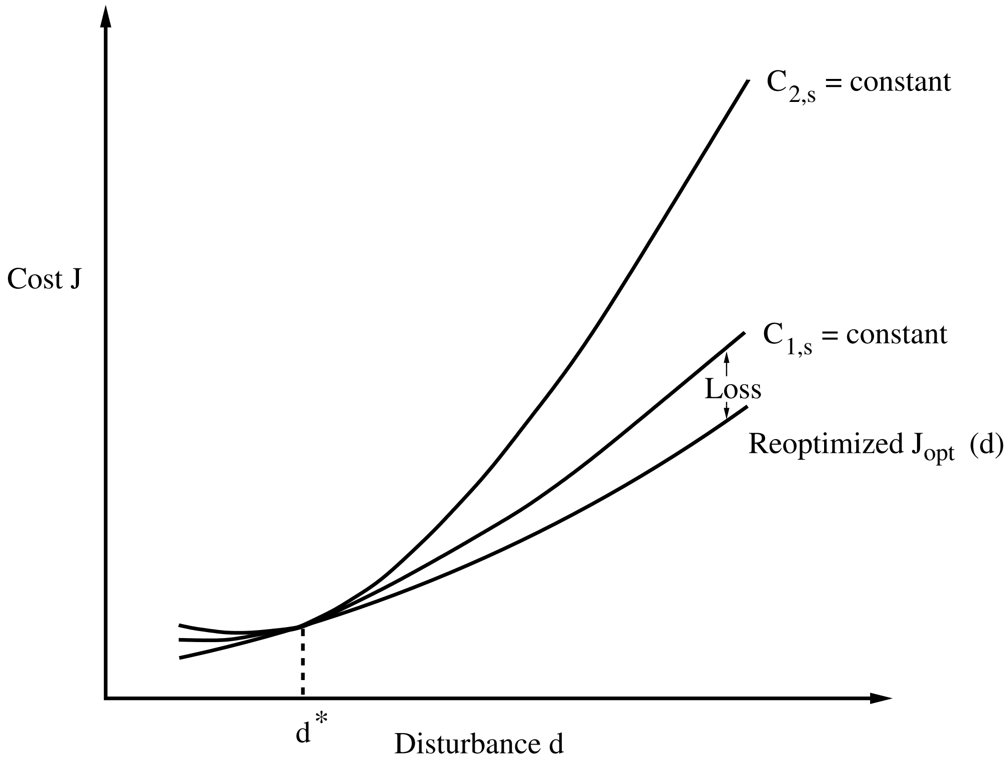
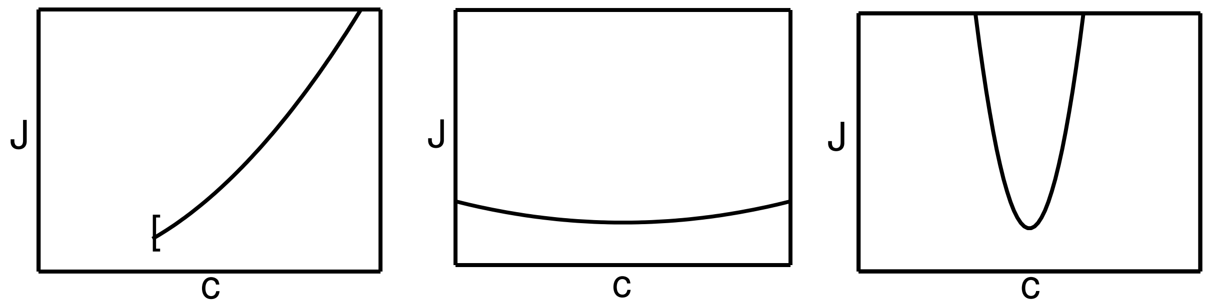


Figure 2: Loss imposed by keeping constant setpoints for the controlled variables



(a) Implementation easy: Active constraint control

(b) Implementation easy: Insensitive to error in c

(c) Implementation difficult: Look for another controlled variable

Figure 3: Implementing the controlled variable

2 Previous work

Inspired by the work of Findeisen *et al.* (1980), the basic idea of self-optimizing control was formulated about twenty years ago by Morari *et al.* (1980). Morari *et al.* (1980) write that "in attempting to synthesize a feedback optimizing control structure, our main objective is to translate the economic objectives into process control objectives. In other words, *we want to find a function* c *of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating conditions.* [...] This means that by keeping the function $c(u, d)$ at the setpoint c_s, through the use of the manipulated variables u, for various disturbances d, it follows uniquely that the process is operating at the optimal steady-state." If we replace the term "optimal adjustments" by "acceptable adjustments (in terms of the loss)" then the above is a precise description of what we in this paper denote a self-optimizing control structure. The only factor they fail to consider is the effect of implementation error $c - c_s$. Morari *et al.* (1980) propose to select the best set of controlled variables based on minimizing the loss ("feedback optimizing control criterion 1"). They also propose that Monte Carlo simulations should be used to evaluate the loss if the disturbances have a probability distribution.

Somewhat surprisingly, the idea of "feedback optimizing control" of Morari *et al.* (1980) has up to now received very little attention. One reason is probably that the paper also dealt with the issue of finding the optimal operation (and not only on how to implement it), and another reason is that the only example in the paper happened to result in an implementation with the controlled variables at their constraints. The constrained case is "easy" from an implementation point of view, because the simplest and optimal implementation is to simply maintain the constrained variables at their constraints ("active constraint control", (Maarleveld and Rijnsdrop 1970)). No example was given for the more difficult unconstrained case, the focus of this paper, where the choice of controlled (feedback) variables is a critical issue. The follow-up paper by Arkun and Stephanopoulos (1980) concentrated further on the constrained case and tracking of active constraints.

At about the same time, Shinnar (1981) published a more intuitive process-oriented approach for selecting controlled variables, and applied it to the control of a fluidized catalytic cracker (FCC). The work may at first seem unrelated, but if one translates the words and notation, then one realizes that Shinnar's ideas are close to the ideas presented in this paper and in Morari *et al.* (1980). The main difference is that Shinnar assumes that the overall objective of the operation is to control a set of "primary" process variables Y_p at their specifications, whereas we in this paper follow Morari *et al.* (1980) and assume that the overall objective is to minimize some economic cost function J. In both cases it is assumed that the overall objective may be indirectly achieved by controlling some other variables at their setpoint; these controlled variables are denoted Y_{cd} by Shinnar (1981) and c by Morari *et al.* (1980) (and in this paper). Shinnar (1981) writes that the controlled variables should "have a maximum compensating effect on Y_p".

The similar later paper by Arbel *et al.* (1996) extended the FCC case study, and introduced the concepts of "dominant variables" and "partial control". The *dominant variables* are the process variables that tend to dominate the process behavior, for example, the temperature in a reactor, and which therefore intuitively may be good candidates as controlled variables, By *partial control* is meant that control of these variables indirectly achieves acceptable control of the primary variables[1]. The authors provide some intuitive ideas and examples for selecting dominant variables which may be useful in some cases, especially when no model information is available. However, it is not clear how helpful the idea of "dominant" variable is, since they are not really defined and no explicit procedure is given for identifying them. Indeed, Arbel *et al.* (1996) write that "the problems of partial control have been discussed in a heuristic way" and that "considerably further research is needed to fully understand the problems is steady-state control of chemical plants". It is believed that the approach presented in this paper, based on

[1]The terms "partial control" and "partially controlled system" are used by other authors (Waller *et al.* 1988) (Skogestad and Postlethwaite 1996) in a more general sense, to mean the system as it is appears from some higher layer in the control hierarchy with some loops already closed (e.g. a plant where the liquid level loops are closed).

using a (steady-state) model to evaluate the (economic) loss, provides an important part of this missing theoretical framework.

Tyreus (1999) provides some additional interesting ideas on how to select dominant variables, partly based on the extensive variable idea of Georgakis (1986) and the thermodynamic ideas of Ydstie, e.g. (Alonso and Ydstie 1996), but again no procedure for selecting such variables are presented. Again, it is believed that a more systematic approach, e.g. based on applying the four requirement for variable selection given in Section 5.2, or (even better) evaluating the loss as discussed Section 5.4, will confirm the recommendations given by Tyreus (1999).

Luyben (1988) introduced the term "eigenstructure" to describe the inherently best control structure (with the best self-regulating and self-optimizing property). However, he did not really define the term, and also the name is unfortunate since "eigenstructure" has a another unrelated mathematical meaning in terms of eigenvalues. Apart from this, Luyben and coworkers (e.g. Luyben (1975), Yi and Luyben (1995)) have studied unconstrained problems, and some of the examples presented point in the direction of the selection methods presented in this paper. However, Luyben proposes to select controlled outputs which minimizes the steady-state sensitive of the manipulated variable (u) to disturbances, i.e. to select controlled outputs (c) such that $(\partial u/\partial d)_c$ is small, whereas we really want to minimize the steady-state sensitivity of the economic loss (L) to disturbances, i.e. to select controlled outputs (c) such that $(\partial L/\partial d)_c$ is small.

