Self-optimizing control of a large-scale plant:
The Tennessee Eastman process

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September 7, 2001

Submitted to Ind.Eng.Chem.Res
Revision June 2001

Abstract

The paper addresses the selection of controlled variables, that is, "what should we control". The concept of self-optimizing control provides a systematic tool for this, and in the paper we show how it may be applied to the Tennessee Eastman process which has a very large number of candidate variables. In the paper we present a systematic procedure for reducing the number of alternatives. One step is to eliminate variables which with constant setpoints result in large losses or infeasibility when there are disturbances (with the remaining degrees of freedom reoptimized).

The following controlled variables are recommended for this process:

- Optimally constrained variables: Reactor level (minimum), reactor pressure (maximum), compressor recycle valve (closed), stripper steam valve (closed) and agitator speed (maximum).
- Unconstrained variables with good self-optimizing properties: 1) Reactor temperature, 2) composition of C in purge and 3) recycle flow or compressor work.

The feasibility of this choice is confirmed by simulations. A common suggestion is to control the composition of inerts. However, this seems to be a poor choice for this process because disturbances or implementation error may give infeasibility.

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1 Introduction

This paper addresses the selection of controlled variables for the Tenessee Eastman process. However, the main objective of the paper is to demonstrate how to select controlled variables for a large-scale process, so the paper should be of interest also for readers without a prior knowledge or interest in the Tenessee Eastman process.

We base the selection on the concept of self-optimizing control using steady state models and steady state economics. "Self-optimizing control" is when an acceptable (economic) loss can be achieved using constant setpoints for the controlled variables, without the need to reoptimize when disturbances occur (Morari *et al.* 1980) (Skogestad and Postlethwaite 1996) (Skogestad 2000*a*). The constant setpoint policy is simple, but it will not be optimal (and thus have a positive loss) due to the following two factors:

1. Disturbances, i.e. changes in (independent) variables and parameters which cause the optimal setpoints to change.
2. Implementation errors, i.e. differences between the setpoints and actual values of the controlled variables (e.g. due to measurement errors or poor control) (Skogestad 2000*a*).

The effect of these factors (the loss) depends on the choice of controlled variables, and the objective is to find a set of controlled variables for which the loss is acceptable.

Downs and Vogel (1993) introduced the Tennessee Eastman challenge problem at an AIChE meeting in 1990. The purpose was to supply the academic community with a problem that contained many of the challenges that people in industry meet. The process has eight components, including four reactants (A, C, D and E), two products (G and H), an inert (B) and a byproduct (F). The reactions are

$$\begin{array}{rcll} \mathrm{A(g) + C(g) + D(g)} & \rightarrow & \mathrm{G(liq)} & \text{(Product)} \\ \mathrm{A(g) + C(g) + E(g)} & \rightarrow & \mathrm{H(liq)} & \text{(Product)} \\ \mathrm{A(g) + E(g)} & \rightarrow & \mathrm{F(liq)} & \text{(Byproduct)} \\ \mathrm{3D(g)} & \rightarrow & \mathrm{2F(liq)} & \text{(Byproduct)} \end{array}$$

The process has four feed streams (A, D, E and C feeds), one product stream and one purge stream. Almost all of the inert (B) enters in the largest C feed which actually contains almost 50% of component A. The process has five major units; a reactor, a product condenser, a vapor-liquid separator, a recycle compressor and a product stripper, see Figure 1. There are 41 measurements and 12 manipulated variables. Detailed data are given in Downs and Vogel (1993). We have based our simulation on the model avaiable at the home page of Ricker (1999). We here study the optimal operation of the base case (mode 1) with a given 50/50 product ratio between components G and H, and a given production rate.

This plant has been studied by many authors, and it has been important for the development of plantwide control as a field. Many authors has used it to demonstrate their procedure for the design of a control system. We here consider the selection of controlled variables.

McAvoy and Ye (1994) proposed to control reactor temperature, reactor pressure, recycle flow rate, compressor work, concentration of B (inert) in purge, and concentration of E in product flow. Ricker and Lee (1995) tested this strategy, finding that the compressor power loop often saturated during transients.

Lyman and Georgakis (1995) recommended a control structure where the following variables are controlled: Reactor temperature, reactor level, recycle flow rate, agitation rate, composition of A, D and E in reactor feed, composition of B (inert) in purge and composition of E in product. Even though they consider the operation cost for the control structure, their structure is not economically optimal since some variables that should be kept at their constraints (like the compressor recycle valve) are used as manipulated variables.

Ricker (1995) considered the steady-state optimal operation of the plant. In all cases, he found that it is optimal to have maximum reactor pressure, minimum reactor level, maximum agitator speed, and minimum steam valve opening. Furthermore, in most cases it is optimal to use minimum compressor recycle valve opening. Ricker (1995) notes that the controlled variables "must be carefully chosen; arbitrary use of feedback control loops should be avoided".

Figure 1: Tennessee Eastman process flowsheet

Ricker and Lee (1995) used nonlinear model predictive control (NMPC), and compared with the multiloop (decentralized) strategy of McAvoy and Ye (1994) which they find performs adequately for many scenarios, but they suggest that compressor power should not be controlled. For these simpler cases the NMPC strategy improves performance, but the difference seems too small to justify the NMPC design effort. On the other hand, for the more difficult cases, the decentralized approach would require multiple overrides to handle all conditions, and nonlinear model predictive control may be preferred.

In another study, Ricker (1996) considered decentralized control and concludes that there is little, if any, advantage to the use of NMPC on this application. His approach is similar to the one in this paper. First, he chooses to control the variables which optimally should be at their constraints ("active constraint control"). Second, he excludes variables for which the economic optimal value varies a lot. He ends up controlling compressor recycle valve position (at minimum), steam valve position (at minimum), reactor level (at minimum), reactor temperature, composition of C in reactor feed, and composition of A in reactor feed. He notes that it is important to determine appropriate setpoint values for the latter three unconstrained variables.

Luyben *et al.* (1997) set the agitation rate and the recycle valve at their constraints, and choose to control the reactor pressure, reactor level, separator temperature, stripper temperature, ratio between E and D feedrates, A in purge, and B (inert) in purge.

Tyreus (1999) uses a thermodynamic approach to select controlled variables. This can provide useful guideliness, but can not in general provide the optimal solution since thermodynamics is independent of cost data. He sets the agitation on full speed, closes the steam valve and the compressor recycle valve, and chooses to control reactor temperature, reactor pressure, reactor level and A in reactor feed and B (inert) in purge flow.

To summarize, most authors do not control all the variables that are constrained at the optimum and therefore do not operate optimally in the nominal case. Most control reactor pressure, reactor level, reactor temperature and composition of B (inert). It is common to control stripper temperature, separator temperature, and composition of C and/or A in reactor feed.

The main objective of this paper is to search systematically for a set of controlled variables, if such a set exists, which results in self-optimizing control for the Tennessee Eastman process. In particular, the issue is to find a good choice for the three unconstrained variables.

2 Self-optimizing control

We here give an introduction to self-optimizing control, and refer to the paper of Skogestad (2000*a*) for more details including a discussion of the related literature (two more recent references not included in Skogestad (2000*a*) are Stephanopoulos and Ng (2000) and Larsson and Skogestad (2000)).

Many people do realize that the selection of controlled variables is actually an issue. But ask the question:

> ”Why are we controlling hundreds of temperatures, pressures and compositions in a chemical plant, when there is no specification on most of these variables? Is it just because we can measure them or is there some deeper reason?”

The main basis for control is that the plant has many degrees of freedom that need to be specified during operation, and the “deeper” reason for selecting a particular set of controlled variables is that it provides “self-optimization” when there are disturbances or other changes in the operating point.

