INTEGRATED OPTIMIZATION AND CONTROL

by

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Abstract

Increased competition in the process industry requires improved operation. One strategy is to use real-time optimization (RTO) based on measured disturbances and process outputs. The optimal solution is usually implemented by updating the setpoints to the control system, which then tries to keep the controlled variables at their given setpoints. Thus, the selection of controlled variables *integrates the optimization and the control* layer.

It is important to select the right controlled variables. First, there are always uncertainty with respect to the true value of the disturbances, so the optimal value of the selected controlled variables should not depend strongly on the disturbances. Second, the operation should not be sensitive to the implementation error in the controlled variables. The ideal situation is to have self-optimizing control where we may use constant setpoint values so that no optimization layer is needed. However, even if we have an optimization layer, it is important to select the right controlled variables in order to reduce the effect of uncertainty.

In the simplest case the setpoints for the controlled variables are fixed at their nominally optimal values. However, because of disturbances this may result in feasibility problems. The main contribution of this thesis is to propose methods to avoid such problems by adjusting the setpoints ("backoff"). Three different implementation policies are considered: (i) Constant nominal setpoints, (ii) constant robust setpoints and (iii) nominal setpoints with online feasibility correction (by use of MPC). A method for selection of controlled variables, based on steady-state economics, is extended to include these approaches. A good choice of controlled variables will reduce the need for logic, model predictive control and/or online optimization and give a simpler and cheaper system.

Another contribution is to provide several detailed case studies. The "backoff" approaches are illustrated on a reactor, separator and recycle process and an evaporation process. A plantwide control design procedure is applied to a combined cycle power plant and a distillation column heat-integrated with an indirect heat pump.

Finally, the thesis discusses whether or not it is best to have many stages in a distillation column. It is found that with fixed setpoints to the top and bottom compositions, few stages gives best controllability with respect to disturbance rejection, whereas many stages gives best controllability with respect to setpoint tracking. However, with the same energy usage it is possible to over-purify the products and many stages always gives better controllability.

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To my parents I dedicate this thesis.

Contents

Chapter 1

Introduction

In this chapter the thesis is restricted, motivated and placed in a wider perspective. An overview of the thesis and its main contributions is given together with a brief discussion of related works.

1.1 Motivation and focus

Increasing demands for efficient operation and utilization of energy and raw materials in chemical processes require better knowledge and understanding of the dynamic and steady-state behavior of the processes in order to design control systems. There is need for more sophisticated controller design procedures to operate the process closer to the optimal operating point in spite of disturbances and environment changes. This is in particular important for integrated processes where unreacted raw materials are recycled and hot process streams are heat exchanged against cold process streams, which gives more complex dynamic and steady-state behavior.

The main contribution of this thesis is to apply a method for self-optimizing control (Skogestad 2000a) to several case studies. The method is somewhat extended to include use of constant robust setpoints ("optimal backoff") and nominal setpoints with online feasibility correction ("flexible backoff").

1.2 Related works

Plantwide control deals with the control philosophy of the overall plant with emphasis on the *structural* decisions (Skogestad 2000a). The structural decisions involved in control system design include the following tasks ((Foss 1973), (Morari 1982), (Skogestad & Postlethwaite 1996)):

1. Selection of controlled variables (variables with setpoints)

2. Selection of manipulated variables

3. Selection of measurements (for control purposes including stabilization)

4. Selection of control configuration (a structure interconnecting measurements/setpoints and manipulated variables)

5. Selection of controller type (controller law specification, e.g. MPC).

A review of plantwide control is given by Larsson & Skogestad (2001) (who also propose a *plantwide control design procedure*).

The selection of *controlled variables* is emphasized in the plantwide control design procedure. We here distinguish between primary and secondary controlled variables. The *primary controlled variables* deal with achieving some overall operational objectives. The *secondary controlled variables* deal with stabilizing and achieving acceptable dynamic performance for the system. The primary and secondary controlled variables have different time scales: Primary controlled variables deal mainly with slow (close to steady-state) actions, while secondary controlled variables deal with fast (dynamic) actions.

The idea of self-optimizing control is to find a set of controlled variables that gives a small loss with constant setpoints in spite of varying disturbances and implementation errors (Skogestad 2001). By finding a set of controlled variables with good self-optimizing properties we may not need online optimization at all. Online optimization may give larger loss due to implementation errors and unmeasured disturbances. Self-optimizing control is discussed in Skogestad (2000a) and Skogestad (2000c).

The idea is applied and developed through several case studies which include a Petlyuk distillation column (Halvorsen, Serra & Skogestad 2000) (Alstad & Skogestad n.d.), a reactor, separator and recycle process (Larsson, Skogestad & Yu 1999), the Tennessee Eastman process (Larsson, Hestetun, Hovland & Skogestad 2001), heat integrated distillation columns (Engelien, Larsson & Skogestad 2001), heat integrated distillation columns with pre-fractionator (Engelien et al. 2001), distillation column (Skogestad 2000b), heat-exchanger networks (Glemmestad, Skogestad & Gundersen 1999) (Lid & Skogestad 2001) and gas-lift allocation optimization (Alstad & Skogestad 2003).

Except from Glemmestad et al. (1999) and Lid & Skogestad (2001) they all used constant nominal setpoints. Glemmestad et al. (1999) used constant robust setpoints and Lid & Skogestad (2001) used nominal setpoints with online feasibility correction.

Halvorsen, Skogestad, Morud & Alstad (2003) and Alstad & Skogestad (n.d.) deal with short-cut methods for selecting controlled variables and with identification of optimal linear combination of measurements to use as controlled variables.

1.3 Thesis overview

Chapter 2-7 contain 6 case studies, whereafter chapter 8 sums up the conclusions. Chapter 3 is supplemented by Appendix A and B. Appendix A contains more details about robust optimization. Appendix B shows an illustrating example of online feasibility correction. Appendix C supplements chapter 5 with the model.

Chapter 2 motivates the need for studying the feasibility problem, which is covered in detail in chapter 3. In chapter 2 we apply a systematic approach (Skogestad 2000a) for selecting controlled variables with constant nominal setpoints for the liquid phase reactor with recycle plant (Wu & Yu 1996). Two cases are considered, i.e. minimizing the operating costs and maximizing the production rate.

Chapter 3 presents the definitions, the optimization problems and the extended method for selecting controlled variables to include constant robust setpoints ("optimal backoff") and nominal setpoints with feasibility correction ("flexible backoff"). The ideas are applied to two processes, the reactor, separator recycle process with given feed (Wu & Yu 1996) in chapter 3 and an evaporation process (Newell & Lee 1989) in chapter 4.

In chapter 5 and 6 the selection of controlled variables based on steady-state economics is considered in the plantwide control perspective. A plantwide control design procedure proposed by Larsson & Skogestad (2001) is applied to two case studies, a combined cycle power plant and a distillation column heat-integrated with an indirect heat-pump (Koggersbøl 1995).

Chapter 7 discusses the controllability of a distillation column as function of the number of trays, respectively with fixed setpoints and fixed energy usage (which allows overpurification).

Chapter 8 sums up the conclusions from the thesis and proposes some directions for further work.

List of publications

Chapter 2:

Larsson, T., Govatsmark, M.S., Skogestad, S. and Yu, C.C.: Control Structure Selection for Reactor, Separator and Recycle Process, Ind. Eng. Chem. Res., **42**, pp.1225-1234.

Chapter 3:

Govatsmark, M.S. and Skogestad, S.: A Method for Selection of Controlled Variables and Robust Setpoints, Proc. of 42nd Scandinavian Simulation Society (SIMS) Conference, October 8-9, 2001, Porsgrunn, Norway, pp. 347-360.

Govatsmark, M.S. and Skogestad, S.: Selection of Controlled Variables and Robust Setpoints, Proc. of IFAC World Congress, Barcelona, 21-26 July 2002, Paper T-Mo-M-11-4.

Chapter 4:

Govatsmark, M.S. and Skogestad, S.: Control Structure Selection for an Evaporation Process, European Symposium on Computer Aided Process Engineering 11, Kolding, Denmark, 27-30 May 2001, Elsevier ISBN 0444507094, pp. 657-662.

Chapter 5:

Govatsmark, M.S., Skogestad, S. and Ma'mun S.: A Plantwide Control Procedure with Application to Control Structure Design for a Gas Power Plant, AIChE Annual meeting, Paper 259f, Indiannapolis, 3-8 Nov. 2002.

Chapter 6:

Govatsmark, M.S., Sobocan, G., Skogestad, S. and Glavic, P.: Application of A Plantwide Control Design Procedure to A Distillation Column with Heat Pump, Proc. Sup. Volume of European Symposium on Computer Aided Process Engineering 13, Lappeenranta, Denmark, 1-4 July 2003, pp. 21-28.

Chapter 7:

Govatsmark, M.S. and Skogestad, S.: Optimal Number of Stages in Distillation with respect to Controllability, European Symposium on Computer Aided Process Engineering 12, den Haag, Netherlands, 26-29 May 2002, Elsevier ISBN 0444511091, pp. 499-504.

Other publications:

Skogestad, S., Halvorsen, I.J., Larsson, T. and Govatsmark, M.S.: Plantwide Control: The Search for the Self-Optimizing Control Structure, Preprints 14th IFAC World Congress, Beijing, July 1999, Vol. N, 325-330.

Sobocan, G., Glavic, P., Govatsmark, M.S. and Skogestad, S.: Control and Dynamics of A Distillation Column with Heat Pump, Sup. Proc. of European Symposium on Computer Aided Process Engineering 12, den Haag, Netherlands, 26-29 May 2002.

Chapter 2

Control Structure Selection for Reactor, Separator and Recycle Process

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Authors: T. Larsson, M.S. Govatsmark, S. Skogestad and C.C. Yu

We consider the control structure selection, with emphasis on ”what to control”, for a simple plant with a liquid phase reactor, a distillation column and recycle of unreacted reactants. Plants of this kind have been studied extensively in the plantwide control literature. Our starting point is a clear definition of the operational objectives, constraints and degrees of freedom. Active constraints should be controlled to optimize economic performance. This implies for this case study that reactor level should be kept at its maximum, which rules out many of the control structures proposed in the literature from being economally attractive. Maximizing the reactor holdup also minimizes the “snowball effect”. The main focus is on the selection of a suitable controlled variable for the remaining unconstrained degree of freedom, where we use the concept of self-optimizing control, which is to search for a constant setpoint strategy with an acceptable economic loss. Both for the case with a given feedrate where the energy costs should be minimized, and for the case where the production rate should be maximized, we find that a good controlled variable is the reflux ratio L/F. This applies to single-loop control as well as multivariable model predictive control.

2.1 Introduction

A common feature of many chemical processes is the presence of recycle. Variations of a plant with reaction, separation and mass recycle, see figure 2.1, have been extensively studied in the literature (with different parameters, with and without a distillation column).

Gilliland, Gould & Boyle (1964) used this plant to study how the dynamics and steady state behavior are changed by the positive feedback introduced by the recycle. Papadourakis, Doherty & Douglas (1987) studied the changes in steady-state RGA for the distillation column caused by introducing the recycle. Price (1993) found that control of internal compositions, either distillate or reactor composition, helps the control of bottom composition. Luyben (1993abc,1994) followed up Gilliland's points and focused on the high sensitivity that

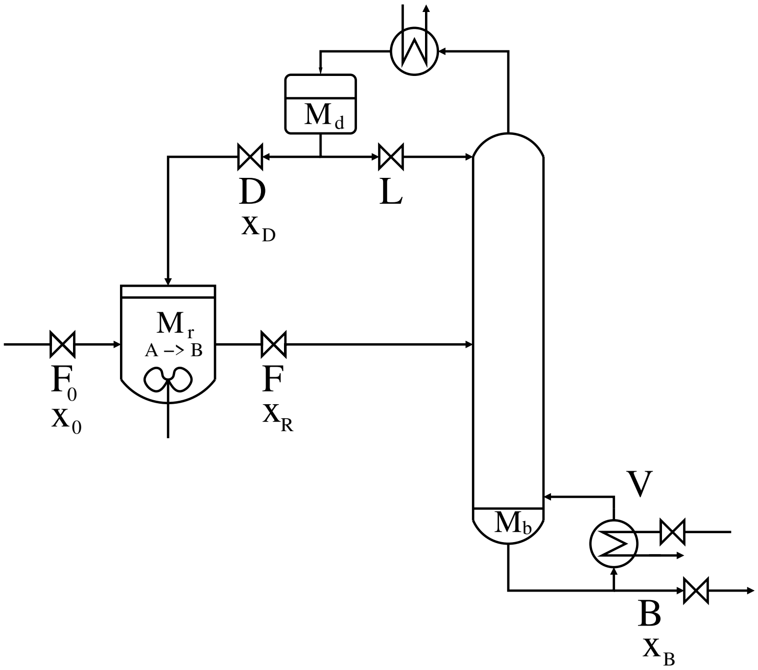

Figure 2.1: Reactor, separator (distillation) and recycle process.

the recycle flowrate in some cases has to the feed-flowrate. He called this the "snowball effect", and as a remedy proposed to let the reactor holdup vary and as a generic rule proposed that "one flowrate somewhere in the recycle loop should be flow controlled" (Luyben 1993b) Wu & Yu (1996) proposed that a better way of avoiding snowballing, was to keep constant reactor composition.

The recycle plant in figure 2.1 has four degrees of freedom at steady state: one for the throughput (feedrate F_0), one for the reactor (holdup M_r) and two for the distillation column (e.g. reflux and boilup), see also table 2.2. In the literature several alternative sets of controlled variables have been proposed for the case with a given feedrate F_0 and given (and controlled) product composition x_B:

- "Conventional" (denoted x_D in the following): Control of M_r and x_D (fixed reactor holdup and "two-point" distillation column control).

- "Luyben's structure" (LS) with varying reactor holdup: Control of F and x_D. (Luyben 1994).

- "Balanced structure I" (with varying reactor holdup): Control of x_r (reactor composition) and x_D. (Wu & Yu 1996).

- "Balanced structure II" (with varying reactor holdup): Control of F/F_0 and x_D. (Wu & Yu 1996).

- "Luyben's rule"(D or F) (Luyben 1993b) applied to case with constant reactor holdup: Control of M_r and D or F (structures CD or CF in Wu & Yu (1996)).

- "Reflux ratio" (L/F): Control of M_r and L/F (this chapter).

Here Luyben's structure (LS) and the balanced structures are "unconventional" in the sense that the reactor level is left floating, which may at first seem impossible. However, the reactor level has a steady-state effect through its effect on the conversion, and will therefore be indirectly given by specifying some other variable, for example, x_r or F. (If desired, for example for safety reasons, one may install a reactor level controller as an inner cascade, with the level setpoint replacing the flow used for level control as a degree of freedom. This will *not* affect the steady-state behavior).

The above works raise some issues that need to be studied further. First, in most of the above works, the overall operational objectives for the plant were not clearly defined. Second, a liquid phase reactor should normally be operated at maximum holdup (liquid level) in order to optimize steady-state economics, whereas the reactor level floats in the "unconventional" structures of Wu & Yu (1996) and Luyben. This has an impact on the steady state economics, an issue that has been overlooked by most researchers so far. Third, "Luyben's rule" of controlling a flow in the recycle loop (D or F) has not been properly substantiated. To the contrary, Wu & Yu (1996) found that the "Luyben structure" (LS) resulted in snowballing in the reactor holdup, and that "Luyben's rule with constant reactor holdup" (D or F) could handle only very small throughput changes.

The objective of this paper is to study in a systematic manner the selection of controlled variables for the reactor with recycle process. To this end we will use the general procedure of Skogestad (2000a), where we first define the economic and operational control objectives and identify the available degrees of freedom. *The goal is to find a self-optimizing control structure where acceptable operation under all conditions is achieved with constant setpoints for the controlled variables.* However, before describing this procedure and applying it to the case study, we discuss in some more detail the so-called snowball effect.

Plant data. The plant and design data are taken from Wu & Yu (1996). The model is simple and assumes a binary feed ($x_0 = 0.9$ mol A/mol and $F_0 = 460$ kmol/h), isothermal reactor with maximum holdup 2800 kmol, and a first-order reaction $A \rightarrow B$ with $k = 0.341$ h^{-1}. The distillation column has 22 stages including reboiler and condenser, liquid feed at stage 13, constant relative volatility $\alpha_{AB} = 2$, and constant molar flows. The purity requirement for the product is $x_B \leq 0.0105$ mol A/mol. From the total mass balance of component A, the nominal reactor concentration is

$$x_r = \frac{F_0(x_0 - x_B)}{kM_r} = \frac{460(0.9 - 0.0105)}{0.341 \cdot 2800} = 0.43 \tag{2.1}$$

2.2 The snowball effect

Luyben (1993a) introduced the term "snowball effect" to describe what can happen, for the recycle process in figure 2.1, in response to an increase in the fresh feedrate F_0. For our process, where all the feed is converted to the product, the increase in F_0 must be accompanied by a corresponding increase in the conversion in the reactor. Assume that we in figure 2.1 have a liquid phase CSTR with a first-order reaction. The amount of A converted in the reactor is then

$$kM_r x_r \quad [\mathrm{molA/s}]$$

We see that there are three options for increasing the conversion (Wu & Yu 1996):

1. Increase the reaction constant k [1/s] (e.g. by increasing the reactor temperature)
2. Increase the reactor holdup M_r [mol]
3. Increase the reactor mole fraction x_r [mol A/mol] of reactant A

We assume here that option 1 (increasing k) is not available.

Option 2 (increasing the reactor holdup) is probably the "default" way of dealing with a feedrate increase when seen from a design person's point of view. More specifically, a design person would increase all extensive variables (including flows) in the process proportionally to F_0, such that the intensive variables (compositions) in the process were kept constant. This is also the idea behind the "balanced" control structures of Wu & Yu (1996). However, changing the reactor holdup (volume) during operation may not be possible, or at least not desirable since for most reactions it is economically optimal to use a fixed *maximum* reactor volume in order to maximize per pass conversion.

Assuming k and M_r constant, the only remaining way to increase conversion is to follow option 3 and increase x_r, which can be done by recycling more unreacted A. However, the effect of this is limited, and the snowball effect occurs because even with infinite recycle D the reactor concentration cannot exceed that of pure A ($x_r = 1$). More precisely, for the process in figure 2.1 the material balance equations for component A and total mass are (Luyben 1994)

$$\text{Overall process}: \quad F_0 x_0 = Bx_B - kM_r x_r; \quad F_0 = B$$

$$\text{Column}: \quad Fx_r = Bx_B + Dx_D; \quad F = B + D$$

Here x_0, x_D and x_B denote the mole fractions of component A in streams F_0, D and B, respectively. By eliminating x_r we find:

$$F = F_0 \frac{kM_r(x_D - x_B)}{kM_r x_D - F_0(x_0 - x_B)} \tag{2.2}$$

If the reactor holdup is large relative to the feedrate, then we have almost complete conversion in one reactor pass and no recycle, so $D \approx 0$ and $F \approx F_0$, that is, the column feedrate F increases linearly with the fresh feedrate F_0. For larger values of F_0, the denominator in (2.2) will approach zero (and x_r will approach x_D), and we will experience "snowballing" with very large increases in D and F in response to only moderate increases in F_0. If the reactor holdup is too small compared to F_0, that is if

$$M_r \leq \frac{F_0(x_0 - x_B)}{kx_D} \tag{2.3}$$

then the desired steady-state is infeasible (even with infinite flow rates for D and F). In practice, because of constraints, the flow rates will not go to infinity. Most likely, the liquid

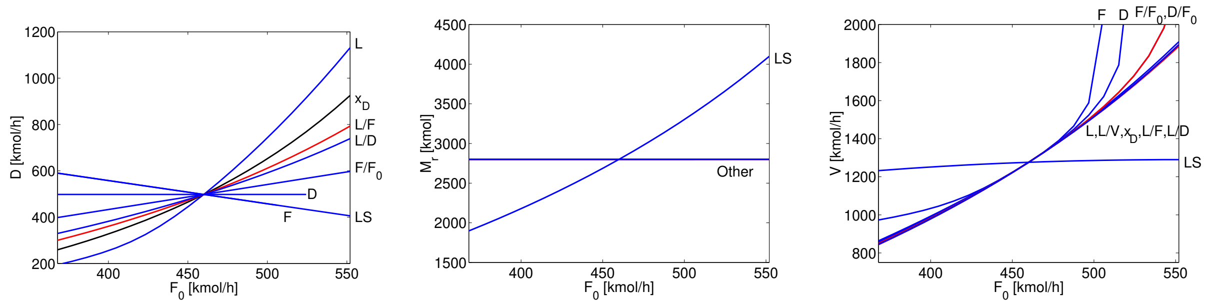

Figure 2.2: Snowballing: Steady-state values of the recycle flow (D), reactor holdup (M_r) and column boilup (V) as a function of feedrate F_0 for alternative control structures.

or vapor rate in the column will reach its maximum value, and the observed result of snowballing will be a breakthrough of component A in the bottom product, that is, we will find that we are not able to maintain the product purity specification (x_B).

To avoid this snowballing, Luyben et al. and Wu & Yu (1996) propose to use a varying reactor holdup (option 2), rather than the "conventional" control structure with constant holdup (option 3). Their simulations confirm that a variable holdup results in less snowballing in D and F, but these simulations are misleading, because they do not consider the reactor holdup. In fact, the Luyben structure (LS), with fixed D or F, may result in snowballing in the reactor holdup (Wu & Yu 1996). This is confirmed by figure 2.2, where we see that an increase in the feedrate may result in:

- Conventional structure (constant x_D) with constant reactor holdup: Snowballing in recycle flow (this is the snowballing considered by Luyben)

- Luyben structure (LS) with varying reactor holdup: Snowballing in reactor holdup

- Luyben rule (constant D or F) with constant reactor holdup: Snowballing inside column.

Actually, the snowballing in the recycle flow with the conventional structure is not even as poor as shown in figure 2.2. This is because we here used an intermediate value for the constant reactor holdup ($M_r = 2800$ kmol), whereas from (2.2) we find that the lowest value of F for a given value of F_0 is when the reactor holdup M_r is at its maximum – so with a fixed *maximum* holdup the conventional structure (x_D) actually gives smaller flows (D and F) than the Luyben structure (LS) in all cases.

In summary, the "snowball effect" is a real operational problem if the reactor (or some other unit in the recycle loop) is "too small", such that we may get close to or even encounter cases where the feedrate is larger than what the reactor (or rather the system) can handle. The "snowball effect" makes control more difficult and critical, but it is not a control problem in the sense it can be avoided by use of control. Rather, it is a design problem which could have been avoided by installing a sufficiently large reactor to begin with. In conclusion, for an existing plant the best remedy against snowballing is to use the maximum reactor holdup.

2.3 General procedure for selecting controlled variables

A plant generally has several operational degrees of freedom (manipulated variables) (there are six for our recycle plant, see table 2.2). The objective of the control system is to adjust these manipulated variables to assist in achieving acceptable operation of the plant. Thus, to design a control system in a systematic manner we first need to define the operational requirements (constraints) and the goal of the operation. In general, we have upper and lower constraints on all extensive variables in a process, and on many intensive variables. The goal of the operation is quantified by defining a scalar cost function J to be minimized. The optimum (minimum value of J) usually lies at some constraints, and usually most of the degrees of freedom are consumed to satisfy these "active" constraints. However, in many cases there are unconstrained degrees of freedom, and the difficult issue is to decide what to control (that is, what to keep at a constant setpoint) in order to satisfy these. If we used optimal setpoints and there were no uncertainty or disturbances, then this choice would not matter. However, there will always be uncertainty and disturbances, and the optimal setpoints for the controlled variables should be insensitive to such changes. In addition, the shape of the objective function should be "flat", so that an implementation error will give a small loss (Skogestad 2000a). To address this in a systematic manner, we will consider the economic loss imposed by keeping a given set of variables constant.

We assume that J is the economic cost, determined mainly by the plant's steady-state behavior, and from Skogestad (2000a) we adopt the following procedure for selecting the controlled variables:

Step 1: Degree of freedom analysis. Determine the degrees of freedom available for steady-state optimization. The easiest way is to count the number of manipulated variables and subtract the number of variables with no steady state that need to be controlled (e.g. reboiler and condenser levels in distillation).

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

Step 3: Identify the important disturbances. Here "disturbances" include process disturbances, implementation errors in the controlled variables (sum of steady-state control error and measurement noise), as well as the effect of changes and errors (uncertainty) in the model.

Step 4: Optimization. The steady-state optimization problem is solved both for the nominal case and for the identified range of disturbances.

Step 5: Identify candidate controlled variables c. Active constraints should normally be controlled, as this optimizes steady-state cost. To select between the remaining unconstrained candidates we proceed to step 6.

Step 6: Evaluation of loss. Evaluate the loss for alternative sets of controlled variables c. Here the loss is the difference between the cost with constant setpoints c_s and the theoretical optimal cost (with setpoints reoptimized for each disturbance d),

$$L = J(c_s, d) - J_{\text{opt}}(d) \tag{2.4}$$

"Self-optimizing" controlled variables c with a small loss L are preferred.

Step 7: Further analysis. Normally several candidates give an acceptable loss, and further analysis may be based on a controllability analysis.

2.4 Selection of controlled variables for the recycle plant

In this section, we use the concept of self-optimizing control, introduced above, to select the controlled variables for the recycle plant. To quantify the goals of operation, we define a scalar economic cost function J to be minimized, or equivalently, a profit function P [$/s] to be maximized. We here select P [$/h] as the difference between the value of the product B and the feed F_0, and subtract the operational costs for distillation and recycling:

$$P = -J = p_{F_0} F_0 - p_V V - p_D D \tag{2.5}$$

Here p_{F_0} [$/mol] is the difference between the product and feedstock prices and we have used $B = F_0$. $p_V V$ is the energy cost related to distillation (since the column has a liquid feed and total condenser, the vapor flows to be evaporated and condensed are approximately the same, and p_V [$/mol] is the sum of the price for reboiling and condensing). The recycle cost $p_D D$ may include costs for pumping and preprocessing (e.g. heating) the stream D. This cost is here neglected, but for gas phase systems with compression the term is usually important.

In general, the optimal way of operating the plant depends on the relative prices. However, for our problem the following two constraints are always active:

- Since the product (mostly B) is more valuable than the feedstock (mostly A), it is optimal to put as much unreacted A into the product as possible, that is, it is always economically optimal to operate with the bottom purity at its constraint (i.e. $x_B = 0.0105$).

- Since there is no economic penalty involved in increasing the reactor holdup, it is optimal for this reaction to keep M_r at its upper bound (i.e., $M_r = 2800$). This maximizes conversion "per pass", which reduces recycle and thereby the load on the distillation column.

We will in the following consider two different cases:

Case I: Given feedrate. With F_0 given and negligible recycling costs ($p_D = 0$), the profit P is only influenced by the energy costs $p_V V$ for heating and cooling in the distillation column. Thus, with a given feedrate F_0, optimal operation is obtained by minimizing the boilup V.

Case II: Variable feedrate. With F_0 as an unconstrained degree of freedom, we find that it is optimal to increase the feedrate F_0 as much as possible (since the profit P increases linearly with F_0 when we increase all other flows in proportion to F_0). However, there are always capacity constraints, and we assume here that the first one to become active is the vapor flow constraint $V \leq V_{max}$ in the distillation column. With $V = V_{max}$ and negligible recycling costs, the profit P is only influenced by the feedrate F_0. Thus, with variable feedrate, optimal operation is obtained by maximizing the feedrate (and production rate) F_0.

All the results in this section are based on a steady-state analysis. Table 2.1 summarizes the results which are further discussed below.

2.4.1 Case I: Given feedrate, minimize operation cost (energy)

Step 1: Degree of freedom analysis. From table 2.2 we see that there are 4 degrees of freedom at steady-state, including F_0.

Step 2: Cost function and constraints. As noted above the objective is to minimize the vapor boilup, i.e. $J = V$. There are constraints on the reactor holdup (M_r), product quality (x_B) and column capacity (boilup V). In addition the feedrate F_0 is given.

Step 3: Disturbances. The main disturbance is in the feedrate F_0, and we consider $\pm 20\%$ changes. We also consider disturbances in the feed composition, $x_0 = 0.9 \pm 0.1$, but these turn out to be of much less importance. The implementation error is assumed to be $\pm 20\%$ in each of the candidate variables, and we also consider a ± 0.002 implementation error (possibly caused by poor dynamic control) in the product composition x_B. (Other possible disturbances, not considered here, include a change in the reaction rate constant k, and a change in the reactor holdup M_r).

Step 4: Optimization. Table 2.3 shows the results of the nominal optimization. As expected, the two constraints on x_B and M_r are active. Since the feedrate F_0 is given, we are then left with one unconstrained degree of freedom.

Step 5: Candidates for control. We choose to control the active constraints in order to optimize operation, i.e. M_r and x_B are controlled. This rules out the “unconventional” structures with variable reactor holdup, including the “Luyben structure” and the “Balanced structures”.

Some of the candidates for the remaining degree of freedom are listed in table 2.1. Two candidate variables have already been eliminated:

- The reactor composition x_r cannot be specified independently and is thus not a candidate for control. This follows from (2.1), since the feed is given (F_0 and x_0) and x_B and M_r are controlled at their constraints.

- The boilup V in the column is not a candidate for control as specifying it below its minimum (optimum) value results in infeasible operation.

	CASE I: MIN. OPERATION COST (ENERGY)		CASE II: MAX. PRODUCTION RATE	
Step 1: Degree of freedom analysis (see table 2.2)				
	Degrees of freedom at steady-state	4	Degrees of freedom at steady-state	4
Step 2: Cost data				
	Objective function		Objective function	
	minimize V		maximize F_0	
	Constraints		Constraints	
	Reactor level $M_r \leq 2800$		Reactor level $M_r \leq 2800$	
	Product quality $x_B \leq 0.0105$		Product quality $x_B \leq 0.0105$	
	Feedrate $F_0 = F_{0,max} = 460$		Vapor boilup $V \leq V_{max} = 1500$	
Step 3: Identify most important disturbances				
	Disturbances		Disturbances	
	Feedrate $F_{0,max} \pm 20\%$		Maximum vapor boilup $V_{max} \pm 20\%$	
	Implementation error $\pm 20\%$		Implementation error $\pm 20\%$	
Step 4: Optimization				
-	Active constraints at the optimum	3	Active constraints at the optimum	3
	M_r, x_B, F_0		M_r, x_B, V	
=	Unconstrained degrees of freedom	1	Unconstrained degrees of freedom	1
	Nominal optimum: V=1276		Nominal optimum: F_0=497.8	
Step 5: Identify candidate controlled variables for unconstrained DOF (c)				
	F, L, D, $\frac{L}{D}$, $\frac{L}{F}$, $\frac{L}{V}$, x_D, $\frac{F}{F_0}$, $\frac{D}{F_0}$		F, L, D, $\frac{L}{D}$, $\frac{L}{F}$, $\frac{L}{V}$, x_D, $\frac{F}{F_0}$, $\frac{D}{F_0}$	
Step 6: Evaluation of loss with constant nominal setpoint, $c = c_s$)				
	Good candidates		Good candidates	
	x_D, L/F, L/D		x_D, L/F, L/D	
	Poor candidates		Poor candidates	
	F, D, L, F/F_0, D/F_0, L/V		F, D, L, F/F_0, D/F_0, L/V	
Step 7: Further analysis.				
	Ratio control (L/F or L/D) is easier than composition control (x_D).			
Conclusion				
	Control $\frac{L}{F}$ or $\frac{L}{D}$ (+ active constraints M_r, x_B, F_0)		Control $\frac{L}{F}$ or $\frac{L}{D}$ (+ active constraint M_r, x_B, V)	

Table 2.1: Summary of self optimizing control analysis.

	Manipulable variables	6
	Product flow B	
	Vapor boilup V	
	Reflux L	
	Recycle (distillate) D	
	Reactor effluent F	
	Feed F_0	
-	Controlled variables with no steady state effect	2
	Condenser level M_D	
	Boiler level M_B	
=	Degrees of freedom at steady state	4

Table 2.2: Degrees of freedom analysis.

	Case I: Min. V	Case II: Max. F_0	
Feedrate F_0	460	497.8	[kmol/h]
Reactor effluent F	958	1113	[kmol/h]
Vapor boilup V	1276	1500	[kmol/h]
Reflux L	778	885	[kmol/h]
Recycle (distillate) D	497	615	[kmol/h]
Recycle composition x_D	0.82	0.83	[mol A/mol]
Bottom composition x_B	0.0105	0.0105	[mol A/mol]
Reactor composition x_r	0.43	0.46	[mol A/mol]
Reactor holdup M_r	2800	2800	[kmol]

Table 2.3: Nominal optimization results for the two cases.

Step 6: Evaluation of the loss. Figure 2.3 shows the loss in energy (i.e., increase in boilup V) imposed by keeping alternative controlled variables fixed at their nominal setpoints. The losses due to implementation errors (third row) and disturbances in F_0 (first row) are quite large for some variables. For example, we see from the first row that with L constant (left plot) a decrease in feedrate by 10%, results in using about 5% more energy than the optimal; this is reduced to less than 0.1% if we keep x_D constant and less than 0.01% if we keep L/F constant (right plot). The disturbances in feed composition x_0 (second row plots) result in very small losses in all cases. The loss due to a backoff in bottom composition from 0.0105 to 0.0085 is about 3% for all structures (last row).

In summary, figure 2.3 shows that control of x_D, L/F or L/D give small losses (right plots), while control of F, D, L, L/V, F/F_0 or D/F_0 give large losses (left plots). In particular, we find that Luyben's rule of fixing one flow in every recycle loop, corresponding to fixing D or F, results in very large losses and even infeasibility, because V goes to infinity when F_0 increases (left plot in second row).

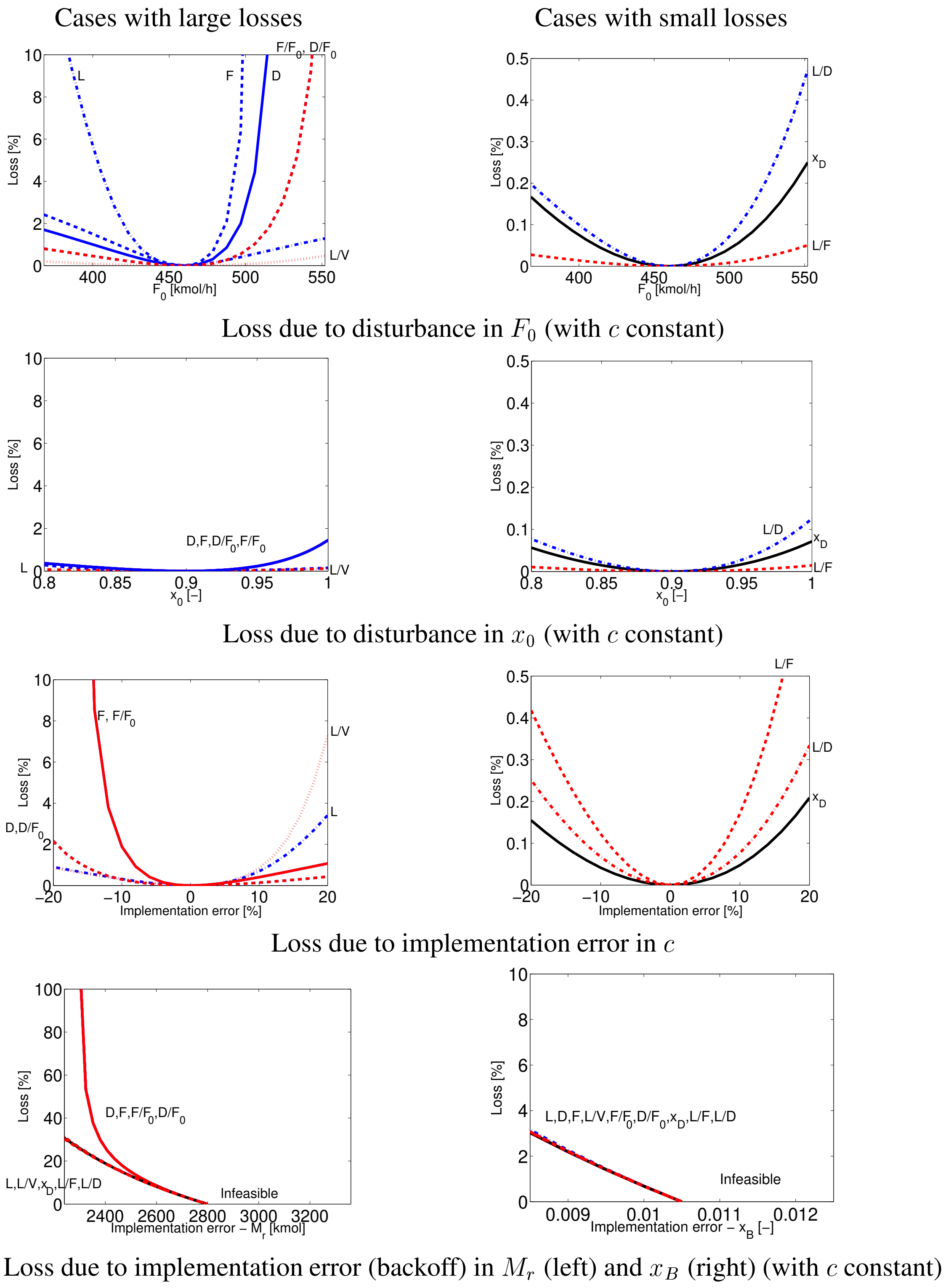

Figure 2.3: Case I: Losses in energy (V) with alternative controlled variables ($F_0 = 460, M_r = 2800, x_B = 0.0105$).

Step 7: Other considerations. The conventional control configuration with maximum reactor holdup (M_r), constant product composition x_B and constant setpoint for the distillate composition (x_D) has very good self-optimizing properties with small economic losses. However, it may be costly to obtain online measurements of x_D, and two-point distillation composition control (of x_D and x_B) is known to be a difficult control problem due to interactions. In any case, the analysis shows that control of the internal distillate composition x_D is not really needed, since in terms of economic loss, control of L/F (or L/D) performs almost equally well. The latter results in a simple control problem and is therefore preferred. Figure 2.4 shows a possible control structure involving the following single loops: $M_r \leftrightarrow F$, $L/F \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

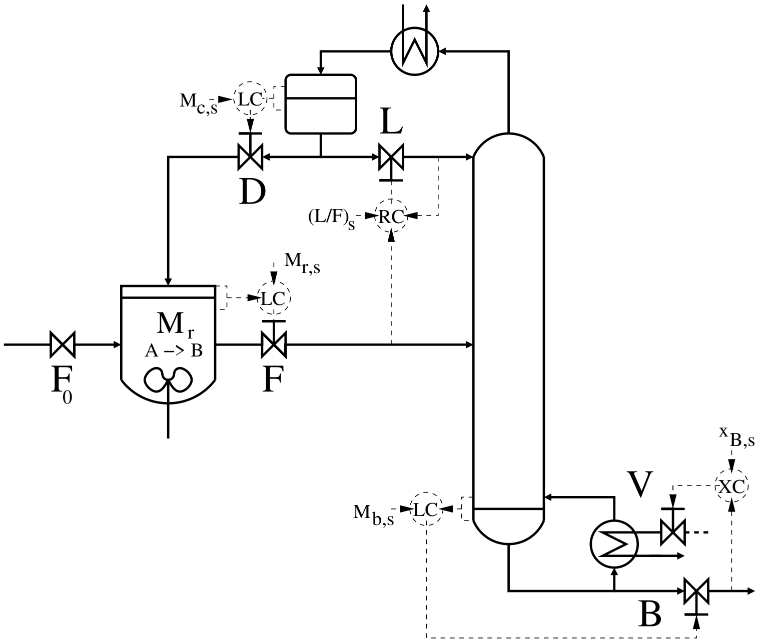

Figure 2.4: Reflux ratio control structure (Case I with given feedrate)

2.4.2 Case II: Maximize the feedrate

We now consider the case where the feedrate is a degree of freedom and should be maximized. This case is of more practical importance, since small losses in production rate usually have a large impact on overall plant economics.

Step 1: Degree of freedom analysis. As before, there are four degrees of freedom at steady state, see table 2.2.

Step 2: Cost function and constraints. The goal here is to maximize the production rate, i.e. to minimize $J = -F_0$, and there are constraints on vapor boilup, reactor holdup and product composition.

Step 3: Disturbances. The main disturbance is in the actual value of the (maximum) boilup V_{max}, which may vary, for example, due to variations in the column pressure or available heat to the column.

Step 4: Optimization. Table 2.3 shows the results from the nominal optimization. We find as expected that all three constraints are active, including the maximum constraint on the vapor boilup. This leaves one unconstrained degree of freedom.

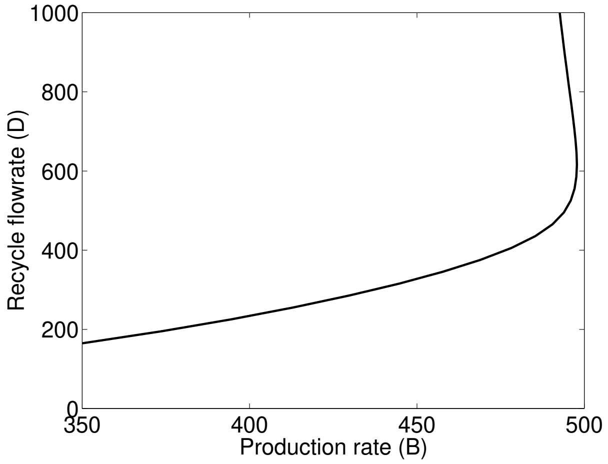

Figure 2.5: Snowballing with V constant: Recycle flow D as a function of production rate $B = F_0$ (Case II, $M_r = 2800$, $x_B = 0.0105$, $V = 1400$).

To understand why the production rate is limited, consider figure 2.5. At low production rates (F_0) there is almost a linear relation between D and F_0. But as F_0 is increased, the load to the distillation column increases ($F = F_0 + D$ increases), and since $V = V_{max}$ is constant we eventually experience "snowballing" with breakthrough of product B in the top of the column. This results in a decrease (rather than the desired increase) in the fraction x_r of A in the reactor, and the production rate drops. This happens at $F_0 = 492.6$ kmol/h (the optimal point).

Step 5: Candidates for control. We consider the same candidate variables as in case I.

Step 6: Evaluation of the loss. Figure 2.6 shows the loss in production rate due to a disturbance in V and due to implementation error. Although the details are different, the results are similar to case I, with small losses for control of x_D, L/F and L/D.

Step 7: Other considerations. Again, since controlling L/F or L/D gives a much easier control problem for the distillation column it will be preferred over control of x_D. A possible control structure is shown in figure 2.7. To be able to handle also case I, we have included a cascade flow control loop where we obtain $F_0 = F_{0,s}$ by adjusting V, but this flow control (FC) loop is not used in case II where we have maximum vapor boilup ($V = V_{max}$).