Fisher *et al.* (1988) discuss selection of controlled variables, mainly focused towards active constraint control. However, somewhat hidden in their HDA example (p. 614) one finds statements about selecting controlled variables which optimal values are insensitive to disturbances (requirement 1 for variable selection presented in this paper).

In his book Rijnsdorp (1991) gives on page 99 a stepwise design procedure for designing optimizing control systems for process units. One step is to "transfer the result into on-line algorithms for adjusting the degrees of freedom for optimization". He states that this "requires good process insight and control structure know-how. It is worthwhile basing the algorithm as far as possible on process measurements. In any case, it is impossible to give a clear-cut recipe here."

Narraway *et al.* (1991), Narraway and Perkins (1993) and Narraway and Perkins (1994)) strongly stress the need to base the selection of the control structure on economics, and they discuss the effect of disturbances on the economics. However, they do not formulate any rules or procedures for selecting controlled variables.

Mizoguchi *et al.* (1995) and Marlin and Hrymak (1997) stress the need to find a good way of implementing the optimal solution in terms how the control system should respond to disturbances, "i.e. the key constraints to remain active, variables to be maximized or minimized, priority for adjusting manipulated variables, and so forth." They suggest that an issue for improvement in today's real-time optimization systems is to select the control system that yields the highest profit for a range of disturbances that occur between each execution of the optimization. This is similar to the ideas presented in this paper.

Finally, Zheng *et al.* (1999) present a procedure for selecting controlled variables based on economic penalties that is similar to the approach presented in this paper (apparently, the work has been performed independently), but they do not consider the implementation error. The procedure is applied to a reactor-separator-recycle system.

In summary, it is clear that many authors have been aware of the importance of the ideas presented in this paper. The main contribution of the present paper is to bring the ideas together and formulate them more clearly, to include the implementation error in the analysis, and to present some good case studies.

3 Degrees of freedom for control and optimization

The number of independent variables for control, N_m, is usually easily obtained from process insight as the number of variables that can be manipulated by external means (which in process control is the number of number of adjustable valves plus the number of other adjustable electrical and mechanical variables).

The number of degrees at freedom for optimization (N_u) is generally less than the number of control degrees of freedom (N_m). We have

$$N_u = N_m - N_0 \tag{1}$$

where $N_0 = N_{m0} + N_{y0}$ is the number of variables with no effect on the cost function J.

N_{m0} **-** number of manipulated inputs (u's), or combinations thereof, with no effect on the J.

N_{y0} **-** number of controlled output variables with no effect on J.

In most cases J depends on the steady-state only, and N_{y0} usually equals the number of liquid levels with no steady-state effect (including most buffer tank levels). However, note that some liquid levels *do* have a steady-state effect, such as the level in a non-equilibrium liquid phase reactor, and levels associated with adjustable heat transfer areas. Also, we should *not* include in N_{y0} any liquid holdups that are left uncontrolled, such as internal stage holdups in distillation columns.

A simple example where N_{m0} is non-zero is a heat exchanger with bypass on both sides, (i.e. $N_m = 2$). However, at steady-state $N_u = 1$ since there is really only one operational degree of freedom, namely the heat transfer rate Q (which at steady-state may be achieved by many combinations of the two bypasses), so we have $N_{m0} = 1$.

Remark on design degrees of freedom. In this paper we are concerned with *operational* degrees of freedom. The *design* degrees of freedom (which is not a concern in this paper) include all the operational degrees of freedom plus all parameters related to the size of the equipment, such as the number of stages in column sections, area of heat exchangers, etc.

4 Optimal operation and its implementation

When controlling a chemical plant our first concern is to stabilize the plant and keep its operation within given constraints. These issues may consume some degrees of freedom (e.g. to stabilize levels with no steady-state effect and to satisfy "active" product specifications), but there will generally be many degrees of freedom u left. What should these be used for?

Loosely speaking, they should be used to "optimize the operation". There may be many issues involved, and to trade them off against each other in a systematic manner we usually quantify a scalar performance (cost) index J which should be minimized. In many cases this index is an economic measure, e.g. the operation cost. For example, J could be of the form

$$J = J_u(u, d) = \int_0^T \phi(u, d) dt \tag{2}$$

where u are the degrees of freedom for optimization, d are time-varying disturbances, and T is the total operation time.

In this paper we will for simplicity use steady-state models and the integration in (2) may be replaced by time-averaging over the various steady-states. The main justification for using a steady-state analysis is that the economic performance is primarily determined by steady-state considerations. The effect of the dynamic control performance can be partly included in the economic analysis by introducing a control error term as an additional disturbance.

Remark. Although we use a steady-state analysis in this paper, it may be extended to truly unsteady-state-processes, like during a grade transition or for a batch process, by using a dynamic model and letting the setpoints c_s be precomputed trajectories as a function of time or of state variables.

4.1 The optimization problem

The optimizing control problem can be formulated as

$$\min_{u} J_u(u,d) \tag{3}$$

subject to the inequality constraints

$$g(u,d) \leq 0 \tag{4}$$

where u are the N_u independent variables we can affect (degrees of freedom), and d are independent variables we can not affect (disturbances). Here the constraints for instance may be

- product specifications (e.g. minimum purity)
- manipulated variable constraints (e.g. nonzero flow)
- other operational limitations (e.g. maximum temperature)

Conflicting constraints may result in a problem without a feasible solution. For example, if we make a product by blending two streams then we cannot achieve a product specification outside the range of feed compositions.

Remark. We have assumed that all dependent (state) variables x have been eliminated such that the cost function and constraints are in terms of the independent variables u and d. However, in some cases it is more convenient to keep the state variables x and corresponding model equations (equality constraints) and formulate the optimization problem as

$$\min_{u} J_x(x,u,d) \tag{5}$$

subject to the constraints

$$g_1(x,u,d) = 0 \tag{6}$$

$$g_2(x,u,d) \leq 0 \tag{7}$$

4.2 Implementing the optimal solution

There are two main issues when it comes to optimizing control. The first is the mathematical and numerical problem of solving the optimization problem in (3) to obtain the optimal operating point. The optimization problem may be very large, with hundreds of thousands of equations and hundreds of degrees of freedom (e.g. for a complete ethylene plant), but with todays computers and optimization methods this problem is solvable, and it is indeed solved routinely today in some plants. The second issue, the focus of this paper, is how the optimal solution should be implemented in practice. Surprisingly, this issue has received much less attention.

To better understand the issues consider the three alternative structures for optimizing control shown in Figure 4:

(a) Open-loop implementation.

(b) Closed-loop implementation with a separate control layer.

(c) Integrated optimization and control.

In the figure the block "process" denotes the process as seen from the optimization layer, so it may actually be a partially controlled plant which includes, for example, stabilizing level loops. This means that the independent variables u for the optimization may include some of the "original" manipulated variables (m) as well as the setpoints used in the lower-layer controllers.

If there were no unmeasured disturbances d then the three implementations would give the same result. The key to understand why the three structures differ, is therefore to consider what happens to the degrees of freedom u in response to a disturbance d (more generally d may include any uncertainty, including errors in the model used for the optimization and control).