The basic idea of self-optimizing control was formulated about twenty years ago by Morari *et al.* (1980) who 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.” The ideas of Morari *et al.* (1980) were further developed by Skogestad (2000*a*) (a somewhat condensed conference version is presented in Skogestad (2000*b*)), who also considered the implementation error and studied several problem cases with an unconstrained optimum. Self-optimizing control is defined as follows:

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

To quantify the loss we must define a a scalar economic cost function J, for example, of the form

$$J(u, d) = \int_0^T \phi(u, d)dt \tag{1}$$

where the independent variables include the degrees of freedom u and the disturbances d. The cost J should be minimized with respect to u subject to satisfying given constraints, including

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

We here assume that the optimization problem is feasible, that is, the constraints are not in conflict such that a solution exists (otherwise, the problem needs to be reformulated). In theory, all the various objectives for plant operation should be included in the cost J and minimizing it should then result in the optimal trade-off between these generally conflicting objectives. In this paper we assume that the economic performance is primarily determined by steady-state considerations and the integration in (1) may be replaced by time-averaging over the various steady-states. The effect of the dynamic control performance can be partly included in the economic analysis by introducing a control error term as part of the implementation error.

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. The term "self-optimizing control" is used when satisfactory economic operation can be achieved with the use of constant setpoints for the controlled variables, that is, without the need for reoptimization when there are disturbances.

To quantify this more precicely, we define the (economic) *loss* L as the difference between the actual value of the cost function and the truly optimal value, i.e.

$$L = J(u, d) - J_{\text{opt}}(d)$$

Truly optimal operation corresponds to $L = 0$, but in general $L > 0$. A small value of the loss function L is desired as it implies that the plant is operating close to its optimum. Self-optimizing control is achieved if an constant setpoint policy results in an acceptable loss L (without the need to reoptimize when disturbances occur). The main issue here is *not* to find the optimal setpoints, but rather to find the right variables to keep constant. The precice value of what is an "acceptable" loss must be selected based on engineering and economic considerations.

The idea of self-optimizing control is illustrated in Figure 2. We see that a loss results when we keep a constant setpoint rather than reoptimizing when a disturbance occurs. For the case in Figure 2 it is better to keep the setpoint c_{1s} constant than to keep c_{2s} constant.

An additional concern with the constant setpoint strategy, is that there is always a difference between the setpoint c_s and the actual value c due to implementation errors caused by measurement errors and imperfect control. To minimize the effect of the errors on the operating cost, the cost surface as a function of c should be as flat as possible. This is illustrated in Figure 3, where we distinguished between three cases when it comes to the actual implementation:

(a) *Constrained optimum.* In this case the optimal cost is achieved when one of the variables is at its maximum or minimum (the figure shows the case when the optimum is obtained for $c = c_{min}$). In this case there is no loss imposed by keeping the variable constant at its "active" constraint. Implementation of an active constraint is usually easy, e.g., it is easy to keep a valve fully open or closed.

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

(c) *Unconstrained sharp optimum.* In this case the cost (operation) is sensitive to the actual value of the controlled variable c and self-optimizing control is not possible. In this case, we would like to find another controlled variable c in which the optimum is flatter.

Thus, the constrained case is easy, because here we select as controlled variables the optimally constrained variables. However, it it not at all clear which variables to select in the *unconstrained case*. Skogestad (2000*a*) recommends that a controlled variable c suitable for constant setpoint control (self-optimizing control) should have the following properties:

Requirement 1. The optimal value of c should be insensitive to disturbances, i.e. $c_{\text{opt}}(d)$ depends only weakly on d.

Requirement 2. The value of c should be sensitive to changes in the manipulated variable u, i.e. the gain $G = \partial y/\partial u$ should be large (equivalently, since $\partial J^2/\partial^2 c = G^{-T} \cdot \partial J^2/\partial^2 u \cdot G^{-1}$, the optimum should be "flat" with respect to the variable c, i.e. $\partial J^2/\partial^2 c$ should be small).

Requirement 3. For cases with two or more controlled variables, the selected variables in c should not be closely correlated.

Requirement 4. The variable c should be easy to measure and control.

The above requirements may be useful for identifying candidate variables, but the requirements are somewhat qualitative and checking them may require quite a lot of computation.

By proper variable scaling, the three first requirements may be combined into the single approximate condition of maximizing the minimum singular value of the gain matrix G (Skogestad 2000*a*).

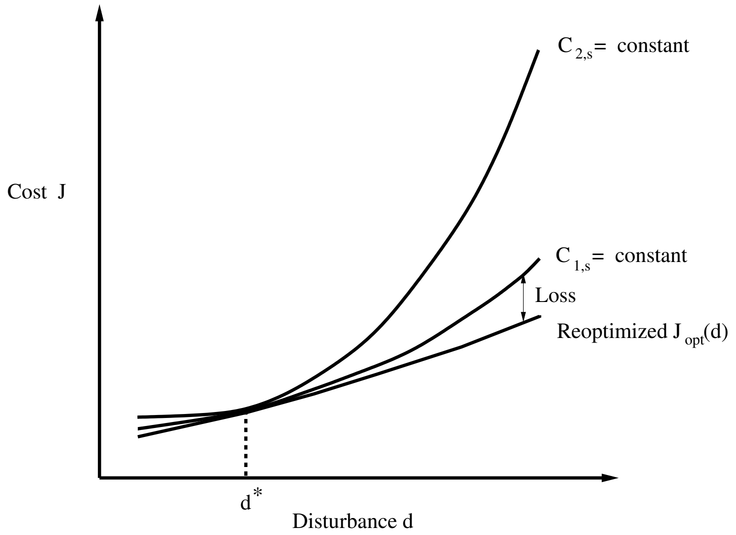
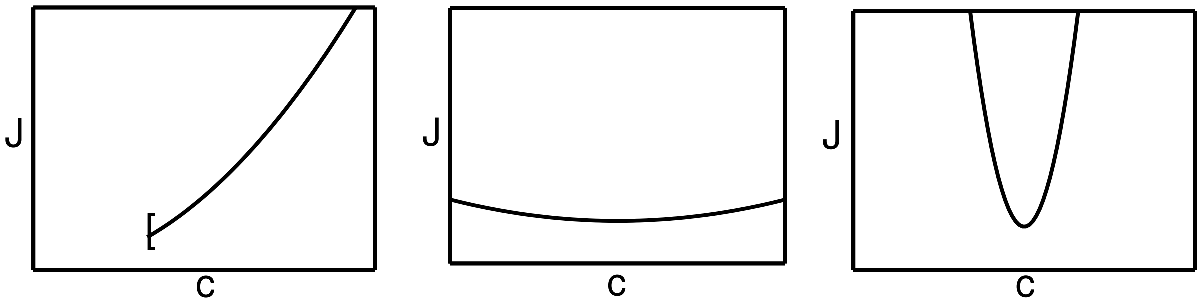


Figure 2: Loss imposed by keeping constant setpoint for the controlled variable



(a) Active constraint control: Implememtation easy

(b) Flat optimum: Implementation easy

(c) Sharp optimum: Sensitive to implementation erros

Figure 3: Implementing the controlled variable

This condition is computationally attractive, but since it only provides local information it may be very misleading in some cases (e.g. see Figure 5 where the minimum occurs very close to infeasibility).

A better and more exact approach is therefore to evaluate the cost function for the expected set of disturbances and implementation errors. We apply here the stepwise procedure for self-optimizing control of Skogestad (2000a). The main steps are:

Step 1 Degree of freedom analysis

Step 2 Definition of optimal operation (cost and constraints)

Step 3 Identification of important disturbances

Step 4 Optimization

Step 5 Identification of candidate controlled variables

Step 6 Evaluation of loss for alternative combinations of controlled variables (loss imposed by keeping constant setpoints when there are disturbances or implementation errors)

Step 7 Final evaluation and selection (including controllability analysis)

Skogestad (2000a) applied this stepwise procedure to a reactor case and a distillation case, but in both cases there were only one unconstrained degree of freedom, so the evaluation in step 6 was managable. However, for the Tennessee Eastman process there are three unconstrained degrees of freedom at the optimum, and a very large number of candidate variables to select from, so it is necessary to do some more effort in step 5 to reduce the number of alternatives. We present below some general criteria that are useful for eliminating controlled variables.