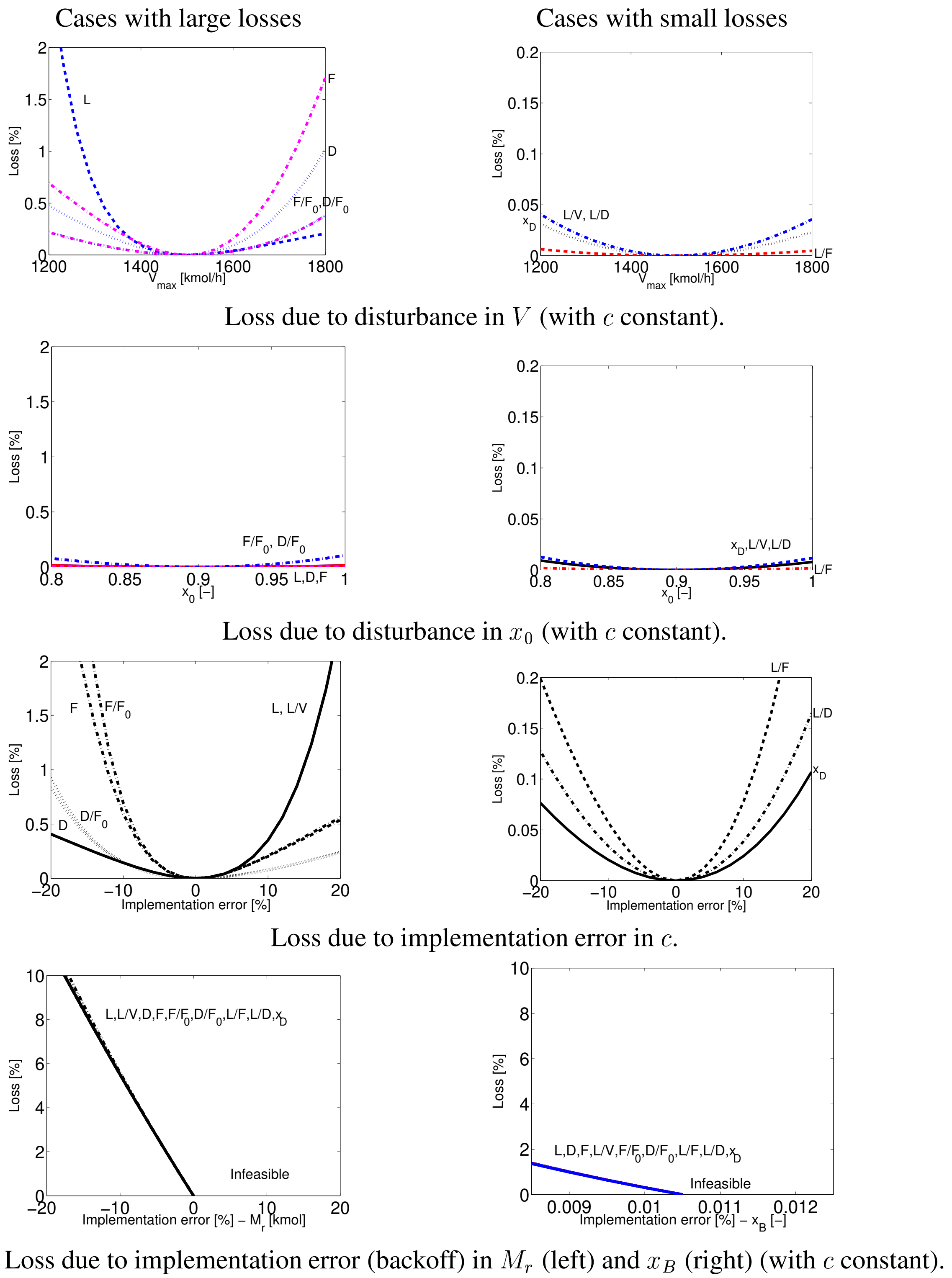

Figure 2.6: Case II: Losses in production rate (F_0) for alternative controlled variables ($V = 1500$, $M_r = 2800$, $x_B = 0.0105$)

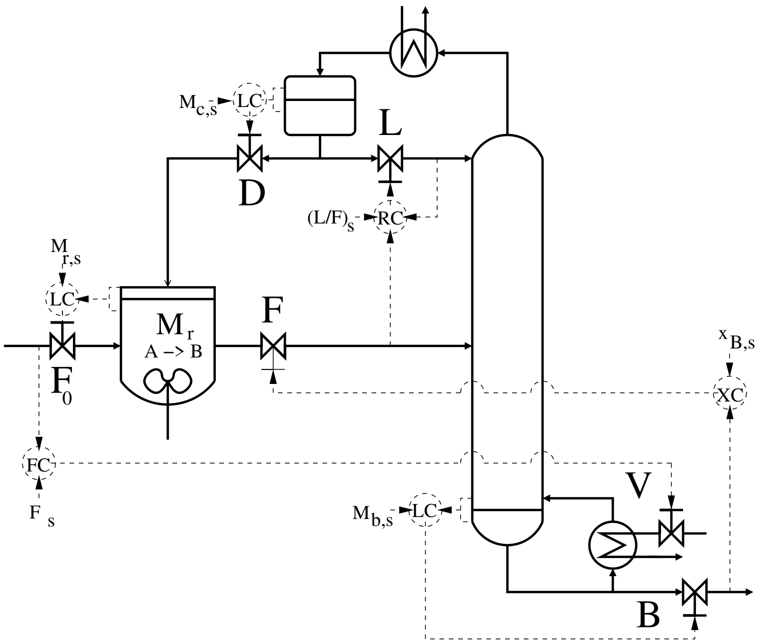

Figure 2.7: Reflux ratio control structure for case II (with flow control loop to handle also case I)

Comment: The same variable, L/F or L/D, turned out to be a good unconstrained controlled variable for both cases I and II. This is generally attractive, as it may reduce the effort in reconfiguring the loops when, for example, the economic conditions change from case I (given production) to case II (maximize production).

2.5 Closed-loop simulations

In figure 2.8 we show for case I (given feedrate F_0, no capacity limit on V) the closed-loop dynamic responses in bottom composition to a 20% increase in feedrate F_0 for the following structures:

Conventional (x_D) : $M_r \leftrightarrow F$, $x_D \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Reflux ratio (L/F) : $M_r \leftrightarrow F$, $L/F \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Luyben rule (F) : $M_r \leftrightarrow D$, F constant, $x_B \leftrightarrow V$, $M_D \leftrightarrow L$ and $M_B \leftrightarrow B$.

Luyben structure (LS) (varying reactor holdup): F constant, $x_D \leftrightarrow L$, $x_B \leftrightarrow V$, $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$.

Note that we have used single-loop controllers and $\leftrightarrow$ means "is paired with" or more precisely "is controlled by". The pairings are based on a relative gain array analysis, and PI-settings are found using the IMC-tuning approach. We selected 0.25 min as the desired closed-loop time constant for the level loops and 2.5 min for the other loops. For the three first structures we have constant maximum reactor holdup, $M_r = 2800$ kmol.

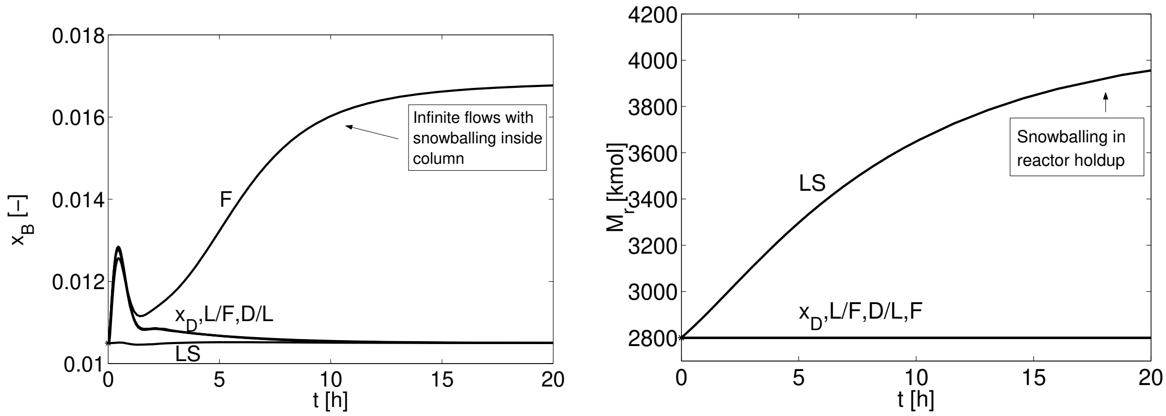

Figure 2.8: Dynamic responses in x_B (left) and M_r (right) to a 20% step increase in F_0 (Case I) for alternatice control structures
x_D : Conventional structure (constant x_D and M_r)
$D/L, L/F$: Reflux ratio structures (constant D/L or L/F and M_r)
F : Luyben rule for case with constant M_r (constant F and M_r)
LS : Luyben structure with varying reactor holdup (constant F and x_D)

The conventional structure and reflux ratio structure yield very similar and acceptable dynamic responses.

The Luyben rule with constant F for the case with constant reactor holdup yields instability. It is not able to maintain the desired bottom composition even for small increases in the feedrate. This confirms the steady-state results in figure 2.3 and the findings of Wu & Yu (1996). This is easily explained: As the feedrate F_0 is increased, we must with constant $F = F_0 + D$ reduce the recycle D to the reactor (which is the opposite of what we would like to do). This results in snowballing inside the distillation column with accumulation of unreacted component A, and operation eventually becomes infeasible.

The Luyben structure (LS) (with varying reactor holdup) clearly yields the best dynamic response in x_B; this is because the varying reactor holdup serves as a surge tanks which helps to smooth (average out) the feedrate disturbance. However, the response in x_B for the Luyben structure is unrealistic since we have allowed the reactor level M_r to exceed its maximum value, and we see from the right plot in figure 2.8 that there is actually a snowballing in the reactor level (Wu & Yu 1996). To guarantee feasibility ($M_r \leq M_{r,max}$) for feedrate changes, we would for the Luyben structure need to "back away" from the reactor level constraint (using a nominal holdup significantly smaller than $M_{r,max}$), which would give non-optimal economic operation with about 50% higher energy usage (V) in the distillation column, or even worse, inability to handle the desired feedrate due to capacity limitations in the distillation column.

On the other hand, if we for the other structures (with constant holdup) introduce a back-off in bottom composition x_B from 0.0105 to 0.0085 (in order to handle the control variations in figure 2.8) then the increase in energy usage (V) is only by about 3% (see lower plot in figure 2.3). Alternatively, we may avoid the need for backoff in x_B (and the resulting 3% energy increase) by using a product tank with mixing to average out the dynamic variations in x_B.

2.6 Discussion

2.6.1 Alternative sets of active constraints

We have in this chapter considered case I with a given feedrate and case II with an unconstrained feedrate, and these resulted in two different control structures. What other cases are there? We here define a "case" in terms of the set of active constraints. For our recycle plant the following four upper constraints are of interest:

$$x_B \leq x_{B,max}, \quad M_r \leq M_{r,max}, \quad F_0 \leq F_{0,max}, \quad V \leq V_{max}$$

Here, as explained earlier, the economic conditions are such that the two first constraints are always active, and at least one of the two latter constraints are active. We are then left with only three cases:

Case I : Constraint on $F_{0,max}$ is active and V is unconstrained. This happens for low values of the available feedrate $F_{0,max}$ (or large values of V_{max}), where it is optimal to process all the available feed while minimizing the value of V.

Case II : Constraint on V_{max} is active and F_0 is unconstrained. This happens for high values of $F_{0,max}$ (or low values of V_{max}), where the available feedrate $F_{0,max}$ exceeds the optimal maximum feedrate.

Case III : Constraints on $F_{0,max}$ and V_{max} are both active. This happens for intermediate values of the available feedrate $F_{0,max}$, provided there is some penalty on recycle, i.e. $p_D > 0$.

The details depend on the cost function $-J = p_{F_0}F_0 - p_V V - p_D D$. The feedrate range where case III is economically optimal is often quite small, especially if recycle costs are small compared to distillation costs. In this chapter we have assumed no recycle costs ($p_D = 0$) and we go directly from case I to case II. For example, with $p_D = 0$ and $V_{max} = 1500$ [kmol/h], we have case I for $F_{0,max} \leq 468.6$ and case II for $F_{0,max} \geq 468.6$. With recycle costs included ($p_D > 0$) it is optimal to use more energy in the distillation column, and we get a region where both constraints are active (case III). For example, with the cost function $-J = F_0 - 0.01V - 0.1D$ (i.e., $p_{F_0} = 1, p_V = 0.01, p_D = 0.1$) and $V_{max} = 1500$, we have case I for $F_{0,max} \leq 468.6$, case III (both constraints active) for $468.6 \leq F_{0,max} \leq 493.2$, and case II for $F_{0,max} \geq 493.2$. Note here that the economic maximum capacity of 493.2 is somewhat less than the achievable maximum capacity of 497.8 [kmol/h].

In the above discussion we have considered the "available feedrate" $F_{0,max}$ (inequality constraint $F_0 \leq F_{0,max}$). For the closely related case with a "given feedrate" ($F_0 = F_{0,max}$)

we have the following: At low feedrates F_0 we have case I with V unconstrained. As the feedrate increases, the boilup V also increases (the change in V for a small change in F_0 may be large if we experience snowballing), and eventually the column reaches its capacity limit (V_{max}). With constant boilup ($V = V_{max}$), it may be possible to increase the feedrate further by reducing the distillate purity x_D and increasing the recycle (case III) , but eventually the column becomes a bottleneck (case II) where it is not feasible to process any more feed while maintaining the given product composition.

Comment: The fact that the distillation column is a bottleneck in case II, does not necessarily mean that production rate can be much increased by increasing its capacity V_{max}, because if the system is close to snowballing, then increasing $M_{r,max}$ is the only effective way of increasing plant capacity.

2.6.2 Decentralized control and reconfiguration of loops

The focus in this paper is to decide on which variables to control, and we have recommended to use the "reflux ratio" structure with control of L/F. The analysis has been based on steady-state economics, and is independent of the actual implementation. However, in the closed-loop simulations we assumed decentralized control, where each controlled variable was paired with a manipulated input. A main problem with decentralized control is that reconfiguration of loops is generally required when the active constraints change. Let us consider this in more detail for our proposed reflux ratio structure.

We have already proposed pairings for cases I and II. In the intermediate case III there are no unconstrained degrees of freedom, that is, the economic optimal control structure is to use all four steady-state degrees of freedom to control the active constraints. A possible control structure for case III is then: $M_r \leftrightarrow F, x_B \leftrightarrow L, F_0 = F_{0,max}, V = V_{max}, M_D \leftrightarrow D$ and $M_V \leftrightarrow B$. Note that the reflux L is here used to control bottom composition. In summary, we then have for the "reflux ratio" structure (in all cases we use $M_D \leftrightarrow D$ and $M_B \leftrightarrow B$):

$$\begin{array}{rllll} \text{Case I}: & M_r \leftrightarrow F & L/F \leftrightarrow L & F_0 = F_{0,max} & x_B \leftrightarrow V \\ \text{Case II}: & M_r \leftrightarrow F_0 & L/F \leftrightarrow L & V = V_{max} & x_B \leftrightarrow F \\ \text{Case III}: & M_r \leftrightarrow F & F_0 = F_{0,max} & V = V_{max} & x_B \leftrightarrow L \end{array}$$

We note that two loops (control of M_r and x_B) need to be reconfigured as we go from case I to case II. To minimize the need for reconfiguration we may use the inflow F_0 to control the reactor level in all cases (this corresponds to setting the production rate at the column bottleneck (V) in all cases). We then get the control structure in figure 2.7:

$$\text{Case I}: \quad M_r \leftrightarrow F_0 \quad L/F \leftrightarrow L \quad F_0 \leftrightarrow V \quad x_B \leftrightarrow F$$

In this case no reconfiguration is required as we go between cases I and II. The disadvantage is that control of feedrate F_0 is indirect so F_0 will deviate from $F_{0,max}$ when the process is disturbed. However, if we have a storage tank for the feed then this does not matter as the variations will average out over time.

2.6.3 Multivariable constraint control (MPC)

To avoid the logic in reconfiguring loops when switching between cases I, II and III, one may use a multivariable controller with explicit handling of constraints (e.g. model predictive control, MPC) that "automatically" reconfigures the control tasks when the active constraints change. However, also here one needs to decide on what variables to setpoint control to satisfy the unconstrained degrees of freedom (cases I and II). Thus, our recommendation of controlling the reflux ratio (L/F) applies also to MPC. The objective of the model predictive controller would then be to control x_B (first priority) and L/F (second priority) at their setpoints (and possibly also the reactor level, condenser level and reboiler level, but we assume these are controlled by a lower-layer level control system), using the degrees of freedom F_0, V and L (assuming here that F, D and B are used for level control in the lower layer), subject to given constraints on F_0 and V. The setpoints which may vary with time, are supplied by the layer above MPC. This may be a steady-state optimizer or an operator.

2.6.4 Economics not important

We have in this study excluded the "unconventional" control structures with variable reactor holdup (Luyben 1994) (Wu & Yu 1996) from being economically optimal. However, with a given feedrate F_0, low energy and recycle costs (p_V and p_D small), and no capacity constraints (V_{max} large), the economic penalty of using $M_r < M_{r,max}$ may be small, and it may be more important to operate the plant as smoothly as possible, for example, to reduce the effect of disturbances on other parts of the plant. In such cases, a variable reactor holdup structure, such as one of the balanced structures of Wu & Yu (1996), may be better, because the reactor is effectively used as a surge tank to "average out" disturbances in the column feedrate. Nevertheless, we do *not* recommend the Luyben structure (LS) (Luyben 1994) with a fixed flow in the recycle loop, since it results in snowballing in the reactor holdup (Wu & Yu 1996); see also figure 2.8. This is also explained since we in response to an increase in feedrate clearly should increase the recycle (and not keep it constant).

2.7 Conclusion

We have presented a systematic approach for selecting controlled variables for the liquid phase reactor with recycle plant. To optimize economics we need to control active constraints. Both for the cases of minimizing operating costs (case I) and maximizing production rate (case II), it is optimal to keep the reactor holdup at its maximum. This makes the Luyben structure (LS) and the two balanced structures of Wu & Yu (1996) economically unattractive. For the unconstrained variables we look for self-optimizing variables where constant setpoints give acceptable economic loss. Both in cases I and II, the reflux ratio (L/F or L/D) appears to be such a variable. In order to avoid the so-called "snowball effect", it has been proposed in the literature to "fix a flow in a liquid recycle loop". However, the rule seems to have limited basis, as it leads to control structures that can handle only small feedrate changes (constant reactor holdup), or that result in large variations in the reactor holdup (variable reactor holdup) (Wu & Yu 1996).

Chapter 3

Selection of Controlled Variables and Robust Setpoints

Based on work presented at the 10th Nordic Process Control Workshop, Åbo, Finland, Aug. 23-25, 2001 and at the 42nd Scandinavian Simulation Society (SIMS) Conference, Porsgrunn, Norway, Oct. 8-9, 2001 and at the 15th International Federation of Automatic Control (IFAC) World Congress, Barcelona, Spain, July 21-26, 2002

The idea of self-optimizing control is “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” (Morari, Arkun & Stephanopoulos 1980). Skogestad (2000a) presents a method for selection of controlled variables, based on steady-state economics. In the simplest case the setpoints for the controlled variables are fixed at their nominally optimal values. However, because of disturbances this may result in feasibility problems, which we here try to avoid by adjusting the setpoints (”backoff”). First, we need to avoid infeasibility in the active constraints (”constraint backoff”) (Perkins, Gannavarapu & Barton 1989). Second, we need to adjust the setpoints of the unconstrained controlled variables. This may be done by offline computation of robust setpoints (”optimal backoff”) or by online feasibility correction (”flexible backoff”). As a case study we consider a reactor-separator-recycle process. For this process the control structures based on Luybens rule (“fix a flow in every recycle loop”) are infeasible if we use the nominal setpoints, but are feasible with reasonable loss if we use robust setpoints.

3.1 Introduction

This chapter is concerned with the *implementation* of an optimal operation policy. We consider a strategy where the optimization layer sends setpoints for the controlled variables to be implemented by the control layer, see figure 3.1.
There are two classes of problems:

- *Constrained*: At the optimal solution all the optimization degrees of freedom are used to satisfy active constraints for all expected disturbances.

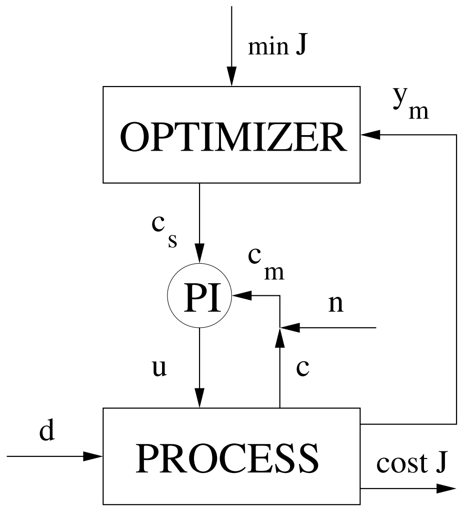

Figure 3.1: A typical optimization system incorporating local feedback: The process is disturbed (d) and the control system tries to keep the controlled variables (c) at their setpoints (c_s). Steady-state optimization based on process measurements (y_m) is performed at regular intervals to track the optimum by updating the setpoints.

- *Unconstrained or partially constrained* (the focus of this chapter): One or more of the optimization degrees of freedom are unconstrained for all or some expected disturbances.

Two important decisions are to be made:

- Decision 1: *Selection of controlled variables (c)*: This is a *structural* decision which is made offline before implementing the control strategy.
- Decision 2: *Selection of setpoints (c_s)* for the controlled variables. This is a *parametric* decision which is done offline or online.

For the constrained variables, active constraint control should be used and the variables lying on the optimally active constraints should be controlled (Maarleveld & Rijnsdorp 1970). To remain feasible it may be necessary to back off from the optimal value of the constraints, for example when the constraints are difficult to measure or difficult to control due to poor dynamics. This is here called "(simple) constraint backoff" and is thoroughly discussed by Perkins and co-workers, e.g. Perkins et al. (1989), Narraway, Perkins & Barton (1991), Narraway & Perkins (1993), Narraway & Perkins (1994), Kookos & Perkins (2002a) and Kookos & Perkins (2002b). An exception to the rule of using active constraint control is when the optimally active constraints may move, and in order to avoid reconfiguration we choose to control unconstrained variables with good self-optimizing properties. Tracking optimally active constraints which are moving due to disturbances is discussed by Arkun & Stephanopoulos (1980).

For unconstrained or partly unconstrained problems the selection of what to control (Decision 1) is crucial. Skogestad (2000a) presents a method based on minimizing the steady-state loss with constant nominal setpoints. However, in many cases the results are sensitive to the magnitude of the disturbances, and we may get infeasibility for large disturbances and implementation errors. This may result in unstable operation. To avoid infeasibility it may be necessary to backoff from the nominal optimum (Decision 2), for example by using robust optimization (Glemmestad et al. 1999). In this case the effect of the ”uncertainty” (disturbances and implementation errors) is reduced both through the selection of controlled variables and their setpoints.

3.2 Some definitions

All further considerations are based on a steady-state analysis, unless stated otherwise. A summary of the notation is shown in table 3.1. All variables are vectors, unless stated otherwise. An element in a vector is denoted with a subscript j. A given operating point is denoted with a subscript i.

3.2.1 Degrees of freedom

The number of *dynamic degrees of freedom* is equal the number of manipulated variables. The number of *steady-state degrees of freedom* can be found by counting the manipulated variables, subtracting the number of variables that need to be controlled but which have no steady-state effect, and subtracting the number of manipulated variables with no steady-state effect. The number of *degrees of freedom for steady-state optimization* (here denoted u) is often equal the number of steady-state degrees of freedom, and this assumption is made in this chapter. The number of *unconstrained steady-state degrees of freedom* is equal the number of steady-state degrees of freedom minus the number of active constraints at the optimum.

3.2.2 Optimal operation

The optimal operation for a given disturbance (d) can be found by solving the following problem:

$$\begin{aligned} &\min_{x,u} J(x,u,d) \\ &f(x,u,d) = 0 \\ &g(x,u,d) \leq 0 \end{aligned} \tag{3.1}$$

The scalar objective function J describes the cost (quality) of operation, f represents the process model and equality constraints, g is the inequality constraints related to operation, u is the independent variables (*manipulated variables* or *inputs*) we can affect, d is the independent variables (*disturbances*) we cannot affect, and x is the internal variables (*states*). The inequality constraints typically include upper and lower bounds on the input and output variables. In addition to the external disturbances d, we must also during actual implementation consider the ”implementation” disturbances (implementation errors d_c and d_g, see later), but these are not included in the above ”open-loop” optimization problem.

Table 3.1: Notation

Δd	deviation from nominal disturbances
Δd_c	deviation from nominal implementation errors in controlled variables
Δd_g	deviation from nominal implementation errors in constraints
b	backoff or setpoint adjustments
b_0	constraint backoff
b_{flex}	flexible backoff
b_{opt}	optimal backoff
c	controlled variables
$\hat{c}$	controlled variables computed online
c_I	controlled variables with high priority
c_{II}	controlled variables with low priority
c_m	measured controlled variables
c_s	setpoints
$c_{s,0}$	nominal setpoints, "corrected" nominally optimal setpoints
c_{flex}	flexible setpoints
$c_{I,flex}$	adjusted setpoints for controlled variables with high priority
$c_{II,flex}$	adjusted setpoints for controlled variables with low priority
$c_{I,s}$	setpoints for controlled variables with high priority
$c_{s,opt}$	optimal setpoints
$c_{s,ref}$	reference values for the setpoints
$c_{s,robust}$	robust setpoints, robustly optimal setpoints
D_c	expected controlled variable implementation error region
D_d	expected disturbance region
D_d^{total}	total feasibility region
D_g	expected constraint implementation error region
$\tilde{D}_{dc}$	expected disturbance and controlled variable implementation error region
$\tilde{D}_{dc}^{c}$	constant setpoint policy feasibility region
$\tilde{D}_{dc}^{c,nom}$	constant setpoint policy feasibility region with nominal setpoints
$\tilde{D}_{dc}^{econ}$	economic disturbance and controlled variable implementation error region
$\tilde{D}_{dcg}$	expected disturbance and implementation error region
$\tilde{D}_{dcg}^{flex}$	feasibility region with online feasibility correction (flexible setpoints)
d	disturbances
d_0	nominal disturbances
d_c	implementation errors in controlled variables
$d_{c,0}$	nominal implementation errors in controlled variables
$d_{c,max}$	maximum expected implementation errors in all controlled variables
$d_{c,max}^*$	maximum expected implementation errors in constrained controlled variables
d_g	implementation errors in constraints
$d_{g,0}$	nominal implementation errors in constraints
$d_{g,max}$	maximum expected implementation errors in constraints
$d_{g,max}^*$	maximum expected implementation errors in active constraints
d_m	measured disturbances
f	equality operational constraints (process/model)
$\hat{f}$	equality operational constraint computed online
$\lvert G(0)\rvert$	scaled steady-state process gain
g	inequality operational constraints
$\hat{g}$	inequality operational constraints computed online
g_m	measured inequality operational constraints

i	operating point
j	element in vector
J	cost
J_c	cost with specific constant setpoint policy
$J_{c,w}$	average cost with specific constant setpoint policy
J_{flex}	cost with flexibel setpoints
J_{opt}	optimal cost
J^*_{opt}	optimal cost with constraint backoff
$J_{opt,w}$	average optimal cost
L	loss
L_{max}	maximum loss
L_w	average loss
n	measurement errors
Q	diagonal weight matrix in online feasibility correction
Q_I	diagonal weight matrix for high priority controlled variables in online feasibility correction
Q_{II}	diagonal weight matrix for low priority controlled variables in online feasibility correction
u	manipulated variables or inputs
u_{flex}	manipulated variables with flexible setpoints
u_{opt}	optimal manipulated variables
u^*_{opt}	”corrected” optimal manipulated variables
w_i	weight for operating point i in the robust optizimation problem
x	internal variables or state variables
$\hat{x}$	internal variables or state variables computed online
x_{opt}	optimal internal (state) variables
x^*_{opt}	optimal internal (state) variables with constraint backoff
x_{flex}	internal (state) variables with flexible setpoints
y	output variables, usually measured
y_m	measured output variables
y_{max}	upper bounds on the output variables
y_{min}	lower bounds on the output variables

3.2.3 Constraints

We distinguish between transient and steady-state constraints, see figure 3.2. (This is similar to batch processes where it is usual to distinguish between path and endpoint/terminal constraints, see e.g. Loeblein, Perkins, Srinivasan & Bonvin (1997).) *Steady-state constraints* may be violated during transients, but not at steady-state or in average, e.g. this could be a product purity constraint. *Transient constraints* must be violated neither in transients nor at steady-state, e.g. this could be a maximum pressure constraint.

We also distinguish between *active constraints* and *inactive constraints*. For a given operating point i an active constraint j satisfies $g_{j,i} = 0$, whereas an inactive constraint j satisfies $g_{j,i} < 0$. Note here that ”optimally active constraints” are usually called simply ”active constraints”.

In most cases we identify a single measured (or estimated) variable y related to each constraint and write (depending on whether g corresponds to a minimum or maximum constraint):

$$g = y - y_{max} \tag{3.2}$$

or

$$g = y_{min} - y \tag{3.3}$$

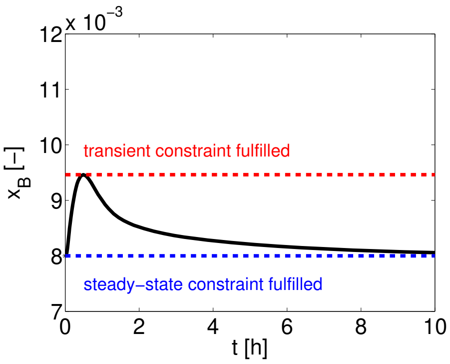

Figure 3.2: Fulfilled steady-state and transient constraint.

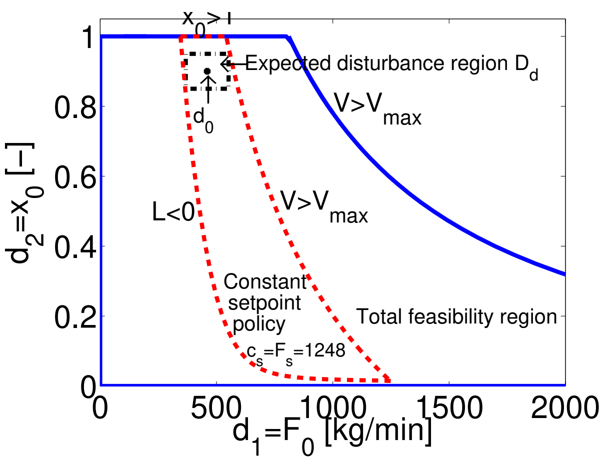

Figure 3.3: Total feasible region (D_d) (solid), feasible region for a constant setpoint policy (controlling F with robust setpoints) ($D^c_d = \{D^{c,robust}_{dc} | d_c = d^*_{c,max}\}$) (dashed) and expected disturbance region (D) (dash-dot).

3.2.4 Controlled variables

We here define the *controlled variables* c as the variables that are specified (kept constant by the control system at steady-state). The controlled variables may consist of manipulated variables, measurements or combinations of measurements and manipulated variables. The number of selected controlled variables is here assumed equal to the number of steady-state degrees of freedom.

We distinguish between *constrained controlled variables* and *unconstrained controlled variables*. A constrained controlled variable is kept constant at an active constraint by the control system.

3.2.5 Uncertainties

Uncertainties in the operation are related to external disturbances (d) and implementation errors (d_c, d_g). Implementation errors may be related to poor control or to errors in the measurements of the controlled variables and constraints.

Disturbances

Disturbances d are independent variables that we cannot affect and that are not related to the control system implementation. These variables may also include uncertainties in the model parameters.

Implementation errors

The implementation error in the controlled variable d_c is the difference between the actual value of the controlled variable c and its setpoint c_s:

$$d_c = c - c_s \tag{3.4}$$

The implementation error d_c may be written as the sum of the measurement error ($c - c_m$) and the control error ($c_m - c_s$), see also figure 3.1. With integral action in the controller, we may often disregard the effect of the dynamic control error. However, even with integral action we may not be able to reach steady-state within the time period of interest, and we then need to include the control error. For controlled variables related to transient constraints we must also include the worst-case dynamic control error (see the work of Perkins et al. (1989)).

Implementation errors in the constraints d_g should be included for the constraints that are measured (g_m) and used by the control system. *The implementation error in the constraint* d_g is the difference between the actual value of the constraint g and the measured or estimated value of the constraint g_m:

$$d_g = g - g_m \tag{3.5}$$

If we have a single measured (or estimated) variable that identifies the constraint (see equation 3.2 or 3.3), then:

$$d_{g,j} = y_j - y_{m,j} \tag{3.6}$$

For a maximum constraint:

$$d_{c,j} = d_{g,j} \tag{3.7}$$

and for a minimum constraint:

$$d_{c,j} = -d_{g,j} \tag{3.8}$$

Expected disturbance and implementation error region

A disturbance d can be expressed as the sum of its nominal value d_0 and some variation $\Delta d \in D_d$:

$$d = d_0 + \Delta d; \quad \Delta d \in D_d \tag{3.9}$$

Similarly, an implementation error in the controlled variables d_c can be expressed as the sum of its nominal implementation error $d_{c,0}$ (usually zero) and some variation $\Delta d_c \in D_c$:

$$d_c = d_{c,0} + \Delta d_c; \quad \Delta d_c \in D_c \tag{3.10}$$

and an implementation error in the constraints d_g can be expressed as the sum of its nominal implementation error $d_{g,0}$ (usually zero) and some variation $\Delta d_g \in D_g$:

$$d_g = d_{g,0} + \Delta d_g; \quad \Delta d_g \in D_g \tag{3.11}$$

The *nominal point* is given by the nominal disturbance (d_0) and the nominal implementation errors ($d_{c,0}$, $d_{g,0}$).

The expected disturbance and implementation error region $\tilde{D}_{dcg}$ = ($\{D_d, D_c, D_g\}$) consists of these expected variations. Note that *"the expected disturbance and implementation error region"* is here often simply called *"the expected disturbances and implementation errors"*. The magnitude of $\tilde{D}_{dcg}$ depends on the considered period. It is largest when the process overall lifetime is considered. Use of online optimization reduces the period and thereby $\tilde{D}_{dcg}$. Note that when using online optimization the nominal point (d_0, $d_{c,0}$,$d_{g,0}$) will change.

Maximum expected implementation errors

The maximum expected implementation error for a controlled variable is:

$$d_{c,max,j} = \max_{\Delta d_{c,j} \in D_{c,j}} |\Delta d_{c,j}| + d_{c,0,j} \tag{3.12}$$

and *the maximum expected implementation error for a constraint* is:

$$d_{g,max,j} = \max_{\Delta d_{g,j} \in D_{g,j}} |\Delta d_{g,j}| + d_{g,0,j} \tag{3.13}$$

The maximum expected implementation error in the constrained controlled variables $d^*_{c,max}$ is equal the maximum expected implementation error in each constrained controlled variable (see equation 3.12) and zero for each unconstrained controlled variable:

$$d^*_{c,max} = \begin{cases} d_{c,max,j} & \forall\ constrained\ controlled\ variables \\ 0 & \forall\ unconstrained\ controlled\ variables \end{cases} \tag{3.14}$$

The maximum expected implementation error in the active constraints $d^*_{g,max}$ is similarly defined:

$$d^*_{g,max} = \begin{cases} d_{g,max,j} & \forall \, active \; constraints \\ 0 & \forall \, inactive \; constraints \end{cases} \tag{3.15}$$

3.2.6 Feasibility

Feasibility

For a set of disturbance variations $\Delta d \in D_d$, operation is feasible if there exist inputs u (and corresponding states x) such that the following constraints are fulfilled for all disturbances:

$$\begin{aligned} f(x,u,d) &= 0 \\ g(x,u,d) &\leq 0 \\ d &= d_0 + \Delta d; \\ \forall \Delta d &\in D_d \end{aligned} \tag{3.16}$$

The set D_d includes the nominal disturbance ($d_0 \in D_d$).

The total feasibility region (D_d^{total}) is the disturbance region where at least one u fulfills the constraints f and g. D_d^{total} is larger than D_d ($D_d \subseteq D_d^{total}$) if we have feasibility.

Feasibility of a specific constant setpoint policy

For a given set of controlled variables c *with setpoints* c_s*, a constant setpoint policy is feasible if the following constraints are fulfilled for all expected disturbances and implementation errors*:

$$\begin{aligned} f(x,u,d) &= 0 \\ g(x,u,d) &\leq 0 \\ c(x,u,d) &= c_s + d_c \\ d &= d_0 + \Delta d; \\ d_c &= d_{c,0} + \Delta d_c; \\ \forall \Delta d \in D_d, \Delta d_c &\in D_c \end{aligned} \tag{3.17}$$

Note that the implementation error in the active constraints are included in d_c, so we do not need to explicitly include implementation errors in the constraints (d_g).

The specific constant setpoint policy feasibility region $\tilde{D}^c_{dc} = \{D^c_d, D^c_c\}$ is the disturbance and implementation error region where the constraints f and g are fulfilled for a specific constant setpoint policy. A specific constant setpoint policy is feasible when the expected disturbance and implementation error region ($\tilde{D}_{dc}$) is a subset of $\tilde{D}^c_{dc}$, i.e. $\tilde{D}_{dc} \subseteq \tilde{D}^c_{dc}$. Note that using online optimization reduces $\tilde{D}_{dc}$ and thereby increases the possibility for achieving feasibility of a specific constant setpoint policy. The specific constant setpoint policy feasibility region for a given implementation error d_c ($\{\tilde{D}_{dc}|d_c\}$) is always a subset of the total feasibility region D_d^{total} for all expected implementation errors d_c, i.e. $\{\tilde{D}_{dc}|d_c\} \subseteq D_d \quad \forall d_c$. This is illustrated in figure 3.3 for a specific example.

3.2.7 Active constraint control

We normally use *active constraint control* (Maarleveld & Rijnsdorp 1970). This implies that if a constraint becomes *optimally active*, we select the corresponding measurement or estimate y_j of the constraint as a controlled variable ($c_k = y_j$). For steady-state constraints we must include the measurement (or estimation) error for the constraint. For transient constraints we must also include the control error (which has been studied in detail by Perkins and co-workers). To ensure feasibility such that the constraints are never violated, the following setpoints for the active constraint controlled variables are used for a minimum constraint:

$$c_{s,j} = y_{min,j} + d_{g,max,j} \tag{3.18}$$

or for a maximum constraint:

$$c_{s,j} = y_{max,j} - d_{g,max,j} \tag{3.19}$$

3.2.8 Loss

For a given choice of controlled variables, the *loss* for a given disturbance (d), implementation error (d_c) and setpoint c_s is (Skogestad 2000a):

$$L(d, d_c, c_s) = J_c(c_s + d_c, d) - J_{opt}(d) \tag{3.20}$$

where

$$J_c(c_s + d_c, d) = J(x(c_s + d_c, d), u(c_s + d_c, d), d) \tag{3.21}$$

Figures 3.4 and 3.5 show the loss as function of the disturbance and implementation error for different sets of controlled variables for a specific example. Note that the losses depend strongly on the selected controlled variables.

The percentage loss $L(\%)$ for a given disturbance (d) and implementation error (d_c) with constant setpoint c_s is:

$$L(d, d_c, c_s)(\%) = \frac{J_c(c_s + d_c, d) - J_{opt}(d)}{J_{opt}(d)} \cdot 100\% \tag{3.22}$$

3.2.9 Self-optimizing control

A set of controlled variables has self-optimizing properties if a constant setpoint policy yields an acceptable loss L for the expected variation in disturbances and implementation errors (Skogestad 2000a).

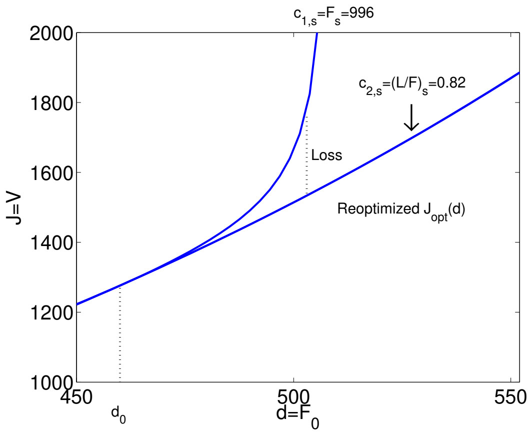

Figure 3.4: Cost as a function of the disturbance with (i) reoptimized setpoint (lower curve) and (ii) two alternative constant setpoint policies (c_1 and c_2). The loss is negligible with c_2 as a controlled variable.

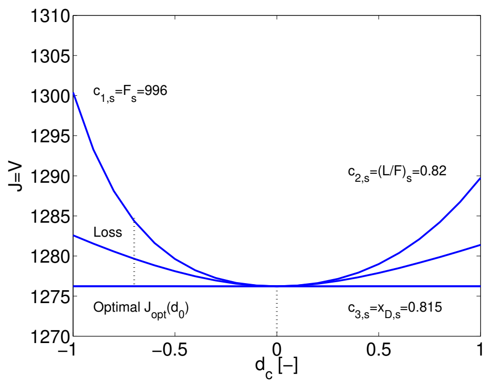

Figure 3.5: Cost as a function of the implementation error. The loss is negligible with c_3 as a controlled variable.

3.2.10 Backoff

Backoff is a setpoint adjustment, which is primarily used to avoid infeasibility, see figure 3.9. More precisely, we define *the backoff (b)* as *the difference between the actual setpoints and some reference values for the setpoints*:

$$b = c_s - c_{s,ref} \tag{3.23}$$

3.3 Optimization problems

3.3.1 Ideal optimization

For a given disturbance (d) the optimal operation (u_{opt} with corresponding x_{opt}) is found by solving the following problem:

$$\begin{aligned} (x_{opt}(d), u_{opt}(d)) = arg[\min_{x,u} J(x,u,d)] \\ f(x,u,d) = 0 \\ g(x,u,d) \leq 0 \end{aligned} \tag{3.24}$$

and we have:

$$J_{opt}(d) = J(x_{opt}(d), u_{opt}(d), d) \tag{3.25}$$

For the nominal case with $d = d_0$, the corresponding optimal setpoints are:

$$c_{s,opt}(d_0) = c(x_{opt}(d_0), u_{opt}(d_0), d_0) \tag{3.26}$$

If we try to implement these setpoints, we will get infeasibility if there are implementation errors (uncertainties) in the (optimally) active constraints. To avoid infeasibility we need to include uncertainties in the optimization as is discussed in the following.

3.3.2 Optimization with constraint backoff ("reoptimized")

The first step in including uncertainties (disturbances and implementation errors) is to introduce constraint backoff ($d^*_{g,max}$, see equation 3.15) to avoid infeasibility caused by implementation error in the constraints that are active at the optimum. The "adjusted" optimal operation (u^*_{opt} with corresponding x^*_{opt}) for a given disturbance (d) is found by solving the following problem (denoted "reoptimized" in the following):

$$\begin{aligned} (x^*_{opt}(d), u^*_{opt}(d)) = arg[\min_{u,x} J(x,u,d)] \\ f(x,u,d) = 0 \\ g(x,u,d) + d^*_{g,max} \leq 0 \end{aligned} \tag{3.27}$$

and we have

$$J^*_{opt}(d) = J(x^*_{opt}(d), u^*_{opt}(d), d) \tag{3.28}$$

For example, assume that we have maximum pressure constraint $p \leq 10$ bar (i.e. $g = p - 10$) and that the implementation (measurement) error for pressure is ± 0.2 bar ($d_{g,max} = 0.2$). In order to guarantee that the actual pressure remains less than 10 bar (feasibility) we must then back off and require $p \leq 9.8$ bar where p is the model pressure. Note that the implementation error may have been accounted for when formulating the constraints, and should then not be counted twice. Also, for input constraints the implementation error is often zero ($d^*_{g,max} = 0$). For example, we are often able to implement exactly the requirement of a closed valve (zero flow) or a fully open valve (maximum flow).

For the nominal case with $d = d_0$, the corresponding "adjusted" nominally optimal setpoints for the controlled variables can be computed by:

$$c_{s,0} = c^*_{opt}(d_0) = c(x^*_{opt}(d_0), u^*_{opt}(d_0), d_0) \tag{3.29}$$

These are hereafter called the *nominal setpoints*. The loss for a given disturbance d and implementation error d_c with constant nominal setpoints $c_{s,0}$ is then:

$$L(d, d_c, c_{s,0}) = J_c(c_{s,0} + d_c, d) - J_{opt}(d) \tag{3.30}$$

For a set of operating points i, the *maximum loss* (in percent) is defined as:

$$L_{max} = \max_i \frac{J_c(c_{s,0} + d_{c,i}, d_i) - J_{opt}(d_i)}{J_{opt}(d_i)} \cdot 100\% \tag{3.31}$$

and the *average loss* or *weighted loss* (in percent) is defined as:

$$L_w = \frac{J_{c,w} - J_{opt,w}}{J_{opt,w}} \cdot 100\% \tag{3.32}$$

where

$$J_{c,w} = \sum_i w_i J_c(c_{s,0} + d_{c,i}, d_i) \tag{3.33}$$

and

$$J_{opt,w} = \sum_i w_i J_{opt}(d_i) \tag{3.34}$$

The corresponding *backoff* is:

$$b_0 = c_{s,0} - c_{s,opt}(d_0) \tag{3.35}$$

Additionally, we have the constraint backoff $d^*_{g,max}$ for the active constraints, see also equation 3.18 or 3.19. This results in an unavoidable additional loss at the nominal operating point, as illustrated in figures 3.6 and 3.7.