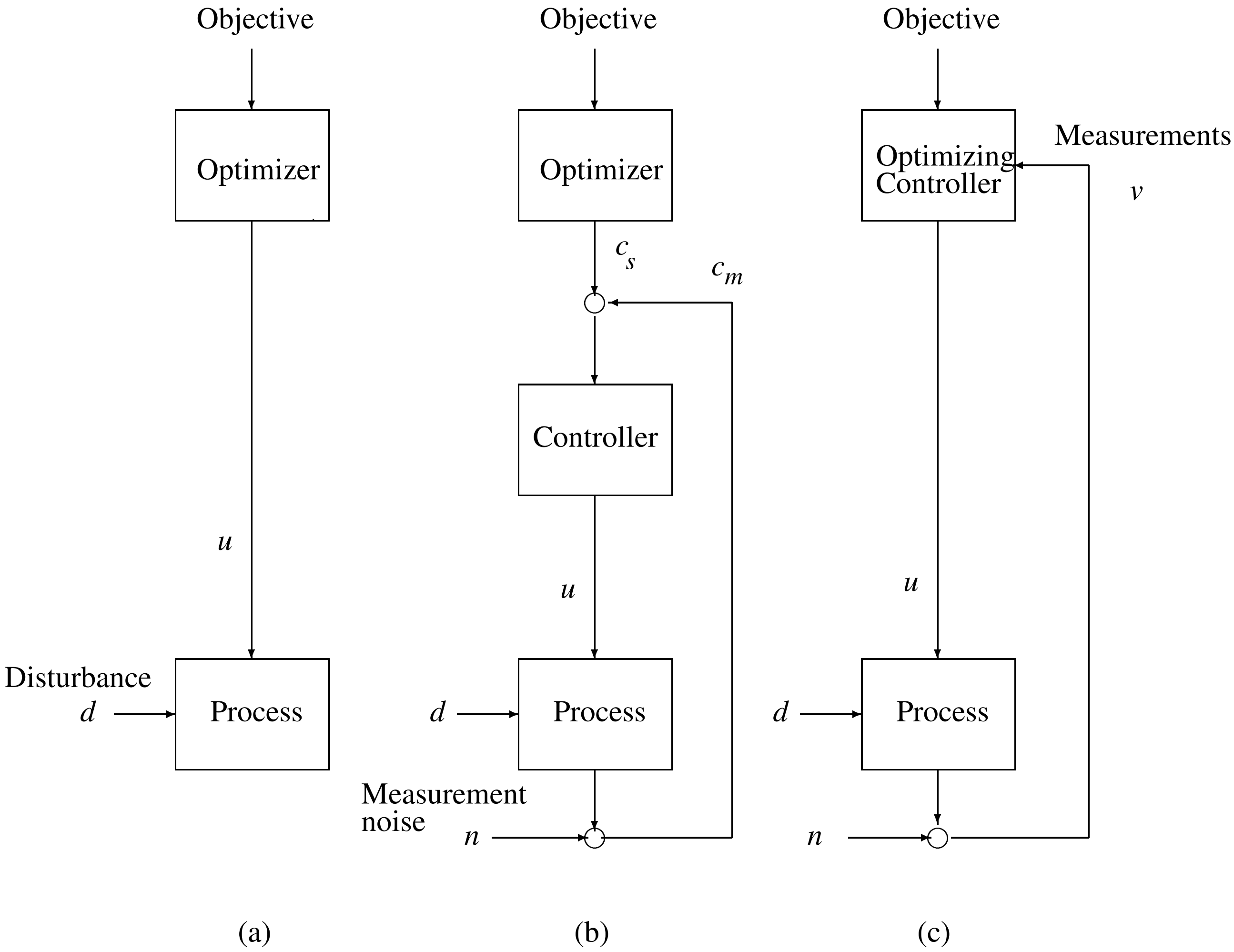


Figure 4: Alternative structures for optimizing control. Structure (b) is studied in this paper

(a) For the open-loop implementation there is no feedback, and u remains unchanged when there is a disturbance d.

(b) For the closed-loop implementation with a separate control layer, the disturbance d affects the measurement c_m, and the controller adjust u so that c_m returns approximately to its setpoint, c_s.

(c) For the integrated optimization and control, all available measurements v (including c_m) are used to identify the disturbance and update the model, and then dynamic on-line optimization is used to recompute a new optimal value for u

In general, the open-loop implementation (a) is not acceptable because there is no attempt to correct for disturbances d.

On the other hand, the centralized implementation in (c) with a single optimizing controller, although optimal from a mathematical point of view, is not likely to be used in practice, even with tomorrows computing power. One important reason is the cost of obtaining a dynamic model; in the centralized controller it is critical that this model is accurate since there are no predetermined links, and the controller must rely entirely on the model to take the right action.

Therefore, in practice, we use the closed-loop implementation (b) where we decompose the control system into separate parts and layers. In the simplest case shown in Figure 4b we may have two layers:

- A steady-state optimization layer which computes the optimal setpoints c_s for the controlled variables, and
- A feedback control layer which implements the setpoints, to get $c \approx c_s$.

In process control applications, the feedback control layer usually operates continuously, whereas the optimization layer (which may be an engineer) recomputes new setpoints c_s only quite rarely; maybe once an hour or once a day (when the plant has settled to a new steady-state). The idea is that by locally controlling the right variables c, we can take care of most of the disturbances, and thus reduce the need for continuous reoptimization. This also reduces the need for model information and tends to make the implementation more robust. On the other hand, it usually implies a performance loss compared to the "true" optimal (centralized) solution, and the challenge is to find a "self-optimizing" control structure (i.e. to find the right controlled variables c) for which the loss L is acceptable.

Comment on active constraint control. In some cases there is no performance loss with the hierarchical structure in Figure 4(b) with a separate optimization and control layer. This is when the optimum lies at some constraints, and we use *active constraint control* where we choose the constrained variables as the controlled variables c (Maarleveld and Rijnsdrop 1970) (Arkun and Stephanopoulos 1980) (Fisher *et al.* 1988). This is a common situation, since if the process model is not too non-linear the optimum operating point is at the intersection of as many constraints as there are degrees of freedom for optimization (Maarleveld and Rijnsdrop 1970). However, in many cases the constraints move depending on the operating point, and a change in the active constraints may require reconfiguration of the control loops. To avoid such an often complicated logic system, we may use in the lower layer a multivariable controller that explicitly handles constraints. In particular, model predictive control (MPC), which has gained widespread use in industry over the last 20 years, provides a simple and efficient tool for tracking active constraints.

4.3 Introductory example

To give the reader some appreciation of the issues, we consider a distillation plant where the plant economics are mainly determined by its steady-state behavior. With a given feed (including given feed rate) and a specified column pressure[2], a conventional two-product distillation column, as shown in

[2]If column pressure is free we often find that the optimal choice is to have maximum cooling corresponding to minimum pressure ("floating pressure control" as suggested by Shinskey (1984)). The reason is that in most cases the relative volatility is improved when pressure is lowered.

Figure 5, has two degrees of freedom at steady state ($N_u = 2$). (From a control point of view the column has $N_m = 5$ degrees of freedom, but two degrees of freedom are needed to stabilize the reboiler and condenser holdups, which have no steady-state effect, and one degree of freedom is used to control the pressure at its given value). The two steady-state degrees of freedom, e.g. selected to be the vapor flow (boilup) V and the distillate flow D,

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

(this is not a unique choice) may be used to optimize the operation of the plant. However the question is: How should the optimal solution be *implemented*, that is, which two variables c should be specified and controlled during operation?

To answer this question in a quantitative manner, we need to define the constraints for the operation and the cost function J to be minimized.

Constraints. We assume that the mole fraction of light component in the distillate product x_D must be above 0.95, $x_D \geq x_{D,min} = 0.95$, and that to avoid flooding the capacity of the column is limited by a maximum allowed vapor load, $V \leq V_{max}$.

Cost function. Rather than minimizing the cost J, it is more natural in this case to maximize the profit $P = -J$, which is the product value minus the feed costs and the operational (energy) costs which are proportional to the vapor flow V,

$$P = p_D D + p_B B - p_F F - p_V V \tag{8}$$

Constrained operation. Let us first consider a case where

- distillate is the more valuable product ($p_D \gg p_B$)
- energy costs are low (p_V is small)

In this case, it is optimal to operate the column at maximum load (to reduce the loss of light component in the bottom) and with the distillate composition at its specification (to maximize distillate flow by including as much heavy component as possible) (Gordon 1986), i.e.

$$V_{\text{opt}} = V_{max}; \quad x_{D,opt} = x_{D,min} = 0.95$$

Thus, the optimum lies at constraints and implementation is obvious: We should select the vapor rate V and the distillate composition x_D as the controlled variables,

$$c = \begin{pmatrix} V \\ x_D \end{pmatrix}; \quad c_s = \begin{pmatrix} V_{max} \\ x_{D,min} \end{pmatrix}$$

In practice, we may implement this using a lower-level feedback control system where we adjust the boilup V to keep the pressure drop over the column (an indicator of flooding, i.e. V_{max}) below a certain limit, and adjust the reflux L (or some other flow, depending on how the level and pressure control system is configured) so that x_D is kept constant.

Unconstrained operation. Next, consider a case where

- bottoms product is the more valuable product ($p_B \gg p_D$)
- energy costs are relatively high (the term $p_V V$ contributes significantly to J)

In this case the optimum may be unconstrained in both variables, and assume for the discussion that

$$V_{\text{opt}} = 0.76 V_{max}; \quad x_{D,opt} = 0.973 > x_{D,min}$$

Implementation in this case is *not* obvious. Some candidate sets of controlled variables are

$$c_1 = \begin{pmatrix} x_D \\ x_B \end{pmatrix}; \; c_2 = \begin{pmatrix} T_{top} \\ T_{btm} \end{pmatrix}; \; c_3 = \begin{pmatrix} V \\ x_D \end{pmatrix}; \; c_4 = \begin{pmatrix} L \\ V \end{pmatrix}; \; c_5 = \begin{pmatrix} L/D \\ V/B \end{pmatrix}$$

and there are many others. Controlled variables c_1 and c_2 will yield a "two-point" control system where we close two loops for quality control; c_3 yields a "one-point" control system where only one quality loop is closed; whereas c_4 and c_5 are "open-loop" policies which require no additional feedback loops (except for the level and pressure loops already mentioned). All of these choices of controlled variables will have different self-optimizing control properties.