3 Problem definition

Step 1. Degrees of freedom analysis. The Tennessee Eastman process has 12 manipulated variables, 41 measurements and 20 disturbances. An analysis, see Table 1, show that at stedy-state two degrees of freedom are lost because we have two liquid levels with no steady-state effect, and two degrees of freedom are consumed to satisfy the equality constraints on the product. We are then left with eight degrees of freedom which may be used for steady-state optimization.

Step 2. Definition of optimal operation. Downs and Vogel (1993) specified the economic cost J [$/h] for the process, which is to be minimized. In simple terms,

$$\begin{aligned} J = (loss\ of\ raw\ materials\ in\ purge\ and\ products) + \\ (steam\ costs) + (compression\ costs) \end{aligned} \tag{2}$$

The first term, related to loss of unreacted raw materials, dominates the cost. All the manipulated variables have associated constraints and there are "output" constraints, including equality constraints on product quality and product rate.

Step 3. Identification of important disturbances. A closer analysis reveals that disturbances 3, 4, 5 and 7 have no steady-state effect on the economics provided we make appropriate use of the available manipulated variables. For example, disturbance 4 (a step in the reactor cooling water inlet temperature), is easily counteracted by increasing the reactor cooling water flowrate; thus this disturbance will have no impact on the economics provided we adjust the cooling rate. Similar arguments can be made for disturbance 3, 5 and 7, provided we manipulate the reactor coolant flow, separator cooling water flow and the C feedrate. Disturbance 6 (loss of feed A) is considered to be so serious that it should be handled by overrides, therefore it is not included in this study.

This leaves only the following three disturbances:

- Disturbance 1: Change in A/C ratio in the C feedstream
- Disturbance 2: Change in fraction of B (inert) in the C feedstream

	Manipulated variables	12
	D feed flow	
	E feed flow	
	A feed flow	
	C feed flow	
	Compressor recycle valve	
	Purge flow	
	Separator liquid flow	
	Stripper liquid product flow	
	Stripper steam flow	
	Reactor cooling water flow	
	Condenser cooling water flow	
	Agitator speed	
-	Levels with no steady state effect	2
	Separator level	
	Stripper level	
-	Equality constraints	2
	Product quality	
	Production rate	
=	Degrees of freedom at steady state	8
-	Active constraints at the optimum	5
	Reactor pressure (maximum)	
	Reactor level (minimum)	
	Compressor recycle valve (closed)	
	Stripper steam valve (closed)	
	Agitator speed (maximum)	
=	Unconstrained degrees of freedom	3

Table 1: Degrees of freedom and active constraints.

- Throughput disturbances: Change in production rate by ± 15 %.

Step 4. Optimization. Ricker (1995) solved the optimization problem using the above cost function and gives a good explanation on what happens at the optimum. At the optimum there are five active constraints (see Tablee 1) and these need to be controlled to achieve optimal operation (at least nominally). We minimized the cost function J with respect to the three remaining unconstrained degrees of freedom, and obtained the same optimal values as given by Ricker (1995). The optimal (minimum) operation cost is 114.323 \$/h in the nominal case, 111.620 \$/h for disturbance 1, and 169.852 \$/h for disturbance 2. A continuation method (Christiansen *et al.* 1996) was used to solve the optimization problem and to generate the cost function surfaces.

The three unconstrained degrees of freedom need to be set during operation, and the main issue, addressed in the next section, is which three variables we should select as controlled variables in a constant setpoints policy such that we achieve acceptable economic loss (self-optimizing control). We define an "acceptable loss" to be 6 \$/h when summed over the four disturbances just mentioned.

4 Candidate controlled variables

We are now at *Step 5: Identification of candidate controlled variables.* This step is the main focus of this paper.

Let us initially *not* make the assumption that we will satisfy specifications or use active constraint control. We then have 12 degrees of freedom, and we want to select 12 controlled variables which are to be controlled at constant setpoints. We can choose from 41 measurements and 12 manipulated variables, so there are 53 candidate variables. Even in the simplest case, where we do not consider variable combinations (such as differences, ratios, and so on), there are

$$\frac{53 \cdot 52 \cdot 51 \cdot 50 \cdot 49 \cdot 48 \cdot 47 \cdot 46 \cdot 45 \cdot 44 \cdot 43 \cdot 42}{12 \cdot 11 \cdot 10 \cdot 9 \cdot 8 \cdot 7 \cdot 6 \cdot 5 \cdot 4 \cdot 3 \cdot 2 \cdot 1} = 2.67 \cdot 10^{11}$$

possible combinations. It is clearly impossible to evaluate the loss with respect to disturbances and implementation errors for all these combinations.

The following criteria are proposed to reduce the number of alternatives. Most of them are rather obvious, but nevertheless we find them useful.

1. Eliminate variables with no effect on the economics (including variables with no steady-state effect). (The value of these variables can be arbitrarily selected and this reduces the number of degrees of freedom and thus the number of controlled variables to be selected. We must, of course, also eliminate the corresponding variables from further consideration as candidate controlled variables.)
2. Equality constraints: The variables directly associated with equality constraints should be controlled. (Again, this reduces the number of controlled variables to be selected, and we must also eliminate the corresponding variables from further consideration.)
3. Active constraint control: We choose to control the active constraints. (Again, this reduces the number of controlled variables to be selected, and we must also eliminate the corresponding variables from further consideration.)
4. Eliminate/group closely related variables
5. Process insight: Eliminate further variables
6. Eliminate single variables which with constant setpoints yield infeasibility or large loss when there are (1) disturbances or (2) implementation errors (with the remaining degrees of freedom reoptimized).
7. Eliminate combinations (pairs, triplets, etc.) of variables that yield infeasibility or large loss
8. Local analysis: Eliminate variables or variable combinations which result in a small value of the minimum singular value of the appropriately scaled gain matrix G (not used in this paper).

After this we enter into the final evaluation for the remaining combinations of variables:

1. Evaluation of disturbance losses
2. Evaluation of implementation losses

We will now apply these critera to our case study.

4.1 Eliminate variables with no effect on the economics

There are two variables with no steady-state effect, namely stripper level and separator level, and their values have no effect on the steady-state economics. This reduces the number of degrees of freedom, and thus controlled variables to be selected, from 12 to 10. The corresponding variables must also be eliminated from further consideration; this eliminates 2 measurements.

Of course, we need to measure and control the two levels to obtain stable operation, but we do not need at this point to make a decison about which manipulated variable we will actually use for this as it does not affect the steady-state cost.

4.2 Equality constraints

The two equality constraints must be satisfied, and this reduces the number of controlled variables to be selected from 10 to 8. The directly related variables may be eliminated from further consideration.

- The stripper liquid flow (product rate) is directly correlated with production rate (which is specified) This eliminates 1 manipulated variable and 1 directly related measurement.
- The separator liquid flow is also strongly correlated with the production rate and should not be kept constant (eliminates 1 manipulated variable)
- The ratio G/H in the product is specified to be 1, and since the product contains mostly G and H this means that there should be about 50% G and 50% H in the product (specified). This eliminates the 2 corresponding related measurements (% G in product and % H in product).
- Put together, the two equality constraints specify the amounts of products G and H. From the stoichometry one may then conclude that none of the four feed streams (A, D, E and C) should be kept constant. However, mainly for illustration, we will retain these variables as degrees of freedom for now, but we will show that they are indeed eliminated based on feasibility and cost considerations.

Note that we do not need at this point to make a decison about which manipulated variables we will actually use to satisfy the equality constraints as this does not affect the steady-state analysis.

4.3 Active constraint control

As mentioned, there are 5 active constraints, and this reduces the number of controlled variables to be selected from 8 to 3.