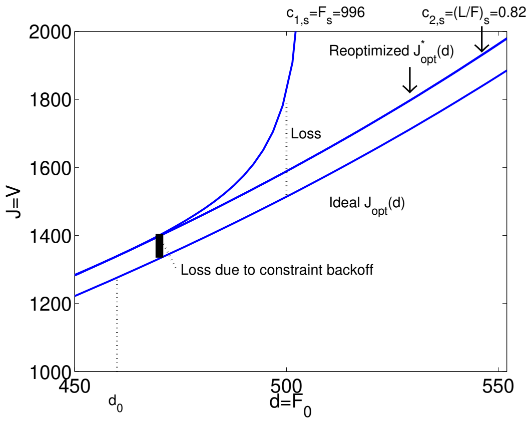

Figure 3.6: Cost as a function of disturbance d with (i) ideal optimization (lower curve), (ii) reoptimization with constraint backoff and (iii) two different constant setpoint policies (c_1 and c_2). The loss is negligible with c_2 as a controlled variable. The loss due to constraint backoff is unavoidable if we want to guarantee feasibility.

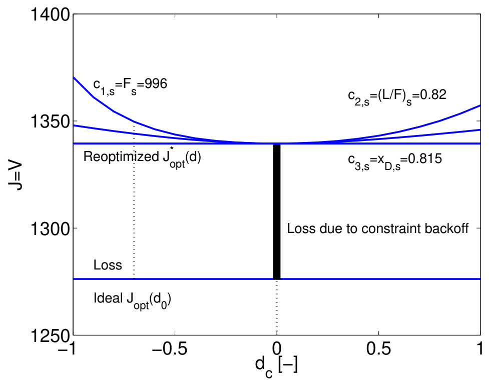

Figure 3.7: Cost as a function of implementation error. The loss is negligible with c_3 as a controlled variable. The additional loss due to constraint backoff is unavoidable.

3.3.3 Robust optimization

The above nominal optimization problem (equation 3.27 with d_0) is relatively easy to solve, and is what we normally would recommend for computing the setpoints for practical implementations. However, these nominal setpoints are generally not the optimal constant setpoints. In particular, this is the case if they may give infeasibility as shown later in the case study. The "truly optimal" constant setpoints may be obtained by including all expected uncertainties (all expected disturbances (d) and implementation errors (d_c)) and evaluate the appropriate average cost.

Let us first consider the simpler problem without implementation errors. This can be regarded as a stochastic optimization problem (Kall & Wallace 1994)[1]:

$$\begin{aligned} "\min_{x,u}" J(x,u,d) \\ f(x,u,d) = 0 \\ g(x,u,d) \leq 0 \\ d = d_0 + \Delta d \\ x \in R^{dimx}; u \in R^{dimu} \end{aligned} \tag{3.36}$$

where Δd is a random vector varying over the set $D_d \subset R^{dimd}$. More precisely, we try to find the input u which when implemented, minimizes an objective function (J) and fulfills a set of constraints (f, g) that are affected by random parameters (Δd).

We here extend this stochastic optimization problem to consider the constant setpoint problem. We must then include the uncertainty related to implementing the optimal solution:

$$\begin{aligned} "\min_{x,u,c_s}" J(x,u,d) \\ f(x,u,d) = 0 \\ g(x,u,d) \leq 0 \\ c(x,u,d) = c_s + d_c \\ d = d_0 + \Delta d \\ d_c = d_{c,0} + \Delta d_c \\ x \in R^{dimx}; u, c_s \in R^{dimu} \end{aligned} \tag{3.37}$$

where Δd and Δd_c are random vectors varying over the sets $D_d \subset R^{dimd}$ and $D_c \subset R^{dimu}$. More precisely, we try to find setpoints c_s which when implemented, minimize an objective function (J) and fulfill a set of constraints (f, g, c) that are affected by random parameters (Δd and Δd_c).

However, the problems above (equations 3.36 and 3.37) are not well defined since the meaning of "min" and the constraints are not clear at all as long as the realization of d and d_c are unknown and may vary. We therefore consider the very similar deterministic problem where we instead of minimizing the expected cost, minimize some "mean" weighted cost ($J_w = \sum_i w_i J(x_i, u_i, d_i)$) while fulfilling the constraints over all expected disturbances (d) and implementation errors (d_c). The problem is infinite dimensional, but we here simplify it by considering a discrete number of operating points ($i = 0, .., m$ where 0 denotes the nominal point and m is the number of "disturbed" operating points). The corresponding *robust optimization problem* was introduced by Glemmestad et al. (1999) to find robust setpoints and evaluate loss, and is defined by:

$$(x_{robust}, u_{robust}, c_{s,robust}) = arg[\min_{x_i,u_i,c_s} \sum_i w_i J(x_i, u_i, d_i)]$$

[1] Kall & Wallace (1994) focus on stochastic optimization problems with recourse to achieve feasibility when the uncertain parameters are known. The recourse problem is not considered here. Feasibility is required for all expected uncertainties (disturbances and implementation errors), while "rare" uncertainties (disturbances or implementation errors) are assumed to be handled by the safety system.

$$\begin{aligned} f(x_i, u_i, d_i) &= 0 \\ g(x_i, u_i, d_i) &\leq 0 \\ c(x_i, u_i, d_i) &= c_s + d_{c,i} \\ d_i &= d_0 + \Delta d_i \\ d_{c,i} &= d_{c,0} + \Delta d_{c,i} \\ \Delta d_i \in D_d, \ \Delta d_{c,i} &\in D_c \end{aligned} \tag{3.38}$$

Note that when using constant robust setpoints no measurements of the uncontrolled constraints are used and the implementation errors in the constraints are not explicitly included. The implementation errors d_g on the active constraints are included in the variables d_c and the constraint backoff is "automatically" included when we obtain c_s. Note also that we need to solve the optimization problem for each candidate set with controlled variables. The robustly optimal setpoints ($c_{s,robust}$) are found from solving the robust optimization problem and are labeled *robust setpoints*. The loss for a given disturbance (d) and implementation error (d_c) with constant robust setpoints is then:

$$L(d, d_c, c_{s,robust}) = J_c(c_{s,robust} + d_c, d) - J_{opt}(d) \tag{3.39}$$

The average and maximum loss with constant robust setpoints are defined similar as for constant nominal setpoints, see equations 3.31 and 3.32. The *optimal backoff* is:

$$b_{opt} = c_{s,robust} - c_{s,0} \tag{3.40}$$

The distribution of operating points (i) and corresponding weights (w_i) in the objective (cost) function can be chosen in different ways. It is clear that the problem becomes very large even for a modest number of operating points. Every new operating point introduces $n_u + n_x$ variables and equality equations, where n_u is the number of manipulated variables and n_x is the number of internal variables. The optimization problem may be solved by using a subspace optimization algorithm, since there are many optimization variables and the degree of freedom for optimization is small (equal the number of controlled variables). Since the optimization problem is nonlinear, relatively few carefully selected operating points should be included to keep the problem not-too-high-dimensional. However, the grid needs to be dense enough to include important nonlinearities, since the feasibility is only guaranteed in the selected operating points and the objective must give a reasonable estimate of the expected cost. The robust optimization problem should be solved offline because it is high-dimensional.

The weights should correspond to a reasonable probability distribution. Preferably, they should be equal the probability for operation in the respective points. This may be quite critical, as use of an incorrect probability distribution (objective function weights and operating points) may give a larger loss than use of nominal setpoints. Using a nominal objective ($w_0 = 1$, $w_i = 0$ when $i \neq 0$) gives zero backoff if the nominal setpoints are feasible.

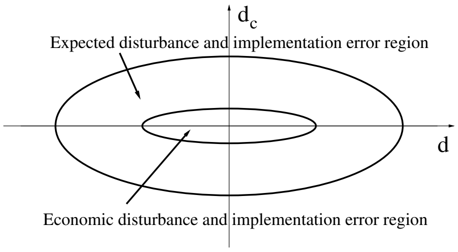

Figure 3.8: Expected disturbance and implementation error region and economic disturbance and implementation error region

Every alternative which is feasible with nominal setpoints, gives unchanged loss with robust setpoints based on a nominal objective. Using an average objective with respect to all operating points considered ($w_i = 1$ for all i) may give a too conservative operation. However, feasibility may be important in a larger region than economics, and this can be handled by defining *the economic disturbance and implementation error region* ($\tilde{D}_{dc}^{econ}$) which is a subset of the expected disturbance and implementation error region ($\tilde{D}_{dc}^{econ} \subseteq \tilde{D}_{dc}$, see figure 3.8), where $w_i = 0$ is used outside the economic disturbance and implementation error region. The constraints must be fulfilled in the expected disturbance and implementation error region, whereas the average cost in the economic disturbance and implementation error region is minimized. Expanding the expected disturbance and implementation error region gives increased losses and increased possibility for infeasibility.

Appendix A contains more details about robust optimization.

3.3.4 Online feasibility correction

A constant setpoint policy may not be feasible, that is, there may not exist any solution to the robust optimization problem, or the constant setpoint policy may be too conservative. Also, the computation load for the robust setpoints may be too heavy. These cases can be handled by adjusting the setpoints online. In practice this may be handled by the steady-state optimization layer in model predictive control (MPC) (Qin & Badgwell 1996), so implementation is straightforward if we have MPC software in place. The main point here is not to present some new algorithm, but to evaluate the resulting operation.

The idea is to keep the operation as close as possible to the nominal setpoints, subject to satisfying the constraints. With *soft prioritization* of the controlled variables, as given by the diagonal weight matrix Q, the resulting online setpoint adjustment problem becomes:

$$\begin{aligned} \min_{u,\hat{x},c_{flex}} \; & (c_{flex} - c_{s,0})^T Q (c_{flex} - c_{s,0}) \\ & \hat{f}(\hat{x}, u, d) = 0 \\ & \hat{g}(\hat{x}, u, d) + d_{g,max} \leq 0 \\ & \hat{c}(\hat{x}, u, d) = c_{flex} \end{aligned} \tag{3.41}$$

The model ($\hat{f}$, $\hat{g}$, $\hat{c}$) used in this online setpoint adjustment is usually linear. Online we usually have measurements of the controlled variables and constraints, and through feedback the operation is updated such that the computed controlled variables ($\hat{c}$) are equal the measured values (c_m) and the computed constraints ($\hat{g}$) are equal the measured constraints (g_m)[2]. Note that a feed-forward solution is possible (in theory), but requires a detailed model and measurements of the disturbances when solving the online setpoint adjustment problem.

For our "offline" analysis of this scheme we will use the nonlinear model. For the analysis we also need to include the implementation errors. The optimization problem used for offline analysis of the online feasibility correction then becomes:

$$
\begin{aligned}
(u_{flex}(d,d_c,d_g), x_{flex}(..), c_{flex}(..)) = arg[\min_{u,x,c_{flex}} (c_{flex} - c_{s,0})^T Q(c_{flex} - c_{s,0})] \\
f(x,u,d) = 0 \\
g(x,u,d) + d_{g,max} - d_g \leq 0 \\
c(x,u,d) = c_{flex} + d_c
\end{aligned}
\tag{3.42}
$$

and we have

$$
J_{flex}(c_{flex} + d_c, d, d_g) = J(x(d_c,d,d_g), u(d_c,d,d_g), d) \tag{3.43}
$$

Since measurements of all constraints (including uncontrolled constraints) are used in the implementation, implementation errors in the constraints (d_g) need to be explicitly included. Except from the inclusion of implementation errors in the constraints, this formulation was used by Lid & Skogestad (2001) to evaluate loss when using model predictive control. The adjusted setpoints, labeled *flexible setpoints* c_{flex}, achieve feasible operation. The loss L for a given disturbance d and implementation errors d_c and d_g with flexible setpoints c_{flex} is then:

$$
L(d, d_c, d_g, c_{flex}) = J_{flex}(c_{flex} + d_c, d, d_g) - J_{opt}(d) \tag{3.44}
$$

The average and maximum loss with flexible setpoints are defined similar as for constant nominal setpoints, see equations 3.31 and 3.32.

Alternatively, we may want *hard prioritization* among the controlled variables. For example variables at active constraints should be kept constant, if possible. The set of controlled variables c is then divided in two subsets c_I and c_{II}:

- c_I: Controlled variables for which no backoff is allowed, if possible (variables with high priority)
- c_{II}: Controlled variables for which backoff is allowed and minimized (variables with low priority).

[2]This requires that the model gains and that the diagonal weight matrix are reasonably selected to avoid instability.

With similar assumptions as for soft prioritization, the resulting operating point for a given disturbance d and implementation errors d_c and d_g can be found.

We first set $c_s = c_{s,0}$ and allow for backoff in the controlled variables with low priority (c_{II}). The resulting optimization problem becomes:

$$\begin{aligned}(u_{flex}(..), x_{flex}(..), c_{flex}(..)) = arg[\min_{x,u,c_{flex}} (c_{II,flex} - c_{II,s})^T Q_{II}(c_{II,flex} - c_{II,s})]\\ f(x,u,d) = 0\\ g(x,u,d) + d_{g,max} - d_g \leq 0\\ c(x,u,d) = c_{flex} + d_c\\ c_{I,flex} = c_{I,s}\end{aligned} \tag{3.45}$$

If there is a solution, the adjusted setpoints c_{flex} give feasibility and are implemented. Otherwise, we allow backoff in the controlled variables with high priority (c_I). The resulting optimization problem becomes:

$$\begin{aligned}(u_{flex}(..), x_{flex}(..), c_{flex}(..)) = arg[\min_{x,u,c_{flex}} (c_{I,flex} - c_{I,s})^T Q_I(c_{I,flex} - c_{I,s})]\\ f(x,u,d) = 0\\ g(x,u,d) + d_{g,max} - d_g \leq 0\\ c(x,u,d) = c_{flex} + d_c\end{aligned} \tag{3.46}$$

If there is no feasible solution to equation 3.46, we need to remove constraints. This is not considered here. If there is a feasible solution, we update the setpoints to the controlled variables with high priority ($c_{I,s} = c_{I,flex}$) and resolve equation 3.45 with the updated setpoints c_s. The adjusted setpoints c_{flex} give feasibility and are implemented.

Note: With hard prioritization among the controlled variables we may need to solve a hierarchy of setpoint adjustment problems online. Hard prioritization among the controlled variables can be generalized to more than two levels of (hard) priority. Online feasibility correction is not restricted to use of nominal setpoints.

The *flexible backoff* is defined as:

$$b_{flex} = c_{flex} - c_{s,0} \tag{3.47}$$

Figure 3.9 shows the optimal backoff and flexible backoff for a disturbance. If the average cost is primarily determined by operation at or close to the nominal point, the use of flexible backoff may give a small loss. The backoff is then just done for ensuring feasibility in some ”extreme” points. However, flexible backoff adjusts the setpoints without considering the actual cost function, so the loss may in some cases be very large. Thus, if these ”extreme” points enter in the average cost, the loss may be large (see figure 3.9). The selection of controlled variables and corresponding setpoints with good self-optimizing properties therefore remains important, also with online feasibility correction.

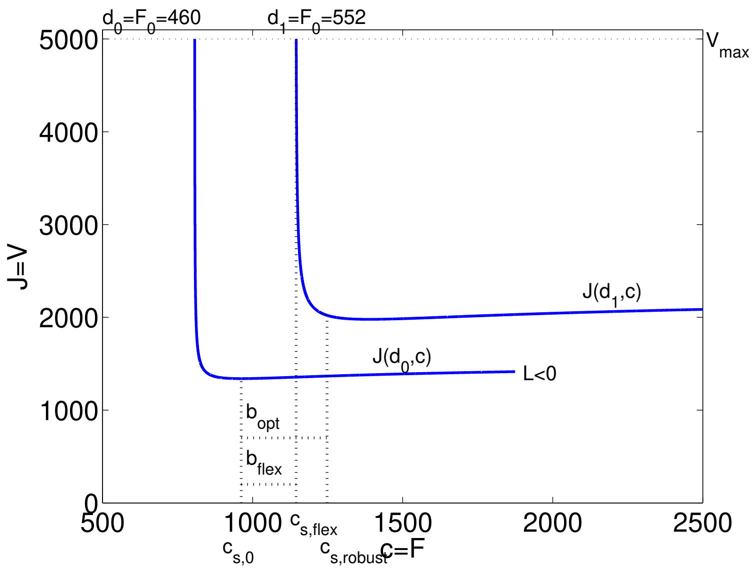

Figure 3.9: Cost (J) as function of the controlled variable (c) at nominal point (d_0, lower curve) and with disturbance (d_1, upper curve). With the setpoint fixed at the nominal optimum ($c_s = c_{s,0}$) we get infeasibility because of disturbances. With optimal backoff ($c_{s,robust} = c_{s,0} + b_{opt}$) we get feasibility and close to optimal operation in both cases. With flexible backoff the setpoint is $c_{s,flex} = c_{s,0}$ at nominal point (d_0) and changes to $c_{s,flex} = c_{s,0} + b_{flex}$ with disturbance (d_1). We get feasibility, but far from optimal operation.

The feasibility region with flexible backoff is discussed in section 3.5.1. Appendix B contains a simple example of using MPC with a linear model, which gives the same solution as the optimization problem used for offline analysis in equation 3.42.

3.4 Example: Reactor, separator and recycle process

We now apply the above ideas to a case study. To select the controlled variables and their setpoints we use an extension of the method of Skogestad (2000a), consisting of the following steps:

1. *Initial system analysis*:
   Identify the number of degrees of freedom, define objective function and constraints, identify main disturbances and measurements, optimize at nominal and for expected disturbances, see equation 3.24.

2. *Identify sets of candidate controlled variables*:
   Eliminate variables with no steady-state effect, use active constraint control, eliminate variables with large losses by using short-cut loss evaluation, eliminate variables based on process insight.

3. *Evaluate the loss for different sets of controlled variables*, using:

   (a) Constant nominal setpoints, see equation 3.29

(b) Constant robust setpoints, see equation 3.38

(c) Nominal setpoints with online feasibility correction (flexible setpoints), see equations 3.45 and 3.46.

4. *Final evaluation and selection of control structure*:
Stabilization, controllability analysis, selection of control configuration and simulation of proposed control structures.

An alternative to the initial screening (step 2) before evaluating the loss (step 3) is to use mathematical programming to find sets of controlled variables which imply small losses. If including a controllability test (step 4) for different controlled variable sets, the selection of controlled variables may be done automatically. With nominal or robust setpoints the selection of controlled variables (step 2 and 3) can be formulated as a standard MINLP-problem.

The process consists of a reactor, a distillation column and a liquid recycle (Papadourakis et al. 1987) and is shown in figure 3.10. We use the model parameters from Wu & Yu (1996).

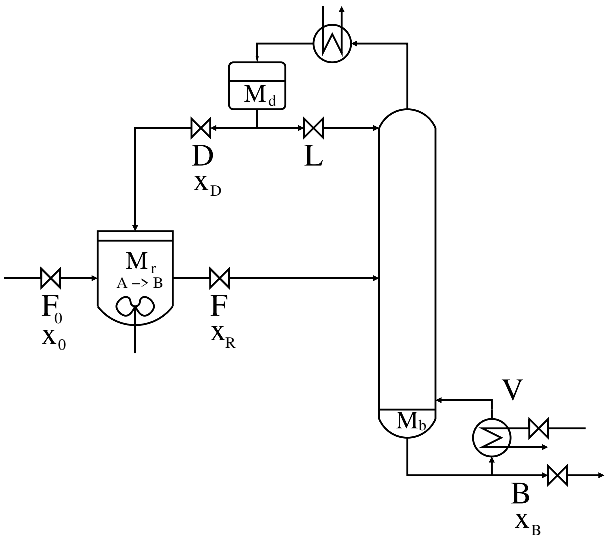

Figure 3.10: Reactor/separator process with liquid recycle

There is no inert in the feed, so no purge is required. In chapter 2 control structure selection with emphasis on identifying promising sets of controlled variables when using constant nominal setpoints under various conditions is considered. We here consider given feedrate (case I in chapter 2). The conclusions from chapter 2 are not changed, though the nominal setpoints are found by using constraint backoff and some extra candidate controlled variables are included.

3.4.1 Initial system analysis

The process has five manipulated variables (valves) which give five degrees of freedom:

$$u_{dyn}^T = [L\ V\ B\ D\ F]$$

However, for stabilization we need to control two variables (the reboiler holdup (M_b) and condenser holdup (M_d)) which have no steady-state effect. We are then left with three degrees of freedom at steady-state. These may be selected as the reactor holdup (M_r), product composition (x_B) and recycle composition (x_D), i.e. $u^T = [M_r\ x_B\ x_D]$. The economic objective is to maximize the profit (the value of the products minus the cost of the utilities and raw materials). Since F_0 is given and there is no purge, it follows that B is given. Furthermore, L depends directly on V, so the economic objective can be simplified to minimize the boilup:

$$J = V$$

The reactor volume (M_r) and boilup flowrate (V) are constrained and there is a product purity specification (x_B):

$$\begin{aligned} 0 \leq M_r &\leq 2800 \\ x_B &\leq 0.0105 \\ V &\leq V_{max} \end{aligned}$$

The reactor volume constraint ($0 \leq M_r \leq 2800$) and boilup flowrate constraint ($V \leq V_{max} = 5000$) are transient constraints whereas the product specification constraint ($x_B \leq 0.0105$) is a steady-state constraint. The main disturbances are feedrate (F_0) and feed composition (x_0):

$$\mathrm{d}^T = [F_0\ x_0] = [460 \pm 92\ \mathrm{kmol/h}\ 0.90 \pm 0.05\ \mathrm{molA/mol}]$$

We consider the following 20 candidate controlled variables (9 manipulated variables and measurements and 11 flow ratios):

$$c^T = [L\ \ V\ \ D\ \ B\ \ F\ \ M_r\ \ x_r\ \ x_B\ \ x_D\ \ \frac{L}{F}\ \frac{V}{F}\ \frac{B}{F}\ \frac{D}{F}\ \frac{V}{L}\ \frac{B}{L}\ \frac{D}{L}\ \frac{B}{V}\ \frac{D}{V}\ \frac{B}{D}\ \frac{F}{F_0}]$$

We will in this chapter *not* consider the use of variable combinations. The implementation errors are initially assumed to be $\pm 10\%$ for the flowrates, $\pm 0.25\%$ (absolute) for the compositions and $\pm 1\%$ for the holdups. The implementation error for the reactor holdup is the sum of expected measurement error and expected (dynamic) control error since the reactor holdup constraint is transient. The implementation error for the product composition is in practice the sum of expected measurement error and steady-state control error. Steady-state optimizations for the nominal point and the corner-points with the expected disturbance variation[3], see equation 3.24, show that the product composition (x_B) and the reactor holdup (M_r) are always at their constraints.

3.4.2 Identify sets of candidate controlled variables

There are 20 candidate controlled variables and three steady-state degrees of freedom. This gives ($20{\cdot}19{\cdot}18/3/2/1 =$) 1140 alternative sets of controlled variables. As a first step we want

[3] We expect that only one disturbance d_j is perturbed from the nominal value at the same time

to reduce the number of candidate sets. We have already eliminated the condenser (M_D) and the reboiler holdup (M_B) which have no steady-state effect. In addition we choose to control the two (optimally) active constraints (c_1=product composition and c_2=reactor holdup). We are then left with 18 candidate controlled variables and 1 steady-state degree of freedom, which give 18 possible sets.

Initial screening is performed by considering the steady-state gain ($\underline{\sigma}(G(0)) = |G(0)|$), which according to the singular value rule (Skogestad & Postlethwaite 1996) should be maximized in order to achieve self-optimizing control. The gain matrix $G(0)$ is obtained with the active constraints kept constant. The candidate controlled variables are scaled with respect to variation in optimal values (absolute value of maximum deviation in the optimal value from the nominally optimal value, $\Delta c_i = \max_D |c_{opt,i}(d) - c_{opt,i}(d_0)|$) and implementation errors. From table 3.2 we see that x_D and L/F are the most promising controlled variables. We note that four candidate variables have a zero gain; B/V, V, x_r and B. This is relatively

Table 3.2: Candidate controlled variables ranked by steady-state gain ($|G(0)|$)

Rank	c_3	$\|G(0)\| \cdot 10^3$
1	x_D	13.1
2	L/F	8.9
3	D/L	7.7
4	D/V	5.8
5	V/L	4.5
6	B/L	4.1
7	V/F	4.0
8	B/D	3.3
9	L	3.0
10	B/F	2.6
11	D	2.6
12	F/F_0	2.5
13	D/F	2.5
14	F	1.9
15	B/V	0
15	V	0
15	x_r	0
15	B	0

easy to explain (see chapter 2): At steady-state the product flowrate must equal the feedrate ($B = F_0$). Thus, keeping the product flowrate (B) constant when the feedrate changes, does not give feasible steady-state operation. The product flow rate (B) is given by the component balance of the product:

$$B = kM_r x_r/(x_B - 1 + x_0)$$

Here M_r and x_B are controlled at their active constraints when, as just noted, $B = F_0$. Thus the reactor composition (x_r) is fixed and can be eliminated as a candidate controlled variable. Since the boilup V in the column is at its minimum, the gain is zero. The boilup V is not a candidate for control because specifying it below its minimum value results in infeasible operation. B and B/V is then eliminated as candidate controlled variables. 14 candidate controlled variables and 1 steady-state degree of freedom still remain, which give 14 possible sets.

3.4.3 Loss evaluation

For the remaining 14 alternative sets we have evaluated the economic loss imposed by using constant setpoints instead of reoptimization. We have also evaluated seven alternatives, discussed in literature, which are not nominally optimal since they do not control the reactor holdup at its constraint. These include the Balanced Structure (BS) with control of x_B, x_r and x_D (Balanced Structure I in chapter 2) and the Luyben Structure (LS) with control of x_B, F and x_D. The nominal point and corner points for expected disturbances and implementation errors are included as operating points with equal weights (w_i). We assume that only one disturbance d_j or implementation error $d_{c,j}$ is perturbed from its nominal value at the same time.

We select to study the following alternatives in more detail:

- x_D or L/F with good self-optimizing properties (small loss in chapter 2)
- F or D which follows Luybens rule
- LS or BS with no control of reactor holdup.

Figures 3.13 and 3.14 show the loss as function of the disturbances and implementation errors with constant nominal setpoints, constant robust setpoints and flexible setpoints for these alternatives. We also compare with reoptimization with constraint backoff ("reoptimized").

(a) Loss evaluation with nominal setpoints

The average and maximum percentage losses with constant *nominal* setpoints based on constraint backoff (see equation 3.29) are listed in table 3.3. The ranking of the alternatives is based on the average loss.

- Control of x_D (figure 3.11) is best, closely followed by L/F (figure 3.12), D/L and D/V, see also chapter 2
- Control of F or D, which follows Luybens rule ("fix a flow in every recycle loop") (Luyben, Tyreus & Luyben 1997), gives infeasibility
- None of the seven alternatives without control of reactor holdup ("below the line" in table 3.3) yield feasible operation for all disturbances.

From figures 3.13 and 3.14 we find:

- The implementation error in the product composition ($d_{c,1}$) gives a significant loss for all alternatives. This is because over-purifying the product increases the boilup rate (energy). Reducing this implementation error ($d_{c,1}$) will give a significant reduction in loss, but will not alter the ranking.

Table 3.3: Average and maximum percentage loss (L_w, L_{max}) with constant nominal setpoints, constant robust setpoints and flexible setpoints for alternative sets of controlled variables.

c_1,c_2,c_3	Nominal setpoints			Robust setpoints			Flexible setpoints				
	$c_{3,s}$	L_w (%)	L_{max} (%)	$b_{3,opt}$	L_w (%)	L_{max} (%)	$b^{max}_{1,flex}$ (%)	$b^{max}_{2,flex}$	$b^{max}_{3,flex}$	L_w (%)	L_{max} (%)
Reoptimized	$c^*_{opt}(d)$	5.16	11.03	–	5.16	11.03	–	–	–	4.97	11.03
x_B,M_r,x_D	0.825	5.22	11.04	0.005	5.21	11.03	0	0	0	5.22	11.04
x_B,M_r,L/F	0.871	5.39	11.24	−0.021	5.35	11.34	0	0	0	5.39	11.24
x_B,M_r,D/L	0.600	5.40	11.15	0.047	5.34	11.35	0	0	0	5.40	11.15
x_B,M_r,D/V	0.375	5.60	11.15	0.026	5.49	11.46	0	0	0	5.60	11.15
x_B,M_r,V/F	1.392	6.05	11.37	−0.037	5.93	11.67	0	0	0	6.05	11.37
x_B,M_r,B/L	0.549	6.31	13.70	0.054	6.05	12.60	0	0	0	6.31	13.70
x_B,M_r,L	837.4	6.68	22.95	−64	6.46	15.87	0	0	0	6.68	22.95
x_B,M_r,V/L	1.600	8.64	41.31	0.206	5.89	12.19	0	0	0	8.64	41.31
x_B,M_r,B/D	0.916	11.2	47.77	−0.140	6.00	11.68	0	0	0	11.2	47.77
x_B,M_r,F/F_0	2.091	inf	inf	0.289	6.22	12.15	0	0	0.1280	36.82	291.78
x_B,M_r,B/F	0.478	inf	inf	−0.056	6.36	12.08	0	0	0.0145	36.87	291.78
x_B,M_r,D/F	0.522	inf	inf	0.061	6.50	12.24	0	0	0.0242	36.89	291.78
x_B,M_r,D	502.0	inf	inf	191	6.79	12.82	0	0	91	26.63	165.24
x_B,M_r,F	962.0	inf	inf	286	7.51	13.90	0	0	183	26.90	165.24
x_B,F/F_0,V/B	–	inf	inf	–	25.87	54.38	0	0.4341	0.6718	9.40	20.28
x_B,F/F_0,x_D	–	inf	inf	–	25.91	54.38	0	0.5971	0.0001	8.24	24.36
x_B,x_D,x_R(BS)	–	inf	inf	–	26.08	54.38	0	0.0868	0	6.36	16.24
x_B,M_r/F,L/D	–	inf	inf	–	26.11	54.38	0	0.7455	0	7.36	27.08
x_B,F/F_0,L/D	–	inf	inf	–	33.13	63.59	0	0.4646	0.0001	10.06	26.59
x_B,F,x_D(LS)	–	inf	inf	–	43.10	94.37	0	183	0.1735	30.84	165.24
V/B,F/F_0,x_D	–	inf	inf	–	45.74	78.75	0.6719	0.4870	0.0321	8.95	28.28

inf: infeasible operation

Constrained variables: $c_{1,s} = x_{B,s} = 0.008$ and $c_{2,s} = M_{r,s} = 2772$

Reoptimized: Reoptimized with constraint backoff, see equation 3.27.

$b^{max}_{j,flex} = \max_i |b_{j,flex,i}|$.

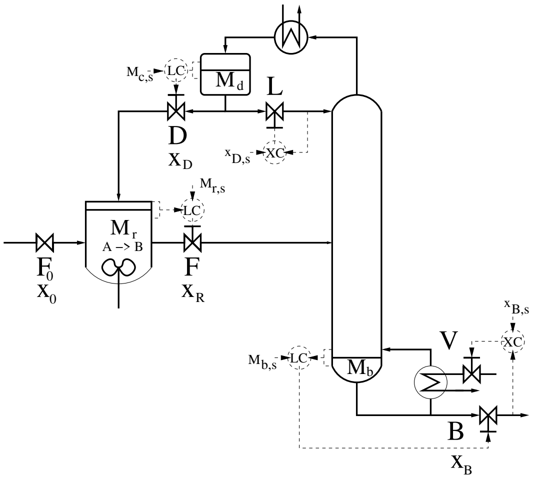

Figure 3.11: Alternative x_D

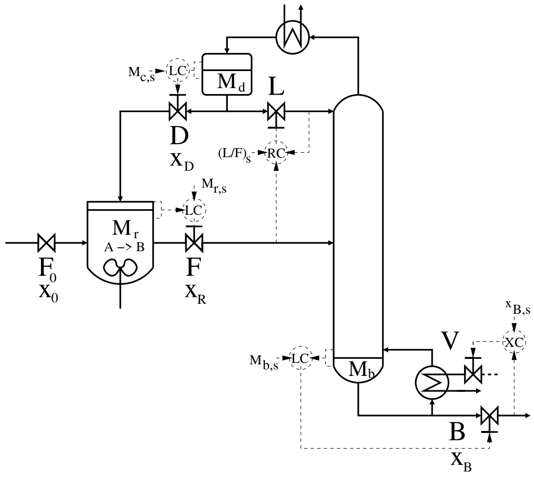

Figure 3.12: Alternative L/F

- Control of F or D (Luybens rule) gives large losses for disturbances in the feedrate (F_0). With feedrates (F_0) larger than 485 for F and 505 for D we get infeasibility.
- Control of structures LS (Luyben structure) or BS (Balanced structure) give large losses with small F_0 and infeasibility with large F_0.

(b) Loss evaluation with robust setpoints

Use of constant nominal setpoints may exclude controlled variables that are workable. We therefore consider the use of constant robust setpoints, see equation 3.38. The average and maximum percentage losses and the backoff in the unconstrained variable with constant *robust* setpoints, are also shown in table 3.3:

- In this case there is no backoff in the constrained controlled variables ($b_{opt,j} = 0$).
- For alternatives that were feasible with constant nominal setpoints, there are only minor changes.
- All alternatives are now feasible, but the loss may be large, especially for the cases "below the line" in table 3.3, where we do not control reactor holdup. However, control of F or D (Luybens rule) which was infeasible with constant nominal setpoints, is now feasible and gives an acceptable loss.

These findings are confirmed by considering figures 3.13 and 3.14. Note that the backoff to achieve feasibility for alternatives which are infeasible with nominal setpoints (e.g. F, D, LS and BS), results in a significant extra loss at the nominal point, although the weighted average loss may be acceptable.

(c) Loss evaluation with flexible setpoints

We will now consider the use of online feasibility correction based on nominal setpoints. We assume hard ranking of the controlled variables (see equations 3.45 and 3.46). The constrained controlled variables have high priority and the unconstrained controlled variables have low priority, for example $c_I = [x_B\ M_r]^T$ and $c_{II} = [F]$ for alternative F. The weight matrices Q_I and Q_{II} are selected as diagonal matrices with one over the expected implementation errors on the diagonal $(1/d_{c,i})$. No implementation error is included for constraints that are not controlled (e.g. M_r for LS and BS). From Table 3.3 we see:

- There is no backoff ($b_{flex} = 0$) for controlled variable alternatives that are feasible with nominal setpoints.
- All considered alternatives are feasible with flexible backoff, but the operation is far from optimal in some cases (much worse than with optimal backoff).
- There are cases where flexible backoff is better than optimal backoff. This is not surprising since optimal backoff uses constant setpoints.

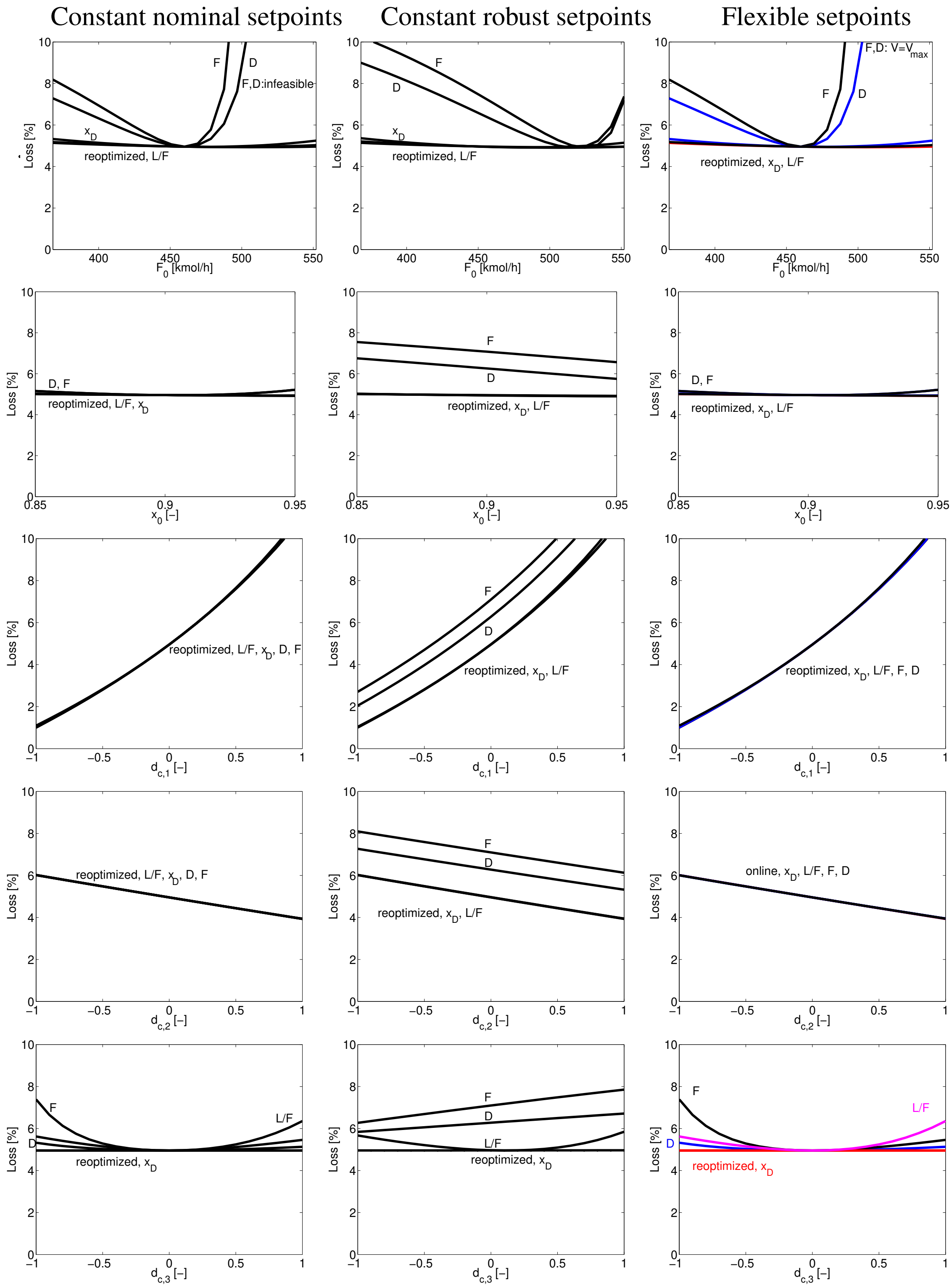

Figure 3.13: Loss as a function of disturbances (F_0, x_0) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) for the "good" controlled variables.

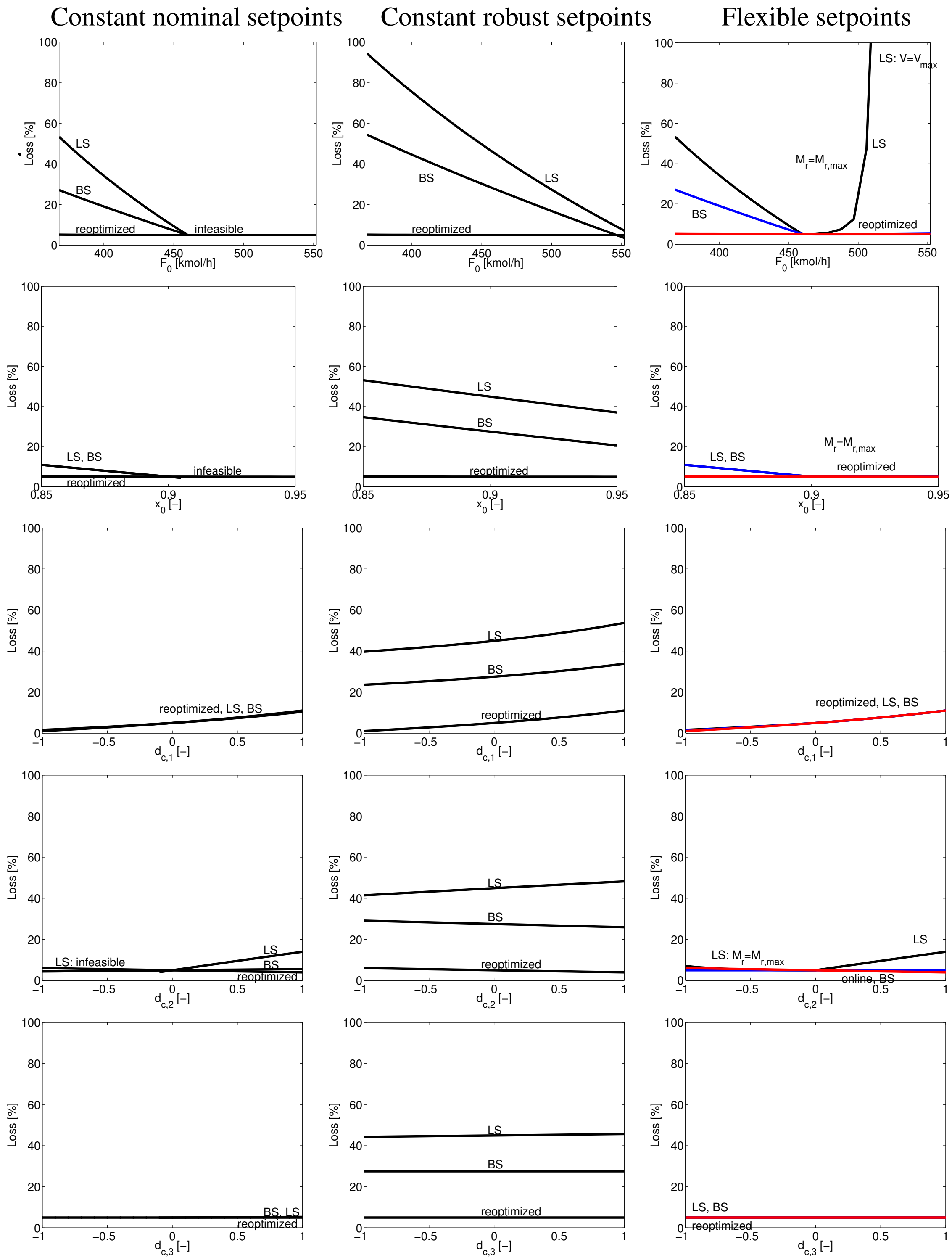

Figure 3.14: Loss as a function of disturbances (F_0, x_0) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) for the "poor" controlled variables.

These findings are confirmed by considering figures 3.13 and 3.14:

- When controlling F or D we avoid infeasibility when the column is saturated at maximum boilup rate at large feedrates ($F_0 > 485$ for F and $F_0 > 505$ for D) by increasing the setpoint D_s or F_s. This corresponds to online reconfiguration and controlling V ($= V_{max}$) at large feedrates. However, the loss is large.

- When controlling BS we avoid violating the maximum reactor holdup constraints at large feedrates ($F_0 > 460$) and large reactant feed fraction ($x_0 > 0.9$) by increasing the setpoint F_s. Alternatively, we may reconfigure online and control the reactor holdup M_r instead of x_r. This corresponds to controlling x_D which gives small losses. Switching the priority of x_D and x_r has no effect, since x_r is given when M_r and x_B are given.

- When controlling LS we avoid violating the maximum reactor holdup constraint at large feedrates ($F_0 > 460$), large reactant feed fractions ($x_0 > 0.9$) and with implementation error in F ($d_{c,2} < 0$), by increasing the setpoint $x_{D,s}$. Alternatively, we may reconfigure online and control the reactor holdup (M_r) instead of the top composition x_D. This corresponds to alternative F which gives large losses at large feedrates F_0. To avoid violating the maximum holdup rate at large feedrates ($F_0 > 520$) we switch to control $V(= V_{max})$ instead of F. By choosing a better weight matrix Q we would avoid violating the maximum reactor holdup constraint by switching to control the reactor holdup M_r instead of F. This corresponds to alternative x_D which gives small losses.

The losses as function of the feedrate with flexible setpoints are also shown in figure 3.15.