At the end of the paper, we study another distillation example, where the optimum is constrained in one variable and unconstrained in the other. We also consider the case where the feed rate is a degree of freedom for the optimization.

5 Selection of controlled variables

In this section we present our procedure for selecting controlled variables, but let us first formulate the problem a bit clearer.

5.1 Problem formulation

Let the "base set" for the N_u available degrees of freedom be denoted u (this is not a unique set), and let d denote the (important) disturbances.Any other variable is then a function of these variables, for example, we can write for the selected N_u controlled variables

$$c = f_u(u, d) \tag{9}$$

Assuming that the set of c's are independent, we can from (9) derive the inverse relationship

$$u = f_c(c, d) \tag{10}$$

where we assume the function f_c exists and is unique. For a given disturbance d we can solve the optimization problem (3) with constraints (4), and if a feasible solution exists obtain the optimal value $u_{\mathrm{opt}}(d)$,

$$\min_{\substack{u \\ g(u,d)\leq 0}} \; J_u(u, d) = J_u(u_{\mathrm{opt}}(d), d) = J_{\mathrm{opt}}(d) \tag{11}$$

However, in actual operation the value of u will differ from the the optimal value $u_{\mathrm{opt}}(d)$, and this results in a **loss** [3] L between the actual operating costs and the optimal operating costs,

$$L = L_u(u, d) = J_u(u, d) - J_{\mathrm{opt}}(d) \tag{12}$$

The magnitude of the loss will depend on the control strategy used for adjusting u during operation, and to understand this better consider the "open-loop" and "closed-loop" strategies. Let d^* denote the nominal value of the disturbance for which the optimization was performed, and let d denote its actual value (during operation). In this paper we use for simplicity the nominal optimal values as setpoints, i.e.

$$u_s = u_{\mathrm{opt}}(d^*); \quad c_s = c_{\mathrm{opt}}(d^*)$$

- In the "open-loop" strategy we attempt to keep u constant at its setpoint u_s (more precisely, $u = u_s + d_u$ where d_u is the implementation error for u)
- In the "closed-loop" strategy we adjust $u = f_c(c, d)$ in a feedback fashion in an attempt to keep c constant at its setpoint c_s (more precisely, $c = c_s + d_c$, where d_c is the implementation error for c)

[3] It is not really necessary to introduce the loss function, and we may instead work directly with the actual cost J. However, the loss provides a better "absolute scale" on which to judge whether a given set of controlled variables c is "good enough", and thus is self-optimizing.

The open-loop policy is often poor; both because the optimal input $u_{\text{opt}}(d)$ depends strongly on the disturbance (so it is not a good policy to keep u_s constant), and because we are not able to implement u accurately (so the implementation error d_u is large).

The question we want to answer is therefore: *What is best choice for the N_u controlled variables c to use in the closed-loop policy?* If we allow for combinations of measurements, then there are infinitely many choices Note that the open-loop policy is included as the special case $c = u$.

We now present three approaches for selecting controlled variables. We first consider the error, $u - u_{\text{opt}}(d)$, and based on this propose four requirements of the controlled variable. We next consider a related method based on maxmizing the minimum singular value. We then consider a more exact stepwise procedure based on explicitly evaluating the loss.

5.2 Requirements for controlled variables

Consider an closed-loop implementation where we attempt to keep c constant at the value c_s. With this implementation the operation may be non-optimal (with a positive loss) due to the presence of a setpoint error and an implementation error.

1. The setpoint error, $e_{cs} = c_s - c_{\text{opt}}(d)$, is the difference between the setpoint and truly optimal value
2. The implementation error, $d_c = c - c_s$, is the difference between the actual value and the setpoint.

These two errors are generally independent; the setpoint error is caused by disturbances (changes in the operating point), whereas the implementation error is caused by measurement error and poor control. The overall error $e_c = c - c_{\text{opt}}(d)$ (which causes a positive loss), is then the sum of the two,

$$e_c = e_{cs} + d_c \tag{13}$$

Clearly, we want e_c to be small. In addition, we would like that a large value of e_c results in only a small value of the "base set" error e_u, that is, we want u to be insensitive to changes in c (or equivalently, we want c to be sensitive to changes in u).

From this, we can derive the following **four requirements for of a good candidate controlled c variable** (also see Skogestad and Postlethwaite (1996), page 404):

Requirement 1. Its optimal value is insensitive to disturbances (so that the setpoint error e_{cs} is small)

Requirement 2. It is easy to measure and control accurately (so that the implementation error d_c is small)

Requirement 3. Its value is sensitive to changes in the manipulated variables u, that is, the gain from u to y is large (so that even a large error in the controlled variable c results in only a small error in u).

Requirement 4. For cases with two or more controlled variables, the selected variables should not be closely correlated.

In short, we should select variables c for which the variation in optimal value and implementation error is small compared to their adjustable range (the range c may reach by varying u) (Skogestad and Postlethwaite (1996), page 408).

As a minor remark we mention that Morari *et al.* (1980) claim that "ideally one tries to select c in such a way such that some or all the elements in c are independent of the disturbances d." This statement is generally *not* true, because we need to be able to detect the disturbances through the variables c. A better requirement is that the *optimal* values of the elements in c are insensitive to disturbances d (requirement 1).

All four requirements should be satisfied. For example, assume we have a mixture of three components, and we have a measurement of the sum of the three mole fractions, $c = x_A + x_B + x_C$. This measurement is always 1 and thus independent of disturbances (so requirement 1 is satisfied), but it is of course not a suitable controlled variable because it is also insensitive to the manipulated variables u (so requirement 3 is not satisfied). Requirement 3 also eliminates variables that have an extremum (maximum or minimum) when the cost has its minimum, because the gain is zero for such variables.

5.3 Minimum singular value

For small variations we may use a linearized relationship between the (remaining) unconstrained degrees of freedom u and any candidate set of controlled variables c.

$$c = Gu \tag{14}$$

Note that any active constraints should be implemented (i.e. kept constant) before obtaining the steady-state gain matrix G. Let $\underline{\sigma}(G)$ denote the minimum singular value of G. If we assume that each controlled variable c has been scaled such that the sum of its optimal range and its implementation error is unity (i.e. $|e_c| = 1$) (this takes care of requirements 1 and 2), and that each "base variable" u has been scaled such that a unit change has the same effect on the cost function J, then we should prefer sets of controlled variable for which $\underline{\sigma}(G)$ is maximized (maximizing the gain takes care of requirement 3 and using the minimum singular value $\underline{\sigma}(G)$ takes care of requirement 4) This condition is derived in Skogestad and Postlethwaite (1996) (page 406). The minimum singular value can also be used as a tool for selecting manipulated inputs variables (Morari 1983), but this is actually an unrelated condition which requires a different scaling of the variables.

Let us briefly go through the derivation of Skogestad and Postlethwaite (1996). For a given disturbance d, a second order Taylor series expansion of the loss around the optimal value $u_{opt}(d)$ gives

$$\Delta L = J(u,d) - J(u_{opt},d) = \frac{1}{2}(u - u_{\text{opt}})^T \left(\frac{\partial^2 J}{\partial u^2}\right)_{\text{opt}} (u - u_{\text{opt}}) \tag{15}$$

(where we have assumed that the problem is unconstrained in u, so that the first-order term $\partial J/\partial u$ is zero.) Thus, the loss depends on the quantity $u - u_{opt}$ which we obviously want as small as possible. Now, for small deviations from the optimal operating point we have that the candidate output variables are related to the independent variables by $c - c_{opt} = G(u - u_{opt})$, or

$$u - u_{opt} = G^{-1}(c - c_{opt}) \tag{16}$$

Since we want $u - u_{opt}$ as small as possible, it therefore follows that we should select the set of controlled outputs c such that the product of G^{-1} and $c - c_{opt}$ is as small as possible. Thus, from Skogestad and Postlethwaite (1996) we have the following rule:

> *Assume we have scaled each variable c such that the expected variation in $c - c_{opt}$ is of magnitude 1 (including the effect of both disturbances and control error), then select the controlled variables c that minimize the norm of G^{-1}, which in terms of the two-norm is the same as maximizing the minimum singular value of G, $\underline{\sigma}(G)$.*

Interestingly, we note that this rule does not depend on the actual expression for the objective function J, but it does enter indirectly through the variation of c_{opt} with d, which enters into the scaling. Also note that in the multivariable case we should scale the inputs u such that the Hessian $\left(\frac{\partial^2 J}{\partial u^2}\right)$ is close to unitary; see Skogestad and Postlethwaite (1996) for details.