Again, the directly related variables should be eliminated from further consideration. We have that 3 of the constraints are related to manipulated variables (compressor recycle valve, stripper steam valve, agitator speed); this eliminates these 3 manipulated variables and also 1 directly related measurement (stripper steam) from further consideration. 2 of the constraints are related to outputs (reactor level and pressure); this eliminates another 2 measurements.

We started with 41 measurements and 12 manipulated variables, from which we wanted to select 12 controlled variables. We are now left with 33 measurements and 7 manipulated variables, from which we want to select 3 unconstrained controlled variables. This gives 9880 possible combinations, which is still much too large.

4.4 Eliminate/group closely related variables

The controlled variables should be independent (requirement 3).

- Six of the remaining manipulated variables are measured (A feed, D feed, E feed, C feed, stripper liquid flow, purge flow) that is, there is a one to one correlation with a measurement (eliminates 6 mesurements).
- The purge and recycle streams have the same composition, and since the recycle stream makes up about 2/3 of the reactor feed it follows that there is only small differences between controlling the purge and reactor feed compositions. We therefore eliminate reactor feed composition (eliminates 6 measurements)

Note that the choice of which variables to keep and which to eliminate was more or less arbitrary, but since the variables are closely related it does not matter very much in the further analysis. The main idea is to keep one variable in each group of related variables.

4.5 Process insight: Eliminate further candidates

Based on understanding of the process some further variables can be excluded form the set of possible candidates for control:

- The pressure drops should be as small as possible, thus with constant (maximum) reactor pressure, the pressures in separator and stripper should be allowed to float (eliminates 2 measurements).
- The condenser and reactor cooling water flowrates should not be held constant, since that would imply a loss for disturbances 4 and 5 (eliminates 2 manipulated variables). For the same reason we should not keep the reactor and separator cooling water outlet temperatures constant (eliminates 2 measurements).

4.6 Eliminate single variables that yield infeasibility or large loss

The idea is to keep a single candidate variable constant at its nominally optimal value, and evaluate the loss for (1) various disturbances and (2) for the expected implementation error for this variable for the "best" case with the remaining degrees of freedom reoptimized. If the loss is large (or even worse, no feasible solution is found), then this variable can be eliminated from further consideration.

Infeasibility. Keeping one of the following four manipulated variables constant results in infeasible operation for disturbance 2 (inert feed fraction): D feed flow, E feed flow , C feed flow (stream 4) and purge flow, see Table 2. This is independent on how the two remaining degrees of freedom are used.

Variable	Nominal value (constant)	Nearest feasible value with disturbance 2
D feed flow [kg/h]	3657	3671
E feed flow [kg/h]	4440	4489
C feed flow [kscmh=k Sm^3/h]	9.236	9.280
Purge flow [kscmh]	0.211	0.351

Table 2: Single variables with infeasibility for disturbance 2 (increase of inert fraction in feed)

This is further illustrated in Figure 4, where we see that the nominally optimal purge rate results in infeasable operation for disturbance 2. We also see from Figure 4 that a small negative implementation error in the purge rate will yield infeasibility.

Loss. We have now left 1 manipulated variable (A feed flow) and 17 measurements. Table 3 shows the loss (deviation above optimal value) for fixing one of these 18 variables at a time, and reoptimizing with respect to the remaning two degrees of freedom. The losses with constant A feed flow and constant reactor feedrate are totally unacceptable for disturbance 1 (eliminates 1 manipulated variable and 1 measurement). In fact, we could have eliminated these earlier based on their close relationship to the product rate equality constraint. The remaining 15 measurements yield reasonable losses. However, we have decided to eliminate variables with a loss larger than 6 $/h when summed for the three disturbances. This eliminates the following 5 measurements: separator temperature, stripper temperature, B (inert) in purge, G in purge, and H in purge.

4.7 Eliminate pairs of constant variables with infeasibility or large loss

We are now left with 11 candidate measurements, that is, $(11 \cdot 10 \cdot 9)/(3 \cdot 2) = 165$ possible combinations of three variables.

The next natural step is to proceed with keeping pairs of variables constant, and evaluate the loss with the remaining degree of freedom reoptimized. However, there are 55 combinations of pairs, so this in itself would be a very large effort. We therefore choose to skip this step in the procedure.

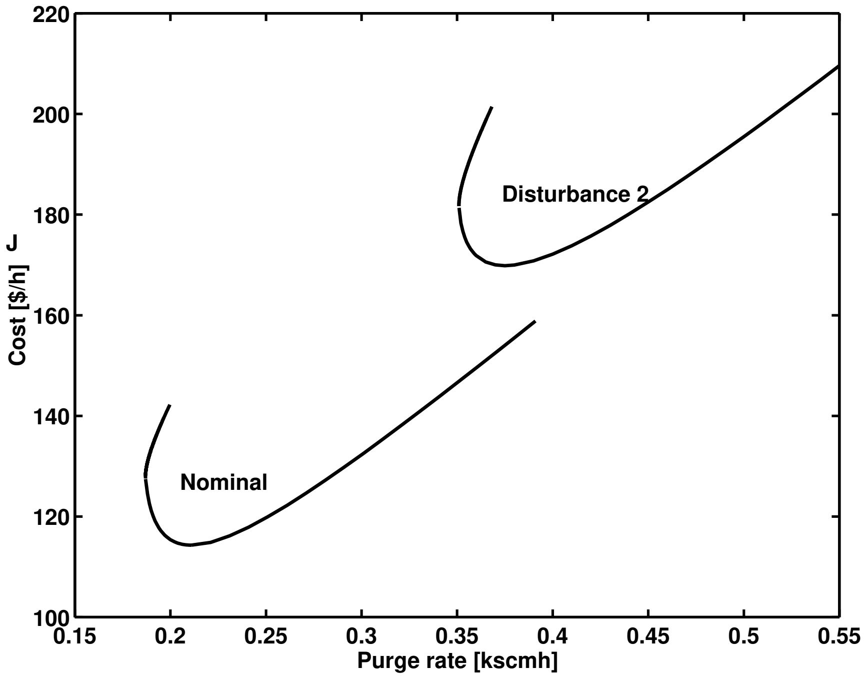


Figure 4: Cost as a function of purge rate (with the remaining two degrees of freedom optimized)

5 Selection of controlled variables

We are now at *Step 6: Evaluation of loss for alternative combinations of controlled variables.* This is done by computing the loss imposed by keeping constant setpoints when there are disturbances or implementation errors.

As mentioned, we are now left with 165 possible combinations of three variables. An initial screening based on computing losses (Hestetun 1999) indicates that one of the three controlled variables should be reactor temperature, which is the only remaining temperature among the candidate variables. Furthermore, reactor temperature is proposed by most authors, and it is normally easy to control, so we will now only consider combinations that include reactor temperature.

A further evaluation shows that we should eliminate % F (byproduct) in purge as a candidate variable, because the optimum is either very "sharp" in this variable, or optimal operation is achieved close to its maximum achievable value (see a typical plot in Figure 5). In either case, operation will be very sensitive to the implementation error for this variable.

5.1 Evaluation of disturbance losses

The losses for the remaining $9 \cdot 8/2 = 36$ possible combinations of 2 variables are shown in Table 4. Note that the recycle flow is the flow from the compressor which is returned to the reactor, and it should not be confused with the compressor recycle valve which we have chosen to keep closed. Not surprising, keeping both the recycle flow and compressor work constant results in infeasibility. This is as expected, because from process insight these two variables are closely correlated (and we should probably have eliminated one of them earlier).

We note that constant % F in product in all cases results in a large loss or infeasibility for disturbance 2. This, combined with the above finding that we should not control % F in purge, leads to the conclusion that it is *not* favorable to control the composition of byproduct (F) for this process.

The following four cases have a summed loss of less than 6 $/h:

Case I. Reactor temperature, Recycle flow, and C in purge (loss 3.8 $/h).