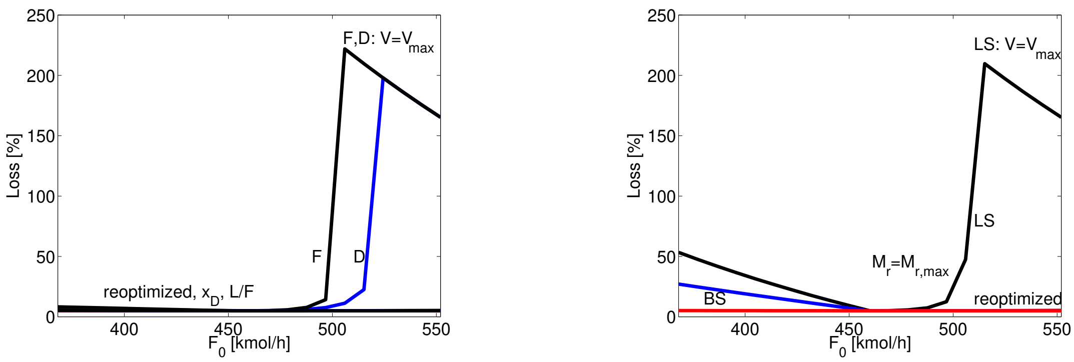

Figure 3.15: Loss with flexible setpoints as a function of disturbance F_0 for "good" controlled variables (left) and "poor" controlled variables (right).

Anyway, the conclusion has not changed. The loss is smaller and control is simpler if we keep x_D or L/F at constant nominal setpoints rather than controlling D or F at constant robust setpoints or controlling BS or LS at flexible setpoints.

3.4.4 Final evaluation and selection of control structure

We will now check the control properties of two alternatives with small losses (x_D and L/F), the two alternatives that follow Luybens rule (F and D) and the two alternatives which do not control the reactor holdup (LS and BS). In designing the control system, we first stabilize the reactor holdup, reboiler holdup and condenser holdup. The controllability analysis reveals no problems for the six alternatives. As the alternatives show small interactions, decentralized control is selected. The pairing of the controlled variables and manipulated variables is based on the steady-state relative gain array (RGA), as shown in table 3.4, where loop 1 and 2 are purely stabilizing loops. Loop 3 and 4 are used to control active constraints.

Table 3.4: Proposed decentralized control structures based on RGA

Alternative	*Loop* 1	*Loop* 2	*Loop* 3	*Loop* 4	*Loop* 5
x_D	$M_b \leftrightarrow B$	$M_d \leftrightarrow D$	$M_r \leftrightarrow F$	$x_B \leftrightarrow V$	$\mathrm{x}_D \leftrightarrow L$
L/F	$M_b \leftrightarrow B$	$M_d \leftrightarrow D$	$M_r \leftrightarrow F$	$x_B \leftrightarrow V$	L/F$\leftrightarrow L$
F	$M_b \leftrightarrow B$	$M_d \leftrightarrow L$	$M_r \leftrightarrow D$	$x_B \leftrightarrow V$	F
D	$M_b \leftrightarrow B$	$M_d \leftrightarrow L$	$M_r \leftrightarrow F$	$x_B \leftrightarrow V$	D
LS	$M_b \leftrightarrow B$	$M_d \leftrightarrow D$	F^1	$x_B \leftrightarrow V$	D/L$\leftrightarrow L$
BS	$M_b \leftrightarrow B$	$M_d \leftrightarrow D$	$x_r \leftrightarrow F^1$	$x_B \leftrightarrow V$	D/V$\leftrightarrow L$

[1]To stabilize the system cascade control may be used with the following inner loop: $M_r \leftrightarrow F$

The SIMC-tunings of Skogestad (2003) are used to select PI control parameters. Simulations are performed with constant nominal and robust setpoints for step changes in the disturbances, feed flow rate (F_0) and feed composition (x_0). Figure 3.16 shows the reactor holdup and the product composition for an increase in the feedrate ($\Delta F_0 = +20\%$) with constant nominal setpoints. Controlling F gives instability in x_B and the Luyben Scheme (LS) gives instability in M_r. Figure 3.17 shows the reactor holdup and the product composition

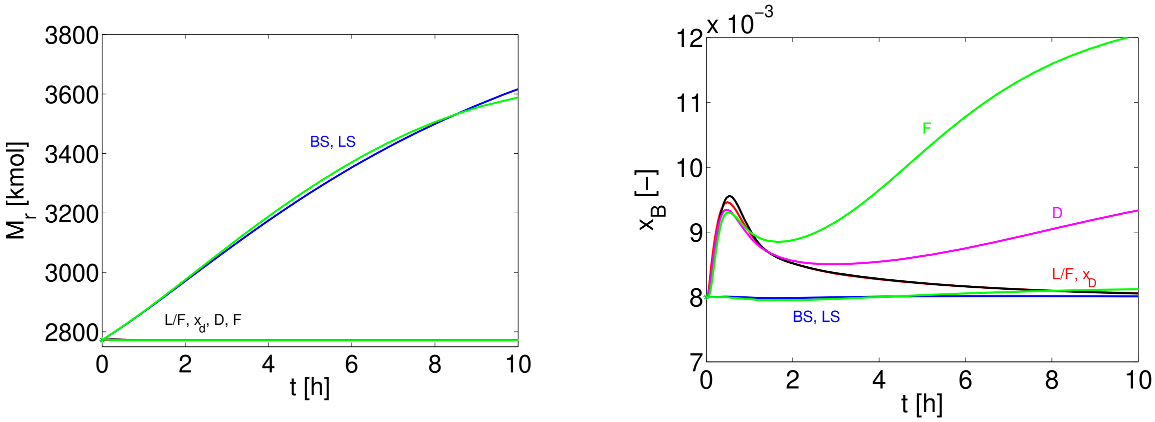

Figure 3.16: Reactor holdup (M_r) (left) and product composition (x_B) (right) when $\Delta F_0 = +20\%$ with nominal setpoints.

for an increase in the feedrate ($\Delta F_0 = +20\%$) with constant robust setpoints. F gives the fastest control and x_D the slowest control.

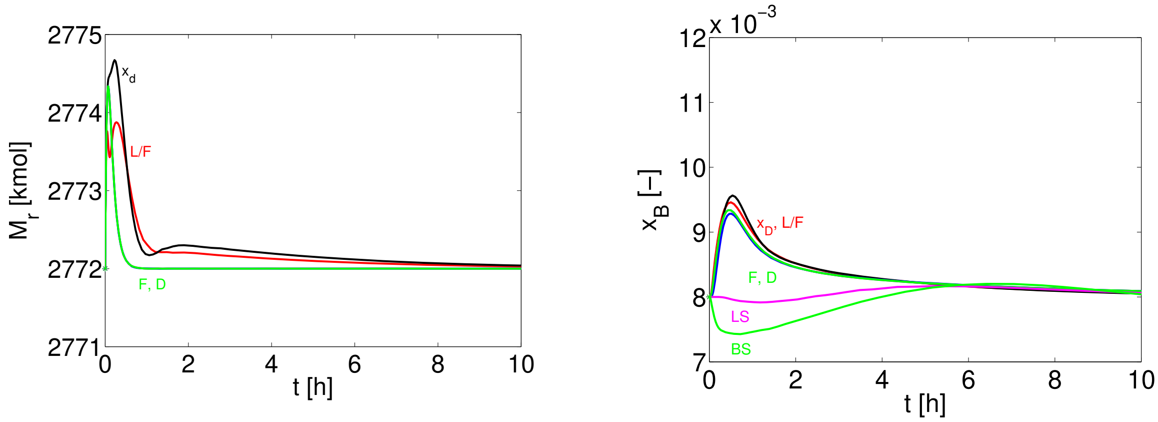

Figure 3.17: Reactor holdup (M_r) (left) and product composition (x_B) (right) when $\Delta F_0 = +20\%$ with robust setpoints.

The control deviations are significantly smaller than the expected implementation errors. If we assume small measurement errors, the study can be performed with some smaller expected implementation errors, which will reduce the economic loss, but not change the ranking.

3.5 Discussion

3.5.1 Feasibility regions

Specific constant setpoint policy

In addition to the economic loss for expected disturbances and implementation errors, the region of feasibility of a specific constant setpoint policy is important. A large feasible region is advantageous as it reduces the need for reconfiguration and thus keeps the control system simple. The choice of controlled variables has a large effect on the region of feasibility. In our case study, controlling L/F with nominal setpoints ($\{\tilde{D}_{dc}^{L/F,nom}|d_c = d_{c,max}^*\}$) gives a much larger feasible region than controlling F with nominal setpoints ($\{\tilde{D}_{dc}^{F,nom}|d_c = d_{c,max}^*\}$), see figure 3.18. The latter alternative is infeasible (see table 3.3) since the region of feasibility does not cover the expected disturbance region (D_d).

Online feasibility correction

The feasibility region with flexible setpoints (online feasibility correction) ($\tilde{D}_{dcg}^{flex}$) is independent of the controlled variables and corresponding setpoints. The feasibility region with flexible setpoints with zero implementation errors is equal the total feasibility region, i.e. $\{\tilde{D}_{dcg}^{flex}|d_c = 0, d_g = 0\}$=$D_d^{total}$. With no implementation errors in the constraints the fea-

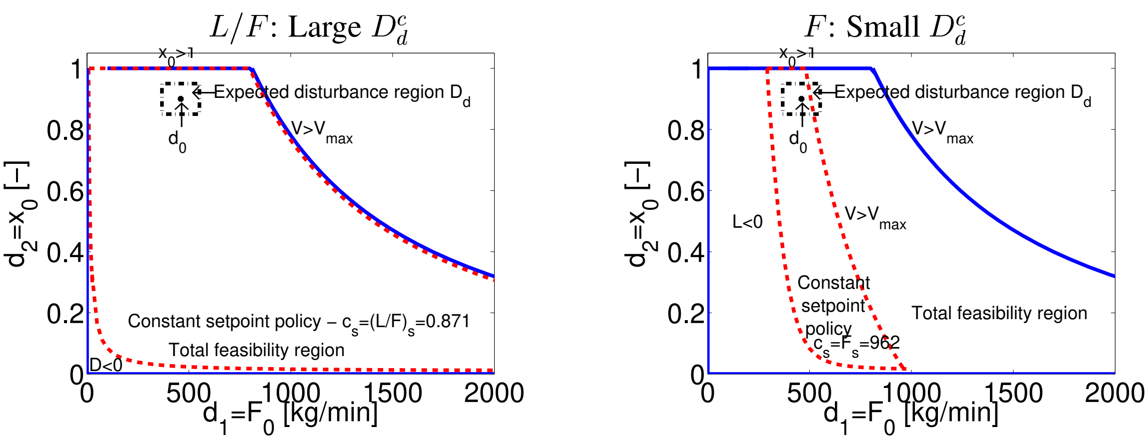

Figure 3.18: The constant setpoint policy feasibility region (dashed) when controlling L/F with nominal setpoints ($D_d^{nom,L/F}$=$\{\tilde{D}_{dc}^{nom,L/F}|d_c = d_{c,max}^*\}$) (left) and when controlling F with nominal setpoints ($D_d^{nom,F}$=$\{\tilde{D}_{dc}^{nom,F}|d_c = d_{c,max}^*\}$) (right).

sibility region with flexible setpoints ($\{\tilde{D}_{dcg}^{flex}||d_{g,j}| \leq |d_{g,max,j}^*|\}$) is larger than a specific constant setpoint policy feasibility region ($\tilde{D}_{dc}^c$), i.e. $\tilde{D}_{dc}^c \subseteq \{\tilde{D}_{dcg}^{flex}||d_{g,j}| \leq |d_{g,max,j}^*|\}$. Note that implementation error in the uncontrolled constraints may make $\{\tilde{D}_{dcg}^{flex}|d_g\}$ not a subset of D_{dc}^{flex} for some d_g. Figure 3.19 illustrates the feasibility region with constant nominal setpoints (left), constant robust setpoints (in the middle) and flexible setpoints (right) for given controlled variables ($c = F$) and with implementation errors $d_{c,max}^*$ and $d_{g,max}^*$. Use of constant nominal setpoints is not feasible (see table 3.3) since the region of feasibility does not cover the expected disturbance region. Use of constant robust setpoints is feasible and the feasible region is increased (and moved) to cover the expected disturbance region. When using flexible setpoints, feasibility is no problem, and the feasibility region is almost equal the total feasibility region.

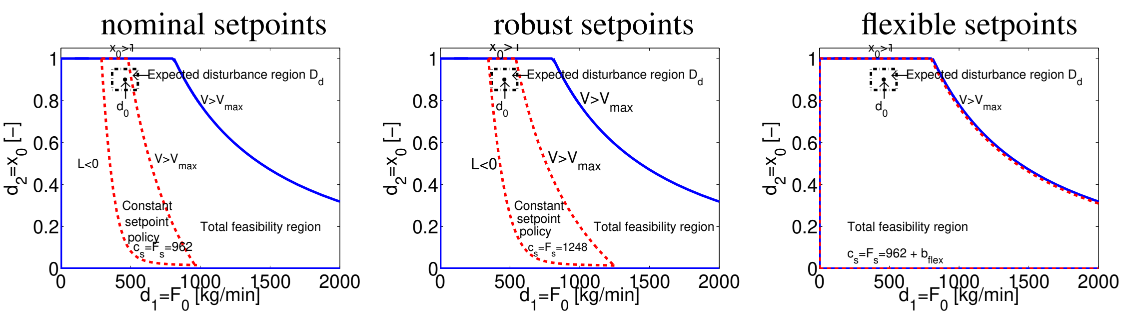

Figure 3.19: The feasibility region (dashed) with constant nominal setpoints (left), constant robust setpoints (middle) and flexible setpoints (right) when controlling F and with implementation errors d_c=$d_{c,max}^*$).

3.6 Conclusion

We have introduced several alternative methods for computing setpoints. The simplest is to use constant nominal setpoints, but this may give large loss in some cases or infeasible operation. One alternative is to find the best constant setpoint (”optimal backoff”) by solving a quite complex robust optimization problem. Another alternative is to allow for online adjustments of the nominal setpoints such that we achieve feasibility (MPC adjustment) (”flexible backoff”).

As a case study we have used a reactor, separator and recycle process. Control of x_D and L/F show the best self-optimizing control properties. Alternatives which follow Luybens rule (F and D), require robust setpoints and give larger loss than x_D and L/F. Alternatives with variable reactor holdup (e.g. Luyben Structure and Balanced Structure) require flexible setpoints and give significantly larger loss than x_D and L/F.

Although the feasibility region and the loss for a specific constant setpoint policy can be reduced by use of logic, model predictive control and/or online optimization, a good choice of controlled variables will reduce the need for these remedies and give a simpler and cheaper system. Note that the required backoff and the corresponding economic loss depend on the selected controlled variables. Thus, the primary issue is to select the right control structure (variables), whereas the backoff is just a setpoint *adjustment* to deal with nonlinearities and infeasibility.

Chapter 4

Control Structure Design for An Evaporation Process

Based on work presented at the 11th European Symposium on Computer Aided Process Engineering (ESCAPE-11), Kolding, Denmark, May 27-30, 2001

A systematic procedure for control structure selection, with emphasis on ”what to control” is applied to the evaporation process of Newell & Lee (1989). Promising sets of controlled variables are selected, based on steady-state economic criteria. The objective is to find sets of controlled variables which with constant setpoints keep the process close to the economic optimum (”self-optimizing control”) in face of disturbances and implementation errors. We here apply both setpoints found by nominal and robust optimization in addition to online feasibility correction. For the most promising sets of economic controlled variables a controllability analysis is performed and control structure selected. Compared to control of x_2, P_2 and F_3 as proposed by Kookos & Perkins (2002a) we find that control of $T_{201} - T_{200}$ in addition to the active constraints gives smaller losses and a simpler system.

4.1 Introduction

Control structure selection consists of selecting controlled variables, manipulated variables, measurements and links between them. A poor choice can give both dynamic and steady-state problems, such as instability, input saturation, operation outside constraints and non-optimal operation. This can be partly counteracted by using logic, model predictive control and online optimization, but the control system then becomes more complicated and costly than necessary. Selecting a good control structure is a precondition for getting a simple, well-behaving control system.

In this chapter we primarily consider the selection of controlled variables and corresponding setpoints to achieve 1) feasible operation and 2) close to optimal operation with respect to steady-state economics. Maarleveld & Rijnsdorp (1970) proposed to control variables at constraints in optimum (”active constraint control”). Arkun & Stephanopoulos (1980) considered tracking of optimally active constraints which vary with the disturbances. Morari et al. (1980) and Skogestad (2000a) identify controlled variables which, when kept constant at their setpoint, automatically keep the operation close to its optimum, such that online optimization may not be needed. Normally, the setpoints are selected as their nominally optimal values. However, this may exclude controlled variables that are workable, and we may not find any feasible sets of controlled variables at all. Backoff, (Perkins 1998), from the nominal operation is sometimes needed in order to obtain feasible operation. We define backoff (or setpoint adjustment) as the difference between the nominally optimal setpoint and the actual setpoint. The actual setpoints are chosen for example to achieve feasible operation when there are disturbances or implementation errors.

We here consider using robust setpoints or flexible setpoints to achieve feasibility. Robust setpoints are determined by robust optimization, which minimizes the nominal steady-state economic criteria, given that we have feasibility (i.e. the constraints are satisfied for all expected disturbances and implementation errors (Glemmestad et al. 1999)). Flexible setpoints (online feasibility correction) are based on the nominal setpoints and setpoint adjustment is done online when needed to avoid infeasibility. In practice, flexible setpoints (online feasibility correction) is implemented by using MPC. Note that the required backoff and corresponding economic loss depend on the selected controlled variables. Thus, the primary issue is to select the right controlled variables, whereas the backoff is just a setpoint *adjustment* to deal with nonlinearities and in particular constraints.

Perkins and co-workers (e.g. Perkins et al. (1989), Narraway et al. (1991), Narraway & Perkins (1993), and Narraway & Perkins (1994)) deal with the selection of control structure based on steady-state economics, but their approach is rather different: They assume that most of the disturbances are handled by the online optimization, which recomputes the setpoints. They do not consider the possibility that these setpoints may be wrong because of model error or unknown disturbances. The only ”uncertainty” they consider is the dynamic control error due to assumed small disturbances which may require backoff from the active constraints to achieve feasibility.

Kookos & Perkins (2002a) applied this method to the evaporation process. The proposed controlled variables are the operating pressure P_2, the product composition x_2 and the recirculating feedrate F_3. In this chapter we will select a control structure for the same process by following a procedure aiming at self-optimizing control.

4.2 Control Structure Selection Procedure

We apply the procedure presented in chapter 3:

1. *Initial system analysis*:
   Identify the number of degrees of freedom, define objective function and constraints, identify main disturbances and candidate controlled variables, optimize at nominal and for expected disturbances, see equation 3.24.

2. *Identify sets of candidate controlled variables*:
   Eliminate variables with no steady-state effect, use active constraint control, eliminate variables with large losses by using short-cut loss evaluation, eliminate variables based on process insight.

3. *Evaluate the loss for different sets of controlled variables*, using:

   (a) Constant nominal setpoints (see equation 3.29)

   (b) Constant robust setpoints (see equation 3.38)

   (c) Nominal setpoints with online feasibility correction (flexible setpoints) (see equations 3.45 and 3.46)

4. *Final evaluation and selection of control structure*:
   Stabilization, controllability analysis, selection of control configuration and simulation of proposed control structures.

4.3 Evaporation Process Case Study

In the evaporation process of Newell & Lee (1989) the concentration of dilute liquor is increased by a vertical heat exchanger with recirculated liquor, see figure 4.1.

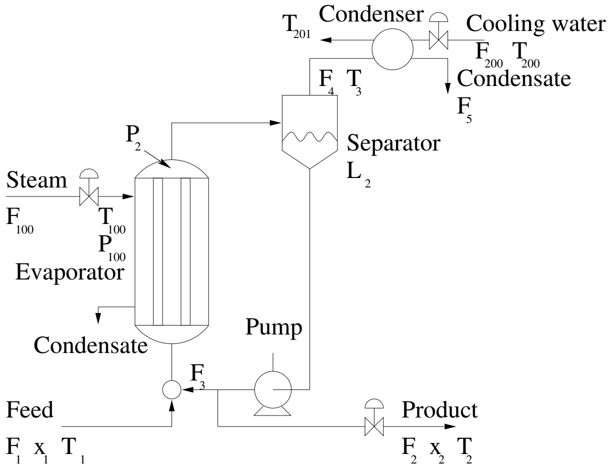

Figure 4.1: Evaporation process

4.3.1 Initial system analysis

The steady-state economic objective is to minimize the operational cost ($\$/h$) related to steam, cooling water and pump work (Wang & Cameron 1994):

$$J = 600F_{100} + 0.6F_{200} + 1.009(F_2 + F_3) \tag{4.1}$$

Process constraints related to product specification, safety and design must be met:

$$x_2 \geq 35\% \tag{4.2}$$
$$40\text{kPa} \leq P_2 \leq 80\text{kPa} \tag{4.3}$$
$$P_{100} \leq 400\text{kPa} \tag{4.4}$$
$$0\ \text{kg/min} \leq F_{200} \leq 400\text{kg/min} \tag{4.5}$$
$$0\ \text{kg/min} \leq F_3 \leq 100\text{kg/min} \tag{4.6}$$

There are four manipulated variables; steam pressure, cooling water flowrate, recirculating flowrate and product flowrate:

$$u^T \ = \ [F_{200}\ P_{100}\ F_3\ F_2] \tag{4.7}$$

One degree of freedom is purely dynamic (the separator level which needs to be stabilized), hence there are three steady-state degrees of freedom. The major disturbances are feedrate, feed concentration, feed temperature and cooling water inlet temperature, with expected variations about $\pm 20\%$:

$$d^T = [F_1\ x_1\ T_1\ T_{200}] = [10 \pm 2\ \text{kg/min} \quad 5 \pm 1\% \quad 40 \pm 8^{\text{o}}\text{C} \quad 25 \pm 5^{\text{o}}\text{C}]. \tag{4.8}$$

The controlled variable candidates are primarily all possible measurements and manipulated variables:

$$y^T = [F_2\ F_3\ F_4\ F_5\ X_2\ T_2\ T_3\ L_2\ P_2\ F_{100}\ T_{100}\ P_{100}\ Q_{100}\ F_{200}\ T_{201}\ Q_{200}] \tag{4.9}$$

In addition we look at some combinations of measurements (or feed-forward improvement of the alternative): Six flowratios (F_2/F_1, F_3/F_1, F_4/F_1, F_5/F_1, F_{100}/F_1, F_{200}/F_1) and one temperature difference ($T_{201} - T_{200}$).

Expected implementation error associated with each variable is: Flowrates $\pm 10\%$, compositions $\pm 1\%(absolute)$, temperature $\pm 1^oC$, pressure $\pm 2.5\%$, flowratios $\pm 22\%$ and temperature differences $\pm 2^oC$. The implementation errors are computed as worst-case error for flowratios and the temperature difference. The model equations are given in Newell & Lee (1989)[1].

The steady-state optimal value at the nominal point for the objective function is $6162\$/h$, corresponding to the following optimal values for the measurements and manipulated variables:

$$y^T_{opt} = [1.4\ 27.7\ 8.6\ 8.6\ 35.0\ 90.9\ 83.4\ 1.0\ 56.2\ 10\ 151.5\ 400\ 365.6\ 230.2\ 45.5\ 330] \tag{4.10}$$

Steady-state optimizations at the nominal point and for extreme values of the expected disturbances yield that two of the constraints; product composition (x_2) and steam pressure (P_{100}), are always active. The last degree of freedom is optimally unconstrained for most disturbances. There is one exception, for low feedrate the last degree of freedom is consumed by the minimum operating pressure constraint.

[1]Newell & Lee (1989) assumed the time lag connected to the slave controllers to be 1.2 min. This seems too large, and we use 0.1 min

4.3.2 Identify sets of candidate controlled variables

There are 22 candidate controlled variables and three steady-state degrees of freedom. We have already eliminated the separator level (L_2) which has no steady-state effect. We choose to control the constraints which are always optimally active ($c_1 = x_2$, $c_2 = P_{100}$). We are then left with 20 candidate controlled variables and 1 steady-state degree of freedom, which gives 20 possible sets. The best economic choice for the last controlled variable is related to the self-optimizing control properties.

The minimum singular value rule (Skogestad & Postlethwaite 1996), is applied to eliminate some of the sets. For one single input the rule is to select the controlled variable with the largest absolute steady-state process gain ($|G(0)|$), when the variables are scaled with respect to the sum of the maximum setpoint error ($\max_d e_{c,s} = \max_d |c_{opt}(d_0) - c_{opt}(d)|$) and the expected implementation error (d_c). Eight of the candidate controlled variables give zero gain: F_2, F_4, F_5, T_{100}, Q_{200}, F_2/F_1, F_4/F_1 and F_5/F_1. They are fixed when the product composition (x_2) and steam pressure (P_{100}) are fixed and are not candidates for control. The seven most promising combinations of economic controlled variables are ranked in table 4.1. Using a short-cut method presented by Mahajanam & Zheng (2000) gives the same ranking.

Table 4.1: Most promising alternative sets of controlled variables based on the scaled steady-state gain $|G(0)|$

Rank	c_1	c_2	c_3	$\|G(0)\|$
1	x_2	P_{100}	T_{201}	0.0150
2	x_2	P_{100}	F_{200}/F_1	0.0135
3	x_2	P_{100}	F_{200}	0.0108
4	x_2	P_{100}	P_2	0.0044
5	x_2	P_{100}	T_2	0.0042
6	x_2	P_{100}	T_3	0.0042
7	x_2	P_{100}	F_3	0.0018
(Newell)	x_2	P_2	F_3	–

In addition we study an alternative proposed and used by Newell & Lee (1989). In this alternative the recirculating flowrate (F_3) is not used as a manipulated variable in the basic control layer. They do not use active constraint control because the last available manipulated variable, cooling water outlet flow (F_{200}), has too small effect on the product composition (x_2). The steam pressure (P_{100}) is not kept on its constraints, but is used to control the product composition (x_2). The cooling water flowrate (F_{200}) is used to control the operating pressure (P_2). This alternative, controlling x_2, P_2 and F_3, is labeled Newell[2].

[2]Kookos & Perkins (2002a) proposed the same controlled variables as Newell & Lee (1989).

4.3.3 Loss evaluation

(a) Loss evaluation with constant nominal setpoints

For the remaining 12 alternatives we compute the loss related to implementing constant nominal setpoints (compared to the truly optimal policy with all three variables re-optimized) for different disturbances and implementation errors. The nominal point and the corner-points for expected disturbances and implementation errors are included as operating points with equal weights (w_i). We assume that only one disturbance d_j or implementation error $d_{c,j}$ is perturbed from its nominal value at the same time. The nominal setpoints are found by

Table 4.2: Average and maximum percentage loss with constant nominal setpoints, constant robust setpoints and flexible setpoints. The nominal setpoint $c_{3,s}$, optimal backoff $b_{3,opt}$ and maximum flexible backoff $|b_{j,flex}|$ are included.

c_3	Nominal setpoints			Robust setpoints			Flexible setpoints			
	$c_{3,s}$	L_w	L_{max}	$b_{3,opt}$	L_w	L_{max}	$b^{max}_{2,flex}$	$b^{max}_{3,flex}$	L_w	L_{max}
reoptimized	$c^*_{opt}(d)$	0.55	1.05	–	0.55	1.05	–	–	0.55	1.05
$T_{201}-T_{200}$	20.48	inf	inf	2.53	0.58	1.08	0	2.53	0.55	1.05
T_{201}	45.48	inf	inf	2.53	0.59	1.08	0	2.53	0.56	1.05
F_{200}/F_1	23.12	inf	inf	−2.44	0.60	1.08	0	2.54	0.56	1.05
P_2	56.63	inf	inf	13.38	1.20	2.73	0	12.93	0.70	1.54
T_2	91.49	inf	inf	7.82	1.20	2.73	0	7.26	0.70	1.54
T_3	83.71	inf	inf	6.78	1.20	2.73	0	6.56	0.70	1.54
F_3/F_1	2.93	inf	inf	0.77	1.22	2.73	0	0.62	0.81	1.54
F_{200}	231.22	inf	inf	–	inf	inf	0	66.55	0.56	1.05
F_{100}/F_1	1.00	inf	inf	–	inf	inf	0	0.21	0.69	1.99
F_3	29.27	inf	inf	–	inf	inf	0	13.28	0.84	2.94
F_{100}	10.04	inf	inf	–	inf	inf	0	2.18	1.22	3.81
Q_{100}	367.57	inf	inf	–	inf	inf	0	79.61	1.22	3.81
Newell	–	inf	inf	–	inf	inf	12.93	11.69	0.72	1.66

inf: infeasible operation

Active constraints: $c_{1,s} = x_{2,s} = 36\%$, $c_{2,s} = P_{100,s} = 390kPa$

Newell: $c_1 = x_2$, $c_2 = P_2$, $c_3 = F_3$ ($c_{1,s} = 36$, $c_{2,s} = 56.63$, $c_{3,s} = 29.27$)

Reoptimized: Reoptimized with constraint backoff, see equation 3.27.

Optimal backoff: $b_{1,opt}$=0, $b_{2,opt}$=0

Flexible backoff: $b^{max}_{1,flex}$=0

$b^{max}_{j,flex}$=$max_i|b_{j,flex,i}|$

optimizing with constraint backoff at nominal point. In addition we evaluated the loss by using reoptimization with constraint backoff. Table 4.2 shows that none of the alternatives are feasible with constant nominal setpoints.

Figure 4.2 shows that the loss for the various controlled variables is most sensitive to disturbances in the feedrate (F_1), the feed composition (x_1) and cooling water inlet temperature (T_{200}), and to implementation errors in the unconstrained variable ($d_{c,3}$). Reducing the implementation error in the product composition ($d_{c,1}$) will give a significant reduction in the loss, but does not alter the ranking. The loss with reoptimization with constraint backoff is primarily caused by implementation errors in the controlled variables ($d_{c,1}$). Controlling F_{200}/F_1,

T_{201} or $T_{201} - T_{200}$ gives infeasibility ($P_2 < P_{2,min}$) at small feedrates (F_1). Controlling F_3, F_3/F_1, P_2, T_2 or T_3 gives infeasibility ($F_{200} > F_{200,max}$) at large feedrates (F_1) or high inlet cooling water temperature (T_{200}). In addition implementation error in F_{200}/F_1 ($d_{c,3}$) gives infeasibility when controlling F_{200}/F_1. Accordingly there are no feasible alternatives using nominal setpoints.

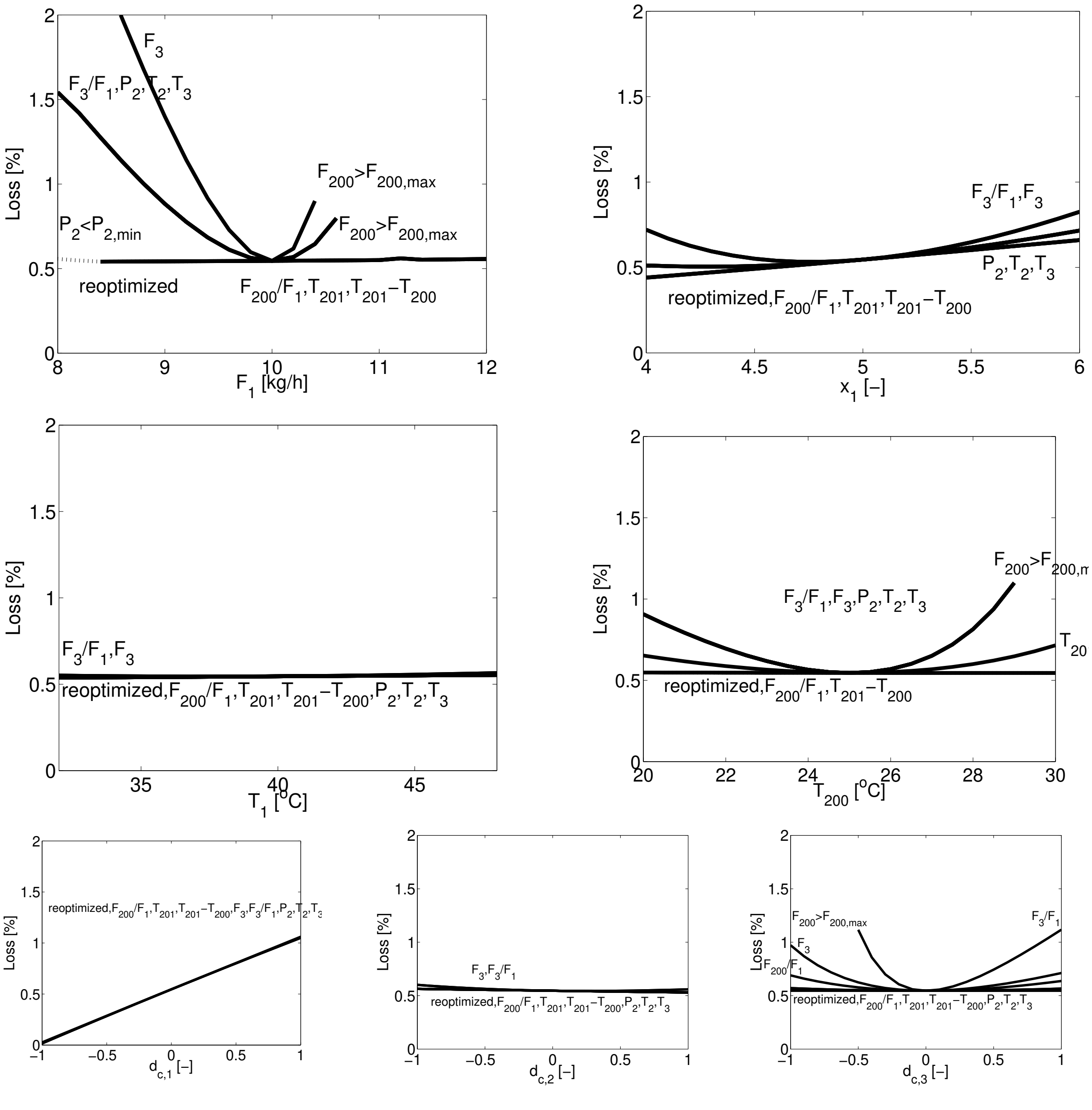

Figure 4.2: Loss as function of disturbances (F_1, x_1, T_1, T_{200}) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) with constant nominal setpoints ($c_{s,0}$).

(b) Loss evaluation with constant robust setpoints

To achieve feasibility we compute the optimal backoff by robust optimization (Glemmestad et al. 1999). The optimal backoff in the unconstrained controlled variable ($b_{3,opt}$) in addition to the average and maximum percentage loss are given in table 4.2. Controlling $T_{201} - T_{200}$ gives the smallest loss, closely followed by controlling T_{201} and F_{200}/F_1. For many of the alternatives (e.g. controlling F_3, F_{200} or Newell) the constraints are so tight that there exists no feasible constant setpoint adjustment offline.

Figure 4.3 shows that there are significant differences between the alternatives even at the nominal point (which is in the middle of the graphs). With robust setpoints the selection of controlled variables are sensitive to disturbances in the feed composition (x_1), the feedrate (F_1) and cooling water inlet temperature (T_{200}) in addition to the implementation error in the unconstrained variable ($d_{c,3}$).

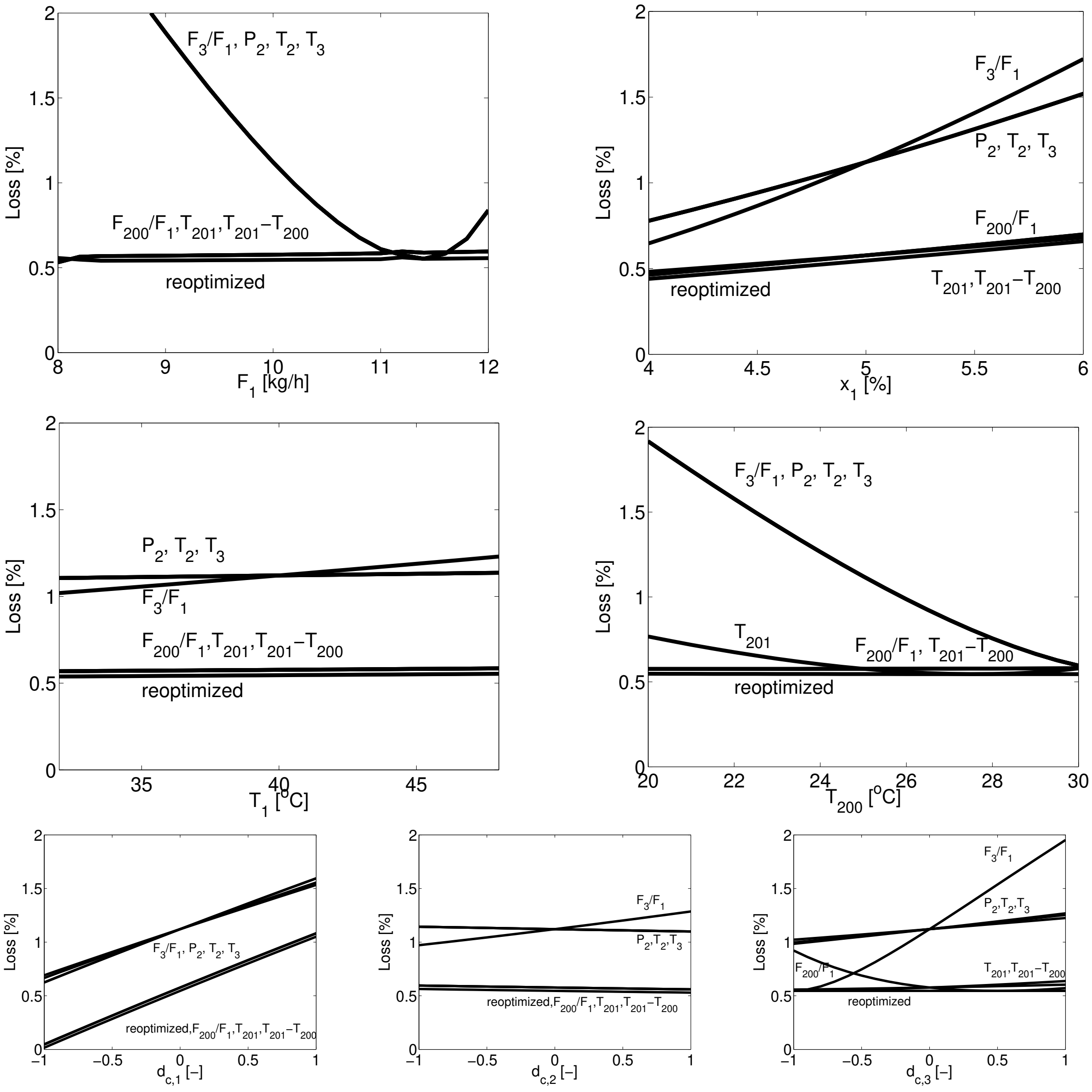

Figure 4.3: Loss as function of disturbances (F_1, x_1, T_1, T_{200}) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) with constant robust setpoints ($c_{s,robust}$).

(c) Loss evaluation with flexible setpoints

An alternative approach is to achieve feasibility by use of online feasibility correction. We assume hard prioritization among the controlled variables. Constrained controlled variables have high priority and unconstrained variables have low priority. The weight matrices Q_{II} and Q_I in equations 3.45 and 3.46 are selected as a diagonal matrix with elements equal to the inverse of the implementation error, $q_{ii} = 1/d_{c,i}$. Table 4.2 shows the maximum backoff in the unconstrained controlled variable ($|b_{3,flex}|$) in addition to the average and the maximum percentage loss when using flexible setpoints. All alternatives are now feasible. For this case study online adjustment of the nominal setpoints (flexible backoff) is always better than using the best constant setpoints (robust setpoints). However, there are only minor improvements compared with using robust setpoints for the best alternatives ($T_{201} - T_{200}$, T_{201}, F_{200}/F_1). The losses are somewhat reduced and are approximately equal to the losses with reoptimization (with constraint backoff). In addition, controlling F_{200} is now feasible and gives a relatively small loss.

Figure 4.4 shows the losses as a function of the expected disturbances and implementation errors, and we have the following comments:

- When controlling $T_{201} - T_{200}$, T_{201}, F_{200}/F_1 or F_{200} we avoid violating the lower operating pressure constraint ($P_{2,min}$) at low feedrates (F_1) by increasing $T_{201,s}$ or $T_{201,s} - T_{200,s}$, or by decreasing $F_{200,s}$ or $F_{200,s}/F_{1,s}$. Alternatively, we can reconfigure online by switching to control $P_2 = P_{2,min}$ when $P_{2,min}$ is violated.

- When controlling P_2, T_2, T_3, F_3 or F_3/F_1 we avoid infeasibility at high feedrates (F_1) and at high cooling water inlet temperature (T_{201}) when F_{200} saturates by increasing $P_{2,s}$, $T_{2,s}$ or $T_{3,s}$, or by decreasing $F_{3,s}$ or $F_{3,s}/F_{1,s}$. Alternatively, we can reconfigure online by switching to control $F_{200} = F_{200,max}$ when F_{200} saturates.

- In the proposed structure of Newell & Lee (1989) several constraints may be violated, and the logic becomes more complicated. For high feedrates and a high inlet cooling water temperature the cooling water flowrate should be kept constant instead of the operating pressure (P_2).

- Alternatives that follow Luybens rule (”Control a flowrate in every recycle”), i.e. Newell and F_3, give significant losses.

4.3.4 Final evaluation and selection of control structure

A controllability analysis was performed for the two most economically promising alternatives, namely control of F_{200}/F_1 and $T_{201} - T_{200}$. Control of T_{201} shows largely the same dynamic properties as controlling $T_{201} - T_{200}$ (except for disturbances in the inlet cooling water temperature T_{200}) and is not explicitly treated. Both alternatives are controllable.

The process is stabilized by controlling the holdup in the separator (L_2) by manipulating

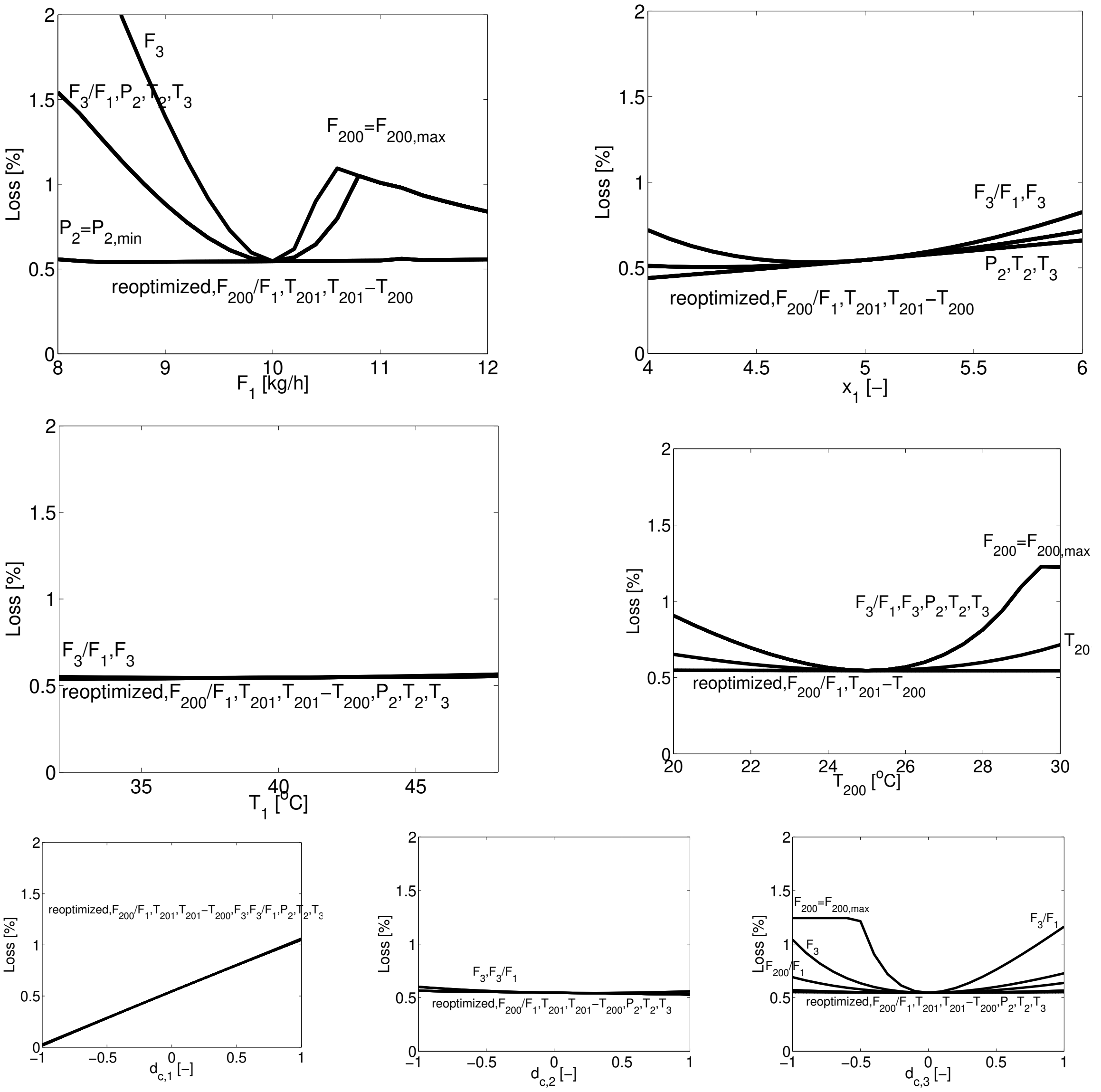

Figure 4.4: Loss as function of disturbances (F_1, x_1, T_1, T_{200}) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) with flexible setpoints ($c_{s,flex}$).

the product flow (F_4). The cooling water temperature difference ($T_{201} - T_{200}$) is paired with the cooling water flowrate (F_{200}). The corresponding relative gain array element is positive at steady-state (0.9368) and close to one at frequencies around the expected bandwidth. The resulting control structures when controlling F_{200}/F_1 or controlling $T_{201} - T_{200}$, respectively are shown in figures 4.5 and 4.6.