The above requirements or use of the minimum singular value may be very useful for identifying good candidate controlled variables. However, for a more exact evaluation one should use the procedure described next. It is based on evaluating the loss imposed by keeping the selected controlled variables constant.

5.4 Stepwise procedure for evaluating the loss

To compare alternative choices for the controlled variables c one may directly evaluate the cost J (or equivalently the loss L which yields more information) for the expected set of disturbances $d \in \mathcal{D}$, and expected set of implementation (control) errors $d_c \in \mathcal{D}_c$. Self-optimizing control is achieved if one with constant values of c (more precisely, $c = c_s + d_c$) obtains an acceptable value of the loss L.

This results in the following procedure for selecting controlled variables c:

Step 1: Degree of freedom analysis. Determine the number of degrees of freedom (N_u) available for optimization, and identify a set of base variables (u) for the degrees of freedom.

Step 2: Cost function and constraints. Define the optimal operation problem by formulating a scalar cost function J to be minimized for optimal operation, and specify the constraints that need to be satisfied.

Step 3: Identify the most important disturbances (uncertainty). These may be caused by

- Errors (uncertainty) in the assumed (nominal) model used in the optimization (including the effect of incorrect values for the nominal disturbances d^* used in the optimization)
- Disturbances ($d - d^*$) (including parameter changes) that occur after the optimization
- Implementation errors (d_c) for the controlled variables c (e.g. due to measurement error or poor control)

From this one defines the set of disturbances $\mathcal{D}$ and set of implementation errors $\mathcal{D}_c$ to be considered. Often it is a finite set of disturbance combinations, for example, consisting of the extreme values for the individual disturbances. In addition, one must determine how to evaluate the mean cost function J_{mean}. There are many possibilities, for example

1. Average cost for a finite set of disturbances (used in this paper)
2. Mean cost from *Monte-Carlo* evaluation of a distribution of d and d_c.
3. Worst-case loss

Step 4: Optimization.

1. First solve the nominal optimization problem, that is, find $u_{\text{opt}}(d^*)$. From this may one also obtain a table with the nominal optimal values for all other variables (including the candidate controlled variables).
2. In most cases (unless it involves too much effort) we then solve the optimization problem for the disturbances d in question (defined in step 3). This is needed to check whether there exists a feasible solution $u_{\text{opt}}(d)$ for all disturbances d, and to find the optimal cost $J_{\text{opt}} = J_u(u_{\text{opt}}, d)$ needed if we want to evaluate the loss. It may also be used in step 5 to identify candidate controlled variables.

Step 5: Identify candidate controlled variables. Typically, these are measured variables or simple combinations thereof. The four requirements presented earlier are useful in identifying good candidates. For example, based on the optimization in step 4, one may look for variables which optimal value is only weakly dependent of disturbances (requirement 1). The variable should also be easy to control and measure (requirement 2), and it should be sensitive to changes in the manipulated inputs (requirement 3). If there is more than one variable, then the selected variables in the set should be independent (requirement 4). Insight and experience, e.g. into what constitute the "dominant" process variables, may also be helpful at this stage, because the possible number of variables, and especially variable combinations, may be extremely large.

Step 6: Evaluation of loss. Compute the mean value of the loss for alternative sets of controlled variables c. This is done by evaluating the loss

$$L_u(u, d) = J_u(u, d) - J_{\text{opt}}(d); \quad u = f^{-1}(c_s + d_c, d) \tag{17}$$

with fixed setpoints c_s for the defined disturbances $d \in \mathcal{D}$ and implementation errors $d_c \in \mathcal{D}_c$. (We usually select the setpoints as the nominal optimal values, $c_s = c_{\text{opt}}(d^*)$, but it is also possible to let the value of c_s be subject to an optimization.)

Step 7: Further analysis and selection. Select for further consideration the sets of controlled variables with acceptable loss (and which thus yield self-optimizing control). These could then be analyzed to see if they are adequate with respect to other criteria that may be relevant, such like the region of feasibility and the expected dynamic control performance (input-output controllability)

5.5 Toy example

Consider a simple "toy example" with one degree of freedom u. The cost function to be minimized is $J_u = (u - d)^2$. We nominally have $d^* = 0$ and the expected disturbance magnitude is $|d| \leq 1$. For this problem we always have $J_{\text{opt}}(d) = 0$ corresponding to $u_{\text{opt}}(d) = d$. We consider three alternative choices for the controlled variable (measurements),

$$c_1 = 0.1(u - d); \quad c_2 = 20u; \quad c_3 = 10u - 5d$$

where the variables have been scaled such that $|d_{ci}| = |c_i - csi| \leq 1, i = 1, 2, 3$ (i.e. same implementation error for all three variables). Since $u_{\text{opt}}(d) = d$, the optimal value of three alternatives as a function of the disturbance are

$$c_{1,opt}(d) = 0; \quad c_{2,opt}(d) = 20d; \quad c_{3,opt} = 5d$$

Nominally $d^* = 0$ and $c_{i,opt}(d^*) = 0$, so we select in all three cases $c_{is} = 0, i = 1, 2, 3$.

Let us first evaluate how the three candidate variables meet the above requirements for controlled variables.

1. *Its optimal value is insensitive to disturbances.* From this point of view, the preferred controlled variable is c_1 (zero sensitivity), followed by c_3 (sensitivity 5) and c_2 (sensitivity 20).
2. *It is easy to control accurately.* There is no difference here since the implementation error d_c is the same for the three variables.
3. *Its value is sensitive to changes in u.* This favors c_2 (gain 20), followed by c_3 (gain 10), whereas variable c_1 (gain 0.1) is very poor in this respect.

In summary, it is not clear from these requirements which controlled variable is the best.

Let us next consider the minimum singular value rule. For the scalar case the minimum singular value is simply the absolute value of the gain G from u to c, so we prefer controlled variables for which the value of $|G|$ is large. We must first scale the variables properly. For c_1 the "unscaled" gain is 0.1, and the scaling factor is $|c_1 - c_{1,opt}| = 1 + 0 = 1$ (the control error is 1 plus the variation in $c_{1,opt}(d)$ due to disturbances which is 0), so the scaled gain is $G_1 = 0.1/|c_1 - c_{1,opt}| = 0.1/1 = 0.1$. Similarly, $G_2 = 20/|c_2 - c_{2,opt}| = 20/|1 + 20| = 0.95$, and $G_3 = 10/|c_3 - c_{3,opt}| = 10/|1 + 5| = 1.67$. Thus, the singular value rule says that c_3 is the best choice (largest gain), quite closely followed by c_2, whereas c_1 is the worst (smallest gain).

Let us finally evaluate the losses (the more exact method). For this simple example they can be evaluated analytically, and we find for the three alternatives

$$L_1 = (10d_{c1})^2; \quad L_2 = (0.05d_{c2} - d)^2; \quad L_3 = (0.1d_{c3} - 0.5d)^2$$

(For example, for c_3 we have $u = (c_3 + 5d)/10$ and with $c_3 = c_{3s} + d_{c3} = d_{c3}$ we get $J_u = (u - d)^2 = (0.1d_{c3} + 0.5d - d)^2$). With $|d| = 1$ and $|d_c| = 1$ the worst-case values of the losses are

$$L_1 = 100; \quad L_2 = 1.05^2 = 1.1025; \quad L_3 = 0.6^2 = 0.36$$

In accordance with the singular value rule, we find that *output c_3 is the best overall choice for self-optimizing control* (with the smallest loss), and c_1 is the worst. Note that with no implementation error ($d_c = 0$) c_1 would be the best, and with no disturbance ($d = 0$) c_2 would be the best.

6 Reactor example

We here illustrate the stepwise procedure for selecting controlled variables with a simple example that can easily be reproduced by the reader. Consider a continuously stirred tank reactor (CSTR) where two irreversible first-order reactions take place

$$A \to B; \quad r_A = k_A x_A \quad [\mathrm{s}^{-1}]$$

$$B \to C; \quad r_B = k_B x_B \quad [\mathrm{s}^{-1}]$$

Component B is the desired product and its concentration as a function of the residence time has a peak value, at which we want to operate the reactor.

Model. Let z_i and x_i denote mole fractions of component i in the feed and reactor, respectively, and let F [mol/s] be the feed rate and M [mol] the reactor holdup. There are only three components, A, B and C, and steady-state material balances yield

$$z_A F - x_A F - k_A x_A M = 0$$

$$z_B F - x_B F + k_A x_A M - k_B x_B M = 0$$

$$x_C = 1 - x_A - x_B$$

The feed contains only components A and C, i.e. $z_C = 1 - z_A$. We consider the following nominal data:

$$z_A = 0.8;\ k_A = 1s^{-1};\ k_B = 1s^{-1};\ F = 1\mathrm{mol/s}$$

Step 1: Degree of freedom analysis

With a given feed rate and feed composition the reactor has one degree of freedom at steady-state, which may be selected as the reactor holdup, i.e

$$u = M \quad [\mathrm{mol}]$$

The value of M should be adjusted to optimize the operation.