Fixed variable	Disturbance 1	Disturbance 2	Throughput +15/-15%
A feed flow *	709.8	6.8	
Reactor feed flow*	53.5	0.5	
Recycle flow	0.0	0.8	0.5 / 0.3
Reactor Temp.	0.0	0.9	1.2 / 0.7
Sep Temp.*	0.0	0.5	4.2 / 2.3
Stripper Temp.*	0.1	0.3	4.3 / 2.3
Compressor Work	0.0	0.6	0.2 / 0.1
A in purge	0.0	0.7	0.4 / 0.2
B in purge*	0.0	7.4	3.1 / 1.6
C in purge	0.0	0.5	0.1 / 0.1
D in purge	0.0	0.0	0.2 / 0.1
E in purge	0.0	0.4	0.0 / 0.1
F in purge	0.0	0.5	0.0 / 0.0
G in purge*	0.0	0.4	4.1 / 2.2
H in purge*	0.0	0.4	4.2 / 2.2
D in product	0.0	0.1	0.2 / 0.1
E in product	0.0	0.0	1.2 / 0.7
F in product	0.0	1.5	1.4 / 0.8

Table 3: Loss [$/h] with one variable fixed at its nominal optimal value and the remaining two degrees of freedom reoptimized. Variables marked with * have a loss larger than 6 $/h.

Case II. Reactor temperature, Compressor work, and C in purge (loss 3.9 $/h).

Case III. Reactor temperature, C in purge, and E in purge (loss 5.1 $/h).

Case IV. Reactor temperature, C in purge, and D in purge (loss 5.6 $/h).

The choice of Ricker (1996), with reactor temperature, A in purge and C in purge, is somewhat less favorable with a summed loss of 9.8 $/h.

5.2 Evaluation of implementation losses

In addition to disturbances, there will always be an implementation error related to each controlled variable, that is, a difference between its setpoint and its actual value, e.g. due to measurement error or poor control. In Figure 6 we plot for "best" case I the cost as a function of the three controlled variables (the plots for case II are nearly identical and are not shown). We see that the optimum is flat over a large range for the three controlled variables, and we conclude that implementation error will not cause a problem.

5.3 Summary

In conclusion, control of reactor temperature, C in purge, and recycle flow or compressor work (cases I or II) results in a small loss for disturbances, has a flat optimum (and is thus insensitive to implementation error), and are therefore good candidates for self-optimizing control.

6 Implementation and analysis of controllability

We are now at *Step 7: Final evaluation and selection.* The analysis up to now is purely based on steady-state economics, and we have said nothing about how the proposed controlled variables should

Case	Fixed variables		Distur-bance 1	Distur-bance 2	Throughput +15%	-15%	Sum
	Recycle Flow	Comp. Work	0.1	Infeas.	Infeas.	40.4	Infeas.
	Recycle Flow	A in purge	0.0	1.2	Infeas.	9.1	Infeas.
I	Recycle Flow	C in purge	0.0	1.9	1.3	0.6	3.8
	Recycle Flow	D in purge	0.0	3.7	4.8	3.0	11.6
	Recycle Flow	E in purge	0.0	3.7	3.1	2.2	9.0
	Recycle Flow	D in prod.	0.2	2.6	38.0	11.9	52.7
	Recycle Flow	E in prod.	0.2	1.5	42.1	12.9	56.5
	Recycle Flow	F in prod.	0.2	37.7	1.8	0.8	40.5
	Comp. Work	A in purge	0.0	1.3	126.0	8.0	135.3
II	Comp. Work	C in purge	0.0	1.8	1.4	0.7	3.9
	Comp. Work	D in purge	0.0	4.0	5.5	3.6	13.1
	Comp. Work	E in purge	0.0	4.0	3.5	2.8	10.3
	Comp. Work	D in prod.	0.2	2.0	40.8	12.8	55.8
	Comp. Work	E in prod.	0.2	1.6	45.3	13.8	60.9
	Comp. Work	F in prod.	0.2	32.8	1.9	0.9	35.8
Ricker	A in purge	C in purge	0.0	2.4	5.3	2.1	9.8
	A in purge	D in purge	0.0	2.3	13.4	5.2	20.9
	A in purge	E in purge	0.0	2.3	10.2	4.6	17.1
	A in purge	D in prod.	0.0	1.6	50.5	10.6	62.7
	A in purge	E in prod.	0.1	1.3	54.6	11.1	67.1
	A in purge	F in prod.	0.1	17.0	4.5	2.1	23.7
IV	C in purge	D in purge	0.0	2.4	2.1	1.1	5.6
III	C in purge	E in purge	0.0	2.4	1.7	1.0	5.1
	C in purge	D in prod.	0.0	1.7	5.1	2.5	9.3
	C in purge	E in prod.	0.0	1.7	5.4	2.7	9.8
	C in purge	F in prod.	0.2	35.6	1.9	1.2	38.9
	D in purge	E in purge	0.0	2.6	77.3	Infeas.	Infeas.
	D in purge	D in prod.	6.2	5.4	52.6	Infeas.	Infeas.
	D in purge	E in prod.	5.5	Infeas.	52.2	Infeas.	Infeas.
	D in purge	F in prod.	0.5	Infeas.	2.4	1.0	Infeas.
	E in purge	D in prod.	4.5	5.3	54.9	Infeas.	Infeas.
	E in purge	E in prod.	3.8	Infeas.	54.3	Infeas.	Infeas.
	E in purge	F in prod.	0.5	Infeas.	1.6	0.9	Infeas.
	D in prod.	E in prod.	0.2	3.2	42.4	Infeas.	Infeas.
	D in prod.	F in prod.	0.2	Infeas.	Infeas.	3.3	Infeas.
	E in prod.	F in prod.	0.2	Infeas.	Infeas.	3.5	Infeas.

Table 4: Loss [$/h] when fixing all three degrees of freedom. Reactor temperature is fixed in all cases.

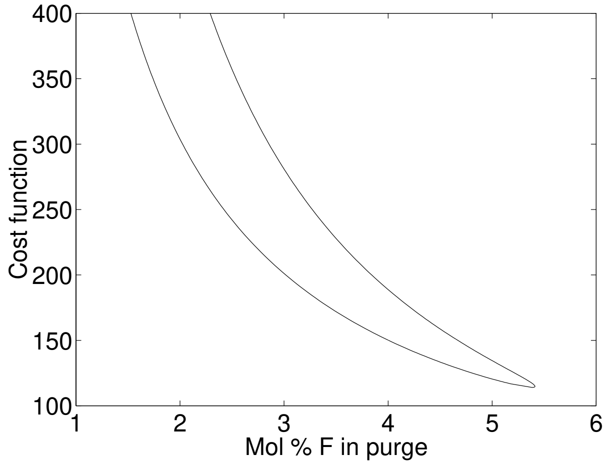


Figure 5: Unfavorable shape of cost function with % F (byproduct) in purge as controlled variable. Shown for case with constant reactor temperature and C in purge.

be implemented. Obviously, this is also an important consideration, as one choice of controlled variables may result in a system that is easy to control, whereas another may result in serious control problems, for example, caused by unstable (RHP) zeros (the multivariable extension of inverse response behavior).

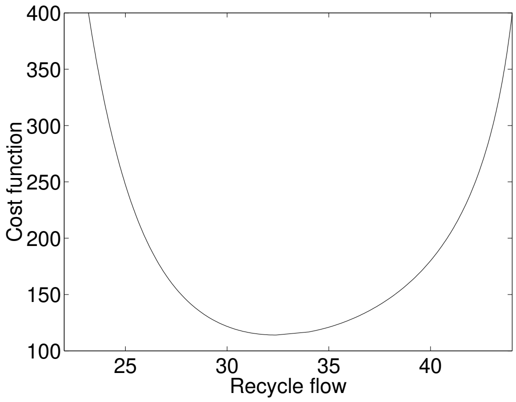
The truly optimal approach would be to solve the whole problem as one big optimization problem, taking into account both economics and control. However, this is intractable for most real problems, and the approach taken in this paper is then preferred. Here we first identify candidate sets of controlled variables with acceptable steady-state economics. We then check the controllability of the best alternative (case I in our case). If it is acceptable, then we have found a viable solution. If it is not acceptable, then we check the remaining candidates. If neither of these turns out to be controllable, then we must relax our requirements on the steady-state economics and consider more candidates.