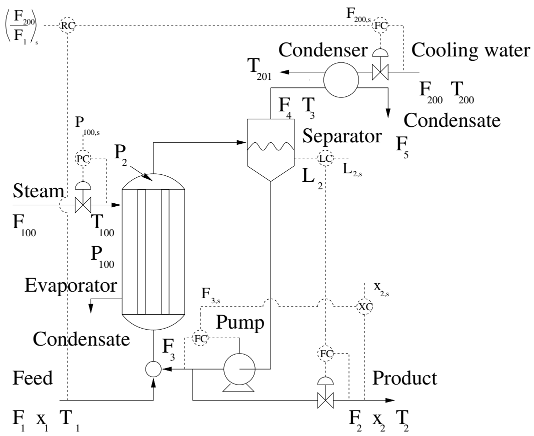

Figure 4.5: Evaporation process with control structure when controlling F_{200}/F_1

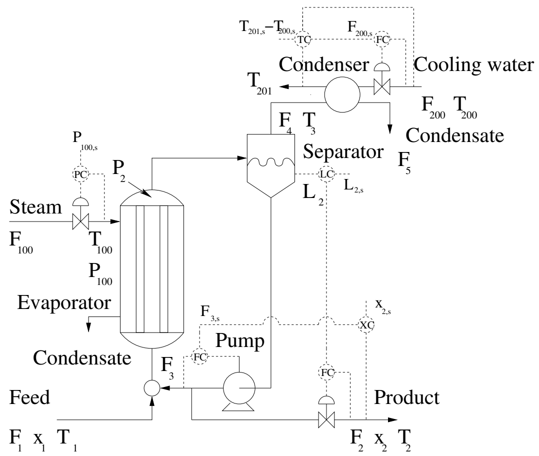

Figure 4.6: Evaporation process with control structure when controlling $T_{201} - T_{200}$

Decentralized controllers were designed by the SIMC tuning method (Skogestad 2003), and nonlinear simulations were performed to verify the controllability of the designs when using robust setpoints. Figure 4.7 shows the product composition (x_2) and evaporator operating pressure (P_2) when controlling F_{200}/F_1 or $T_{201} - T_{200}$ with robust setpoints in response to a 20% disturbance in the feedrate.

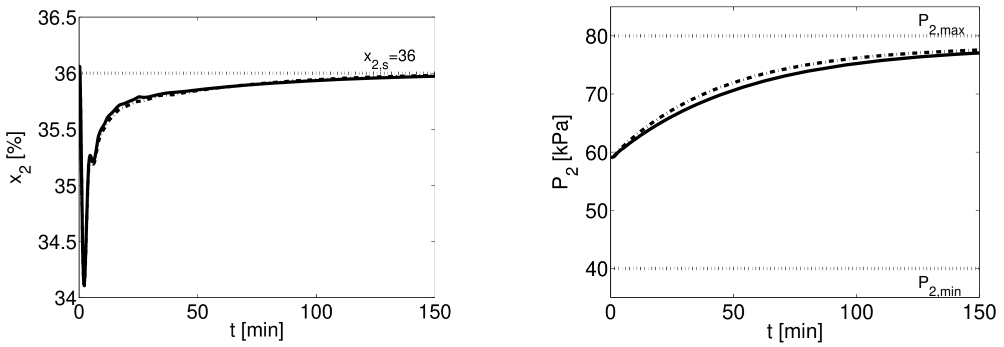

Figure 4.7: x_2 and P_2 when controlling either F_{200}/F_1 (solid) or $T_{201} - T_{200}$ (dashed) with constant robust setpoints and F_1 increased with 20% (from 10 kg/s to 12 kg/s).

4.4 Conclusion

A systematic procedure for control structure selection, with emphasis on ”what to control”, has been demonstrated on an evaporation process. Controlling $T_{201} - T_{200}$ gives the smallest economic loss both when using robust setpoints and flexible setpoints. To avoid computing flexible setpoints online (or reconfigure online) we propose to use robust setpoints. Controlling $T_{201} - T_{200}$ with robust setpoints in addition to active constraints shows acceptable control behavior. Compared with the structure of Kookos & Perkins (2002a) with control of x_2, P_2 and F_3, the losses are smaller and the system is simplier since online feasibility correction is not required.

Chapter 5

Application of a Plantwide Control Design Procedure to a Combined Cycle Power Plant

Based on work presented at the American Institute of Chemical Engineers (AIChE) Annual Meeting, Indiannapolis, US, Nov. 3-8, 2002 and at the 11th Nordic Process Control Workshop, Trondheim, Norway, Jan. 9-11, 2003

Plantwide control deals with the structural decisions of the control system for an overall plant. Usually these decisions are based on experience and engineering insight. In this chapter we apply the plantwide control design procedure of Larsson & Skogestad (2001) to a combined cycle power plant. The process has one unconstrained steady-state degree of freedom at its optimal operating point. We find that control of the super-heater gas inlet temperature in addition to the variables at active constraints gives the smallest loss, only 0.16% larger than reoptimization with constraint backoff. Controlling the super-heater inlet temperature partly decouples the operation of the gas turbine and the steam turbine cycle.

5.1 Introduction

A chemical plant, including a power plant, may have thousands of measurements and control loops. In practice, the control system is usually divided into several layers, separated by time scale, including

- scheduling (weeks)
- site-wide optimization (day)
- local optimization (hour)
- supervisory (predictive, advanced) control (minutes)
- regulatory control (seconds).

The layers are linked through the controlled variables, where the setpoints are computed by the upper layer and implemented by the layer below. An important issue is the selection of these variables.

Plantwide control deals with the structural decisions of the control system for an overall plant. Usually these decisions are based on pure experience and engineering insight. A typical control system incorporating local feedback and online optimization is shown in figure 5.1. A recent review of the literature on plantwide control and a plantwide control design procedure can be found in Larsson & Skogestad (2001). In this paper we apply the procedure to a combined cycle power plant. A systematic approach to plantwide control starts by formulating the operational objectives. This is done by defining a cost function J that should be minimized with respect to the optimization degrees of freedom, subject to a given set of constraints.

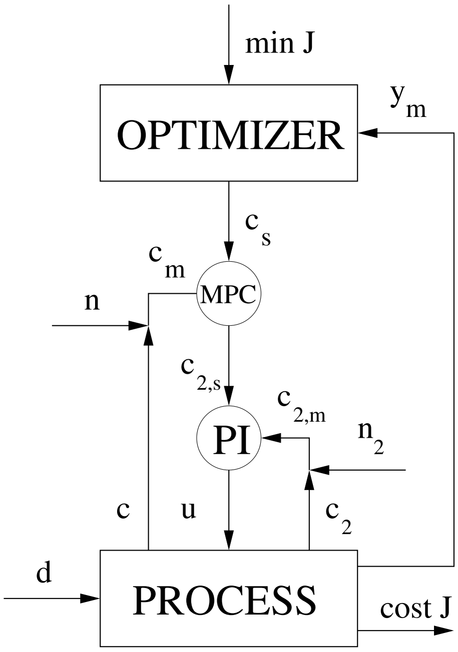

Figure 5.1: A typical control system incorporating local feedback and online optimization: The process is disturbed (d) and a regulatory control layer (here: PI-controller) tries to reject fast disturbances by keeping the secondary controlled variables (c_2) at their setpoints ($c_{2,s}$) by updating the manipulated variables (u). A supervisory control layer (here: MPC) tries to reject slow disturbances by keeping the primary controlled variables (c) at their setpoints (c_s) by updating the setpoints to the secondary controlled variables ($c_{2,s}$). Steady-state optimization based on process measurements (y_m) is performed at regular intervals to track the optimum (minimize the cost J) by updating the setpoints to the supervisory control layer (c_s).

5.2 Plantwide Control Design Procedure

The plantwide control design procedure is divided in two main parts:

I. Top-down analysis, including definition of operational objectives and consideration of degrees of freedom available to meet these. Steps:

1. Selection / identification of manipulated variables

2. Degrees of freedom analysis

3. Selection of primary controlled variables c (based on steady-state economics)

4. Selection of production rate manipulator.

II. Bottom-up design of the control system, starting with stabilizing the process. Steps:

5. Structure of regulatory control layer (including selection of secondary controlled variables, c_2.)

6. Structure of supervisory control layer (including MPC applications)

7. Structure of optimization layer

8. Validation of proposed control structure.

The procedure is generally iterative and may require several loops through the steps, before converging at a proposed control structure.

A very important issue is the selection of the controlled variables c. First, we need to select the "primary" controlled variables c directly related to ensuring optimal economic operation (step 3 above). We propose to:

- Control active constraints
- Select unconstrained controlled variables so that with constant setpoints the process is kept close to its optimum in spite of disturbances and implementation errors.

The selection procedure involves the following sub-steps:

Step 3.1 Determination of degrees of freedom for optimization

Step 3.2 Definition of optimal operation (cost and constraints)

Step 3.3 Identification of important disturbances

Step 3.4 Optimization (nominally and with disturbances)

Step 3.5 Identification of candidate controlled variables

Step 3.6 Evaluation of loss for alternative combinations of controlled variables (loss imposed by keeping constant setpoints when there are disturbances or implementation errors)

Step 3.7 Evaluation and selection of primary controlled variables (including controllability analysis).

Second, we need to select ”secondary” controlled variables c_2 which are needed in order to achieve satisfactory regulatory control (step 5 above). The selection of these consists of the following sub-steps:

Step 5.1 Control unstable or integrating liquid levels

Step 5.2 Control other unstable modes, e.g. for an exothermic reactor

Step 5.3 Control variables which would otherwise ”drift away” due to large disturbance sensitivity. This involves controlling extra local measurements which can be used for local disturbance rejection (including ”linearization” of the process).

5.3 Combined Cycle Power Plant Case Study

In this chapter we apply the plantwide control design procedure to a simple combined cycle power plant shown in figure 5.2. The plant produces electric power and consists of a gas

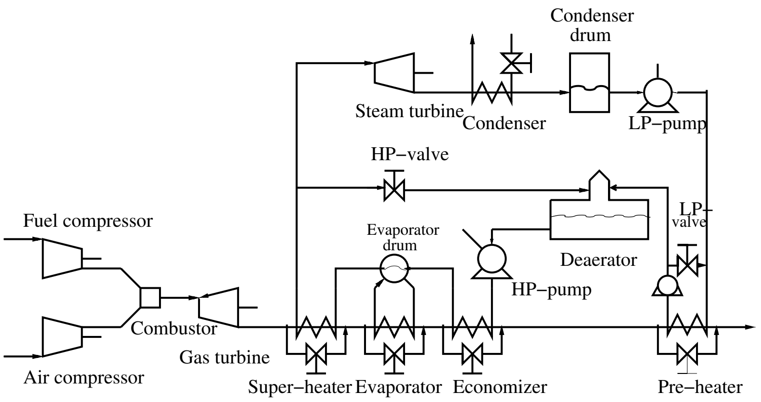

Figure 5.2: A simple combined cycle power plant process

turbine and a steam turbine cycle. In the gas turbine compressed natural gas (fuel) and air react in the combustor to flue gas with high temperature. The flue gas is expanded in the turbine[1] and electric power is produced. The exhaust gas still has high temperature and in the steam turbine cycle it is heat-exchanged with water to produce steam. The steam is expanded through the steam turbine and more electric power is produced.

The process is a single pressure combined cycle with a back-pressure steam turbine (see also figure 3.4 in Bolland (1990)). In addition, we have included a fuel compressor and bypasses around the super-heater, evaporator, economizer and pre-heater. The gas turbine, steam turbine, fuel compressor, air compressor and electric generator are assumed to be connected

[1]This turbine is here called the gas turbine, but often the term ”gas turbine” denotes the whole system with compressor, combustor and turbine.

on a single shaft, but with gears so that the fuel and air compressor speeds can be selected independently. The high pressure ratio over the turbines results in choked flow, which implies that the turbine flowrate is independent of the turbine speed. Since the turbine speed has only a minor effect on the operation with our assumptional constant efficiency, we have not included extra gears to allow the turbine speeds be selected independently. The turbine speeds are therefore equal to the electric generator speed, which is given by the frequency of the electric network. More details can be found in the diploma works of Gronnaess (2001) and Saue (2002).

5.3.1 Manipulated variables

The process has eleven manipulated variables (fuel compressor speed, air compressor speed, super-heater bypass, evaporator bypass, economizer bypass, pre-heater bypass, LP pump work, LP recycle flowrate, HP recycle flowrate, HP pump work and cooling water flowrate), see table 5.1.

Table 5.1: Manipulated variables and degrees of freedom

	Manipulated variables		11
	Fuel compressor speed	$\omega_{c,fuel}$	
	Air compressor speed	$\omega_{c,air}$	
	Super-heater bypass	F_{super}	
	Evaporator bypass	F_{evap}	
	Economizer bypass	F_{econ}	
	Pre-heater bypass	F_{pre}	
	LP pump work	$W_{p,LP}$	
	LP recycle flowrate	F_{LP}	
	HP recycle flowrate	F_{HP}	
	HP pump work	$W_{p,HP}$	
	Cooling water flowrate	F_{cw}	
$-$	Levels with no steady-state effect		2
	Condenser drum holdup	M_{cond}	
	Evaporator drum holdup	M_{evap}	
$-$	Other constraints and specifications		$1/2$
	Deaerator pressure	P_d	
	Net electricity load (case I)	$W_{net,s}$	
	Fuel feedrate (case II)	F_{fuel}	
$=$	Number of steady-state degrees of freedom		$8/7$

5.3.2 Degrees of freedom analysis

There are 11 dynamic degrees of freedom, see table 5.1. However, there are two holdups which need to be controlled but which have no steady-state effect. This then consumes two degrees of freedom. In addition, the deaerator pressure is given (1 atm) and this leaves eight steady-state degrees of freedom. Also, there may be a constraint on the feed or production rate (case I and case II) which consumes one degree of freedom, and we are then left with only seven steady-state degrees of freedom.

5.3.3 Primary controlled variables

Degrees of freedom for optimization

The number of degrees of freedom for optimization is equal to the number of steady-state degrees of freedom, which in our case is seven or eight, see table 5.1.

Definition of optimal operation

Economic objective
The economic objective during operation is to minimize the cost J. This is the costs of the utility and raw materials minus the value of the electric power:

$$J = p_{fuel}F_{fuel} + p_{air}F_{air} + p_{cw}F_{cw} - p_{el}W_{net} \tag{5.1}$$

The net electric power is:

$$W_{net} = W_{t,gas} + W_{t,steam} - W_{c,fuel} - W_{c,air} - W_{p,LP} - W_{p,HP} \tag{5.2}$$

We here consider three different cases:

- Given net electricity production W_{net} (case I)
- Given fuel feedrate F_{fuel} (case II)
- No specification on net electricity production and free fuel feedrate (case III)

In the following we assume free air and cooling water (with no cost). This is reasonable for Norwegian conditions. The objective for case I with a given net electricity production can then be simplified to minimize the use of fuel (natural gas).

$$J_I = F_{fuel} \tag{5.3}$$

Similarly, the objective for case II can be simplified to maximize the net electricity production:

$$J_{II} = -W_{net} \tag{5.4}$$

Finally, the objective for case III can be simplified to minimizing:

$$J_{III} = -p_{el}/p_{fuel}W_{net} + F_{fuel} \tag{5.5}$$

The price ratio p_{el}/p_{fuel} in Norway today is approximately 0.038 kg/MJ ($p_{el} = 0.15\ NOK/kWh$ and $p_{fuel} = 0.7\ NOK/Sm^3$). However, in this case study we use a value of $0.1\ kg/MJ$.

All three cases will probably occur during the plants life cycle, so we would like to find a control structure for each case which allows for a simple switch between them. Case III is especially relevant because of the liberation of the energy market, e.g. (Ferrari-Trecate, Gallestey, Stothert, Hovland, Letizia, Spedicato, Morari & Antoine 2002). We will therefore mostly concentrate on case III.

Constraints

The most important constraints are summarized below:

$$T_{comb} \leq 1500^oC \quad (5.6)$$
$$T_{w,pre,n} \geq 63^o \quad (5.7)$$
$$T_{w,super,1} \leq 550^oC \quad (5.8)$$
$$F_{cw} \leq F_{cw,max} \quad (5.9)$$
$$F_{LP,valve} \leq F_{LP,valve,max} \quad (5.10)$$
$$f_{surge,comp,flue}(P_{comb}/P_{flue}, N_{comp,flue}, F_{flue}) \leq 0 \quad (5.11)$$
$$f_{surge,comp,air}(P_{comb}/P_{air}, N_{comp,air}, F_{air}) \leq 0 \quad (5.12)$$
$$P_{comb} \leq 150\ bar \quad (5.13)$$
$$P_{w,evap} \leq 220\ bar \quad (5.14)$$
$$P_{w,deaerator} = 1\ bar \quad (5.15)$$

In addition all flowrates should be non-negative. The temperature constraints are steady-state constraints which means that short-term transient violations of the temperature constraints are acceptable. The other constraints are transient constraints which must be satisfied at all times.

Identification of important disturbances

Table 5.2: Disturbances with expected variations

Disturbance	Nominal value	Expected variation	Unit
Fuel feed pressure (P_{fuel})	20	± 4	bar
Fuel feed temperature (T_{fuel})	10	± 2	^oC
Air feed pressure (P_{air})	1	± 0.01	bar
Air feed temperature (T_{air})	10	± 10	^oC
Cooling water temperature (T_{cw})	10	± 5	^oC
Flue gas outlet pressure (P_{flue})	1	± 0.01	bar
Net electricity production(W_{net})(case I)	1100	± 100	MW
Fuel feedrate (F_{fuel})(case II)	25	± 5	kg/s

The nominal values and expected variations for the disturbances are given in table 5.2. The most important disturbance for case I is the net electricity production (W_{net}) and for case II the fuel feedrate (F_{fuel}). For case III the disturbance with largest effect on the optimum is the air inlet temperature (T_{air}). Other disturbances, which have not been considered in this case study, include the frequency of the electric net and the ambient temperature.

Table 5.3: Optimal operation for different fuel feedrates (F_{fuel}).

F_{fuel} $[kg/s]$	W_{net} $[MW]$	$-J_{III}$ $[kg/MJ]$	η [%]	DOFs (I,II,III)	Active constraints	Comment
33.2921	846.4637	51.3542	50.72	$0,0,1$	1,2,3,4,6,7,8,9	Active constraint change, max η
35	889.5541	53.9554	50.70	$0,0,1$	1,2,3,4,7,8,9	
37.0449	941.4737	57.1025	50.70	$0,0,1$	1,2,3,4,5,6,7,9	Active constraint change
40	1010.9215	61.0922	50.42	$0,0,1$	1,2,3,4,5,6,7	
45	1121.1309	67.1131	49.70	$0,0,1$	1,2,3,4,5,6,7	
49.4784	1195.3742	70.0590	48.20	$0,0,1$	1,2,3,4,5,6,7	Optimum for case III
50	1199.7787	69.9779	47.87	$0,0,1$	1,2,3,4,5,6,7	
50.6697	1202.2403	69.5543	47.34	$0,0,1$	1,2,3,4,5,6,7	Max W_{net}
52.1408	1042.8165	52.1409	39.90	$0,0,1$	1,2,3,4,5,6,7	Max F_{fuel}

J_{III}: Profit for case III

DOF: no. of unconstrained degrees of freedom (for cases I, II and III)

W_{net}: net electricity production

η: efficiency = net electricity production W_{net}/total reaction enthalpy H_{rx}

Active constraints: 1: Max gas turbine inlet temperature (eq. 5.6), 2: Max cooling water flowrate (eq. 5.9), 3: Min HP recycle steam flowrate, 4: Min super-heater bypass flowrate, 5: Min evaporator bypass flowrate, 6: Min economizer bypass flowrate, 7: Max LP recycle flowrate (eq. 5.10), 8: Max steam turbine inlet temperature (eq. 5.8), 9: Max steam evaporator pressure (eq. 5.14)

Steady-state optimization

We have optimized the operation for different fuel feedrates and present in table 5.3 the resulting number of unconstrained degrees of freedom and active constraints and corresponding net electricity production. Cases I and II have no unconstrained steady-state degrees of freedom, while case III has one.

At high flowrates the gas turbine inlet temperature is at its maximum of 1500^oC. The HP recirculating flowrate is always at its minimum. The cooling water flowrate and the LP recirculating flowrate are always at their maximum. The bypasses around the super-heater, the evaporator and the economizer are always closed. The optimally active constraints are changed when the fuel feedrate drops below 38.4267 kg/s.

The optimum for case III is obtained with a fuel feedrate of 49.4784 kg/s and a net electricity production of 1195 MW. The objective function J is then 70.0590.

The maximum electricity production is achieved with a fuel feedrate of 50.6697 kg/s. The net electricity production is then 1202 MW.

The maximum achievable fuel feedrate is 52.1408 kg/s. The net electricity production is then 1043 MW.

The maximum efficiency η is 0.5072, which is achieved with a fuel feedrate equal 33.2921 kg/s and a net electricity production equal 846 MW. The optimally active constraints have then changed; the maximum steam turbine inlet temperature is active instead of the minimum high pressure recirculating flowrate.

We have also performed optimization for case III with respect to different disturbances. The optimally active constraints do not change. Expected disturbances in the air inlet temperature have the largest effect on the optimal operation.

Identification of candidate controlled variable sets

We consider the following candidate controlled variables:

$$c^T = [u \;\; p \;\; F \;\; T \;\; Q \;\; W \;\; N \; F_R] \tag{5.16}$$

Here u denotes the manipulated variables. The remaining are measured or combined variables: p is the pressure, F is the flowrate, T is the temperature, Q is the duty, W is the work, N is the compressor speed and F_R is the flowratio. The 89 candidate controlled variables are shown in table 5.4.

The implementation errors are initially assumed to be $\pm$ 10% for flowrates, $\pm$ 2.5% for pressures, $\pm$ 1 ^oC for temperatures, $\pm$ 30% for duties, $\pm$ 30% for work and $\pm$ 10% for compressor speed. An exception is combustor temperature (T_{comb}) which is very high and the implementation error is expected to be $\pm$ 10 ^oC.

For cases I and II there are no unconstrained degrees of freedom at the optimum. Because we expect the fuel feedrate to always exceed 38.4287 kg/s the optimally active constraints will not change. We therefore select to control the following active constraints (see table 5.3): Maximum gas turbine inlet temperature (1), maximum cooling water flowrate (2), minimum high-pressure recirculating flowrate (3), maximum low-pressure recirculating flowrate (4), no super-heater bypass (5), no evaporator bypass (6) and no economizer bypass (7).

For case III we control the same active constraints, but in addition the production rate is an unconstrained degree of freedom. So we need to select one more controlled variable. An initial screening of the 89 candidate controlled variables is performed by evaluating the steady-state gain ($|G(0)|$) where $G(0)$ is obtained with the active constraints kept constant. The candidate controlled variables are scaled with respect to variation in optimal values (maximum deviation from the nominally optimal value, $\Delta c_i = \max_D |c_{opt,i}(d) - c_{opt,i}(d_0)|$) and implementation errors. According to the singular value rule (Skogestad & Postlethwaite 1996) the steady-state gain should be maximized. The super-heater gas inlet temperature ($T_{g,super,1}$) seems to be the most promising variable, see table 5.4. Candidate controlled variables with a zero gain have either no steady-state effect or are not independent of the specified active constraints. A small value of the steady-state gain may indicate feasibility problems for larger disturbances, but since this is a local analysis it may not necessarily be the case.

Table 5.4: Initial screening of candidate controlled variables (c_2). Ranked by the (scaled) steady-state gain ($|G(0)|$).

Rank	c_2	$\|G(0)\|$
1	$T_{g,super,1}$	7.6936
2	$T_{g,super,2}$	7.6898
3	$T_{g,super,3}$	7.6839
4	$T_{g,super,4}$	7.6748
5	$T_{g,super,5}$	7.6613
6	$T_{g,super,6}$	7.6417
7	$T_{w,super,1}$	7.6405
8	$T_{g,super,7}$	7.6148
9	$T_{w,super,2}$	7.6035
10	$T_{w,super,3}$	7.5437
11	$T_{g,evap,1}$	7.5419
12	$T_{g,evap,2}$	7.4616
13	$T_{w,super,4}$	7.4464
14	$T_{g,evap,3}$	7.3748
15	$T_{w,super,5}$	7.2858
16	$T_{g,evap,4}$	7.2828
17	$T_{g,evap,5}$	7.1868
18	$T_{g,evap,6}$	7.0886
19	$T_{w,super,6}$	7.0168
20	$T_{g,evap,7}$	6.9897
21	$T_{g,econ,1}$	6.8679
22	$T_{g,econ,2}$	6.6881
23	$T_{w,super,7}$	6.5726
24	$T_{g,econ,3}$	6.4145
25	$T_{w,econ,6}$	6.1383
26	$T_{w,evap}$	5.9777
27	$T_{g,econ,4}$	5.9528
28	$T_{w,econ,5}$	5.9329
29	$T_{w,econ,7}$	5.6884
30	$P_{g,comb}$	5.4713
31	$T_{w,econ,4}$	5.3397
32	$T_{g,econ,5}$	5.0688
33	$P_{w,evap}$	4.6744
34	$T_{w,econ,3}$	4.2523
35	$F_{g,pre,bypass}$	3.8911
36	$P_{w,cond}$	3.6352
37	$T_{g,econ,6}$	3.5759
38	$T_{g,pre,7}$	2.8786
39	$T_{g,pre,6}$	2.6817
40	$N_{air,dim}$	2.6644
41	$T_{g,pre,5}$	2.4641
42	$F_{g,air}$	2.3358
43	$F_{g,econ}$	2.2931
44	$F_{g,evap}$	2.2931
45	$F_{g,super}$	2.2931
46	$F_{g,gasturbin}$	2.2931
47	$T_{w,econ,2}$	2.2232
48	$T_{g,pre,4}$	2.1113
49	$T_{w,econ,1}$	2.0919
50	$T_{g,pre,3}$	1.7340
51	$T_{w,cond}$	1.5724
52	$F_{g,pre}$	1.5391
53	$W_{comp,air}$	1.4687
54	$W_{comp,fuel}$	1.4496
55	Q_{super}	1.3846
56	$T_{g,pre,2}$	1.3670
57	$F_{w,pump,LP}$	1.2288
58	$F_{w,pump,HP}$	1.2288
59	$F_{w,pump,HP}$	1.2288
60	$F_{w,evap}$	1.2288
61	$F_{w,super}$	1.2288
62	$F_{w,steamturbine}$	1.2288
63	$W_{gas,turbine}$	1.0653
64	$T_{g,pre,1}$	1.0101
65	$F_{g,fuel}$	0.9587
66	$N_{fuel,dim}$	0.9587
67	$W_{pump,HP}$	0.9494
68	$T_{g,econ,7}$	0.6635
69	$W_{steam,turbine}$	0.6568
70	$F_{g,fuel}/F_{g,air}$	0.6211
71	Q_{econ}	0.4638
72	Q_{cond}	0.4525
73	$W_{pump,LP}$	0.4347
74	Q_{pre}	0.3704
75	Q_{evap}	0.3620
76	$T_{w,pre,6}$	0.1102
77	$T_{w,pre,6}$	0.0922
78	$T_{w,pre,5}$	0.0741
79	$T_{w,pre,4}$	0.0558
80	$T_{w,pre,3}$	0.0373
81	$F_{w,pre}$	0.0207
82	$T_{w,pre,2}$	0.0187
83	$F_{g,econ,bypass}$	0.0000
84	$F_{g,evap,bypass}$	0.0000
85	$F_{g,super,bypass}$	0.0000
86	$F_{w,valve,LP}$	0.0000
87	$F_{w,valve,HP}$	0.0000
88	$T_{w,pre,1}$	0.0000
89	$T_{w,deaerator}$	0.0000

Evaluation of loss

For case III, we evaluate for the alternative candidate controlled variable sets the economic loss imposed by using constant setpoints instead of re-optimization (with no implementation errors). The average cost and loss with constant nominal setpoints are shown in table 5.5 for the 54 feasible alternatives. We have evaluated the loss with expected disturbances in the inlet air temperature and expected implementation errors in the combustor temperature.

Table 5.5 shows that for the feasible alternatives the loss related to the disturbances (d) is rather small. The loss related to the implementation error in the optimal active constraint, the combustor temperature (T_{comb}) ($d_{c,1}$), is significant, but largely independent of the controlled variables. In any case, there is much money to be gained by reducing the implementation error related to the combustor temperature. The difference in loss between the alternatives is mainly due to the implementation error in the unconstrained controlled variable. Temperatures and pressures give significantly smaller losses than the other unconstrained controlled variables.

Figure 5.3 shows the loss for six selected sets of controlled variables. Again we find that the main differences in the loss are due to the implementation error in the unconstrained controlled variable. We see that control of the super-heater gas inlet temperature ($T_{g,super,1}$) gives the smallest loss, which is only 0.16% larger than with reoptimization with constraint backoff. The inclusion of constraint backoff is necessary to achieve feasibility. Physically, controlling the super-heater inlet temperature, which is the pinch temperature in the steam cycle, simplifies the operation of the plant by partly decoupling the gas and steam cycle operation.

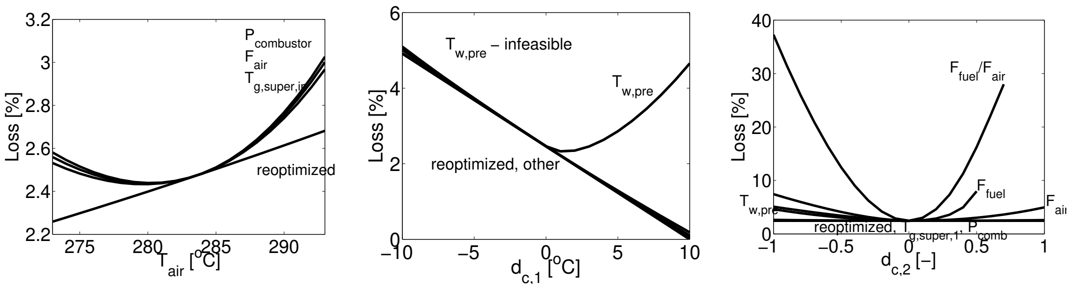

Figure 5.3: Loss as function of disturbances in the air feed temperature (T_{air}), implementation error in controlling the combustor temperature T_{comb} ($d_{c,1}$) and implementation error in the unconstrained controlled variable ($d_{c,2}$).

The through-put is limited by the required deaerator pressure and the bypass structure. The alternatives which are infeasible (and not shown in table 5.5), mostly have problems with limited through-put for an increase in the air inlet temperature (disturbance) and / or implementation error related to the unconstrained controlled variable.

Table 5.5: Cost and loss for feasible candidate controlled variables (c) for case III with constant nominal setpoints.

Rank	c_1	c_2	$c_{s,1}$	$c_{s,2}$	$J_w(d)$	$J_w(d_{c,1})$	$J_w(d_{c,2})$	J_w	$L_w(\%)$
-	ideal optimization (eq.3.24)		$c_{opt,1}(d)$	$c_{opt,2}(d)$	70.1595	70.0590	70.0590	70.0877	–
-	reoptimized (eq.3.27)		$c^*_{opt,1}(d)$	$c^*_{opt,2}(d)$	68.3165	68.5945	68.3339	68.4034	2.40
1	$T_{g,comb}$	$T_{g,super,1}$	1490	738.4425	68.2449	68.2798	68.3286	68.2915	2.56
2	$T_{g,comb}$	$T_{g,super,2}$	1490	738.1387	68.2450	68.2795	68.3285	68.2914	2.56
3	$T_{g,comb}$	$T_{g,super,3}$	1490	737.6457	68.2451	68.2791	68.3284	68.2913	2.56
4	$T_{g,comb}$	$T_{w,econ,}$	1490	521.2845	68.2213	68.3302	68.3007	68.2912	2.56
5	$T_{g,comb}$	$T_{g,super,4}$	1490	736.8455	68.2453	68.2785	68.3282	68.2911	2.56
6	$T_{g,comb}$	$T_{g,super,5}$	1490	735.5469	68.2456	68.2775	68.3280	68.2909	2.56
7	$T_{g,comb}$	$T_{w,super}$	1490	735.3269	68.2453	68.2779	68.3277	68.2908	2.56
8	$T_{g,comb}$	$T_{g,super,6}$	1490	733.4393	68.2462	68.2758	68.3276	68.2904	2.56
9	$T_{g,comb}$	$T_{w,super}$	1490	733.0823	68.2456	68.2765	68.3271	68.2903	2.56
10	$T_{g,comb}$	$T_{g,super,7}$	1490	730.0188	68.2471	68.2732	68.3270	68.2898	2.57
11	$T_{g,comb}$	$T_{w,super}$	1490	729.4393	68.2462	68.2742	68.3261	68.2896	2.57
12	$T_{g,comb}$	$T_{w,econ,}$	1490	564.9546	68.2148	68.3350	68.2961	68.2894	2.57
13	$T_{g,comb}$	$T_{w,super}$	1490	723.5270	68.2472	68.2702	68.3244	68.2882	2.57
14	$T_{g,comb}$	$T_{g,evap,1}$	1490	718.6409	68.2504	68.2636	68.3252	68.2875	2.57
15	$T_{g,comb}$	$T_{w,super}$	1490	713.9315	68.2491	68.2628	68.3211	68.2857	2.57
16	$T_{g,comb}$	$T_{g,evap,2}$	1490	708.5846	68.2537	68.2529	68.3231	68.2848	2.57
17	$T_{g,comb}$	$T_{w,econ,}$	1490	460.9243	68.2246	68.3266	68.2757	68.2840	2.57
18	$T_{g,comb}$	$T_{g,evap,3}$	1490	699.6965	68.2571	68.2413	68.3205	68.2817	2.58
19	$T_{g,comb}$	$T_{w,super}$	1490	698.3585	68.2528	68.2471	68.3143	68.2803	2.58
20	$T_{g,comb}$	$T_{w,econ,}$	1490	596.5496	68.2020	68.3360	68.2698	68.2785	2.58
21	$T_{g,comb}$	$T_{g,evap,4}$	1490	691.8407	68.2604	68.2287	68.3176	68.2782	2.58
22	$T_{g,comb}$	$T_{g,evap,5}$	1490	684.8974	68.2637	68.2153	68.3143	68.2743	2.59
23	$T_{g,comb}$	$T_{g,evap,6}$	1490	678.7606	68.2668	68.2014	68.3106	68.2702	2.59
24	$T_{g,comb}$	$P_{g,comb}$	1490	4289495	68.2073	68.3307	68.2309	68.2674	2.60
25	$T_{g,comb}$	$T_{w,super}$	1490	673.0842	68.2611	68.2085	68.2975	68.2669	2.60
26	$T_{g,comb}$	$T_{g,evap,7}$	1490	673.3367	68.2697	68.1871	68.3066	68.2658	2.60
27	$T_{g,comb}$	$T_{g,econ,1}$	1490	671.0885	68.2729	68.1712	68.3010	68.2606	2.61
28	$T_{g,comb}$	$T_{g,econ,2}$	1490	667.9811	68.2777	68.1454	68.2915	68.2519	2.62
29	$T_{g,comb}$	$T_{g,econ,3}$	1490	663.6861	68.2852	68.1001	68.2740	68.2361	2.64
30	$T_{g,comb}$	$T_{w,evap}$	1490	632.0651	68.2795	68.1027	68.2567	68.2303	2.65
31	$T_{g,comb}$	$T_{w,econ,}$	1490	619.4084	68.1701	68.2920	68.1545	68.2239	2.66
32	$T_{g,comb}$	$F_{g,pre,bypass}$	1490	1081.7586	68.2186	68.3349	68.0055	68.2074	2.68
33	$T_{g,comb}$	$T_{g,econ,4}$	1490	657.7496	68.2982	68.0078	68.2357	68.2025	2.69
34	$T_{g,comb}$	$P_{w,evap}$	1490	18443043	68.2795	68.1027	68.0009	68.1572	2.75
35	$T_{g,comb}$	$T_{g,econ,5}$	1490	649.5443	68.3234	67.7602	68.1263	68.1077	2.83
36	$T_{g,comb}$	$P_{w,cond}$	1490	2758.3129	68.2853	68.0591	67.5059	68.0049	2.97
37	$T_{g,comb}$	$F_{g,air}$	1490	1877.2604	68.2237	68.3354	66.7168	67.8408	3.21
38	$T_{g,comb}$	$F_{g,econ}$	1490	1925.9941	68.2082	68.3351	66.6735	67.8239	3.23
39	$T_{g,comb}$	$F_{g,evap}$	1490	1925.9941	68.2082	68.3351	66.6735	67.8239	3.23
40	$T_{g,comb}$	$F_{g,super}$	1490	1925.9941	68.2082	68.3351	66.6735	67.8239	3.23
41	$T_{g,comb}$	$F_{g,gasturbin}$	1490	1925.9941	68.2082	68.3351	66.6735	67.8239	3.23
42	$T_{g,comb}$	$N_{air,dim}$	1490	759.1992	68.3823	68.3354	66.7168	67.8861	3.14
43	$T_{g,comb}$	$W_{compfuel}$	1490	7647527	67.7918	68.3146	64.0736	66.9563	4.47
44	$T_{g,comb}$	$F_{g,pre}$	1490	844.2354	68.2568	68.1975	63.2473	66.8196	4.66
45	$T_{g,comb}$	$W_{compair}$	1490	2399731637	68.4136	68.3343	61.7553	66.4772	5.15
46	$T_{g,comb}$	Q_{super}	1490	28559883	68.2478	68.2695	60.8696	66.1582	5.61
47	$T_{g,comb}$	$F_{w,pumpLP}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
48	$T_{g,comb}$	$F_{w,pumpHP}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
49	$T_{g,comb}$	$F_{w,pumpHP}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
50	$T_{g,comb}$	$F_{w,evap}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
51	$T_{g,comb}$	$F_{w,super}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
52	$T_{g,comb}$	$F_{w,steamturbin}$	1490	148.3785	68.2875	68.0414	59.4146	65.6887	6.28
53	$T_{g,comb}$	$W_{gasturbin}$	1490	3397557688	68.2031	68.3246	56.7562	64.9860	7.28
54	$T_{g,comb}$	W_{pumpHP}	1490	2721519	68.2831	68.0764	50.0754	63.0291	10.07

$J_w(d)$: Average cost for disturbances in the air temperature.

$J_w(d_{c,1})$: Average cost for implementation errors in the combustor temperature.

$J_w(d_{c,2})$: Average cost for implementation errors in the unconstrained controlled variable.

J_w: Average cost for considered disturbances and implementation errors.

Since the loss when controlling the super-heater gas inlet temperature is only marginally larger than with reoptimization with constraint backoff, the possible improvement by finding other combinations of variables to control is not very large and is not considered here. Using constant robust setpoints or flexible setpoints (online feasibility correction) (see chapter 3) is also not considered here.

5.3.4 Production rate manipulator

One step in the procedure of Larsson & Skogestad (2001) is to identify the bottlenecks and production rate manipulator. However, we are here primarily dealing with a gas phase system, and finding the production manipulator is not so important. The through-put on the gas side is determined in the gas turbine (nozzles equation is used since the flow is choked). The through-put in the steam turbine cycle is determined by the flow through the steam turbine (nozzles equation is used because the flow is choked).

5.3.5 Structure of regulatory control layer

Stabilization
The levels in the evaporator drum and the condenser drum need to be stabilized. The deaerator drum is much larger than the other drums, and since we have a closed system controlling the deaerator drum level is not needed. At large pressure ratios the steam turbine flowrate is given, independent of the steam turbine speed. Since the steam turbine flowrate is the inlet flowrate to the condenser drum, we select to stabilize the condenser drum level by manipulating the outlet flowrate, i.e. the low-pressure pump flowrate. Since the steam turbine flowrate gives the outlet flowrate to the evaporator drum level, we select to stabilize the evaporator drum level by manipulating the inlet flowrate, i.e. the high-pressure flowrate pump.

Local disturbance rejection
Local flow controllers are used for achieving local disturbance rejection. Flow controllers are implemented by manipulating the valve openings, compressor speeds or pump effects. These loops are not included in our study.

5.3.6 Structure of supervisory control layer

Decentralized control
We want to control the gas turbine inlet temperature (T_{comb}), the super-heater gas inlet temperature ($T_{g,super,1}$) and the deaerator pressure ($P_{w,deaerator}$):

$$y^T = [T_{comb}\ T_{g,super,1}\ P_{w,deaerator}] \tag{5.17}$$

Available manipulated variables are the fuel feedrate (F_{fuel}), the air feedrate (F_{air}) and the pre-heater bypass flowrate ($F_{g,pre,bypass}$).

$$u^T = [F_{fuel}\ F_{air}\ F_{g,pre,bypass}] \tag{5.18}$$

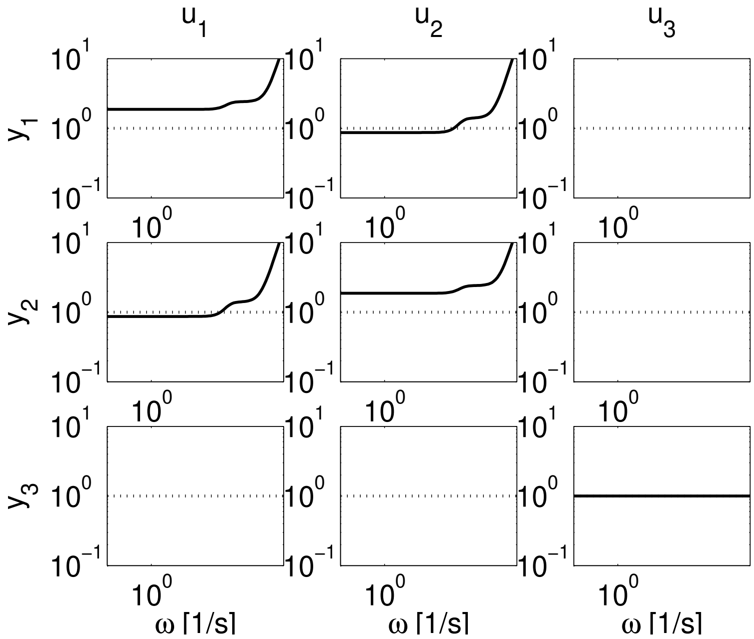

Figure 5.4: Frequency-dependent RGA ($\Lambda(j\omega)$)

The frequency dependent relative gain array (RGA) is shown in figure 5.4. Pairing the deaerator pressure with the pre-heater bypass flowrate gives no two-way interactions with the other loops. The other two pairings are not so clear. Pairing on the diagonal elements gives the smallest RGA-number, see figure 5.5. We then avoid pairing on the negative elements in the steady-state RGA:

$$\Lambda(0) = \begin{bmatrix} 1.8674 & -0.8674 & 0.0000 \\ -0.8674 & 1.8674 & 0.0000 \\ -0.0000 & 0.0000 & 1.0000 \end{bmatrix} \tag{5.19}$$

Model predictive control (MPC)
Because the selected alternative has no problems with violation of uncontrolled constraints, neither in transients nor at steady-state, MPC is not required.