Step 2: Cost function and constraints

In this example component B is the desired product and the objective is to maximize the concentration of B, i.e. we choose the cost function

$$J = -100 \cdot x_B$$

(in most cases we would recycle unreacted A, but this is not the case in this example). We would like to find a controlled variable which results in a mean loss of less than 0.5 when there are disturbances.

There are no extra constraints, except for physical constraints such as $0 \leq M < \infty$.

Step 3: Disturbances

We will consider the following disturbances (errors):

- d_1: Feed rate reduced by 30%
- d_2: Feed fraction of A reduced from 0.8 to 0.6
- d_3: Feed fraction of A increased from 0.8 to 10.0
- d_4: Rate constant k_A increased by 50%
- d_5: Rate constant k_B increased by 50%
- d_c: Implementation error for the controlled variable, e.g., due to measurement error: see step 5.

The mean loss is here chosen as the average of the loss resulting from each of these six disturbances (one at a time).

Step 4: Optimization

For many reactors it is optimal to operate with maximum holdup M, for example, this would be the case if the objective were to maximize the production or concentration of component C. However, in our case we want to maximize the concentration of intermediate product B which goes through a maximum as we increase the holdup M (see Figure 6 which shows the cost function $J = -100x_B$ as a function of M).

From the above model, we find that the optimal holdup and corresponding optimal compositions in the nominal case are:

$$\text{Nominal optimum :} \quad M = 1.0\text{mol}; \quad x_A = 0.4, x_B = 0.2, x_C = 0.4$$

corresponding to $J = -100x_B = -20$. When there are disturbances, the optimal values change as given in Table 1.

Step 5: Candidate controlled variables

As mentioned, the reactor has one steady-state degree of freedom during operation. How should this degree of freedom be set, i.e., which variable should be kept constant? The following candidates for the controlled variable c are suggested

- $c_1 = M$ (holdup)
- $c_2 = M/F$ (residence time)
- $c_3 = x_A$
- $c_4 = x_B$
- $c_5 = x_C$
- $c_6 = x_B/x_A$
- $c_7 = \theta_1 = x_A + 2x_B + 3x_C$ (a property variable)
- $c_8 = \theta_2 = x_A + 3x_B + 2x_C$ (a property variable)

Alternatives 1 and 2 are open-loop policies (with feedforward action from F for c_2), whereas the other are feedback policies. These are essentially the available measurements in the reactor. The property variables in alternatives 7 and 8 may represent a boiling temperature, a viscosity, a refraction index or similar. We select the setpoint for each variable as its nominally optimal value.

We need to identify the implementation error d_c for each of the candidate controlled variables. Assuming that the implementation error is mainly to due to measurement errors and that the measurement error is 10% for M and F, and 5% for the mole fractions, we use the following values for d_c:

- M: 10%
- M/F: 20%
- x_A, x_B and x_C: 5%
- x_A/x_B: 10%
- θ_1 and θ_2: 0.1 unit (about 5%)

Which controlled variable is preferred? It seems clear that it will be better to keep M/F rather than M constant, because the optimal residence time M/F is independent of the feed rate, whereas the optimal value of the holdup M clearly depends on the feed rate. It is also rather obvious that a policy based on keeping x_B constant is most likely to fail, because x_B goes through a maximum as we increase M, and if we specify a value of x_B above this maximum, then operation is infeasible. However, otherwise it is not at all clear, even in this simple case, what the best choice of the controlled variable is.

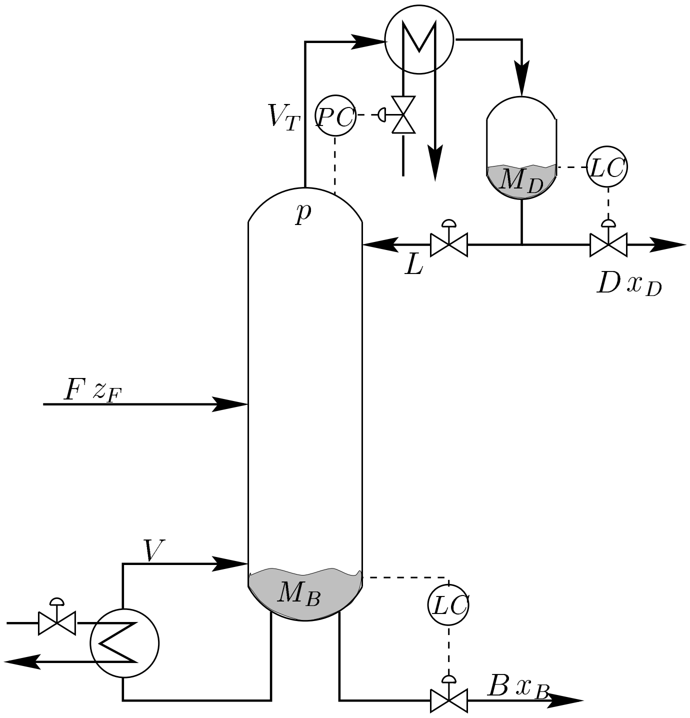


Figure 5: Typical distillation column controlled with the LV-configuration

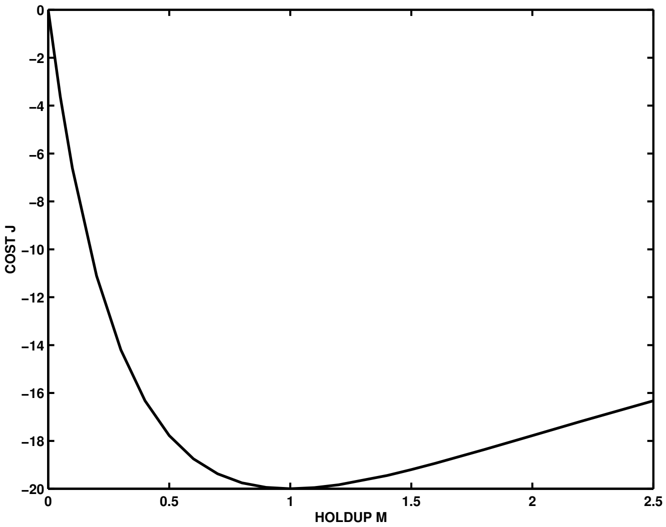


Figure 6: Reactor case study: Cost function J as a function of holdup M

Step 6: Evaluation of loss

To compare the alternatives, we compute the loss $L = J - J_{\text{opt}}$ with each of the candidate variables kept constant at its nominal optimal value. The results are given in Table 2 for the 8 candidate variables and the 6 disturbances. Disturbance d_c represents the implementation error and the loss in this case is evaluated with $c = c_s + d_c$. For example, for $c_2 = M/F$ we have $c_{2s} = 1.0$ and $d_c = 0.2 \cdot 1.0 = 0.2$ (20% error) and fixing $M/F = 1.0 + 0.2 = 1.2$ (rather than the optimal value of 1.0) results in a loss of 0.17 (see Table 2).

We see from Table 2 that the loss is quite small (to the acceptable value of 0.5) in most cases, but in some cases there is no feasible solution (marked as inf. in the table). As expected, this is the case if we specify $x_B = 0.2$ as this is higher than the maximum achievable. But note that infeasibility may occur for most choices of controlled variables if the disturbance is sufficiently large. For example, if we specify $x_A = 0.4$ then we would obviously get infeasibility when $z_A < 0.4$. Note that there is usually no "warning", in terms of a large value of the loss, as we approach infeasibility.

For this specific example, the implementation error turns out to be less important. However, in many cases it may be a critical factor which eliminates otherwise good candidate controlled variables.

Step 7: Selection of controlled variable

Most engineers would probably attempt to control some composition if such measurements were available, and indeed we find that keeping the variable $c_6 = x_B/x_A$ at 0.5 is the ideal choice when there are disturbances in z_A (see Table 1). However, keeping $x_B/x_A = 0.5$ results in rather large losses when there are disturbances in the rate constants, resulting in an average loss of 0.74 (larger than our desired value of 0.5). Keeping $x_A = 0.40$ gives a large loss when z_A changes, but the loss is smaller for other disturbances, so the average loss is 0.52 (just above the acceptable). As expected, keeping $x_B = 0.2$ results in infeasibility in some cases, and also keeping $x_C = 0.4$ results in infeasibility when z_A is too low. Keeping θ_1 constant gives a large loss when there is a disturbance in z_A, whereas θ_2 is somewhat sensitive to implementation errors. In summary, from Table 2 we see that none of the composition measurements ($x_A, x_B, x_C, x_B/x_A$) or property measurements (θ_1, θ_2) result in an acceptable average loss of 0.5 or less.