A procedure for controllability analysis is given on page 246 in Skogestad and Postlethwaite (1996). It is based on first obtaining a linearizing model, and then checking if the disturbances in questions may be rejected with the available inputs taking into account the presence of RHP-zeros, etc. However, we were not able to obtain a linearized model of the effect of the disturbances for the Tennessee Eastman process. Partly for this reason, and partly because most engineers are more convinced by closed-loop simulations, we will here use the "simulation approach" for evaluating the controllabilty.

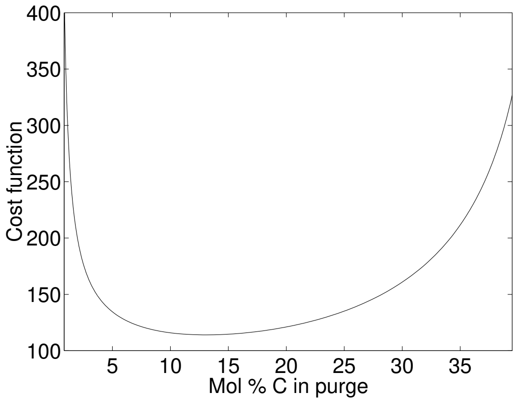
In the "simulation approach" we propose a particular control structure, tune the controllers, and show with simulations that control is acceptable. Note that model uncertainty should generally be included in these simulations. If we use decentralized control (as we do) then model uncertainty is generally less critical, as a decentralized controller does not really make much use of the plant model. If we can find a particular tuning with acceptable control, then we can conclude that the plant is controllable, at least for the disturbance and uncertainty scenario considered. However, the simulation generally approach suffers from the problem that it depends on the particular tunings and disturbances used in the simulations, and this may make it difficult to draw definite conclusions.

7 Simulation of proposed control structure

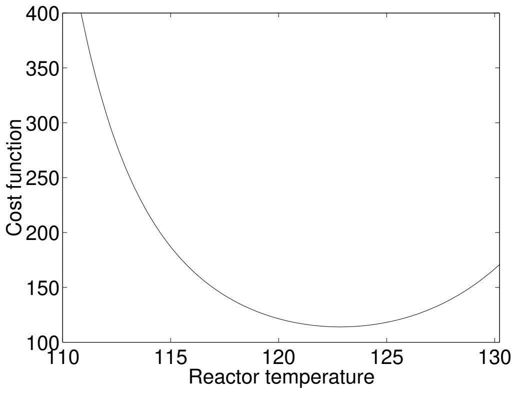
We here consider control of the plant using the controlled variables with the best steady-state economics (case I). We propose a decentralized control system, and show by simulations that acceptable control is indeed possible.



(a) Constant reac.T and C in purge



(b) Constant reac.T and recycle flow



(c) Constant C in purge and recycle flow

Figure 6: Optimum is relatively flat for case I

7.1 Decentralized control structure

Our first attempt was to design a decentralized control structure follows the procedure of Larsson and Skogestad (2000) (the heading numbers below refers to Table 1 in that paper). The resulting structure and PI tunings are given in Table 5.

1. Controlled variables

Let us summarize the above results (case I). From the degrees of freedom analysis in Table 1 we know that there are 12 manipulated variables. However, 2 of these degrees of freedom are consumed to control liquid levels with no steady-state effect:

1. Separator level
2. Stripper level

Furthermore, there are 2 equality constraints,

3. Production rate (given)
4. Ratio between G and H in product (given)

To operate optimally there are 5 active constraints. Three are related to manipulated inputs,

5. Compressor recycle valve (closed)
6. Stripper steam valve (closed)
7. Agitator speed (maximum)

whereas two are related to outputs,

8. Reactor level (maximum)
9. Reactor pressure (minimum)

There are then 3 remaining unconstrained degrees of freedom which may be used to optimize the operation. Based on the above steady-state economic analysis we propose to control the following three variables at their nominally optimal setpoints (case I) in order to achieve self-optimizing control:

10. Reactor temperature
11. % C in purge
12. Recycle flow

Three of the above "controlled variables" are manipulated inputs (5,6 and 7) and these need no further consideration in terms of control. However, a strategy for controlling the remaining 9 variables must be found, and in terms of decentralized control this implies that each controlled variables must be paired with one the remaining 9 manipulated inputs, which are: Separator liquid flow, stripper liquid product flow, C feed flow, D feed flow, E feed flow, purge flow, reactor cooling water flow, A feed flow, and condenser cooling water flow.

In addition, we may need to close some loops for stabilization or to improve local disturbance rejection, but the setpoints for these "inner" loops may be used as degrees of freedom so this does not effect the above steady-state analysis, although it may affect the selecting of the control structure (pairing of variables).

2. Production rate

Where should the throughput be set? This is a very important choice, as it determines the structure of the remaining inventory control system.

In our case, the most obvious choice is to use the stripper liquid flow which is the product stream. However, this stream is most likely needed for stabilizing the stripper level which has no steady-state effect. The production rate must therefore be set upstream, and in the decentralized scheme we will use largest of the four feed streams, which in this case is the C feed flow.

Another rather obvious choice for adjusting the production rate is to use the total feed rate, i.e., the sum of the four feed streams. However, this does not give a decentralized control scheme and will be considered later in the improved control structure.

3a. Regulatory control layer: Stabilization

There are two integrating liquid levels which may be stabilized as follows (here the symbol $\leftrightarrow$ means "is paired with" or more precicely "is controlled by"):

1. Separator level $\leftrightarrow$ Separator liquid flow

2. Stripper level $\leftrightarrow$ Stripper liquid product flow

In addition, the exothermic reaction results in an instability in the reactor system, but it is easily stabilized as follows (McAvoy and Ye 1994) (Havre and Skogestad 1998):

10'. Cooling water outlet temperature $\leftrightarrow$ Cooling water flow

Note that this loop introduces the setpoint for the reactor cooling water outlet temperature as a new degree of freedom, i.e. it replaces the cooling water flow as a manipulated variable when seen from the layer above.

3b. Regulatory control layer: Local disturbance rejection

In general, we use extra local measurements in inner cascades to improve local disturbance rejection, for example, use of flow controllers based on measuring the flow is very common. However, as a first try we will not use any inner cascades here (except for the temperature controller 10' which we introduced for stabilizing the reactor).

4. Supervisory control layer: Decentralized control

We still have 7 variables (3, 4 and 8 to 12 in the above list) that need to be controlled at given setpoints using the remaining 7 manipulated variables.

As a first attempt, we use decentralized control and base the pairings on a relative gain array (RGA) analysis of the stabilized 7×7 system. The main rules for the RGA-analysis are (e.g. (Skogestad and Postlethwaite 1996)):

1. Avoid pairing on negative RGA-elements at steady-state.
2. Prefer pairing on RGA-elements close to 1 (with the other elements close to 0) at the bandwith frequency.

The best pairings according to these rules for loops 3, 4, 8, 9, 10, 11 an 12 are as given in Table 5. Note that the RGA-analysis recommends that production rate should be controlled using the C feed flow, which is the largest feed stream. With these pairings the magnitudes of the "paired" RGA-elements at frequency 0.5 rad/h (corresponding to a closed-loop response time of about 2 h) range from about 0.29 (loop 11) to 1.6 (loop 9), indicating that there are significant interactions. This is also expected based on physical insight. For example, if we change the production rate (setpoint loop 3), then we will need to change all the flows, introducing interactions into most of the other loops.