5.3.7 Structure of optimization layer

The loss improvement by introducing online optimization when we control the inlet gas temperature, is less than 0.16%, see table 5.5, so online optimization is not needed.

5.3.8 Validation of proposed control structure

Figure 5.6 shows the selected control structure for case III. Stabilization is performed by controlling the evaporator drum level and condenser drum level by manipulating the flowrate

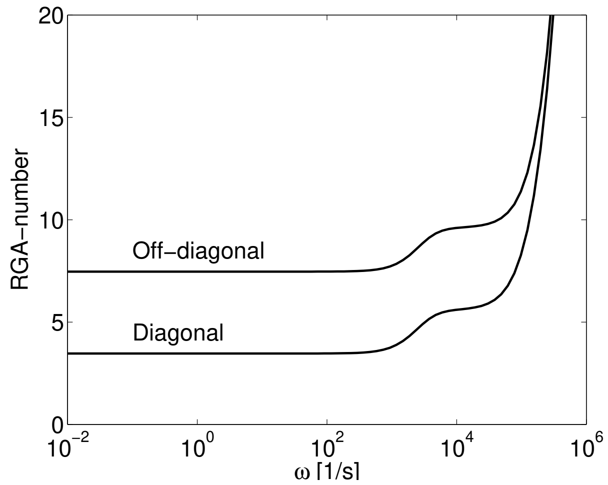

Figure 5.5: Frequency-dependent RGA-number ($||\Lambda(j\omega) - I||_{sum}$)

through the HP pump and the LP pump, respectively. The gas turbine inlet temperature is controlled by manipulating the fuel feedrate, and the deaerator temperature is controlled by manipulating the pre-heater bypass flowrate. The super-heater gas inlet temperature is controlled by manipulating the air feedrate. When the net electricity production is given (case I), the fuel feedrate is used to control the net electricity production instead of the super-heater gas inlet temperature, see figure 5.7. The gas turbine inlet temperature is now controlled by the air feedrate. When the fuel feedrate is given (case II), the super-heater gas inlet temperature is no longer controlled, see figure 5.8. The gas turbine inlet temperature is controlled by manipulating the air feedrate.

We finally validate the proposed control structure for case III by performing nonlinear simulation. The controllers are tuned by using SIMC-tuning rules (Skogestad 2003). The desired closed-loop time constants (τ_c) are selected equal 0.01 s for the inlet gas turbine temperature controller and the super-heater gas inlet temperature controller, 120 s for the deaerator pressure controller and 10 s for the level controllers. Figure 5.9 shows the responses in controlled variables (the gas turbine inlet temperature, the super-heater gas inlet temperature and the deaerator pressure) and the corresponding manipulated variables (fuel feedrate, air feedrate and pre-heater bypass flowrate) for a step in the feed air temperature of 10^oC. The disturbances have only minor effect on the operation. The initial control errors in the gas turbine inlet temperature and the super-heater gas inlet temperature are large, $+40^oC$ and $+14^oC$ respectively. The temperature constraints are steady-state constraints so the constraint violations during fast transients are acceptable.

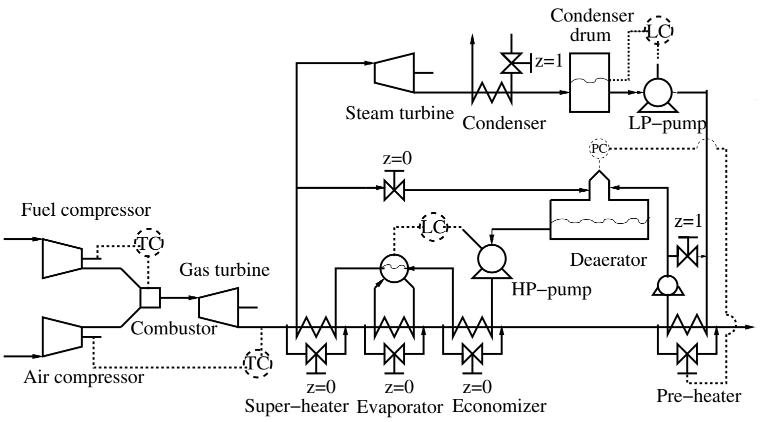

Figure 5.6: Combined cycle power plant process with proposed control structure for case III

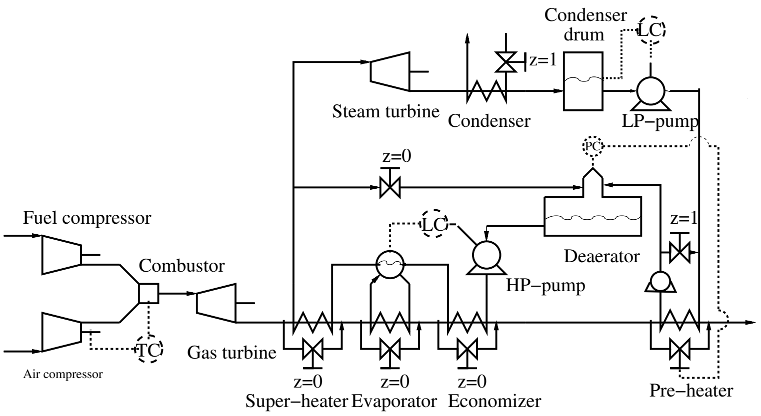

Figure 5.7: Combined cycle power plant process with proposed control structure for case I

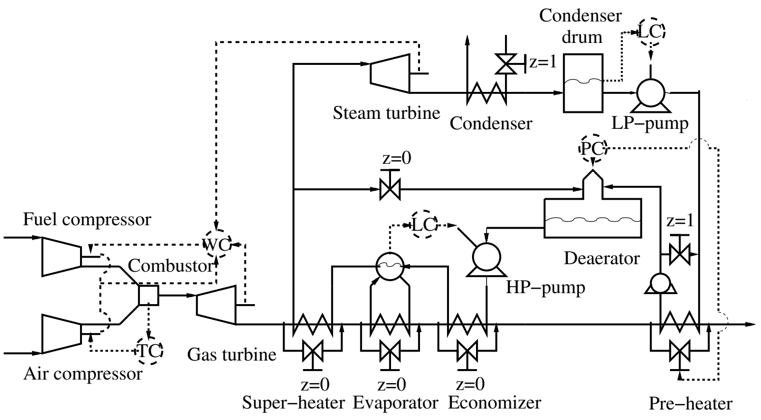

Figure 5.8: Combined cycle power plant process with proposed control structure for case II

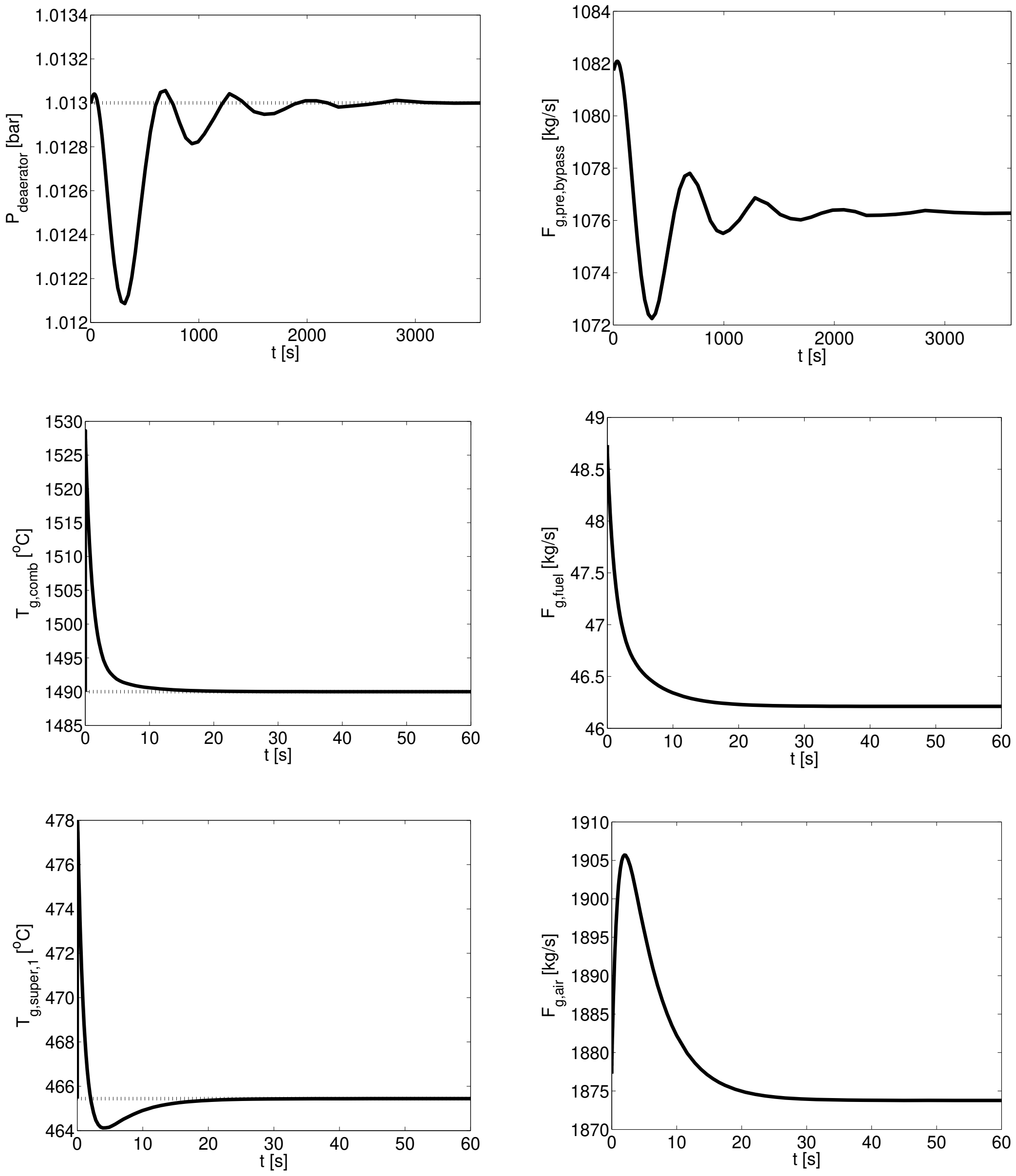

Figure 5.9: The deaerator pressure, pre-heater bypass flowrate, combustor temperature, fuel feedrate, super-heater gas inlet temperature and air feedrate response when increasing the feed air temperature with 10^oC

5.4 Conclusion

A systematic procedure for plantwide control design has been demonstrated on a combined cycle power plant. The selection of the primary controlled variables is the most important step in the procedure.

The process has one unconstrained steady-state degree at its optimal operation. We find that controlling the super-heater gas inlet temperature in addition to the variables at active constraints at optimum gives the smallest loss, which is only 0.16% larger than reoptimization with constraint backoff. Controlling the super-heater inlet temperature partly decouples the operation of the gas turbine and the steam turbine cycle.

The disturbances have rather small effects on the optimal operation of the process. The implementation errors related to the controlled variables have significantly larger effect. The main difference in loss between the alternatives comes from the implementation error for the unconstrained controlled variables. Control of temperatures and pressures give significantly smaller losses than other candidate controlled variables.

Chapter 6

Application of a Plantwide Control Design Procedure to a Distillation Column with Heat Pump

Based on work presented at the 13th European Symposium on Computer Aided Process Engineering (ESCAPE-13), Lappeenranta, Finland, June 1-4, 2003

In this chapter we apply the plant-wide control design procedure of Larsson & Skogestad (2001) to a distillation column with a heat pump (Koggersbøl 1995). A top-down analysis is performed to select primary controlled variables based on the ideas of self-optimizing control and to identify bottlenecks. A bottom-up design is then performed to design the control system, including the selection of extra measurements (secondary controlled variables) for stabilization and local disturbance rejection. We find that controlling the temperature at stage 4 (T_4) in addition to the active constraints gives a simple system with close-to-optimal operation.

6.1 Introduction

Distillation consumes a large a large fraction of the energy in the chemical process industries. Consequently, there is a significant incentive to improve the energy efficiency in distillation. Use of heat pumps is one way to improve the energy efficiency. The most widely used cycle for heat pumps is direct vapor recompression (Salim, Sadasivam & Balakrishnan 1991). Luyben (1992) examines the dynamics and control of direct vapor recompression. However, we here want to study distillation with indirect heat pump. Except from work done at the Denmark Technical University by Jorgensen and co-workers the literature covering dynamics and control of indirect heat pump, is rather limited.

Figure 6.1 shows the control structure for the distillation column with indirect heat pump proposed by Li, Gani & Jorgensen (2003). The reboiler holdup is controlled by manipulating the bottom product rate, the condenser tank holdup is controlled by manipulating the reflux rate and the condenser holdup at the heat pump side is controlled by manipulating

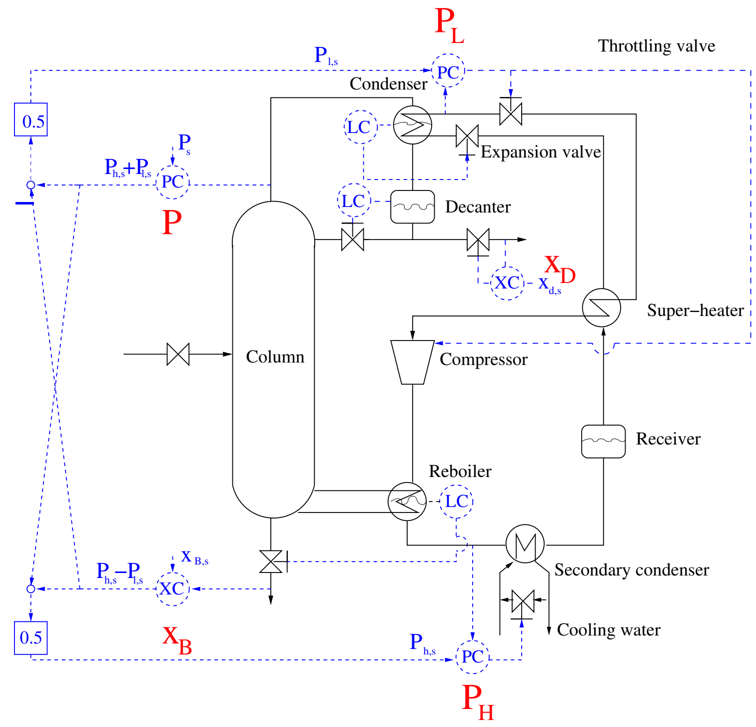

Figure 6.1: Distillation column with heat pump with proposed control structure in literature

the expansion valve opening. The heat pump cycle is stabilized by controlling the high heat pump pressure (p_H) by manipulating the cooling water recirculation valve opening. The low pressure in the heat pump (p_L) is controlled by manipulating the cooling capacity. The cooling capacity is determined by the number of active compressor cylinders and the pressure drop across the throttling valve opening. The capacity was adjusted by using the number of cylinders and fine adjustment was performed with the throttling valve. The sum of setpoints to the high and low pressure in the heat pump is then used as manipulated variable to control the column pressure p. The difference between the high pressure and low pressure in the heat pump is then used as manipulated variable to control the bottom composition x_B. The top composition x_D is controlled by manipulated the distillate flowrate D.

In this paper we apply the plantwide control design procedure of Larsson & Skogestad (2001) and find that it gives the structure shown in figure 6.2. More details related to the procedure itself are presented in chapter 5.

6.2 Distillation Column with Heat Pump Case Study

Methanol and 2-propanol are separated in a distillation column with 11 theoretical stages (in addition to the condenser) and with the feed at stage number 6 (from the bottom) (Koggersbøl 1995). The distillation column is heat-integrated by using the heat pump to ”upgrade” the ”heat” generated in the condenser so it may be used in the reboiler. A secondary condenser is included in the heat pump.

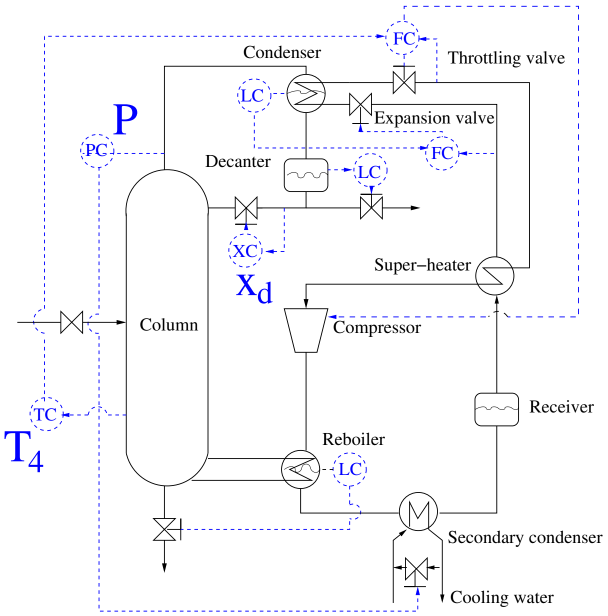

Figure 6.2: Distillation column with heat pump with proposed control structure

6.2.1 Manipulated variables

The process has 9 manipulated variables. These are the feed valve, reflux valve, distillate valve, bottom product valve, expansion valve, throttling valve, compressor speed, number of active compressor cylinders and cooling water valve.

6.2.2 Degrees of freedom analysis

There are 9-3-2-1=3 steady-state degrees of freedom: Three holdups (condenser and reboiler holdup in the column and condenser holdup in the heat pump) need to be controlled, but have negligible steady-state effect. This consumes 3 degrees of freedom. The effect of changing the compressor speed, throttling valve opening and number of active cylinders in the compressor are similar (all change the work supplied), and this consumes 2 degrees of freedom. Finally, the feedrate is given, and this consumes 1 degree of freedom.

6.2.3 Primary controlled variables

Degrees of freedom for optimization

The degrees of freedom for optimization are the three steady-state degrees of freedom.

Definition of optimal operation

The economic objective during operation is to maximize the profit, which in this case is the value of the products minus the costs of the utility and raw materials. We assume that the value of the top product is twice that of the bottom product and feed, that the cooling water is free and that the price ratio between the compressor work and the top product is 0.001 mol/W. Maximizing the profit P is equivalent to minimizing the cost $J = -P$. The objective function to be minimized is then: $J = -D + 0.001W_{comp}$.

There are constraints on the top composition ($x_D \geq 0.95$), bottom composition ($x_B \leq 0.10$), maximum column pressure ($p \leq 2$ bar), minimum pressure column ($p \geq 0.5$ bar), weeping ($V \geq V_{min}(p, T)$) and flooding ($V \leq V_{max}(p, T)$). In addition there are some safety limits on the high pressure in the heat pump ($p_H \leq 16$ bar) and low pressure in the heat pump ($p_L \leq 6$ bar). The composition constraints (x_D, x_B) are steady-state constraints and violation during transients are accepted. The other constraints (p, p_L, p_H, V) are transient constraints and can be violated neither during transients nor at steady-state.

Identification of important disturbances

The feedrate ($F = 51.27 \pm 10.25$ mol/min) and the feed composition ($z_F = 0.5 \pm 0.1$) are the most important disturbances.

Steady-state optimization

The optimal operating point is obtained by minimizing J with respect to the three degrees of freedom for various values of the disturbance, see Table 6.1. The constraints on the pressure (p) and the top composition (x_D) are both active at the optimum and this does not change for the expected disturbances.

Table 6.1: Optimal operation for nominal and expected variations in disturbances.

	L $[\frac{mol}{min}]$	V $[\frac{mol}{min}]$	D $[\frac{mol}{min}]$	B $[\frac{mol}{min}]$	x_B $[-]$	T_B $[^oC]$	p_L $[bar]$	p_H $[bar]$	T_L $[^oC]$	T_H $[^oC]$	J $[mol/min]$
Nominal	145.6	171.6	25.83	25.44	0.0433	66.1	3.91	8.58	44.6	75.3	24.6946
F=41.02	119.8	140.7	20.69	20.32	0.0418	65.8	4.01	8.53	45.4	75.0	19.8109
F=61.52	170.0	201.2	30.94	30.58	0.0447	66.3	3.81	8.63	43.7	75.6	29.5538
z=0.4	156.4	177.1	20.29	30.98	0.0399	66.2	3.89	8.61	44.4	75.4	19.1002
z=0.6	130.9	162.3	31.38	19.89	0.0476	65.9	3.94	8.55	44.8	75.1	30.3385

For all cases: x_D=0.95, p=0.5bar and T_D=48.98^{o}C. Nominal point: F=51.27 mol/min, $z_F = 0.5$.

Identification of candidate controlled variables

We select to control the two active constraints; top product composition ($c_1 = x_D$) and minimum column pressure ($c_2 = p$). This leaves one unconstrained degree of freedom, so one additional controlled variable needs to be selected. Single temperatures and compositions at different column stages are selected as candidates. The following implementation errors are assumed: ± 0.01 mole fraction units for compositions (except ± 0.005 for x_D), $\pm 2.5\%$ for pressure and $\pm 0.2K$ for temperatures.

Loss evaluation

For the alternative sets of controlled variables we evaluate the economic loss imposed by using constant setpoints instead of re-optimization (with no implementation errors). The loss is evaluated at the nominal point and at corner-points for each disturbance and implementation error. In table 6.2 the average cost, average percentage loss and maximum percentage loss are shown for different sets of controlled variables. The applied setpoints, found by optimization at nominal point with safety margins (equal the expected implementation errors), are included for the optimal active constraints (simple back-off). The alternatives are rather insensitive to disturbances, while implementation errors have some effect. Controlling the composition at stage three ($c_3 = x_3$) in addition to x_D and p gives the smallest loss but a small loss is also achieved with a constant temperature, for example, T_4. Using robust setpoints or flexible setpoints (online feasibility correction) is not considered here.

Selection of controlled variables

We select to control the temperature at stage 4 ($c_3 = T_4$), since measuring a temperature in the column is probably easier than measuring a composition and the loss for controlling T_4 is not much larger than for controlling x_3.

Table 6.2: Nominal setpoints (c_s), average objective (J_w), average percentage loss (L_w) and maximum percentage loss (L_{max}) for different sets of controlled variables

Rank	c_1	c_2	c_3	$c_{1,s}$	$c_{2,s}$	$c_{3,s}$	J_w	$L_w(\%)$	$L_{max}(\%)$
-	ideal opt. (eq.3.24)			$c_{opt,1}(d)$	$c_{opt,2}(d)$	$c_{opt,3}(d)$	24.6969	–	–
-	reoptimized (eq.3.27)			$c^*_{opt,1}(d)$	$c^*_{opt,2}(d)$	$c^*_{opt,3}(d)$	24.4762	0.89	1.83
1	x_D	p	x_3	0.9550	51250	0.1206	24.4662	0.93	1.86
2	x_D	p	x_2	0.9550	51250	0.0755	24.4645	0.94	1.85
3	x_D	p	x_4	0.9550	51250	0.1840	24.4636	0.94	1.87
4	x_D	p	T_4	0.9550	51250	336.4207	24.4595	0.96	1.84
5	x_D	p	T_3	0.9550	51250	337.8033	24.4591	0.96	1.84
6	x_D	p	T_2	0.9550	51250	338.8453	24.4552	0.98	1.83
7	x_D	p	x_5	0.9550	51250	0.2674	24.4551	0.98	1.88
8	x_D	p	T_5	0.9550	51250	334.6892	24.4545	0.98	1.85
9	x_D	p	$x_1 = x_B$	0.9550	51250	0.0450	24.4535	0.99	1.85
10	x_D	p	T_1	0.9550	51250	339.6092	24.4486	1.01	1.83
11	x_D	p	T_6	0.9550	51250	332.7065	24.4371	1.05	1.93
12	x_D	p	x_6	0.9550	51250	0.3670	24.4281	1.09	2.65
13	x_D	p	T_7	0.9550	51250	330.8500	24.4274	1.09	1.95
14	x_D	p	x_7	0.9550	51250	0.4629	24.4201	1.12	2.65
15	x_D	p	T_8	0.9550	51250	328.6717	24.3985	1.21	2.17
16	x_D	p	x_8	0.9550	51250	0.5820	24.3920	1.23	2.85

6.2.4 Production rate manipulator

Bottlenecks

The bottleneck of the overall process is assumed to be upstream of the heat-integrated distillation column, so the feedrate is the production bottleneck.

6.2.5 Structure of regulatory control layer

Linearization
The throttling valve at the compressor inlet is strongly nonlinear in its response. The behavior is linearized by controlling the compressor flowrate (F_{comp}) by manipulating the throttling valve opening and the number of active compressor cylinders. More precisely, the compressor flowrate should be controlled by using parallel control: A fast P-controller which manipulate on the throttling valve opening and a relatively slow PI-controller which manipulate on the number of active cylinders. The nonlinear behavior related to the expansion valve is linearized by controlling the expansion valve flowrate ($F_{e,valve}$) by manipulating the expansion valve opening.

Stabilization
The levels in the condenser (decanter) and reboiler in the column side must be stabilized. The reboiler holdup is controlled by manipulating the bottom product flowrate B and the condenser level is stabilized by manipulating the distillate flowrate D. In addition the holdup in the heat pump is stabilized by controlling the condenser level in the heatpump by manipulating the expansion valve flowrate.

6.2.6 Structure of supervisory control layer

The aims of the supervisory control layer are to keep the selected controlled variables ($c_1 = x_D$, $c_2 = p$ and $c_3 = T_4$) at constant setpoints.

Decentralized control
In the supervisory layer, the cooling water valve opening ($\alpha_{cv,8}$) is used to control the pressure (p), the reflux flowrate (L) is used to control the top composition (x_D) and the compressor flowrate ($F_{comp,s}$) is used to control the temperature at stage 4 (T_4). Control of the pressure p and either top composition x_D or temperature of stage 4 (T_4) is necessary to avoid that the plant drifts away from its desired operating point when disturbances occur. In practice control of p and x_D may be included in the regulatory control layer.

Multivariable control
A multivariable controller should be evaluated, since the interactions are strong and the desired bandwidth for the controllers (x_D- and T_4-controller) are approximately equal.

Model predictive control (MPC)
Because the selected alternative has no problems with violation of uncontrolled constraints, neither during transients nor at steady-state, there is no need to consider use of MPC.

6.2.7 Structure of optimization layer

With control of T_4 and the active constraints, the loss is not much larger than the loss when we use "reoptimization" with constraint backoff. Online optimization is therefore not needed.

6.2.8 Validation of selected control structure

The resulting control structure is shown in figure 6.2, and it has been validated by nonlinear simulations. P/PI-controllers were tuned using the SIMC-tuning rules (Skogestad 2003) with a desired closed loop constants of 0.1 min for the holdup controllers, 1 min for the pressure controller and 5 min for the composition and temperature controller. Results of the nonlinear simulations to steps in the feedrate ($\Delta F = \pm 20\%$) and feed composition ($\Delta z_F = \pm 0.1$) are shown in figure 6.3. The figure shows the column pressure (p), the top composition (x_D) and the temperature at stage 4 (T_4) for a step in the feedrate equal $\pm 20\%$. The control performance is acceptable since the control deviations are small compared to the expected implementation errors.

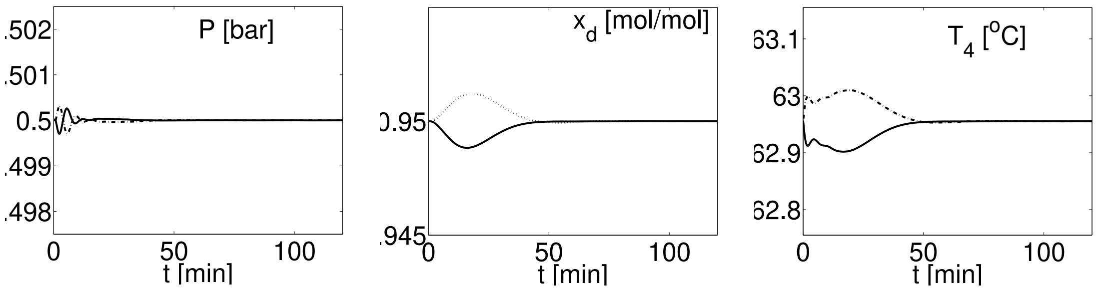

Figure 6.3: Column pressure (p), top composition (x_D) and temperature at stage 4 (T_4) for steps in the feedrate (F). (Solid shows a 20% increase in F and dashed shows a 20% decrease in F.)

6.3 Discussion

6.3.1 Comparing with control structure proposed in literature

Based on the economic objective used here, control of the temperature at stage 4 (T_4) has slightly better self-optimizing properties than control of the bottom composition. This is seen by comparing rank 4 and rank 9 in table 6.2. Even more important, control of T_4 is easier from a dynamic point of view.

By controlling the flowrate using the trottling valve the process is linearized and faster control in the regulatory control layer is possible than by controlling the heat pump pressures. This is because the process dynamic related to the controlling the flowrates are faster than the dynamic related to the control of the heat pump pressures. With faster regulatory control faster supervisory control is in practice possible.

6.3.2 Optimal placement of controlled variable in column

The optimal placement in the column of the controlled variable (temperature) with respect to steady-state economics depends on both the implementation error and the disturbances. The disturbances have the smallest effect when the controlled variable is placed at the end of the column (e.g. T_1 or x_1), because the whole column is then used to ”filter” the disturbances. On the other hand, the effect of the implementation error is smallest when the controlled variable is placed where the column profile is steepest (e.g. T_6 or x_7). The best placement of the controlled variable with respect to both the disturbances and the implementation error is somewhere between (e.g. T_4 or x_3), see figure 6.4 and figure 6.5. Havre (1998) used

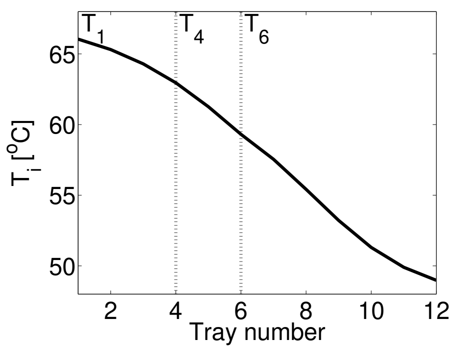

Figure 6.4: Temperature profile in the distillation column

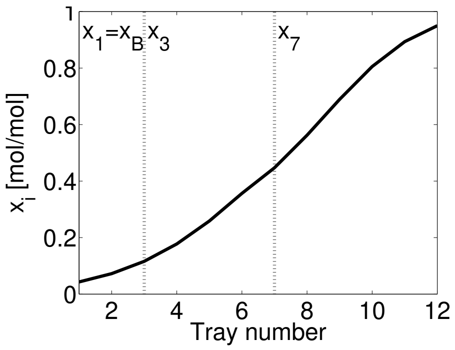

Figure 6.5: Composition profile in the distillation column

the same argumentation for selecting stages for temperature control, though the objective was somewhat different, namely to minimize the steady-state control error in the top- and bottom-composition.

6.4 Conclusion

A systematic procedure for selecting a plantwide control structure has been demonstrated on a distillation column with heatpump. The selection of the primary controlled variables is the most important step in the procedure. We find that controlling the temperature at stage 4 (T_4) in addition to the active constraints gives a simple system with close to optimal operation.

Chapter 7

Optimal Number of Stages in Distillation with respect to Controllability

Based on work presented at the 12th European Symposium on Computer Aided Process Engineering (ESCAPE-12), The Hague, The Netherlands, May 26-29, 2002

The central question to be examined in this chapter is if it is best with respect to controllability to have a large or small number of stages in a distillation column when the objective is to have dual composition control. With fixed setpoints to the top and bottom compositions, few stages gives the best controllability with respect to disturbance rejection, whereas many stages gives best controllability with respect to setpoint tracking. However, this comparison is unfair as the energy usage (V) is much higher with few stages. With the same energy usage (V) it is possible to over-purify the products and many stages is always better in terms of controllability. The reason for these findings is that controllability is improved by (i) increasing the number of stages (with fixed internal flows), and (ii) increasing the internal flows.

7.1 Introduction

We want to evaluate if it is best to have a large or a small number of stages in a distillation column with respect to controllability. We do not here consider design costs. The study is for dual composition control where we have a given purity specification in the top and in the bottom of the column. The conventional LV-configuration is used for stabilizing the condenser and reboiler holdups.

Skogestad (1997) claims that it is better for controllability to have many stages. He writes: *How should the column be designed to make feedback control easier? In terms of composition control, the best is probably to add extra stages. This has two potential advantages:*

1. *It makes it possible to over-purify the products with only a minor penalty in terms of energy cost; recall the expression for* $V_{min} = \frac{1}{1-\alpha}F$ *which is independent of the purity. The control will then be less sensitive to disturbances.*

2. *If we do not over-purify the products, then with "too many" stages a pinch zone will develop around the feed stage. This pinch zone will effectively stop composition changes to spread between the top and bottom part of the column, and will therefore lead to a decoupling of the two column ends, which is good for control.*

However, this finding is not confirmed by Meeuse & Tousain (2001) who claim, based on optimal design of LQG controllers, that it is better to have few stages. The objective of this chapter is to study this issue in more detail.

7.2 Column data

A distillation column separating a two-component feed mixture is studied, see figure 7.1. The model details are described in Skogestad (1997). We assume that the feed is given.

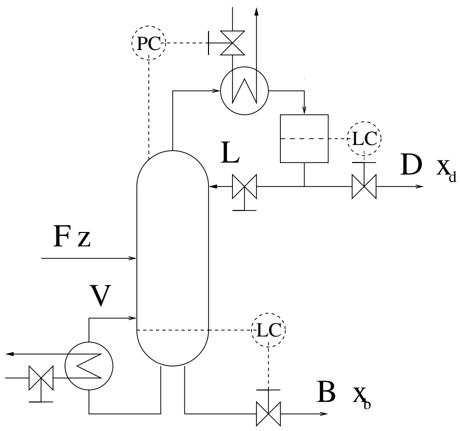

Figure 7.1: One-feed two-product distillation column

With the indicated conventional control configuration for pressure and levels (see figure 7.1), the two remaining manipulated variables are the reflux flowrate (L) and the vapor boilup flowrate (V). The selected controlled variables are the composition of light component in the top product (x_D) and the composition of light component in the bottom product (x_B). The expected setpoint variations are 0.99 ± 0.01 for the top composition (x_D) and 0.01 ± 0.01 for the bottom composition (x_B)[1]. The disturbances are feed flow rate ($F = 1 \pm 0.1$ kmol/min) and feed composition ($z_F = 0.5 \pm 0.05$). The feed is assumed to be saturated liquid ($q_F = 1$). The number of stages is varied between 25 (just above the minimum number of stages for the given separation) and 71. The feed stage is at the middle. The column data are summarized in table 7.1. The nominal holdup is kept approximately constant at 20.5 kmol in the entire column, independent of number of stages (this is obviously not realistic as the holdups will

[1] It is obviously not possible to achieve $x_D = 1$ or $x_B = 0$. Actually, the setpoint changes are applied to the linearized model, and for the nonlinear model the allowed setpoint variations are then approximately x_D = 0.98 to 0.995 and x_B = 0.005 to 0.02

Table 7.1: Column data

Controlled variables (y)	x_D	0.99	$kmol/kmol$
	x_B	0.01	$kmol/kmol$
Manipulated variables (u)	L	$2.0 - 21.5$	$kmol/min$
	V	$2.5 - 22.0$	$kmol/min$
Disturbances (d)	F	1 ± 0.1	$kmol/min$
	z_F	0.5 ± 0.05	$kmol/kmol$
Key hydraulic parameters	M_i	$20.5/N_T$	$kmol$
	M_d	0.5	$kmol$
	M_b	0.5	$kmol$
	τ_L	0.063	$min/stage$
	$\sum_i M_i$	20.5	$kmol$
Thermodynamic data	α	1.5	$-$
Number of stages	N_T	$25 - 71$	$-$
Feed stage number	N_F	$13 - 36$	$-$

increase when the flows increase). Note from figure 7.2 that the energy usage, as expressed by the boilup V, decreases dramatically as we increase the number of stages, from $V/F = 22.0$ with 25 stages to $V/F = 2.5$ with 75 stages. This is important for the column operation, but energy usage is otherwise not taken into account in the following analysis. Note also that in this chapter the controlled variables (x_D, x_B) are denoted outputs and the manipulated variables (L, V) are denoted inputs.

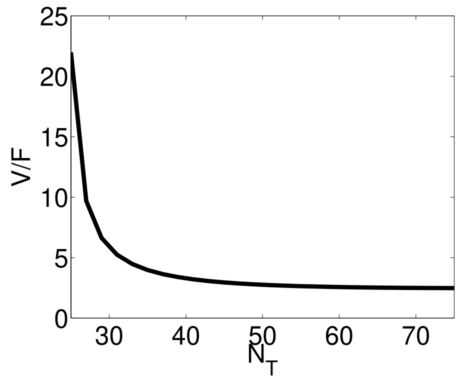

Figure 7.2: Nominal boilup as function of number of stages with fixed product purities ($x_D = 0.99$, $x_B = 0.01$).

7.3 Open-loop responses

The nonlinear open-loop output (x_D, x_B) responses for $\pm$ 10 % step changes in the inputs (L, V) and in the disturbances (F, z_F) for different number of stages are shown in figures 7.3 and 7.4. Figure 7.3 shows the whole open-loop response which is seen to be strongly nonlinear. However, for control purposes the initial response is of main interest, and this is shown in figure 7.4. We find that:

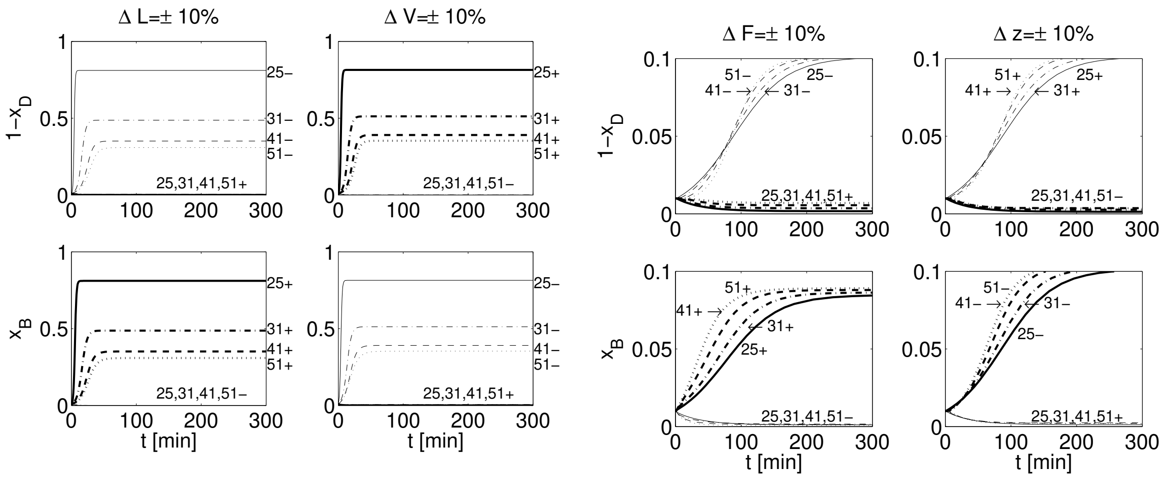

Figure 7.3: Open-loop output responses for steps in inputs (left side) and disturbances (right side)

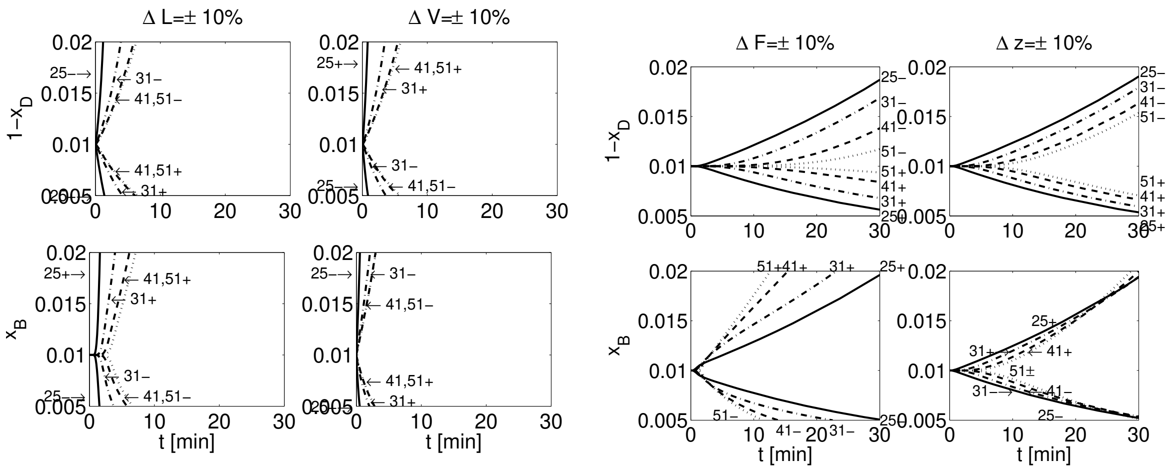

Figure 7.4: Initial open-loop output responses for steps in inputs (left side) and disturbances (right side)

- The inputs (L, V) have a much faster and larger effect with few stages. This is mainly because a 10% input change is much larger in absolute units with few stages because the flows are much larger (see figure 7.2)
- Initially, the disturbances (F, z) have a larger effect with few stages.
- However, at longer time scale the effect of disturbance is larger with many stages.

Note that the fastest control is required for x_B with disturbances in F, where many stages requires somewhat faster control than few stages.

Table 7.2: Maximum expected or acceptable deviation used to scaling

Output error	y_{max}	=[0.01 0.01]^T
Setpoints	r_{max}	=[0.01 0.01]^T
Inputs	u_{max}	=u_{nom} (varies, see figure 7.2)
Disturbances	d_{max}	=[0.10 0.05]^T

7.4 Controllability analysis

To evaluate the inherent performance limitations with different number of stages, we use some simple linear controllability measures (Skogestad & Postlethwaite 1996). A linear model ($y = Gu + G_d d$, $\tilde{r} = Rr$) is obtained by linearizing the nonlinear model at the nominal point (d_{nom}^T=$[F\ z_F]$=$[1\ 0.5]$, y_{nom}^T=$[1 - x_D\ x_B]$=$[0.01\ 0.01]$). G is the process gain matrix, G_d is the disturbance gain matrix and R is the diagonal matrix that includes the maximum expected setpoint changes ($R_{ii} = r_{max,i}/y_{max,i}$). The variables ($d^T$=$[\Delta F\ \Delta z_F]$, y^T=$[\Delta x_D\ \Delta x_B]$, u^T=$[\Delta L\ \Delta V]$, r^T=$[\Delta x_{D,s}\ \Delta x_{B,s}]$) are scaled such that a ± 1 variation corresponds to an allowable/expected change from the nominal value. More precisely, the scaled variables are obtained by dividing the change by the maximum change for each variable as given in table 7.2.

The frequency dependent process gains ($g_{ij}(j\omega)$) in figure 7.5 and disturbance gains ($g_{dij}(j\omega)$) in figure 7.6 confirm the time responses:

- With few stages the inputs (L, V) have a larger effect.
- Fastest control is required for x_B with disturbances in F. Somewhat faster control is required with many stages.

The required bandwidth for rejecting the effect of disturbances (ω_d) in F for x_B is approximate 0.1 min^{-1}. This is much higher than bandwidths for reference tracking, which are about ω_r=$1/30$ min^{-1}. The expected bandwidths for the wanted controllers are then expected somewhat above 0.1 min^{-1}.

The relative gain array (RGA) is used to assess the (two-way) interactions and the sensitivity to input uncertainty for multivariable control. The frequency dependent RGA (Λ) for a square system G is $\Lambda(\omega) = G(j\omega) \times [G^{-1}(j\omega)]^T$ where the symbol $\times$ denotes element-by-element multiplication. Figure 7.7 shows that the RGA-values for the 1,1-element, and thus the two-way interactions, are much higher with few stages, especially at low frequencies. The 1,1-element at steady-state is 3995 with 25 stages, 164 with 31 stages, 36 with 41 stages and 15 with 51 stages. Large interactions (around the expected bandwidth) indicate high sensitivity to input uncertainty and thereby reduced control performance. This confirms the result ("potential advantage 2") of Skogestad (1997). Note that the RGA-number ($||RGA - I||_{sum}$) gives the same conclusion, see figure 7.8.