Somewhat surprisingly, the "open-loop" policy where we keep the holdup $M = 1.0$ results in very small losses for all disturbances, except when there is a disturbance in the feed rate F where the loss is 0.6. The sensitivity to feed rate disturbances is eliminated if we include "feedforward" action from the feed rate F and instead keep the residence time M/F constant, but there is a penalty in terms of a larger implementation error. In conclusion, the simplest and best strategy for the example is to keep constant the holdup M (average loss 0.18) or the residence time M/F (average loss 0.10).

Of course, also other considerations, such as the cost of instrumentation and controllability (dynamic performance) should be considered when making the final choice. Fortunately, the "open-loop" policy of keeping $c_1 = M$ constant is good in this respect, as it involves only a simple level control system with no expected control problems besides the implementation (measurement) error which was already included in the analysis.

Another case: No C in feed

Above we assumed that the feed contained components A and C, but consider next a different case where the feed contains component B rather than component C. Otherwise all the data is the same. Variable x_A here replaces x_B/x_A as the ideal variable with respect to disturbances in z_A (this can be proven analytically), and keeping x_A constant also yields small losses when there are other disturbances. Therefore, in this case the loss is smallest (0.18) when x_A is constant; it is 0.20 with θ_1 constant; 0.32 with x_C constant; 0.81 with M/F constant; 0.89 with M constant; 1.09 with θ_2 constant; whereas keeping x_B constant or x_B/x_A constant results in infeasibility (Skogestad *et al.* 1999). Thus we find, somewhat surprisingly, that the ranking is almost reversed compared to that found with C in the feed.

Disturbance	J	M	$\frac{M}{F}$	x_A	x_B	x_C	$\frac{x_B}{x_A}$	θ_1	θ_2
Nominal	-20.00	1.00	1.00	0.40	0.20	0.40	0.50	2.00	1.80
$d_1 : F = 0.7$	-20.00	0.70	1.00	0.40	0.20	0.40	0.50	2.00	1.80
$d_2 : z_A = 0.6$	-15.00	1.00	1.00	0.30	0.15	0.55	0.50	2.25	1.85
$d_3 : z_A = 1.0$	-25.00	1.00	1.00	0.50	0.25	0.25	0.50	1.75	1.75
$d_4 : k_A = 1.5$	-24.24	0.82	0.82	0.36	0.24	0.40	0.67	2.04	1.88
$d_5 : k_B = 1.5$	-16.16	0.82	0.82	0.44	0.16	0.40	0.37	1.96	1.72

Table 1: Optimal values for reactor case study

Disturbance	Loss with $M = 1.0$	Loss with $\frac{M}{F} = 1.0$	Loss with $x_A = 0.4$	Loss with $x_B = 0.2$	Loss with $x_C = 0.4$	Loss with $\frac{x_B}{x_A} = 0.5$	Loss with $\theta_1 = 2.0$	Loss with $\theta_2 = 1.80$
Nominal	0	0	0	0	0	0	0	0
$d_1 : F = 0.7$	0.62	0	0	0	0	0	0	0
$d_2 : z_A = 0.6$	0.00	0.00	1.67	inf.	15.0*	0	3.35	0.36
$d_3 : z_A = 1.0$	0.00	0.00	1.00	5.00	1.75	0	1.39	0.28
$d_4 : k_A = 1.5$	0.24	0.24	0.24	4.24	0	1.39	0.06	0.82
$d_5 : k_B = 1.5$	0.16	0.16	0.16	inf.	0	2.83	0.04	0.72
d_c : impl. error	0.05	0.17	0.05	inf.	0.05	0.20	0.29	1.72
Average loss	0.18	0.10	0.52	inf.	2.80*	0.74	0.86	0.65
Ranking	2	1	3	8	7	5	6	4

inf. denotes infeasible operation

* At the limit to infeasibility ($M/F = 0$) for z_A=0.6.

Impl.error: $M = 1.1, M/F = 1.2, x_A = 0.42, x_B = 0.21, x_C = 0.42, x_B/x_A = 0.55, \theta_1 = 2.1, \theta_2 = 1.9$

Table 2: Loss for reactor case study

Conclusion

We have considered alternative controlled variables for a reactor case study. In one case (with C in feed) the residence time was the best controlled variable, whereas in another case (no C in feed) the concentration of component A was the best choice. It is not easy to explain physically why the particular variables are preferred in the two cases. This shows that it may be difficult to rely on physical insight, e.g. about "dominant" variables, when selecting controlled variables. Instead, one should evaluate the (economic) performance of the plant, to see which choice of controlled variable keeps the operation closest to the optimal when there are disturbances.

7 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 is "column D" of Skogestad and Morari (1988) and represents a propylene-propane splitter where propylene (light component) is taken overhead as a final product with at least 99.5% purity ($x_D \geq 0.95$), whereas unreacted propane (heavy component) is recycled to the reactor for reprocessing. We assume there is no capacity limit in the column. (We will later study separately the case where $V \leq V_{max} = 10$ kmol/min and the implications this has on the operation of the column.)

Step 1: Degree of freedom analysis

As mentioned in the introductory example, for a given feed rate the column has two operational 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 introduces prices for all streams entering and exiting the column and consider the following profit function P which should be maximized (i.e. $J = -P$)

$$P = p_D D + p_B B - p_F F - p_V V \tag{18}$$

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 unneccessary reprocessing of light component reduces the overall capacity of the plant; this dependency is not really important but it it realistic).

We assume that the nominal feed rate is given at $F = 1$ kmol/min (alternatively, we could introduce the constraint $F \leq F_{max} = 1$ kmol/min, but it is optimal to have $F = F_{max}$ in this case). With $F = 1$

[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_c: 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 will consider implementation errors for the other selected controlled variable (see below).

Step 4: Optimization

In Table 3 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 ($x_D = 0.996$). In addition, we have considered the effect of a higher price for the distillate product ($p_D = 30$) and a five times higher energy price ($p_V = 0.5$).

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 columns has no capacity constraints, and the efficiency is assumed independent of the column load.

Step 5: Candidate controlled variables

It is clear that one of the controlled variables should be the distillate composition, x_D. This follows since the optimal solution is always obtained when the product purity specification for the most expensive product is "active", i.e. in our case when $x_D = 0.995$. We are then left with one "unconstrained" degree of freedom which we want to specify by keeping a controlled variable at a constant value.

From Table 3 we see that, except in the last case with a much higher energy price, the optimal bottom composition stays fairly constant around $x_B = 0.04$. This indicates that a good strategy for implementation may be to control x_B at a constant value of 0.04. However, there 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 alternative controlled variables are considered (in addition to x_D which should always be kept constant at its lower limit of 0.995):

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

We consider implementation errors of about 20% in all variables, including x_D. From Table 3 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 of from physical insight which variable to prefer. We will therefore evaluate the loss.

Step 6: Evaluation of loss

In Table 4 we show for $F = 1$ [lmol/min] the loss $L = P_{\rm opt} - P$ [$/min] when each of the six candidate controlled variables are kept constant at their nominally optimal values. Recall that we would like the loss to be less than 0.04 [$/min] for each disturbance. We have the following comments to the results given in Table 4:

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. However, use of L/F or V/F as controlled variables is 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.
10. We have not computed the effect of changes in prices in Table 4, because these do not effect column behavior, so all alternatives behave the same (with the same loss). Thus, if there are price changes, then one must recompute new optimal values for the variables.

Step 7: Selection of controlled variables

From Table 4 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 used[4] to keep $x_D = 0.995$.
- $L/F = 15.07$ is kept constant.

Alternative control system.

- L is used to keep $x_D = 0.995$.
- $V/F = 15.70$ is kept constant.

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

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

Disturbance	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	0.637	15.594	16.232	24.47	4.443
$p_D = 30$	0.995	0.035	0.641	15.714	16.355	24.51	
$p_V = 0.5$	0.995	0.138	0.597	11.026	11.623	18.47	

Nominal values: $F = 1, z_F = 0.65, q_F = 1.0, p_D = 20, p_V = 0.1$

Table 3: Optimal operating point (with maximum profit P/F) for distillation case study

Disturbance	$x_B = 0.04$	$D/F = 0.639$	$L = 15.065$	$L/F = 15.065$	$V/F = 15.704$	$L/D = 23.57$
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: $x_B = 0.048, D/F = 0.766, L = 18.08, L/F = 18.08, V/F = 18.85, L/D = 28.28$

Uacceptable loss (larger than 0.04) shown in bold face

Table 4: Loss [$/min] for distillation case study.