Dynamic simulations show that this simple decentralized control systems performs acceptably for most of the disturbances given by Downs and Vogel (1993), including setpoint changes in the production rate and in the G/H ratio. The PI controllers were initially tuned individually based on Ziegler-Nichols method, and were then implemented and retuned sequentially, starting with the fast loops. A typical response for a combination of disturbances is shown in Figure 7. We note that a disturbance in the A/C ratio in the C feed stream (disturbance no. 1) increases the % C in the purge stream which through loop

Loop	Controlled variable	Manipulated variable	Gain K_c	Integral time τ_I
1	Separator level	Separator liquid flow	-2.5	200 min
2	Stripper level	Stripper liquid product flow	-0.5	300 min
3	Production rate	C feed flow	0.005	3 min
4	Product ratio G/H	D feed flow	2	150 min
5		Compressor recycle valve: closed		
6		Stripper steam valve: closed		
7		Agitator speed: maximum		
8	Reactor level	E feed flow	5	1200 min
9	Reactor pressure	Purge flow	-1	90 min
10	Reactor temperature	Setpoint cooling water outlet temp.	5	1 min
10'(stab)	Cooling water outlet temperature	Reactor cooling water flow	-10	6 min
11	% C in purge	A feed flow	-5	500 min
12	Recycle flow	Condenser cooling water flow	-3	200 min

Table 5: Decentralized control structure

11 increases the A feed flow. This causes increased reactor pressure, but it remains inside the limit of 2895 kPa.

7.2 Improved control structure with some decoupling

The above decentralized control structure works, but it is quite interactive and it is sensitive to some disturbances because inner flow controllers are not included. Our "improved" control structure with some decoupling is given in Table 6. It is very similar to that of Ricker (1996), but we had to make some modifications since he controls A in purge instead of recycle flow. The main idea is to introduce physical decoupling by (1) using the total feed flow to control the production rate, and (2) using the D/E feed flow ratio to control the product ratio G/H (as is reasonable from the stoichiometry). In addition, flow controllers are implemented to improve local disturbance rejection.

The dynamic response with this control structure is significantly better. This is illustrated by the dynamic simulations shown in Figure 8. As before, the disturbance in the A/C ratio in the C feed stream, increases % C in the purge stream which through loop 11 reduces the C feed flow. However, the total feed flow is constant (loop 3), so all the other flows are increased to compensate for this, and there is almost no interactions into the other loop. For example, the reactor pressure remains almost constant.

The responses to other disturbances are also very good, and simulations (not included) show that they are generally similar to or slightly better than the reponses of Ricker (1996) which was the basis for our improved structure.

In conclusion, the dynamic simulations show that the set of controlled variables with the best self-optimizing properties in terms of steady-state economics (case I), is controllable. It is possible to achieve acceptable control with a simple decentralized control structure, but performance is improved markedly by introducing some simple "decoupling" elements such as use of total feed flow as a manipulated variable.

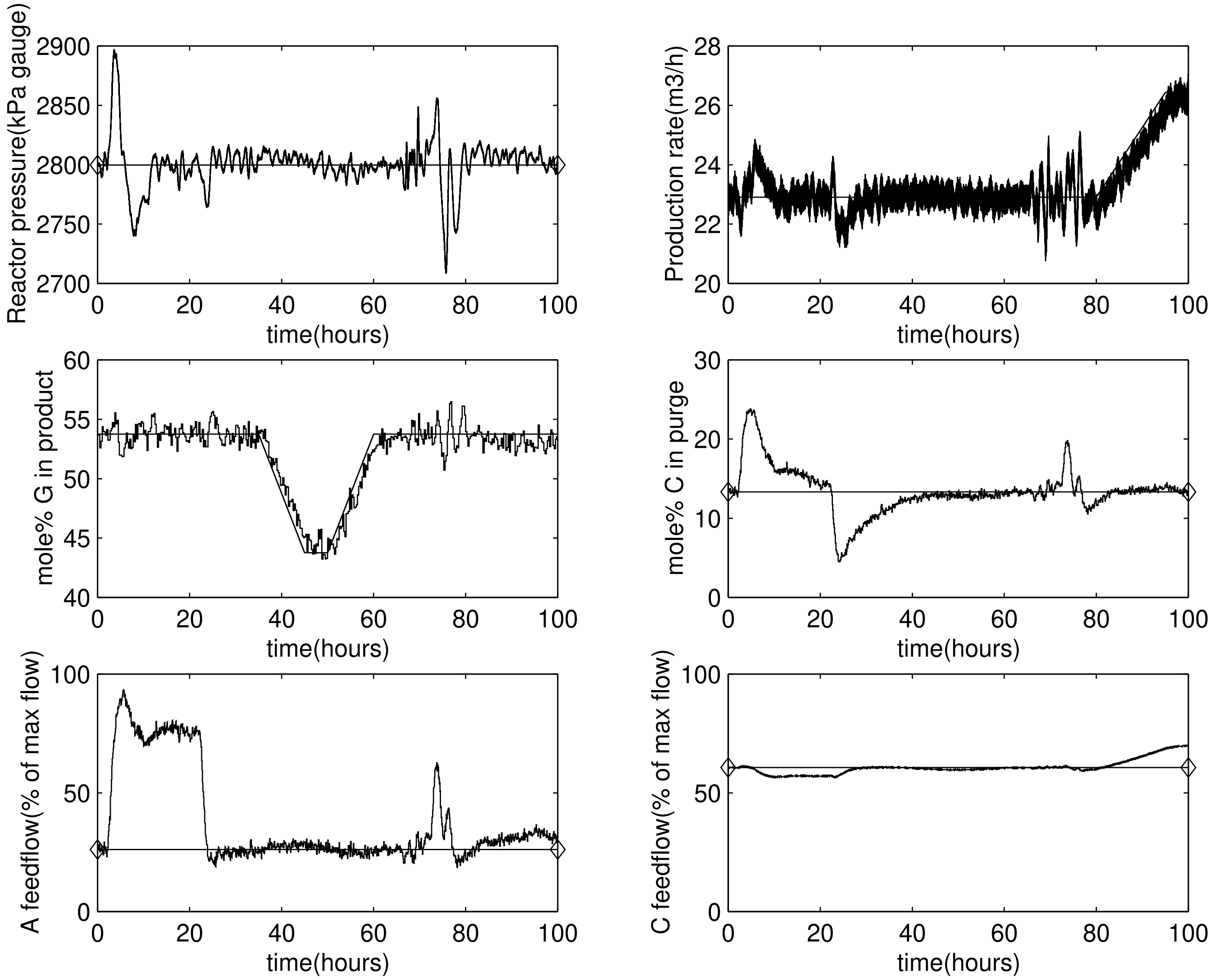


Figure 7: Decentralized control structure.
$t = 0 - 22$ h: Disturbance (no.1) in A/C ratio in C feed
$t = 35 - 45$ h: Ramp down setpoint in % G in product
$t = 50 - 60$ h: Ramp up setpoint in % G in product
$t = 65 - 70$ h: Disturbances (nos. 12 and 15) in reactor cooling water
$t = 70 - 75$ h: Disturbance (no.8) in A,B,C feed composition
$t = 80 - 95$ h: Ramp up setpoint for production rate