There are no unstable (RHP) poles or unstable (RHP) zeros.

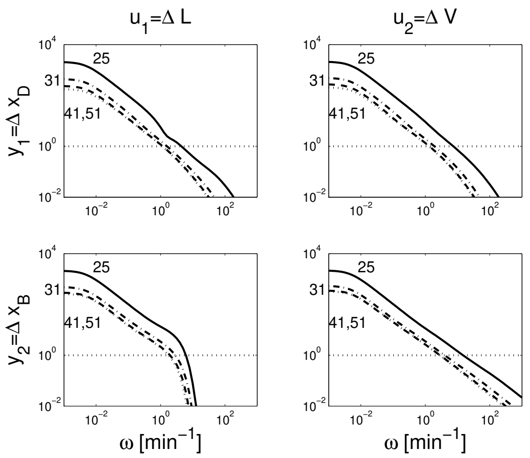

Figure 7.5: Process gains ($G(j\omega)$)

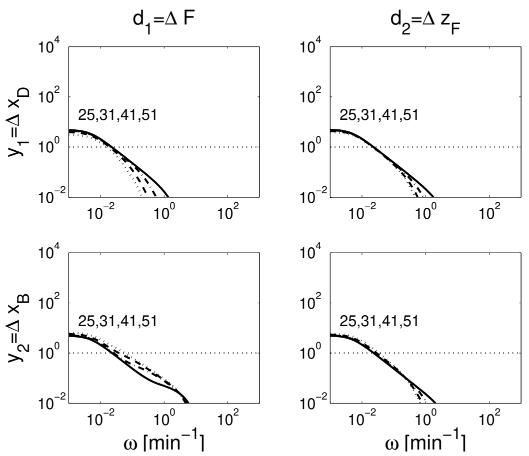

Figure 7.6: Disturbance gains ($G_d(j\omega)$)

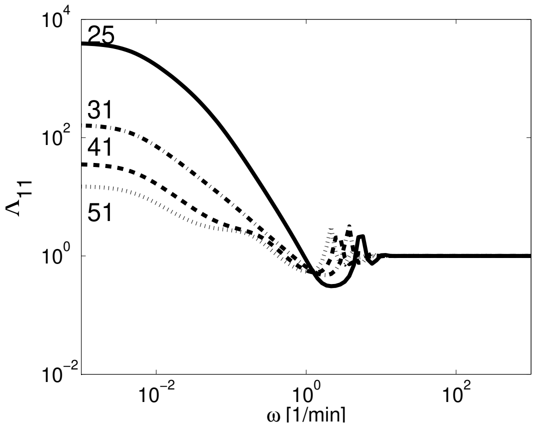

Figure 7.7: 1,1-element in the RGA

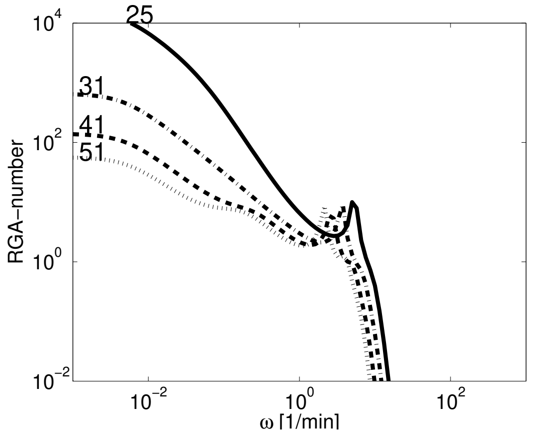

Figure 7.8: RGA-number ($||RGA - I||_{sum}$)

The inputs required for perfect control (with respect to disturbance rejection and reference tracking) are $u = G^{-1}Rr - G^{-1}G_d d$. The elements in the scaled matrices $G^{-1}R$ and $G^{-1}G_d$ should be less than 1 in the frequency range where control is needed. From figure 7.9 we find that there are no problems with input saturation related to disturbance rejection. Note that input usage around the expected bandwidth is larger with many stages than with few stages. From figure 7.10 we find that with reference tracking input saturation is a problem with 25 stages. Note that at low frequencies input usage for reference tracking with few stages is larger than with many stages.

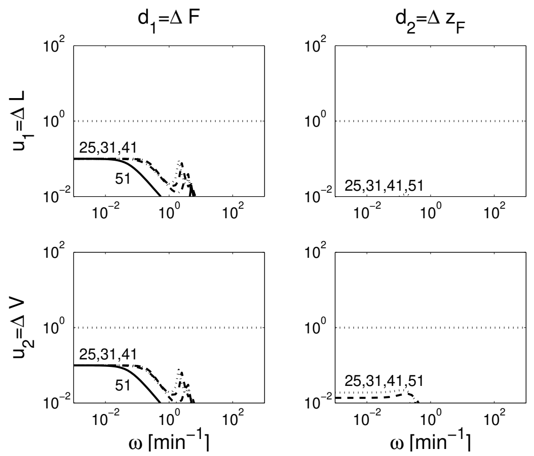

Figure 7.9: Input usage with perfect disturbance rejection ($G^{-1}G_d(j\omega)$)

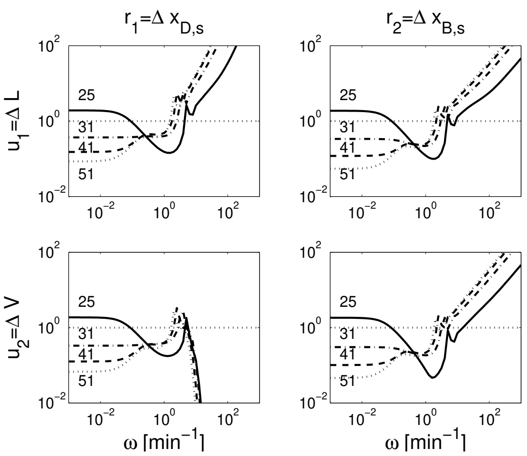

Figure 7.10: Input usage with perfect reference tracking ($G^{-1}R(j\omega)$)

7.4.1 Decentralized control

To analyze the use of decentralized control on this system we consider the closed-loop disturbance gain (CLDG) and the performance relative gain array (PRGA) (Skogestad & Postlethwaite 1996). x_D is controlled by manipulating L and x_B is controlled by manipulating V (we then avoid pairing on a negative steady-state RGA-element). The RGA-number confirms that there are large two-way interactions, see figure 7.8. The CLDG ($\tilde{G}_d$) yields the effect of disturbances under decentralized control and is defined as $\tilde{G}_d(s) = \tilde{G}(s)G^{-1}(s)G_d(s)$ where $\tilde{G}$ is a diagonal matrix consisting of the diagonal elements of G ($\tilde{G}$=diag$\{g_{ii}\}$). The closed-loop disturbance gains $\tilde{g}_{dij}$ in figure 7.11 indicates that many stages gives the best disturbance rejection at low frequencies. This is a contrast to the open-loop disturbance gains g_{dij} where we only found minor differences with various number of stages. The differences in $\tilde{g}_{dij}$ may be explained by that decentralized control is sensitive to interactions, which are especially strong with few stages. At medium and higher frequencies there are only minor differences in $\tilde{g}_{dij}$. As expected, there are no problems with input saturation with disturbance rejection because $\tilde{g}_{dij}$ are smaller than the corresponding diagonal process gains g_{ii}, i.e. $|g_{ii}| > |\tilde{g}_{dij}| \forall i, j$ when $|\tilde{g}_{dij}| > 1$.

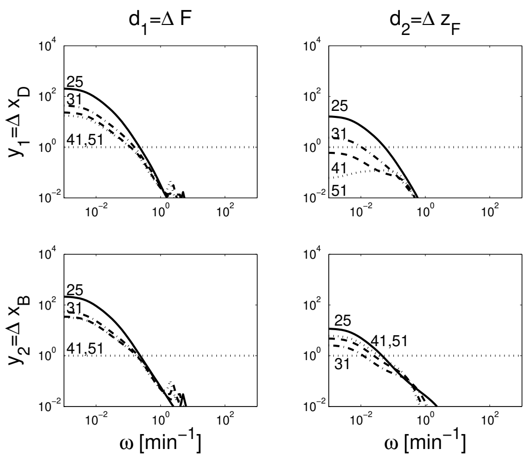

Figure 7.11: CLDG ($\tilde{G}_d$)

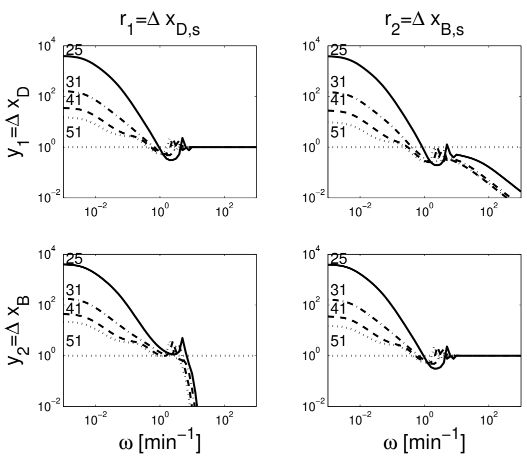

Figure 7.12: PRGA (Γ)

The PRGA ($\Gamma(s) = \tilde{G}(s)G^{-1}(s)$) yields the effect of setpoint changes and one-way interactions under decentralized control. Again we find that many stages is better (see figure 7.12). As expected, we get input saturation for reference tracking with 25 stages since the PRGA-elements (γ_{ij}) are larger than the corresponding diagonal process gains at low frequencies ($|g_{ii}| < \gamma_{ij}, \forall i, j$ with $\omega < 0.01$).

Figure 7.11 shows that the required bandwidth for rejecting the disturbances (ω_d) in F with decentralized control is about $1/3\ min^{-1}$ for both outputs. Since the required bandwidth for rejecting disturbances in z and for reference tracking (say $\omega_r = 1/30\ min^{-1}$) is lower, the expected bandwidth for a decentralized controller must be somewhat above $1/3\ min^{-1}$. The phase lag in the diagonal process gain elements indicates no problem with achieving the expected bandwidth. Note that neglected dynamics in the model (e.g. measurement dynamics) may give problems with the phase lag. A time delay up to $\theta = 1/\omega_d$ =3 min (e.g., related to neglected dynamics) is acceptable.

7.5 μ-optimal controller analysis

The control objective is to keep the product compositions within ± 0.01 (mole fraction units) from their desired values. To check whether this is even possible we design an optimal controller for the linear plant, taking into account expected disturbances, setpoint changes and model uncertainty (diagonal input and output uncertainty).

7.5.1 Setup

Figure 7.13 shows the block diagram used for this analysis. Model uncertainty is included both as input and output uncertainty. This setup is primarily based on Lundstrom & Skogestad (1995). K is the controller. G' is the overall plant model which consists of the disturbance

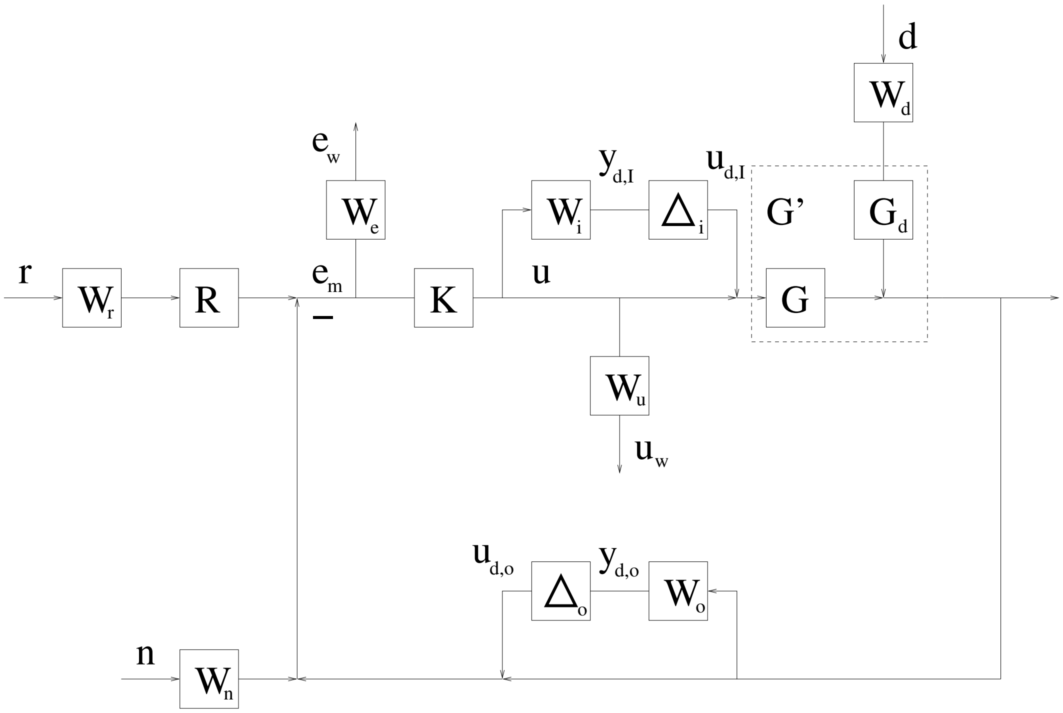

Figure 7.13: Block diagram for μ-analysis

gain G_d and the process gain G. G' has two outputs y (x_D and x_B) and four inputs u (L, V, F and z_F). R is a diagonal matrix that includes the maximum expected setpoint changes. W_r, W_d and W_n are weight matrices for setpoints r, disturbances d and measurement noise n. W_e and W_u are weights respectively on deviation from desired setpoints e and manipulated variables u. Model uncertainty is represented by $W_i\Delta_i$ which models input uncertainty, and $\Delta_o W_o$ which models output uncertainty. Δ_i and Δ_o are any diagonal matrices with H_∞-norm less than one. The weighting matrices are diagonal with elements as following below. For the reference tracking weight we use:

$$w_r = 1/(\tau_r s + 1) = 1/(30s + 1) \tag{7.1}$$

The reference weight gives that a reference change should follow a first order response with time constant equal 30 min. For the disturbance weight we use:

$$w_d = 1 \tag{7.2}$$

which means that the controller should reject disturbances for all frequencies. For the measurement noise weight we use:

$$w_n = 10^{-4} \tag{7.3}$$

High frequency measurement noise is assumed handled by the output uncertainty weight. For the output weight we use:

$$w_e = (\frac{\tau_{cl}}{M_s}s + 1)/(\tau_{cl}s + A) = (0.5s + 1)/(s + 10^{-4}) \tag{7.4}$$

τ_{cl} ($= 1$ min) is the closed-loop response time, and M_s ($= 2$) is the maximum allowed peak of the sensitivity function. In practice integral action is necessary when A is very small. We use $A = 10^{-4}$. For the input weight we use

$$w_u = (\tau_u s)/(\frac{\tau_u}{M_\infty}s + 1) = s/(10s + 1) \tag{7.5}$$

The input weight gives a penalty at high frequencies or fast changes in input usage. The input gain penalty is 10 % at high frequencies ($M_\infty = 0.1$). The weight gives a penalty related to a time constant less or equal 1 min ($\tau_u = 1$ min). For the input gain uncertainty we use

$$w_i = (\tau_i s + M_{i,0})/(\tau_i/M_{i,\infty}s + 1) = (0.5s + 0.2)/(0.25s + 1) \tag{7.6}$$

The input gain uncertainty is 20 % at low frequencies ($M_{i,0}$ = 0.2) and increases to 200% at high frequencies ($M_{i,\infty}$ =2). The weight allows for a time delay of 0.5 min at the inputs (τ_i = 0.5 min). For the output we use

$$w_o = (\tau_o s + M_{o,0})/(\tau_o/M_{o,\infty}s + 1) = s/(0.5s + 1) \tag{7.7}$$

The output gain (or measurement uncertainty) is assumed equal zero at low frequencies ($M_{o,0} = 0$) and increases to 200% at high frequencies ($M_{i,\infty} = 2$). The weight allows for a time delay of 1 min in each measurement (τ_o = 1 min). A summary of the weights is shown in figure 7.14.

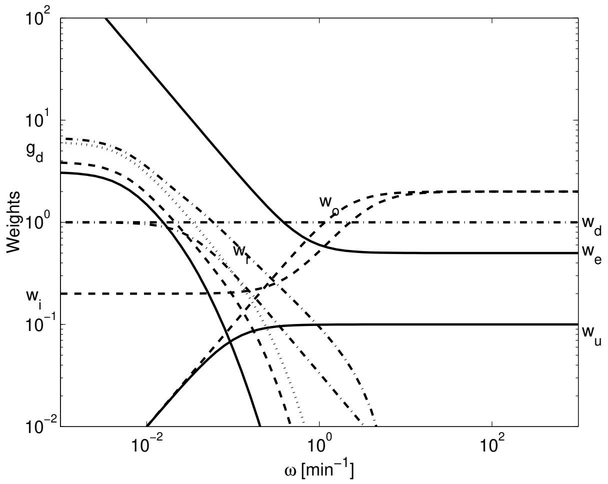

Figure 7.14: Weights

For the system in figure 2, μ_{NP} is the H-infinity norm of the transfer function from the scaled inputs $[r\ d\ n]$ to the scaled outputs $[e_w\ u_w]$, or equivalently tells us by which factor the performance weights must be reduced to have the scaled errors less than 1. μ_{RP} tells by which factor the uncertainty and performance weights must be reduced to give the worst-case scaled errors less than 1. In summary, μ_{NP} and μ_{RP} should be as small as possible, and preferably less than 1.

Table 7.3: μ-optimal controller and SIMC-tuned PI-controllers analysis for different number of stages

N_T/N_F	V/F	μ-optimal		SIMC-tuned PI	
		μ_{NP}	μ_{RP}	μ_{NP}	μ_{RP}
$25/13$	22.0	0.6769	1.327	792.5	792.6
$31/16$	5.25	0.7243	1.043	61.08	61.30
$41/21$	3.21	0.7552	0.994	19.20	19.42
$51/26$	2.73	0.7735	0.9975	12.92	13.13
$61/31$	2.56	0.7662	0.9913	11.59	11.83
$71/36$	2.49	0.7802	1.003	12.71	12.96

7.5.2 μ-optimal controller

The μ-optimal controller minimizes the structured singular value μ_{RP} for the system. The μ-optimal controller is designed by DK-iteration (Doyle, Wall & Stein 1982). The results are summarized in table 7.3. Nominally, the performance (μ_{NP}) is somewhat better with few stages. However, model uncertainty is an important consideration for distillation, and μ_{RP} decreases and robust performance is improved until we reach about 40 stages where the performance remains constant.

This can be explained by the fact that with uncertainty the decoupling effect of multivariable controllers are reduced.

7.5.3 SIMC-tuned PI-controller

To confirm the above results for a more practical controller, we consider single-loop PI-control of top and bottom composition. x_D is controlled by manipulating L and x_B is controlled by manipulating V. We use the SIMC PI-tuning rules (Skogestad 2003) to find the proportional gain (K_c) and integral time (τ_I):

$$K_c = \frac{1}{k^{'}(\theta + \tau_c)} \tag{7.8}$$

$$\tau_I = 4(\theta + \tau_c) \tag{7.9}$$

Here $k^{'}$ is the initial increase of the time response to a unit step in the input, θ is the time delay and τ_c is the desired closed-loop response time (tuning parameter). The desired closed-loop time (τ_c) is selected equal the expected delay ($\tau_c = \theta = 0.5\ min + 1\ min = 1.5\ min$). A μ-analysis of the SIMC-tuned PI-controllers shows that these controllers give good stability properties, but the performance is rather poor with μ_{NP} and μ_{RP} well above 1. Nevertheless we see from table 7.3 that performance is improved (μ_{NP} and μ_{RP} is smaller) as we increase the number of stages.

This is explained by the fact that decentralized controllers are sensitive to interactions.

7.6 Nonlinear simulations

To check the control behavior for different number of stages, simulations with the nonlinear model using the SIMC-tuned PI-controllers were performed. No dynamics related to the measurements or the inputs are included in the simulations. Figure 7.15 shows the outputs for a step in F. With few stages the peak of the control errors are smaller, but outputs return slower to their setpoints than with many stages. Note that we get a steady-state offset with 25 stages. Figure 7.16 shows the outputs to a step in z. The response in x_B is best with few stages, whereas the response in x_D it is best with many stages. Except from the initial closed-loop response in x_D with a disturbance in F, the initial closed-loop responses can be explained by the initial open-loop responses (i.e. no control). The initial closed-loop response in x_D with a disturbance in F is opposite that of the initial open-loop response. This can be explained by the interactions with the x_B-controller: Fast control of x_B is required to reject the increase in F, and this is done by increasing V which increases x_D. With a given bandwidth for the x_B-controller (independent of the number of stages, $\omega_B = 0.5/\theta$) the control error in x_B and then the use of V is larger for many stages which give larger initial increase in x_D. The shorter settling time with many stages can be explained by the fact that the interactions are smaller at low frequencies. Note that for all disturbances the control errors are far inside the acceptable control error for all number of stages.

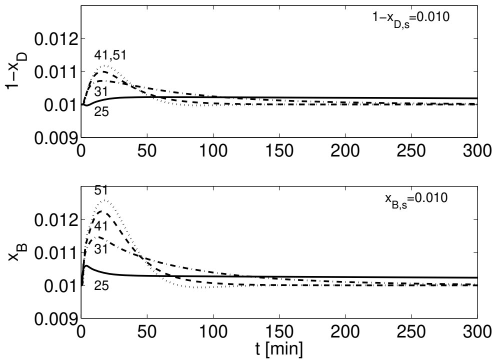

Figure 7.15: Output responses to 10% increase in F with SIMC-tuned PI-controllers.

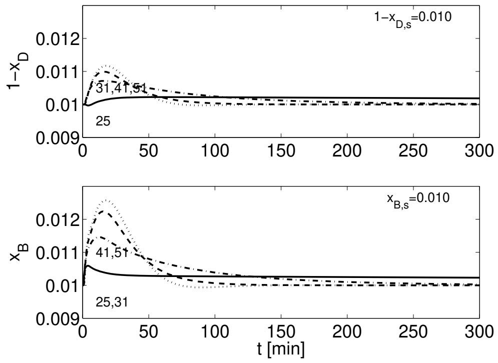

Figure 7.16: Output responses to 10% increase in z_F with SIMC-tuned PI-controllers.

Figures 7.17 and 7.18 show the responses to steps in the setpoints. Here we find that many stages gives much better responses, especially in terms of the settling time. As expected the setpoints are not achieved at steady-state with 25 stages. The initial responses are similar since the bandwidth is equal and given by the expected delay in the measurements and inputs. As for the disturbances, shorter settling time with many stages is explained by smaller interactions.

Note that the nonlinear simulations correlate well with the μ-analysis where the output weights at low frequencies are selected large, such that achieving short settling time is prioritized.

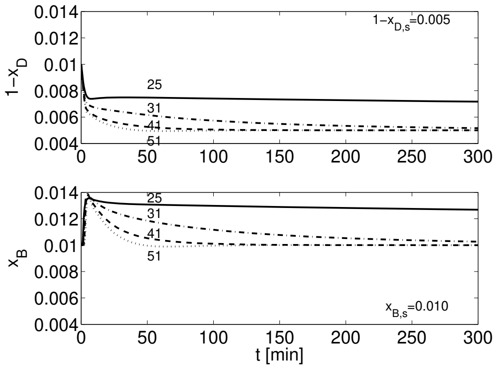

Figure 7.17: Output responses with a setpoint change in $x_{D,s}$ from 0.990 to 0.995 with SIMC-tuned PI-controllers.

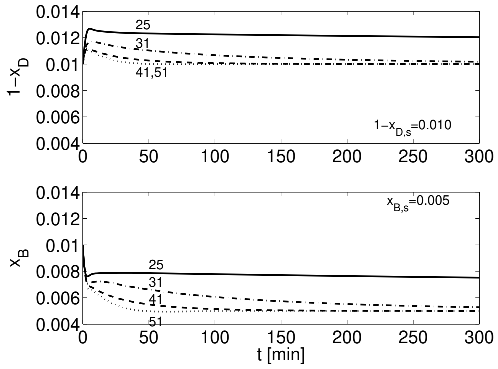

Figure 7.18: Output responses with a setpoint change in $x_{B,s}$ from 0.010 to 0.005 with SIMC-tuned PI-controllers.

7.7 Over-purification of the products

Until now we have compared columns that have had very different internal flowrates and correspondingly very different energy usages. With few stages we need large internal flowrates (large energy usage) to achieve the product specifications, while with many stages the internal flowrates approach a minimum, see figure 7.2. We have in fact to consider two factors: (i) The number of stages and (ii) the size of internal flowrates. A large number of stages gives smaller interactions, while large internal flowrates give a larger (and faster) effect of the inputs and initially improved "damping" of the disturbances. With given setpoints these two factors are competing, since few stages results in large internal flows and many stages results in small internal flows. A probably fairer comparison is to keep the energy usage constant for all number of stages. This will allow for over-purification at the top and bottom composition for cases with many stages ("potential advantage 1" of Skogestad (1997)).

The top and bottom composition setpoints for a different number of stages are determined by keeping constant internal flowrates in the column at the nominal point ($F = 1\ kmol/min$, $z_F = 0.5 kmol/kmol$). Table 7.4 shows the resulting product composition for two cases: with $V/F = 2.73$ kmol/min and $V/F = 22.0$ kmol/min. $V/F = 22.0$ kmol/min gives an overpurified operation. To make the gain more linear we take the logarithm of the top and bottom composition (Skogestad 1997). The controllers are tuned with the SIMC-controller tuning rules. No delay or dead time in the measurements are included in the simulations. Figure 7.19 shows the output responses to a 10% increase in F and figure 7.20 shows the output responses to a 10% increase in z when the nominal boilup is equal 22.0 kmol/min. We find that many stages is much better. We are far from violating the output constraints, and the disturbances in F have neglectable effect on the outputs. Figure 7.21 shows the output

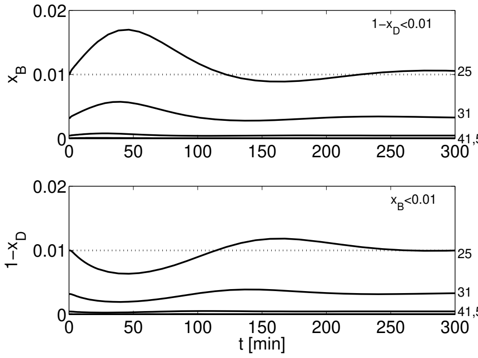

Figure 7.19: Responses with over-purification for a 10% increase in F. Nominal boilup V=22.0 kmol/min in all cases.

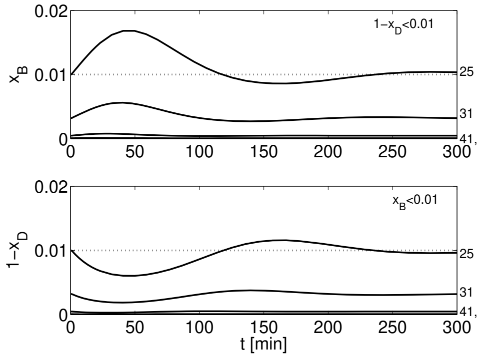

Figure 7.20: Responses with over-purification for a 10% increase in z_F. Nominal boilup V=22.0 kmol/min in all cases.

responses to a 10% increase in the feedrate and figure 7.22 shows the output responses to a 10% increase in the feed composition when the nominal boilup is $V = 2.73$ kmol/min. Few stages are much worse, and we are far from fulfilling the constraints and the disturbances have significant effect on the top and bottom compositions. In conclusion, in terms of con-

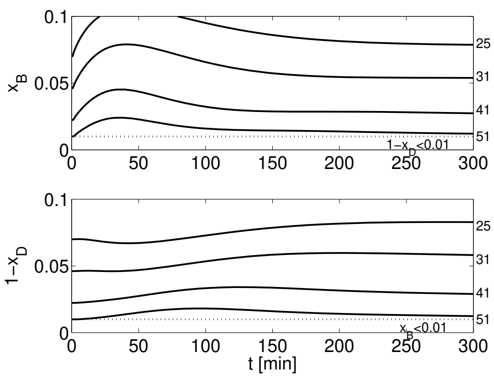

Figure 7.21: Responses with over-purification for a 10% increase in F. Nominal boilup V=2.73 kmol/min in all cases.

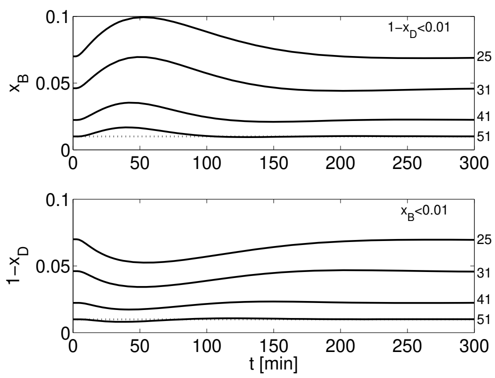

Figure 7.22: Responses with over-purification for a 10% increase in z_F. Nominal boilup V=2.73 kmol/min in all cases.

trollability analysis it is clearly better to have as many stages as possible and over-purify the top and bottom product.

Table 7.4: Top and bottom composition for different number of stages when using $V = 2.73$ kmol/min and $V = 22.0$ kmol/min

N_T/N_F	$V/F = 2.73$		$V/F = 22.0$	
	x_D	x_B	x_D	x_B
$25/13$	0.0701	0.0701	0.0100	0.0100
$31/16$	0.0462	0.0462	0.0032	0.0032
$41/21$	0.0224	0.0224	$4.75 \cdot 10^{-4}$	$4.75 \cdot 10^{-4}$
$51/26$	0.0100	0.0100	$7.02 \cdot 10^{-5}$	$7.02 \cdot 10^{-5}$
$61/31$	0.0041	0.0041	$1.04 \cdot 10^{-5}$	$1.05 \cdot 10^{-5}$
$71/36$	0.0015	0.0015	$1.53 \cdot 10^{-6}$	$1.53 \cdot 10^{-6}$

7.8 Conclusion

With fixed setpoints to the top and bottom compositions few stages gives the best controllability for disturbance rejection whereas many stages gives the best controllability for setpoint tracking. However, this comparison is unfair as the energy usage (V) is much higher with few stages. With the same energy usage (V) it is possible to overpurify the products when we have many stages, and then we get better controllability with many stages.

Chapter 8

Concluding remarks and further work

8.1 Concluding remarks

8.1.1 Self-optimizing control

We have presented a systematic approach for selecting controlled variables for a liquid phase reactor with recycle plant. To optimize economics we need to control active constraints. Both for the cases of minimizing operating costs with given feedrate (case I) and maximizing production rate with free feedrate (case II), it is optimal to keep the reactor holdup at its maximum. This makes the Luyben structure (LS) and the two balanced structures of Wu & Yu (1996) economically unattractive. For the unconstrained variables we look for self-optimizing variables where constant setpoints give acceptable economic loss. Both in cases I and II, the reflux ratio (L/F or L/D) appears to be such a variable. In order to avoid the so-called "snowball effect", it has been proposed in the literature to "fix a flow in a liquid recycle loop". However, the rule seems to have limited basis, as it leads to control structures that can handle only small feedrate changes (constant reactor holdup), or that result in large variations in the reactor holdup (variable reactor holdup) (Wu & Yu 1996).

We have extended the systematic approach for selecting controlled variables by introducing several alternative methods for computing setpoints. The simplest is to use constant nominal setpoints, but this may give large loss in some cases or infeasible operation. One alternative is to find the best constant setpoint ("optimal backoff") by solving a quite complex robust optimization problem. Another alternative is to allow for online adjustments of the nominal setpoints such that we achieve feasibility ("flexible backoff"). Although the feasibility region can be increased and the loss for a specific constant setpoint policy can be reduced by use of logic, model predictive control and/or online optimization, a good choice of controlled variables will reduce the need for these remedies and give a simpler and cheaper system. Note that the required backoff and the corresponding economic loss depend on the selected controlled variables. Thus, the primary issue is to select the right control structure (variables), whereas the backoff is just a setpoint *adjustment* to deal with nonlinearities and infeasibility. As a case study we have used a reactor, separator and recycle process (Wu & Yu 1996) and an evaporation process (Newell & Lee 1989).

For the reactor, separator and recycle process, control of x_D and L/F show the best self-optimizing control properties. Alternatives which follow Luybens rule (F and D), require robust setpoints and give larger loss than x_D and L/F. Alternatives with variable reactor holdup (e.g. Luyben Structure and Balanced Structure) require flexible setpoints and give significantly larger loss than x_D and L/F.

For the evaporation process, control of $T_{201} - T_{200}$ gives the smallest economic loss both when using robust setpoints and flexible setpoints. To avoid computing flexible setpoints online (or reconfigure online) we propose to use robust setpoints. Controlling $T_{201} - T_{200}$ with robust setpoints shows acceptable control behavior. Compared with control of x_2, P_2 and F_3 (Kookos & Perkins 2002a) control of $T_{201} - T_{200}$ in addition to the active constraints gives smaller losses and a simpler system since online feasibility correction is not required.

8.1.2 Plantwide control

A systematic procedure for plantwide control design (Larsson & Skogestad 2001) is applied to a combined cycle power plant and a distillation column with heat pump (Koggersbøl 1995). The plantwide control design procedure consists of top-down analysis (including definition of operational objectives and consideration of available degrees of freedom) and bottom-up design of the control system (starting with stabilizing the process). The top-down analysis consists of identifying manipulated variables, a degree of freedom analysis and selection of primary controlled variables (based on economics) and production rate manipulator. The bottom-up design consists of selecting the structure of the regulatory layer (including selection of secondary controlled variables) and the structure of the supervisory layer (including MPC-applications) and proposes whether online optimization should be used. The control structure should be validated by nonlinear simulations.

The combined cycle power plant (considered here) has one unconstrained steady-state degree at optimal operation. Controlling the super-heater gas inlet temperature in addition to the variables at active constraints at optimum gives the smallest loss (only 0.16% larger than reoptimization with constraint backoff). Controlling the super-heater inlet temperature partly decouples the operation of the gas turbine and the steam turbine cycle. In this case the disturbances have rather small effect on the optimal operation of the process. The implementation errors connected to the controlled variables have significantly larger effect. The main difference in loss between the alternatives comes from the implementation of the unconstrained controlled variables. Temperatures and pressures give significantly less loss than the other candidate controlled variables.

For the distillation column with heat pump we find that controlling the temperature at stage 4 (T_4) in addition to the active constraints gives close to optimal operation (self-optimizing control). Compared with Koggersbøl (1995) we propose to linearize the process with controlling the compressor flowrate instead of the low pressure in the heat pump cycle. This gives better performance of the regulatory control layer (faster control) and simplifies the control system (does not need a hierarchy with pressure controllers).

8.1.3 Controllability

With fixed setpoints to the top and bottom compositions few stages in a distillation column gives best controllability for disturbance rejection, whereas many stages gives best controllability to setpoint tracking. However, this comparison is unfair as the energy usage (V) is much higher with few stages. With the same energy usage (V) it is possible to overpurify the products when we have many stages, and then we get better controllability with many stages.

8.2 Directions for future work

8.2.1 Model uncertainty

The effect of model uncertainty when selecting controlled variables based on economics should be studied in more detail. We here divide the model errors in *parametric model errors* and *structural model errors*. Parametric model errors (uncertain estimates of model parameters) can be treated as disturbances. Structural model errors, e.g. as a result of model simplifications, are more difficult to handle. The structural model errors can be found by comparing the applied model with a more detailed model (or measurements), and a conservative approach is to treat them as implementation errors. For future research in this area, a good start may be the work of Marlin and co-workers, e.g. Forbes, Marlin & MacGregor (1994).

8.2.2 Mathematic programming approach

Identification of candidate controlled variables by use of mixed integer programming (MINLP) should be tested. The problem formulation is easy, but a good solver need to be found.

8.2.3 More case studies

More case studies should be performed to improve the understanding and help the development of suitable tools for plantwide control. Many good industrial examples are presented in Luyben, Tyreus & Luyben (1998), e.g. the vinyl acetate process, the isomerization process and the HDA process.

8.2.4 Improvement of presented case studies

Identifying candidate controlled variables

Methods for identifying optimal linear combinations of measurements as controlled variables (Halvorsen et al. 2003) (Alstad & Skogestad n.d.) should be tested.

Robust optimization

Glemmestad et al. (1999) presented two methods for avoiding robust optimization online, either by (i) using nominal optimization online and some constant backoff or (ii) using nominal optimization with some safety margins online. It would have been interesting to include more disturbance and implementation error regions for the reactor, separator and recycle process and for the evaporation process, and study these two methods in more detail.

Combined cycle power plant

The combined cycle power plant process in chapter 5 should be simplified and standardized:

- Replace the fuel compressor with valve and assume that the fuel feed pressure is always higher than the combustor pressure.
- Consider a two-shaft combined cycle power plant.
- Remove the deaerator pressure constraint.

The model should be improved by including more dynamics, and a more systematic literature review should be presented.

Appendix A

Robust optimization

We here discuss robust optimization in more detail. First, we discuss the sensitivity to changing the distribution of operating points and the corresponding weights in the objective criteria for different sets of controlled variables. Second, we give some advice about solving the robust optimization problem.

A.1 Selecting operating points and objective weights

The setpoints should be selected in order to minimize the expected operating cost with respect to disturbances and implementation errors, which are uncertain parameters with some probability distribution. We here distinguish between expected variations in the disturbances and implementation errors that the control system should handle and rare and extreme ("unexpected") variations that should be handled by some safety system (and may in the worst case result in shut-down).

We focus on *expected* variation in disturbances and implementation errors: Robust optimization finds setpoints which fulfill the constraints and minimize the expected operating cost for expected disturbances and implementation errors. Note that if the operating cost for "extreme" disturbances and implementation errors dominates, e.g. they result in shut-down, the objective should be changed to minimize the cost with "extreme" disturbances and implementation errors (e.g. minimize the probability for shut-down). In the case studies we have assumed that:

- The expected variations in disturbances and implementation errors are given by some range.
- Only one disturbance or implementation error is perturbed from nominal point at a time.
- Feasibility is ensured if we get feasibility in the nominal point and the corner-points.
- The average cost in the considered operating points gives a good estimate of the real operating cost.

A better approach than using the average loss of the considered operating points is to evaluate the loss with respect to a large number of random disturbances and implementation errors (operating points) based on the assumed probability distribution ("Monte Carlo simulations"). The expected loss should then be computed for say the 99% operating points with the smallest loss. If more than say 1% of the operating points are infeasible, the approach (the specific constant setpoint policy) is infeasible. Note that robust setpoints can then also give infeasibility.

We now want to discuss robust optimization if the disturbances and implementation errors are uncertain parameters with a given probability distribution and the probability for being in the expected disturbance and implementation error region is larger than say 99%. We want to discuss how the selection of operating points and corresponding weights in the objective function affects the solution with respect to feasibility, loss and setpoint adjustment, and discuss the dimension of the robust optimization problem. In addition we want to consider how the selection of operating points and weights affects the ranking of the alternatives.

Using many operating points is preferred in order to guarantee feasibility and get a good estimate of the expected operating cost for the expected variation in disturbances and implementation errors. However, using many operating points gives a high-dimensional nonlinear optimization problem. The grid of operating points and corresponding objective function weights should therefore be selected carefully in order to get a not-too-high-dimensional optimization problem, which includes the most important nonlinearities[1] and when solved, "guarantees" feasibility and minimizes the actual expected operating cost.

The reactor-separator-recycle process (see chapter 3) is used to illustrate some aspects of selecting different distribution of operating points and corresponding weights in the objective function for different sets of controlled variables. First, we consider a constant expected disturbance and implementation error region and change the objective weights and number of operating points. Second, we consider increasing the expected disturbance and implementation error region.

A.1.1 Constant expected disturbance and implementation error region

We here assume that the expected region for each disturbance or implementation error is constant and only one disturbance or implementation error is perturbed from the nominal point at a time. We look at three different approaches: *Flat cost*, *nominal cost* and *economic region*.

For the *flat cost* and *nominal cost* approaches we include the nominal point and the cornerpoints for the expected disturbances and implementation errors, see figure A.2. While all the operating points are equally weighted in the objective for the *flat cost* approach, only the cost in the nominal point is included in the objective (nominal objective) for the *nominal*

[1] Nonlinearities in the model are important for achieving feasibility, while both nonlinearities in the model and in the probability distribution are important for achieving a good estimate of the expected operating cost.

cost[2] approach. For the *economic region* approach we distinguish between an expected disturbance and implementation error region and an economic disturbance and implementation error region. In the expected disturbance and implementation error region the constraints are fulfilled, and in the economic disturbance and implementation error region the costs are computed and averaged. The corner-points are included as operating points in both regions, see figure A.3. Note that the *flat cost* and the *nominal cost* approach are special cases of the *economic region* approach. For the *flat cost* approach the economic region is selected equal the expected disturbance and implementation error region. For the *nominal cost* approach the economic region is selected equal the nominal point. Note also that the *economic region* approach gives the best approximation of the real probability distribution, see figure A.1, and thereby the best robust setpoints (with smallest expected operating cost).

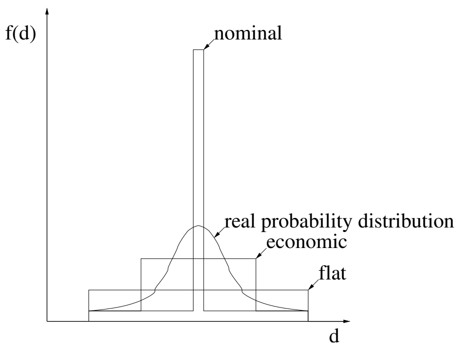

Figure A.1: Probability distributions

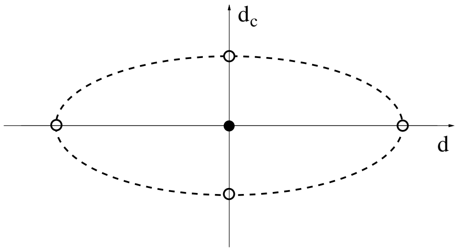

Figure A.2: Operating points with flat and nominal cost (all points are included in the economic region for the flat objective and filled point is included in the economic region for the nominal objective).

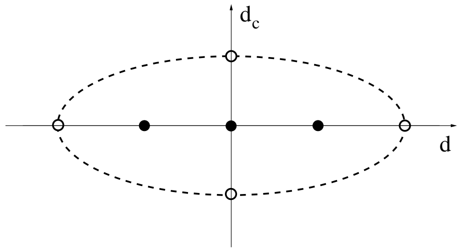

Figure A.3: All operating points are included in the expected disturbance and implementation error region, while the filled points are included in the economic disturbance and implementation error region.

The reactor-separator-recycle process has 2 disturbances (F_0,x_0) and 3 controlled variables (c_1, c_2, c_3) with implementation errors. The expected disturbances are $F_0 = 460 \pm 92$ and

[2]Using robust setpoints based on *nominal cost* we achieve feasibility for the expected disturbance and implementation error region with minimal cost related to the needed backoff at nominal point. *Nominal cost* should be used when the probability for being close to nominal point is large. However, using online feasibility correction may then give smaller loss.

Table A.1: Average percentage loss (L_w) with constant nominal setpoints and constant robust setpoints based on the flat cost, nominal cost and economic region approach.