Another case: Column with capacity limitations

Above we assumed that the feed rate was given and that the column had no capacity limit. However, all columns have a capacity limit, and this will obviously affect its operation. To understand this better, consider a column with the additional capacity constraint on the vapor flow (boilup),

$$V \leq V_{max} = 10 \quad [kmol/min]$$

We also assume that the feed rate F to the column is not "given" but rather "available". This situation may be handled by introducing the constraint

$$F \leq F_{max}$$

where we will treat the available feed rate F_{max} as a parameter. Otherwise, the specifications and cost data are as above. For this problem we then have three steady-state degrees of freedom (e.g., F, V and D) and three constraints (on F, V and x_D). The constraint on x_D is always active, whereas we find that the effect of the other two constraints depends on the value of F_{max}.

Let us first recall the case studied above with no capacity limitations, for which we found $(V/F)_{\text{opt}} = 15.70$ (nominally) corresponding to $x_B = 0.04$. With $V_{max} = 10$ this operation is optimal for $F \leq V_{max}/(V/F)_{\text{opt}} = 10/15.70 = 0.637$ [kmol/min]. Is this the largest feed rate we should accept? No, some more careful thinking reveals that if we have reached $V = V_{max}$, and are free to decide on the feed rate, then we should try to optimize P/V (instead of P/F as done above). With the given column data, we find that $(P/V)_{\text{opt}} = 0.331$ [\$/kmol] is obtained when $x_B = 0.09$, $V/F = 12.77$ and $L/F = 12.15$. Thus, with $V_{max} = 10$ [kmol/min], the optimal profit is obtained with a feed rate of $F_{\text{opt}} = 10/12.77 = 0.783$ [kmol/min], which is then the largest feed rate we should accept.

Let us try to explain this in words. The distillate is the most valuable product, so to maximize its flow we want to have it as "unpure" as possible (this also saves energy), i.e. we keep its purity at the minimum specification ($x_D = 0.995$ in our case). To maximize the distillate flow we also want to avoid putting light component into the bottom product, so we want the bottom product as "pure" as possible. However, this costs energy (V), and we have that the optimum trade-off in our case is obtained for x_B about 0.04. This applies as long as there are no capacity limitations within the column, but if the vapor flow V exceeds its maximum value, then we are forced to put more light component (i.e. a larger fraction of the feed) into the bottom product. For cases where the bottom product is worth less than the feed (as in our case), we will eventually loose money by forcing more feed through the column and the column becomes a real bottle-neck for the overall plant (this occurs for $x_B = 0.09$ in our case),

In summary, when we introduce the constraint $V_{max} = 10$ [kmol/min] and include the feed rate F as a degree of freedom, we have the following three cases depending on the available feed rate F_{max}:

1. **Low available feed rates**; $F_{max} \leq 0.637$ [kmol/min]). This is the case we studied above where it is optimal to operate the column below its vapor capacity limit and to keep $F = F_{max}$. Thus, the optimal solution is unconstrained in one variable, and the nominally optimal value of x_B is 0.04.

   Proposed control system.

   - L is used to keep $x_D = 0.995$ (active constraint).
   - V is adjusted to keep $V/F = 15.70$ constant
   - F is kept at its maximum available value F_{max} (active constraint).

   This is the "alternative control system" proposed above, but is chosen here because we can use the same composition controller as for cases 2 and 3 (below).

2. **Intermediate available feed rates**; $0.637 < F_{max} < 0.783$ [kmol/min]. It is optimal to operate at maximum vapor capacity $V = V_{max} = 10$ [kmol/min], and to process as much feed as possible, i.e. $F = F_{max}$. With $x_D = 0.995$ there are then no remaining degrees of freedom (i.e. all degrees of freedom are consumed for "active constraint control"). As F_{max} is increased from 0.637 to 0.783, the optimal value x_B of increases from 0.04 and 0.09.

   Proposed control system.

- L is used to keep $x_D = 0.995$ (active constraint).
- V is kept at $V_{max} = 10$ (active constraint).
- F is kept at its maximum available value F_{max} (active constraint).

3. **Large available feed rates**; $F_{max} > 0.783$ [kmol/min]). It is optimal to operate the column at maximum vapor capacity $V = V_{max} = 10$ [kmol/min], and to maintain acceptable bottom purity we should *not* process all the available feed, i.e. it is optimal keep keep $F = 0.783 < F_{max}$ (the nominally optimal value of x_B is 0.09 in this case). In this case the column is a bottleneck for the overall plant throughput.

   Proposed control system.

   - L is used to keep $x_D = 0.995$ (active constraint).
   - V is kept at $V_{max} = 10$ (active constraint).
   - F is adjusted to keep $V/F = 12.77$ constant (alternatively, we may keep $F = 0.783$ constant, but using V/F is better if the value of V_{max} changes)

The three above cases for the available feed rate can easily be implemented in a single control system using simple logic.

In summary, the distillation case study shows the importance of selecting the right controlled variables when implementing the optimal solution, and how the column may limit the maximum throughput of the plant. The analysis was mostly based on economic considerations (loss), but the bottom composition x_B was excluded as a controlled variable based on other considerations, namely the cost of measurement and controllability.

We note that the implementation error was not important in this case study, but we stress that it should be included in the analysis. For example, the implementation error is the main reason why we rarely select temperatures near the column ends as controlled variables (because the measurement error is too large compared to its sensitivity).

8 Discussion

8.1 Region of feasibility

In this paper we have evaluated the (economic) *loss* for disturbances of a given magnitude. Another important issue to consider is the region of feasibility (stability) (Zheng *et al.* 1999). We could evaluate *feasibility loss*, defined as the difference between the disturbance region where feasible operation is possible (using the optimal u) and the disturbance region we can handle with constant values of c, to be as small as possible.

For example, consider a case where there is an inequality constraint on an input variable which optimally is active only under certain conditions (disturbances), but this constrained input variable is *not* included as a controlled variable. Here one must be careful to avoid infeasibility during implementation, for example, there may be a disturbance such that the specified value of the controlled variable can only be achieved with a nonphysical value of the input (e.g. a negative flowrate).

The on-line optimization is usually for simplicity based on the nominal disturbance (d^*), and two approaches to avoid infeasibility in such a case are to

1. use "back-offs" for the setpoints during implementation (Narraway *et al.* 1991), or
2. add "safety margins" to the constraints during the (nominal) optimization

One approach for obtaining the values for the back-offs or safety margins may be to solve a "robust optimization problem" (Glemmestad 1997)) where one considers all possible disturbances. There is clearly a need for more research in this area.

A third, and better approach in terms of minimizing the loss, is to track the active constraint. In particular, model predictive control is very well suited and much used for tracking active constraints.

However, even if we track active constaints, we still need to select the unconstrained controlled variables, so the analysis presented in this paper is still needed.

8.2 Additional examples

Additional example for selecting controlled variables are available in a number of publications and Ph.D. theses, e.g.

- Ph.D. thesis of Morud (1995), chapter 8: CSTR with chemical reaction
- Glemmestad *et al.* (1999) and Ph.D. thesis of Glemmestad (1997): Application to heat exchanger networks; special emphasis on feasibility issues.
- Ph.D. thesis of Havre (1998): Application to selection of temperature location in distillation.
- Halvorsen and Skogestad (1998) and Halvorsen and Skogestad (1999): Application to integrated Petlyuk distillation columns.

The Petlyuk distillation example is particularly interesting because in this case the choice of controlled variables makes a big difference (whereas the differences for the rather simple examples presented in this paper admittedly were quite small).

9 Conclusion

The focus in this paper has not been on finding the optimal operation policy, but rather on how to *implement* it in a simple manner in the control system. The idea is to find a set of controlled variables c which, when kept at constant setpoints, indirectly lead to near-optimal operation (with acceptable loss). This is denoted "self-optimizing" control.

To assist in selecting good candidate variables one should look for variables that satisfy the following requirements:

Requirement 1. Its optimal value is insensitive to disturbances

Requirement 2. It is easy to measure and control accurately

Requirement 3. Its value is sensitive to changes in the manipulated variables

Requirement 4. For cases with two or more controlled variables, the selected variables should not be too closely correlated.

In addition, we have presented a systematic procedure for selecting controlled variables based on evaluating the loss $J - J_{\rm opt}$ for possible disturbances. The procedure requires a steady-state process model and a clear definition of the cost function J to be minimized during operation (obviously, without such a cost function one cannot judge what operation is the best). The procedure was applied to three example; to a simple "toy" example, to a somewhat academic CSTR example, and finally to a more realistic distillation column example.

One problem is that in general it not is clear offhand if a self-optimizing structure exists, and going through the various alternatives, for example using the given procedure, can be quite tedious. On the other hand, since the issue of finding good controlled variables is a *structural* problem, then we often find that a good structure obtained for a particular case, also works well on another similar process case with different parameter values. Thus, if we can actually find a self-optimizing structure for a process, then it is almost like an invention (and may pobably even be patented).

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