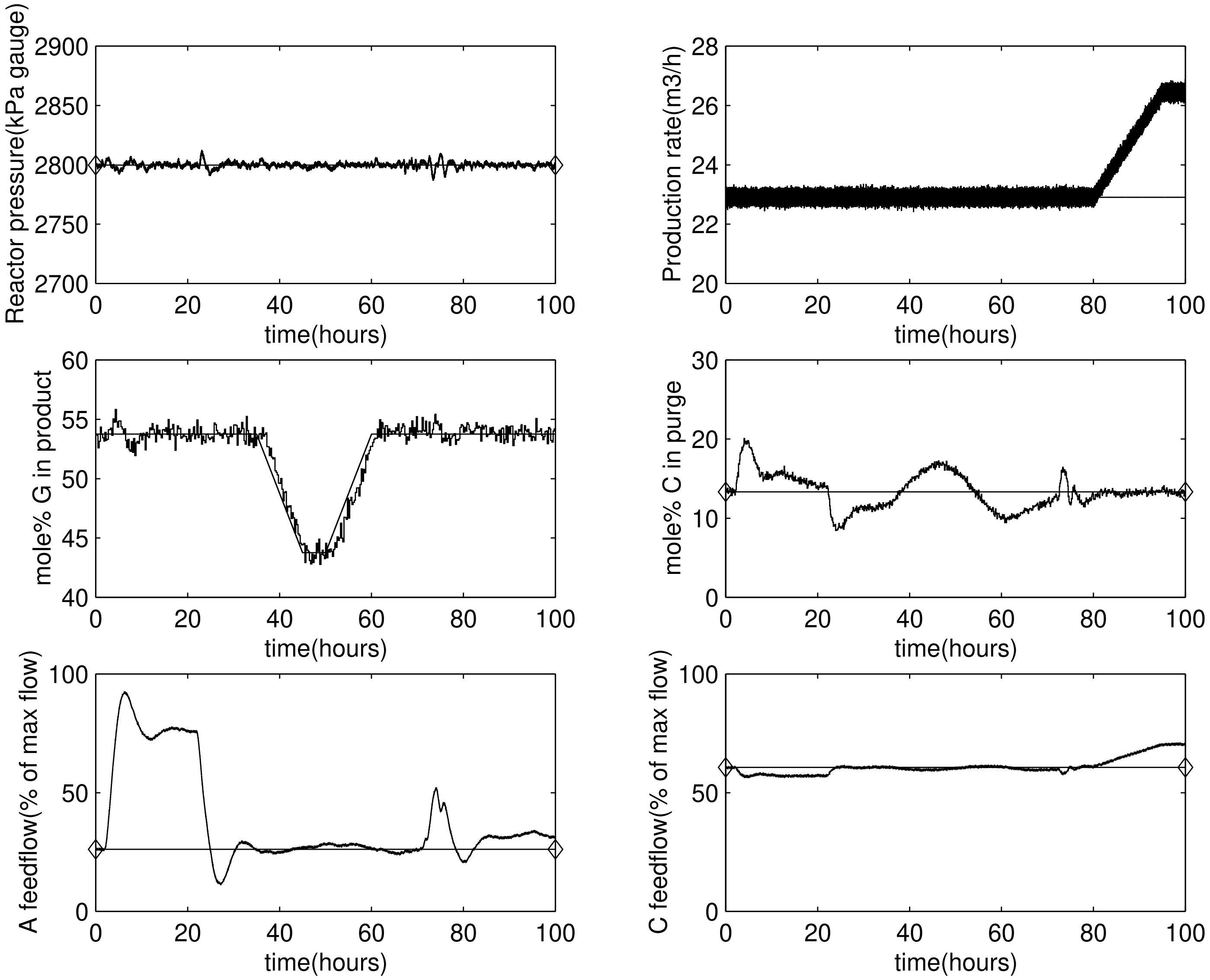


Figure 8: Improved control structure with some decoupling. (same disturbances and setpoint changes as in Figure 7)

Loop	Controlled variable	Manipulated variable	Gain K_c	Integral time τ_I
1	Separator level	Separator liquid flow	-0.001	200 min
2	Stripper level	Stripper liquid product flow	-0.0002	200 min
3	Production rate	Total feed flow	$3.2^\dagger$	120 min
4	Product ratio G/H	D/E feed flow ratio	$-0.032^\dagger$	100 min
5		Compressor recycle valve: closed		
6		Stripper steam valve: closed		
7		Agitator speed: maximum		
8	Reactor level	Setpoint sep. temperature (loop 8')	0.8	60 min
8'(casc)	Separator temperature	Condenser cooling water flow	-4	15 min
9	Reactor pressure	Purge flow	-0.0001	20 min
10	Reactor temperature	Reactor cooling water flow	-8	7.5 min
11	% C in purge	C feed flow	0.0009	562 min
12	Recycle flow	A feed flow	0.00125	120 min

Table 6: Improved control structure with some decoupling
In addition: Inner cascade flow controllers with pure integral action on all flows.
† Decoupling: Tunings are with implementation strategy of Ricker (1996)

8 Discussion

8.1 Should inert composition be controlled?

A common suggestion is that it is necessary to control the inert composition (in our case, mole fraction of component B) in order to (indirectly) control the inventory of inert components (Luyben *et al.* 1997) (McAvoy and Ye 1994) (Lyman and Georgakis 1995) (Tyreus 1999). However, recall that we eliminated B in purge at an early stage because it gave a rather large loss for disturbance 2 (see Table 3). Moreover, and more seriously, we generally find that the shape of the economic objective function as a function of inert composition is very unfavorable, with either a sharp minimum or with the optimum value close to infeasibility. A typical example of the latter is shown in Figure 9. In conclusion, we do not recommend to control inert composition. The inventory of inert in the system is in our case indirectly controlled, for example, by controlling the reactor pressure and recycle flow.

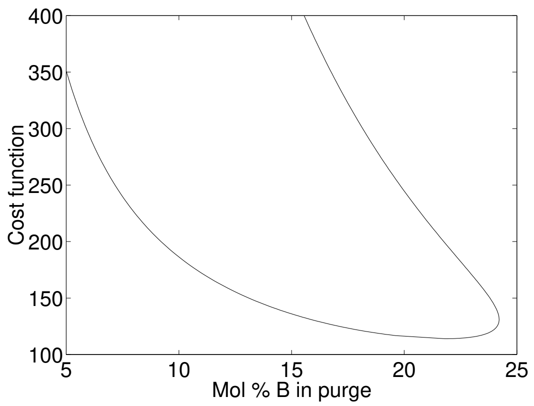


Figure 9: Typical unfavorable shape of cost function with B (inert) in purge as controlled variable (shown for case with constant reactor temperature and C in purge).

8.2 Combinations of variables

In the paper we have presented a number of criteria for reducing the number of alternatives. Note that the number of alternatives would have been much larger if we also had considered combinations of variables, such as sums, differences, ratios and so on.

However, note that combinations between already selected variables do not need to be considered as they do not affect the economic loss analysis presented in this paper. For example, assume we have selected the two temperatures T_1 and T_2 as controlled variables. Then the steady-state disturbance effect will be the same if we choose to keep T_1 and T_2 constant, or if we choose to keep, say, $T_1 - T_2$ and T_2 constant. However, the effect of the implementation error may differ if we have direct measurements of the combined variables, and this may offer some advantage, for example, if we have an accurate measurement of the difference $T_1 - T_2$.

Similarly, manipulated variable combinations and inner cascade controllers do not affect the analysis. For example, the use of the total feed rate as a manipulated variable in the improved control scheme has a dynamic effect, but no steady-state effect, because the controlled variables we keep constant at steady state are the same for the two schemes.

9 Conclusion

In this study of the Tennessee Eastman process, we have focused on the selection of the controlled variables using the concept of self-optimizing control, that is, to achieve acceptable loss with constant setpoints in the face of disturbances and implementation errors. The conclusion is that in addition to the constrained variables, we should control reactor temperature, C in purge and recycle flow or compressor work.

A very common suggestion is that it is necessary to control the inert composition. However, this choice may lead to serious operational problems as demonstrated by Figure 9, and in a more careful evaluation we did not find any favorable combination that included the inert composition.

Note that a systematic approach as taken in this paper may result in a control scheme which is not an obvious choice even for a trained control engineer. For example, during the review of the first version of this paper, where we had not included dynamic simulations to confirm the feasibility of the proposed controlled variables, one reviewer wrote that "it may be impossible to design such a plantwide scheme" whereas another wrote that "this reviewer is convinced that the final control scheme suggsted in this paper will not work either in simulation or in practice". Nevertheless, in this paper we have confirmed using dynamic simulation the feasibility of the proposed control structure.

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Simulink files are available at:
http://www.chembio.ntnu.no/users/skoge/diplom/diplom00/Hovland/
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