Rank	c_1,c_2,c_3	nominal setpoints		robust setpoints nominal cost		robust setpoints flat cost		robust setpoints econ. region	
		$c_{3,s}$	$L_w(\%)$	$b_{opt,3}$	$L_w(\%)$	$b_{opt,3}$	$L_w(\%)$	$b_{opt,3}$	$L_w(\%)$
-	reoptimized	$c^*_{opt}(d)$	5.16	–	3.62	–	5.16	–	4.97
$1, 1, 1, 3$	x_b,M_r,x_d	0.825	5.22	0	3.62	0.005	5.21	0	4.99
$2, 1, 3, 1$	x_b,M_r,L/F	0.871	5.39	0	3.62	-0.021	5.35	0	4.97
$3, 1, 2, 4$	x_b,M_r,D/L	0.600	5.40	0	3.62	0.047	5.34	0	5.00
$4, 1, 4, 4$	x_b,M_r,D/V	0.375	5.60	0	3.62	0.026	5.49	0	5.00
$5, 1, 6, 1$	x_b,M_r,V/F	1.392	6.05	0	3.62	-0.037	5.93	0	4.97
$6, 1, 8, 7$	x_b,M_r,B/L	0.549	6.31	0	3.62	0.054	6.05	0	5.06
$7, 1, 11, 12$	x_b,M_r,L	837.4	6.68	0	3.62	-64	6.46	0.09	5.56
$8, 1, 5, 4$	x_b,M_r,V/L	1.600	8.64	0	3.62	0.206	5.89	0	5.00
$9, 1, 7, 8$	x_b,M_r,B/D	0.916	11.2	0	3.62	-0.140	6.00	0	5.21
$-, 10, 10, 9$	x_b,M_r,B/F	0.478	inf	-0.015	3.69	-0.056	6.36	0	5.22
$-, 11, 12, 10$	x_b,M_r,D/F	0.522	inf	0.024	3.79	0.061	6.50	-0.02	5.24
$-, 12, 9, 11$	x_b,M_r,F/F_0	2.091	inf	0.125	3.83	0.289	6.22	0.02	5.26
$-, 13, 13, 13$	x_b,M_r,D	502.0	inf	90	4.07	191	6.79	90	5.60
$-, 14, 14, 14$	x_b,M_r,F	962.0	inf	182	4.84	286	7.51	182	6.19
$-, 15, 15, 16$	x_b,F/F_0,V/B	–	inf	–	25.87	–	25.87	–	26.61
$-, 15, 16, 16$	x_b,F/F_0,x_d	–	inf	–	25.87	–	25.91	–	26.61
$-, 15, 17, 15$	x_b,x_r,x_d(BS)	–	inf	–	25.87	–	26.08	–	26.60
$-, 15, 18, 16$	x_b,M_r/F,L/D	–	inf	–	25.87	–	26.11	–	26.61
$-, 19, 19, 19$	x_b,F/F_0,L/D	–	inf	–	33.13	–	33.13	–	33.91
$-, 20, 20, 20$	x_b,F,x_d(LS)	–	inf	–	43.09	–	43.10	–	43.78
$-, 21, 21, 21$	V/B,F/F_0,x_d	–	inf	–	45.74	–	45.74	–	46.60

inf: infeasible with constant setpoint policy

Constrained variables: $c_{1,s} = x_{B,s} = 0.008$ and $c_{2,s} = M_{r,s} = 2772$

Reoptimized: Reoptimized with constraint backoff, see equation 3.27.

$x_0 = 0.90 \pm 0.05$. For the *economic region* approach the economic region is selected equal $F_0 = 460 \pm 46$, $x_0 = 0.90 \pm 0.025$ and zero implementation errors. Using the nominal or flat cost gives $2 \cdot 2 + 3 \cdot 2 + 1 = 11$ operating points, $11 \cdot 56 + 5 = 621$ optimization variables, $11 \cdot 56 + 2 = 618$ equality constraints and $11 \cdot 10 = 110$ inequality constraints. Using the economic region gives $2 \cdot 4 + 3 \cdot 2 + 1 = 15$ operating points, 845 optimization variables, 842 equality constraints and 150 inequality constraints in the optimization problem.

Table A.1 shows the average loss when using nominal setpoints and robust setpoints based on respectively nominal cost, flat cost and economic region approach for different sets of controlled variables. The nominal setpoint and optimal backoff for the different approaches are included for the unconstrained variable. Note that the average loss when using robust setpoints based on nominal cost or economic region cannot be compared with the average loss when using nominal setpoints or robust setpoints based on flat cost, since their losses are based on different operating points and objective function weights. Table A.1 shows:

- Use of robust setpoints gives more feasible alternatives than using nominal setpoints. Robust setpoints with nominal cost, flat cost or economic region approach give here the same feasible alternatives.

- No robust setpoints exist for some alternatives, e.g. V and B. A constant setpoint policy for the set of controlled variables is then not feasible. Feasibility and robust setpoints may be achieved with a smaller expected disturbance and implementation error region, e.g. for V. Feasibility and robust setpoints may not be achieved at all if the controlled variables are dependent, e.g. for B.

- For all feasible alternatives with nominal setpoints (e.g. x_D, B/D), the robust setpoints based on the nominal cost approach are equal the nominal setpoints and have the same loss when evaluated with respect to the same operating points and objective function weights. For all infeasible alternatives with nominal setpoints (e.g. F and D), robust setpoints based on the nominal cost approach may give feasibility and minimize the loss related to backoff at nominal point.

- For all feasible alternatives with nominal setpoints (e.g. x_D, B/D), the robust setpoints based on the flat cost (or economic region) approach are different from the nominal setpoints, and the loss is reduced[3]. Robust setpoints based on the flat cost (or economic region) approach are used both to achieve feasibility and to reduce the loss.

- The top ranking of the controlled variables alternatives are rather insensitive to which approach the robust setpoints are based on.

Figure A.4 shows the loss when using robust setpoints based on the three approaches, for different disturbances and implementation errors for alternative L/F (small loss with nominal setpoints, left column) and alternative F (infeasible with nominal setpoints, right column):

- For L/F there are only minor differences in loss for the different approaches, and the loss is similar to loss with reoptimization with constraint backoff.

- For F there are significant differences in loss. The losses for the nominal and economic approach are relatively small in the economic region, but large outside the economic region.

A.1.2 Varying expected disturbance and implementation error region

We here assume that the expected region for each disturbance and the expected region for the implementation error for each controlled variable are constant[4], but more than one disturbance (or implementation error) may be perturbed from the nominal point at the same time. We look at three different cases:

- In case I we expect that only one disturbance or implementation error is perturbed from the nominal point at a time, see figure A.2 (equals the flat cost approach in the previous section).

- In case II we expect that two or more disturbances can be perturbed from the nominal point at a time, while only one implementation error can be perturbed from the nominal point at a time (but never coincide with a disturbance), see figure A.5.

[3] We assume a better estimate of the expected operating cost.

[4] If the size of each region is increased, the loss will increase and in worst case feasibility will not be achieved.

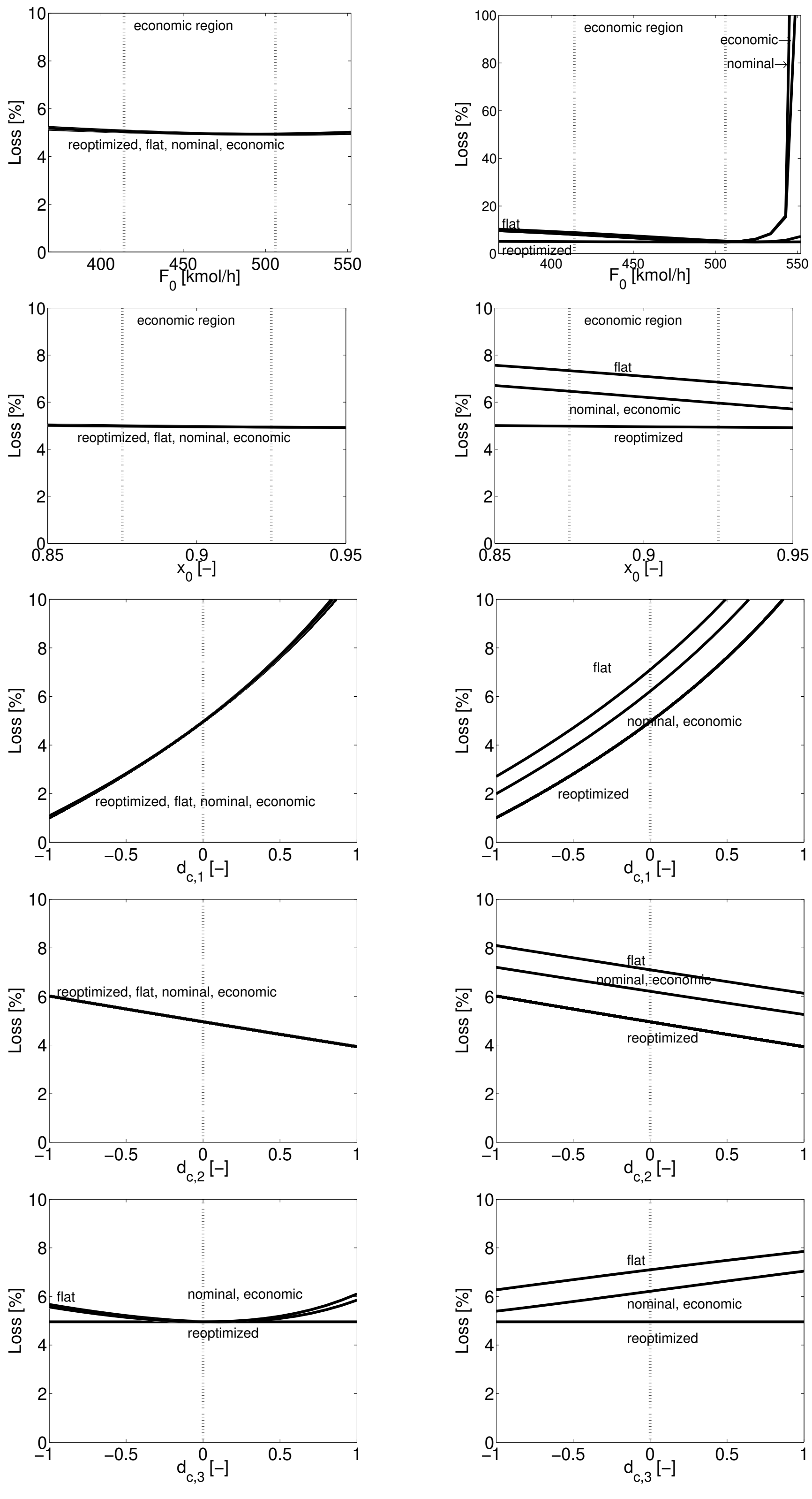

Figure A.4: Loss as function of disturbances (F_0, x_0) and implementation errors ($d_{c,1}$,$d_{c,2}$,$d_{c,3}$) for constant robust setpoints based on the flat cost, nominal cost and economic approach when controlling L/F (left column) and F (right column).

- In case III we expect that every disturbance and implementation error can occur at the same time, see figure A.6.

Note that for all cases we just consider the nominal point and the corner-points for each disturbance and each implementation error, and the selected operating points are equally weighted in the objective function (averaged).

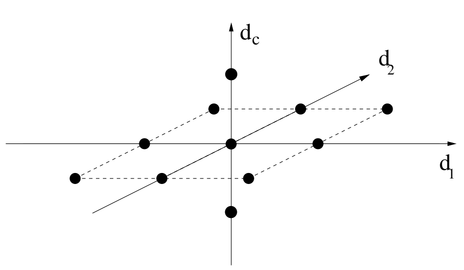

Figure A.5: Operating points when more disturbances can happen at the same time (all points are included in the economic objective).

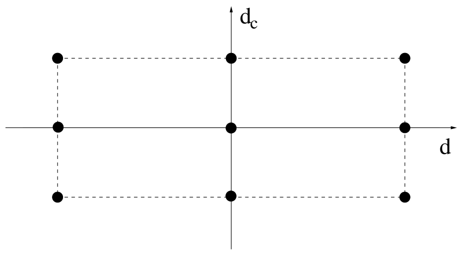

Figure A.6: Operating points when all disturbances (d) and implementation errors can happen at the same time (all points are included in the economic objective).

For the reactor-separator-recycle process (with 2 disturbances and 3 controlled variables with implementation errors) we get $2 \cdot 2 + 3 \cdot 2 + 1 = 11$ operating points for case I, $2^3 + 3 \cdot 2 + 1 = 15$ operating points for case II and $3^5 = 243$ operating points for case III. The optimization problem for case III is high-dimensional. 243 operating points give 13613 optimization variables, 13610 equality constraints and 2430 inequality constraints. The number of combinations should be reduced by just including the most important disturbances and implementation errors in the robust optimization.

Table A.2 shows the average and maximum loss for different alternatives for case I and case II:

- The expected disturbance and implementation error region is larger for case II than for case I, which increases the loss and the backoff.
- The increases in loss and backoff are largest for alternatives with an already large loss and backoff.
- Increasing the expected disturbance and implementation error region does not here change the ranking of the alternatives.

Note that if the expected disturbances and implementation errors are further increased, achieving feasibility by robust optimization may become impossible.

Increasing the feasible region results in increased probability for normal operation, but also increases the nominal and average loss with normal operation. Increasing the economic region results in increased nominal loss, but hopefully reduced average loss for normal operation (i.e. a better estimate of the real operating cost).

Table A.2: Average and maximum percentage loss (L_w, L_{max}) with constant robust setpoints for case I and II.

Rank	c_1,c_2,c_3		robust setpoints - case I			robust setpoints - case II		
		$c_{3,s}$	$b_{opt,3}$	$L_w(\%)$	$L_{max}(\%)$	$b_{opt,3}$	$L_w(\%)$	$L_{max}(\%)$
-	reoptimized	$c^*_{opt}(d)$	–	5.16	11.03	–	5.14	11.03
1, 1	x_b,M_r,x_d	0.825	0.005	5.21	11.03	0.010	5.23	11.03
3, 2	x_b,M_r,L/F	0.871	−0.254	5.35	11.34	−0.024	5.27	11.36
2, 3	x_b,M_r,D/L	0.600	−0.371	5.34	11.35	0.067	5.34	11.45
4, 4	x_b,M_r,D/V	0.375	0.026	5.49	11.46	0.031	5.43	11.53
6, 5	x_b,M_r,V/F	1.392	−0.037	5.93	11.67	−0.024	5.71	11.56
8, 7	x_b,M_r,B/L	0.549	0.054	6.05	12.60	0.046	6.01	12.47
11, 12	x_b,M_r,L	837.4	−64	6.46	15.87	−162	7.00	13.77
5, 6	x_b,M_r,V/L	1.600	0.206	5.89	12.19	0.192	5.75	12.12
7, 8	x_b,M_r,B/D	0.916	−0.140	6.00	11.68	−0.216	6.33	12.40
10, 10	x_b,M_r,B/F	0.478	−0.056	6.36	12.08	−0.070	6.44	12.52
12, 11	x_b,M_r,D/F	0.522	0.061	6.50	12.24	0.072	6.50	12.58
9, 8	x_b,M_r,F/F_0	2.091	0.289	6.22	12.15	0.359	6.33	12.52
13, 13	x_b,M_r,D	502.0	191	6.79	12.82	280	7.20	13.83
14, 14	x_b,M_r,F	962.0	286	7.51	13.90	299	8.57	17.52
15, 16	x_b,F/F_0,V/B	–	–	25.87	54.38	–	33.55	73.51
16, 17	x_b,F/F_0,x_d	–	–	25.91	54.38	–	33.60	73.51
17, 18	x_b,x_r,x_d(BS)	–	–	26.08	54.38	–	33.71	73.51
18, 15	x_b,M_r/F,L/D	–	–	26.11	54.38	–	28.37	59.68
19, 19	x_b,F/F_0,L/D	–	–	33.13	63.59	–	34.29	74.47
20, 20	x_b,F,x_d(LS)	–	–	43.10	94.37	–	51.69	119.35
21, 21	V/B,F/F_0,x_d	–	–	45.74	78.75	–	53.12	98.94

inf: infeasible with constant setpoint policy

Constrained variables: $c_{1,s} = x_{B,s} = 0.008$ and $c_{2,s} = M_{r,s} = 2772$

Reoptimized: Reoptimized with constraint backoff, see equation 3.27.

A.2 Some advise about solving the robust optimization problem

- Use a model that is sparse and has analytical gradients.
- Use a subspace optimization algorithm (e.g. snopt in Tomlab) since the robust optimization problem has many optimization variables and few degrees of freedom for optimization.
- Use good initial values based on optimization in nominal point and for expected disturbances.
- Always check that the solution is physically reasonable.

Appendix B

Online feasibility correction

We illustrate how online feasibility correction can be done for a simple process, using MPC with linear models (Muske & Rawlings 1993) where feedback is included by updating the model biases. First, we show the iterations by symbols and indicate which requirements need to be fulfilled. Second, we show the iterations numerically in a simple toy example.

B.1 Illustrating example

We will now illustrate how online feasibility correction can be done on a simple process when using MPC with linear models (Muske & Rawlings 1993) and feedback is included through bias-updating. We will comment on what is required for this iteration to end up with the same solution as the online feasibility correction problem.

To keep the example simple we assume:

- No dynamics in the process
- All states (x) are eliminated by substitution
- No measurement of disturbances
- No measurement error in controlled variables ($c_m = c$) or constraints ($g_m = g$)
- Soft prioritization among all controlled variables (by selecting Q).

At the starting point the constraints are fulfilled ($g_0 = g(u_0, d_0) < 0$) and the controlled variables are at their setpoints ($c_0 = c(u_0, d_0) = c_s$). The linear model for the constraints and controlled variables are found (e.g. by making step responses) at the starting point. With no measurement error in the controlled variables ($\hat{c}_0 = c_0$) and constraints ($\hat{g}_0 = g_0$) we get:

$$\begin{aligned}\hat{g} &= g_0 + G_g(u - u_0) \\ \hat{c} &= c_0 + G_c(u - u_0)\end{aligned} \tag{B.1}$$

Feedback is included through updating the bias for each model:

$$\begin{aligned} b_g &= g_m - \hat{g}_{old} \\ b_c &= c_m - \hat{c}_{old} \end{aligned} \tag{B.2}$$

With no measurement errors ($g_{m,0} = g_0$, $c_{m,0} = c_0$) and no model error at the starting point ($g_{m,0} = g_0$, $c_{m,0} = c_0$), the biases are equal zero ($b_{g,0} = 0$, $b_{c,0} = 0$). By solving the following problem online:

$$\begin{aligned} \min_{u,c_{flex}} & (c_{flex} - c_s)^T Q (c_{flex} - c_s) \\ g_0 + G_g(u - u_0) + b_{g,1} &\leq 0 \\ c_0 + G_c(u - u_0) + b_{c,1} &= c_{flex} \end{aligned} \tag{B.3}$$

we find that $\hat{u}_0 = u_0$, $\hat{g}_0 = g_0$ and $\hat{c}_0 = c_0$. $u_0 = \hat{u}_0$ is implemented at time step 0 ($k = 0$).

The disturbances are perturbed[1]:

$$d_1 = d_0 + \Delta d \tag{B.4}$$

which results in that some of the constraints g are violated (and/or some of the controlled variables c are not at setpoint anymore).

The constraints and controlled variables are measured:

$$\begin{aligned} g_{m,1} &= g(u_0, d_1) \\ c_{m,1} &= c(u_0, d_1) \end{aligned} \tag{B.5}$$

and the biases are updated:

$$\begin{aligned} b_{g,1} &= g_{m,1} - \hat{g}_0 \\ b_{c,1} &= c_{m,1} - \hat{c}_0 \end{aligned} \tag{B.6}$$

New manipulated variables $\hat{u}_1$ are computed by solving the following problem online:

$$\begin{aligned} \min_{u,c_{flex}} & (c_{flex} - c_s)^T Q (c_{flex} - c_s) \\ g_0 + G_g(u - u_0) + b_{g,1} &\leq 0 \\ c_0 + G_c(u - u_0) + b_{c,1} &= c_{flex} \end{aligned} \tag{B.7}$$

The computed constraints and controlled variables are then:

$$\begin{aligned} \hat{g}_1 &= g_0 + G_g(\hat{u}_1 - u_0) \\ \hat{c}_1 &= c_0 + G_c(\hat{u}_1 - u_0) \end{aligned} \tag{B.8}$$

[1] Alternatively the setpoints are perturbed, $c_s = c_s + \Delta c_s$

$u_1 = \hat{u}_1$ is implemented at time step 1 ($k = 1$).

$\vdots$

$u_{k-1} = \hat{u}_{k-1}$ is implemented at time step $k - 1$.

The constraints and controlled variables are measured:

$$\begin{aligned} g_{m,k} &= g(u_{k-1}, d_1) \\ c_{m,k} &= c(u_{k-1}, d_1) \end{aligned} \tag{B.9}$$

and the biases are updated:

$$\begin{aligned} b_{g,k} &= g_{m,k} - \hat{g}_{k-1} \\ b_{c,k} &= c_{m,k} - \hat{c}_{k-1} \end{aligned} \tag{B.10}$$

New manipulated variables $\hat{u}_k$ are computed by solving the following problem online:

$$\begin{aligned} \min_{u, c_{flex}} (c_{flex,k} - c_s)^T Q (c_{flex,k} - c_s) \\ g_0 + G_g(u - u_0) + b_{g,k} \leq 0 \\ c_0 + G_c(u - u_0) + b_{c,k} = c_{flex} \end{aligned} \tag{B.11}$$

The computed constraints and controlled variables are then:

$$\begin{aligned} \hat{g}_k &= g_0 + G_g(\hat{u}_k - u_0) \\ \hat{c}_k &= c_0 + G_c(\hat{u}_k - u_0) \end{aligned} \tag{B.12}$$

$u_k = \hat{u}_k$ is implemented at time step k.

If the process gains do not change sign and the model gains have the same sign as the process gains and are not too small compared with the process gains, we get:

$$\begin{aligned} \lim_{k \to \infty} b_{g,k} = 0 \\ \lim_{k \to \infty} b_{c,k} = 0 \end{aligned} \tag{B.13}$$

and find the minimum of the online feasibility correction problem (if there exists a feasible solution and the process is convex):

$$\begin{aligned} \min_{u, c_{flex}} (c_{flex} - c_s)^T Q (c_{flex} - c_s) \\ g(u, d_1) \leq 0 \\ c(u, d_1) = c_{flex} \end{aligned} \tag{B.14}$$

i.e.:

$$\lim_{k \to \infty} u_k = u^*, \quad \lim_{k \to \infty} c_{flex,k} = c^*_{flex}$$

Example:

A toy example (Skogestad 2000a) is extended with an inequality constraint and is used as a numerical illustration. The problem has one degree of freedom u. The cost function to be minimized is $J = (u-d)^2$ and the following constraint should be fulfilled: $0.5u+d-0.5 \leq 0$. We nominally have $d = 0$ and consider a disturbance of magnitude $|d| \leq 1$. This gives the following optimization problem:

$$\begin{aligned} &\min_u (u-d)^2 \\ &0.5u + d - 0.5 \leq 0 \\ &d \in [-1, 1];\ u \in R \end{aligned}$$

At the nominal point $d = 0$ the optimum is unconstrained and we have $u = 0$ and $J = 0$. With $d = 1$ the optimum is constrained and we have $u = -2$ and $J = 9$. We consider the controlled variable $c = 0.1(u - d)$ with nominal setpoints ($c_s = 0$). The nominally optimal solution is $u = 0$ (when $d = 0$). We use a constant setpoint policy with controlled variable $c = u - d$ with nominal setpoint $c_s = 0$. At start we are in nominal point ($d = 0$) where the constraint is fulfilled ($g_0 = g(u = 0, d = 0) = -0.5 < 0$) and the controlled variable is at setpoint $c_0 = c(u = 0, d = 0) = 0$. The disturbance is then perturbed ($d = 1$). We consider three cases, using three different models:

Case I. Correct model gains: $\hat{g} = -0.5 + 0.5u$, $\hat{c} = 0.1u$

Case II. Too large model gains: $\hat{g} = -0.5 + 1.5u$, $\hat{c} = 0.2u$

Case III. Too small model gains: $\hat{g} = -0.5 + 0.35u$, $\hat{c} = 0.05u$

The measurements, computed values and biases for the controlled variables and constraints are shown as function of time for the three cases in figure B.1. In addition computed controlled variables and constraints from solving the online feasibility correction scheme used for offline analysis ($c_{flex}(d = 1)$=-0.2, $u_{flex}(d = 1)$=-1) are included. Using correct model

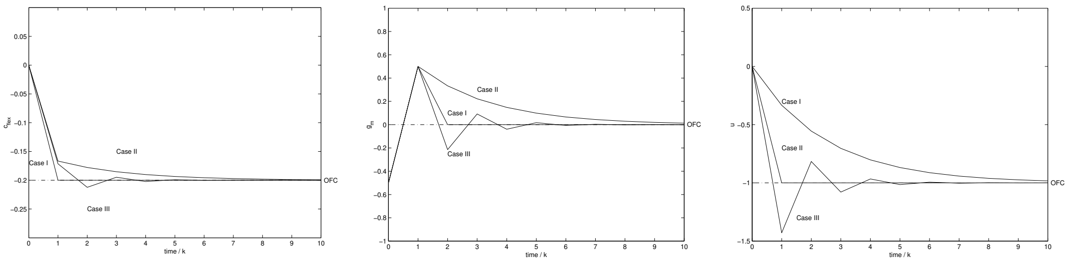

Figure B.1: The flexible setpoints (c_{flex}), measured constraints (g_m) and input u as function of time for case I, II and III.

gains (case I) we arrive at the online feasibility correction solution in one step. Using too large model gains (case II) or too small model gains (case III) we arrive at the online feasibility correction solution, but require more iterations. If reducing the model gains further for case III, we get instability and the online feasibility correction solution is not obtained.

Appendix C

Combined Cycle Power Plant Model

C.1 Process description

The combined cycle power plant is here used to produce electric power and consists of a gas turbine cycle and a steam turbine cycle, see figure C.1. In the gas turbine cycle compressed

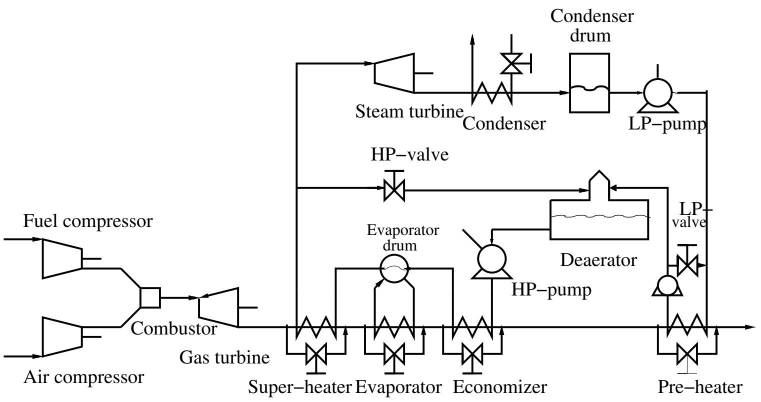

Figure C.1: A combined cycle power plant process

natural gas and air react in the combustor to flue gas with high temperature. The flue gas is expanded in the gas turbine and electric power is produced. The exhaust gas has still high temperature and in the steam cycle the exhaust gas is heat-exchanged with water producing steam. The steam is expanded through the steam turbine and more electric power is produced.

The deaerator is included to reduce the amount of oxygen in the steam / water. The HP-recirculating flowrate is included to improve the deaerator pressure control. The LP-recirculating flowrate is included to make it possible to avoid too low water inlet temperature to the pre-heater. The heat-exchanger bypasses are included to optimize the heat-exchanger network. The fuel gas compressor is included to optimize the combustor pressure.

C.2 Model assumptions

We want a model which can be used to plantwide control purposes. The model needs to be functioning for steady-state optimization and dynamic proposes all over the plant. We need a nonlinear, first principle model.

The model is based on first principles: Mass- and energy balances are used.

Instead of modeling valves with valve equation we assume fast flow controllers which manipulate the valve openings and the flowrates are used as manipulated variables. This gives a more linear and numeric robust model. Missing dynamics can be replaced by including filter on the flowrates.

We assume ideal gas on the gas / flue gas side and use the ideal gas law to compute the combustor pressure.

In the steam cycle the vapor holdup is neglected. We assume phase equilibrium. The pressure is then equal the saturated pressure which is computed by Clausius-Clapeyron equation.

We have neglected all other dynamics than in the heat-exchangers and in the combustor. We should include more dynamics in the gas turbine part - the combustor holdup is small and does not give the sufficient contribution of the dynamics in the gas turbine.

Since the pressure drop is large we expect choked flow. The flowrate through the turbine is then independent of the turbine speed and computed by using nozzle equation. The polytropic efficiency to the turbine is assumed constant.

Compressor maps give the relation between pressure ratio over the compressor and scaled flowrate for different compressor speeds. In addition the compressor efficiency is given as function of pressure ratio and scaled flowrate. We here use a simplified compressor map where the scaled flowrate is proportional to the compressor speed. This is acceptable for high flowrates.

Compressor and turbine work are computed based on the assumption of polytropic compression and expansion.

Specific heat capacities are assumed independent of temperature and composition.

In the combustor we assume that methane and oxygen react and produce water and carbondioxyd. Complete and momentary combustion of the methane is assumed in the combustor.

C.3 Model equations

All computations are done on mass-basis except in the combustor where mol-basis is used.

C.3.1 Enthalpy

Pure components in vapor phase at temperature T_{ref} (and pressure P_{ref}) are used as reference state for the gas side (fuel, air and flue gas). On the steam side water in liquid phase at temperature T_{ref} (and pressure P_{ref}) is used as reference state.

The enthalpy on the gas side (on mass basis) is computed by:

$$h_g = c_{p,g}(T - T_{ref}) \tag{C.1}$$

$c_{p,g}$ is the specific heat capacity for the gas and depends on the composition of the gas:

$$c_{p,g} = \sum_i c_{p,i} x_i \tag{C.2}$$

The enthalpy on mol-basis:

$$h_{n,g} = \sum_i c_{p,i} x_i (T - T_{ref}) \tag{C.3}$$

The enthalpy for water (on mass basis) is:

$$h_l = c_{p,l}(T - T_{ref}) \tag{C.4}$$

The enthalpy for steam /vapor (on mass basis):

$$h_v = c_{p,v}(T - T_{ref}) + h_{vap}(T_{ref}) \tag{C.5}$$

$h_{vap}(T_{ref})$ is the vaporization enthalpy at the reference temperature T_{ref}, and $c_{p,v}$ is the vapor specific capacity.

The reaction enthalpy at temperature ($h_r(T)$) is:

$$h_r(T) = h_r(T_{ref}) + \sum_i n y_i c_{p,i} (T - T_{ref}) \tag{C.6}$$

Internal energy (u) is computed equally, except that c_v is used instead of c_p. We have here assumed $c_v = c_p$.

C.3.2 Compressor

We assume that the scaled flowrate ($F_{dim} = F T_{in}^{0.5} / P_{in}$) is proportional to the compressor speed ($N_{dim} = N / T_{in}^{0.5}$):

$$F_{dim} = k N_{dim} \tag{C.7}$$

k is the proportional constant. This assumption is acceptable for large flowrates. The polytropic efficiency depends on the pressure ratio (P_{out}/P_{in}) over the compressor and the scaled flowrate (F_{dim}). This relation is described by a quadratic function:

$$\eta = \Delta x^T D^T A D \Delta x + \eta_{ref} \tag{C.8}$$

x is a column vector with $x_1 = F_{dim}$ and $x_2 = P_{out}/P_{in}$. Δx is the difference between x and the reference x_{ref} ($\Delta x = x - x_{ref}$). A, D, η_{ref} and x_{ref} are adjustable parameters. This gives a simplified compressor map. An example of a simplified compressor map is given in figure C.2.

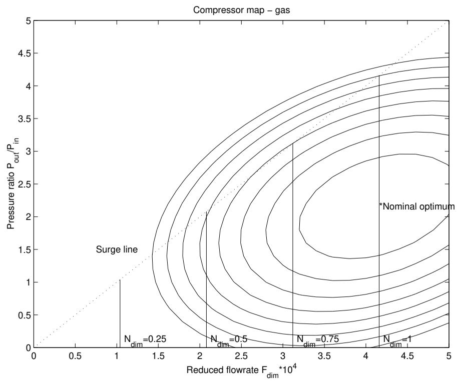

Figure C.2: Simplified compressor map

We assume polytropic compression and compute the outlet temperature (T_{out}) by:

$$T_{out} = T_{in}\left(\frac{P_{out}}{P_{in}}\right)^{\frac{\gamma-1}{\gamma\eta}} \tag{C.9}$$

η is the polytropic efficiency. γ is a coefficient which is computed by:

$$\gamma = \frac{c_p M}{c_p M - R} \tag{C.10}$$

c_p ($= \sum_i c_{p,i} x_i$) is the specific heat capacity. The compressor work (W) is then computed by:

$$W = F c_p (T_{out} - T_{in}) \tag{C.11}$$

C.3.3 Combustor (on mol-basis)

In the combustor methane and oxygen react and produce water and carbondioxyd:

$$CH_4 + 2O_2 \rightarrow 2H_2O + CO_2$$

We assume a momentary and complete reaction of methane (surplus of oxygen), which gives the following reaction rate (R_n):

$$R_n = F_{n,fuel} x_{fuel,methane} \tag{C.12}$$

$F_{n,fuel}$ is the molar fuel flowrate and $x_{fuel,methane}$ is the mole fraction of methane in the fuel gas. The combustor component balances are:

$$\frac{dn_{comb,i}}{dt} = F_{n,fuel} x_{fuel,i} + F_{n,air} x_{air,i} - F_{n,comb} x_{comb,i} + R_n \tag{C.13}$$

$n_{comb,i}$ is the molar holdup of component i in the combustor. F_n is the molar flowrate for fuel, air and flue (from the combustor) gas and is computed from the mass flowrate (F):

$$F_n = \frac{F}{M^T x} = F / \sum_i M_i x_i \tag{C.14}$$

x_i is the mole fraction in the fuel, air and flue gas flowrate. The combustor and flue gas composition is computed by:

$$x_{flue,i} = x_{comb,i} = \frac{n_{comb,i}}{\sum_i n_{comb,i}} \tag{C.15}$$

The energy balance for the combustor gives:

$$\frac{dU_{comb}}{dt} = F_{n,fuel} h_{n,g,fuel} + F_{n,air} h_{n,g,air} - F_{n,flue} h_{n,g,flue} + R_n h_{rx} \tag{C.16}$$

U (=$\sum_i n_i c_{p,i}(T_{flue} - T_{ref})$) is the internal energy and h_r is the reaction enthalpy at temperature T_{comb}. Reordering the energy balance gives the combustor / flue temperature explicitly:

$$c_p^T n_{comp} \frac{dT_{comb}}{dt} = F_{n,fuel} c_p^T x_{fuel} (T_{fuel} - T_{comb}) + F_{n,air} c_p^T x_{air} (T_{air} - T_{comb}) + R_n h_r \tag{C.17}$$

C.3.4 Turbine

Since the speed is assumed given, the flowrate through the turbine (F) is computed by nozzle equation:

$$F = F_{ref} (P_{in} \rho_{in} / P_{in,ref} / \rho_{in,ref})^{0.5} \tag{C.18}$$

P_{in} is the inlet pressure and ρ_{in} is the inlet density. ref refers to the corresponding values at the design point. Since we assume ideal gas, the inlet pressure can be computed by using the ideal gas law:

$$\rho_{in} = \frac{P_{in} M}{R T_{in}} \tag{C.19}$$

T_{in} is the inlet temperature and M $(= \sum_i M_i x_i)$ is the mole weight.

We assume polytropic expansion and compute the outlet temperature (T_{out}) by:

$$T_{out} = T_{in} \left(\frac{P_{out}}{P_{in}}\right)^{\frac{(\gamma-1)\eta}{\gamma}} \tag{C.20}$$

η is the polytropic efficiency (we assume it to be constant). γ is a coefficient which is computed by:

$$\gamma = \frac{c_p M}{c_p M - R} \tag{C.21}$$

c_p ($= \sum_i c_{p,i} x_i$) is the specific heat capacity. The turbine work (W) is then computed by:

$$W = F c_p (T_{in} - T_{out}) \tag{C.22}$$

C.3.5 Super-heater

The super-heater is modeled as co-current heat-exchanger, see Mathisen (1994), and is shown in figure C.3.

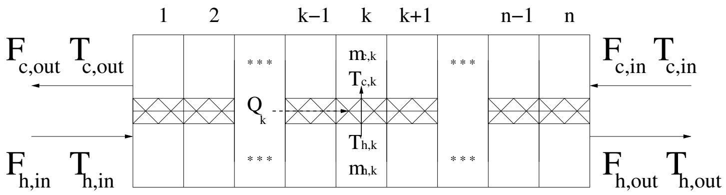

Figure C.3: Heat exchanger model I

Ideal mixing is assumed in each stage and the heat transfer at stage k is:

$$Q_k = UA(T_{h,k} - T_{c,k})/n \tag{C.23}$$

U is the heat transfer coefficient, A is the total heat transfer area (A), n is number of stages, $T_{h,k}$ is the temperature at the hot side at stage k and $T_{c,k}$ is the temperature at the cold side at stage k. The heat transfer coefficient depends on the (vapor) flowrate:

$$U = U_{ref}(F_h/F_{h,ref})^m \tag{C.24}$$

Energy balance for a stage k on the hot side:

$$\frac{dU_{h,k}}{dt} = F_h h_{h,k-1} - F_h h_{h,k} - Q_k \tag{C.25}$$

$U_{h,k}$ is the internal energy at the hot side at stage k, F_h is the mass flowrate at the hot side, $h_{h,k-1}$ is the inlet enthalpy to stage k on the hot side and $h_{h,k)}$ is the outlet enthalpy from stage k on the hot side. The internal energy in cell k on the hot side is:

$$U_{h,k} = (m_h c_{p,h} + m_{h,s} c_{p,s})/n \tag{C.26}$$

Metal (s) is included on the hot side to give a more correct model with respect to dynamic behavior. Reordering the energy-balance gives:

$$(m_h c_{p,h} + m_{h,s} c_{p,s})/n \frac{dT_{h,k}}{dt} = (F_h c_{p,g}(T_{h,k-1} - T_{h,k}) - Q_k \quad \text{(C.27)}$$

We have here assumed that the composition in the heat-exchangers is equal the composition in the combustor (no problem since the dynamics in the vapor phase in neglectable compared to other dynamics).

Energy-balance for cell k on the cold side:

$$\frac{dU_{c,k}}{dt} = F_c h_{c,k+1} - F_c h_{c,k} + Q_k \quad \text{(C.28)}$$

Reordering the energy balance gives:

$$(m_c c_{p,c} + m_{c,s} c_{p,s})/n \frac{dT_{c,k}}{dt} = F_c h_{c,k+1} - F_c h_{c,k} + Q_k \quad \text{(C.29)}$$

C.3.6 Evaporator and evaporator drum

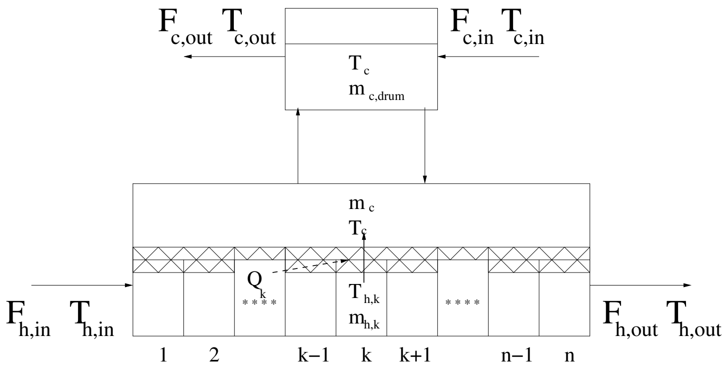

Figure C.4: Heat exchanger model II (heat-exchanger with drum)

The evaporator with drum is shown in figure C.4. The co-current heat-exchanger is modeled with one cell at the water side (cold side). The temperature in the drum is equal the temperature in the cell. On the hot side we assume n cells with ideal mixing. The heat transfer from cell k on the hot side to the cold side is:

$$Q_k = UA(T_{h,k} - T_c)/n \quad \text{(C.30)}$$

U is the heat transfer coefficient, A is the total heat transfer area (A), n is number of stages, $T_{h,k}$ is the temperature at the hot side at stage k and $T_{c,k}$ is the temperature at the cold side at stage k. The heat transfer coefficient depends on the flowrate at the hot side:

$$U = U_{ref}(F_h/F_{h,ref})^m \quad \text{(C.31)}$$

The total heat transfer from hot side to cold side is:

$$Q = \sum_k Q_k \tag{C.32}$$

Mass-balance for the evaporator drum:

$$\frac{dm_{drum}}{dt} = F_{c,in} - F_{c,out} \tag{C.33}$$

Since we assume a cubic geometry, the relation between the mass and the level can be expressed by:

$$m_{drum} = \rho_l A_d l_{drum} \tag{C.34}$$

Reordering the mass-balance gives:

$$\frac{dl_{drum}}{dt} = \frac{dm_{drum}}{dt}/(\rho_l A_d) \tag{C.35}$$

Energy-balance for the cold side:

$$\frac{dU_c}{dt} = F_{c,in}h_{c,in} - F_c h_c + Q \tag{C.36}$$

Reordering the energy balance gives:

$$(m_c c_{p,c} + m_{c,s}c_{p,s} + m_{drum}c_{p,c})\frac{dT_c}{dt} = F_{c,in}(h_{l,c,in} - h_{l,c}) - F_c(h_{v,c} - h_{l,c}) \tag{C.37}$$

Energy balance for the cell k on the hot side:

$$\frac{dU_{h,k}}{dt} = F_h h_{h,k-1} - F_h h_{h,k} - Q_k \tag{C.38}$$

Reordering the energy-balance gives:

$$(m_h c_{p,h} + m_{h,s}c_{p,s})/n\frac{dT_{h,k}}{dt} = F_{h,k-1}h_{g,k-1} - F_{h,k}h_{g,k} - Q_k \tag{C.39}$$

We have here neglected the effect of varying composition in the gas holdup in the heat exchangers.

C.3.7 Economizer

The economizer model is equal the super-heater model.

C.3.8 Pre-heater

The pre-heater model is equal the super-heater model.

C.3.9 Condenser and condenser drum

The condenser and condenser drum is similar to the evaporator and evaporator drum. The only difference is that the hot and cold side have changed position.

C.3.10 Mixer

Mass balance for a mixer when we assume constant mass holdup in the mixer:

$$F_{out} = F_{in,1} + F_{in,2} \tag{C.40}$$

Energy balance for a mixer:

$$\frac{dU}{dt} = F_{in,1}h_{in,1} + F_{in,2}h_{in,2} - F_{out}h_{out} \tag{C.41}$$

Reordering the mass balance gives:

$$mc_{p,g}\frac{dT_{out}}{dt} = F_{in,1}h_{in,1} + F_{in,2}h_{in,2} - F_{out}h_{out} \tag{C.42}$$

C.3.11 Deaerator

Mass balance for the deaerator:

$$\frac{dm_{deaerator}}{dt} = F_{pre} + F_{HP,valve} - F_{HP,pump} \tag{C.43}$$

$m_{deaerator}$ is the mass holdup in the deaerator, F_{pre} is the inlet mass flowrate from the pre-heater, $F_{HP,valve}$ is the inlet mass flowrate through the HP-valve and $F_{HP,pump}$ is the outlet mass flowrate through the HP-pump. We assume that the deaerator is shaped as a box, and the liquid level in the deaerator ($l_{deaerator}$) is then found by:

$$l_{deaerator} = \frac{m_{deaerator}}{\rho_l A_{deaerator}} \tag{C.44}$$

ρ_l is the liquid density and $A_{deaerator}$ is the area.

Energy balance for the deaerator:

$$\frac{dU_{deaerator}}{dt} = F_{pre}h_{l,pre} + F_{HP,valve}h_{v,HP-valve} - F_{HP-pump}h_{l,HP-pump} \tag{C.45}$$

$U_{deaerator}$ is the internal energy, F is the mass flowrates and h is the mass specific enthalpies.

Reordering the energy balance gives:

$$m_{deaerator}c_{p,l}\frac{dT_{deaerator}}{dt} = F_{pre}(h_{pre} - h_{l,deaerator}) + F_{HP-valve}(h_{v,HP-valve} - h_{l,deaerator}) \tag{C.46}$$

C.3.12 Pump

Since the liquid gives incompressible flow, the pump work (W_p) is computed by:

$$W_p = (P_{out} - P_{in})F/\rho \tag{C.47}$$

P_{out} is the outlet pressure, P_{in} is the inlet pressure, F is the flowrate through the pump and $/\rho$ is the (liquid) density. The outlet temperature (T_{out}) can be computed from the energy-balance over the pump:

$$T_{out} = T_{in} + W_p c_p/F \tag{C.48}$$

T_{in} is the inlet temperature and c_p is the specific heat capacity.

C.3.13 Valve

The valves are not modeled, since we want improved numeric properties (linearization of the process, less stiff system). Instead we assume that the flowrate is perfectly controlled by manipulating the valve opening. The flowrate is then specified directly.

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