Pre-Diploma Thesis

# Robust Switching Strategies in Self-Optimizing Tracking Control

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# Abstract

Self-optimizing control is when acceptable performance can be achieved using pre-computed references and with no need to re-optimize when disturbances occur. For linear steady state processes, several methods to identify self-optimizing control structures have been developed recently.

For many industries, however, unsteady state processes become more and more important. A typical example is batch distillation. This thesis extends the idea of self-optimizing control to such tracking problems.

The main difference is that the optimal input trajectories in batch processes often contain a finite number of jump discontinuities. These divide the batch into several intervals and for each interval exists one self-optimizing controller. It is now very important to activate the next controller at the right time as failure to do so may lead to infeasibility. Hence, good feedback-based switching laws are desirable.

A promising candidate is the so-called nullspace method which is examined first. It is found, that a linear combination of states does not lead to acceptable results. Therefore, an alternative switching strategy that uses indirect information about the disturbance is presented. In combination with simple PI-type continuous controllers, self-optimizing control for this particular nonlinear batch process becomes possible and leads to good results.

# Acknowledgment

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# Chapter 1

# Introduction

## 1.1   Background and Motivation

Distillation is one of the oldest and the most commonly used separation method in the chemical process industries (Bausa and Tsatsaronis, 2001). Its importance is easily illustrated: more than 90% of all separations for product recovery and purifications in the United States are done by distillation columns, following capital investments of at least 8 billion U.S. dollars (Humphrey, 1995).

From simple apparatuses for spirit and perfume production to today's modern industrial distillation plants, distillation processes have been studied and improved extensively. While early apparatuses were operated batch-wise, continuous operation of distillation processes has become predominant in most large-scale industries today. However, with increasing demands for special, high-purity products in the pharmaceutical and fine chemical industries, the advantages of batch distillation have been rediscovered in recent decades (Sørensen, 1994).

The main advantage of batch distillation plants is their flexibility. The same plant can handle wide ranges of product amounts, feed compositions or even totally different production recipes. Moreover, and contrary to continuous distillation, only a single batch distillation column is needed to recover multiple components from a feed charge.

From a control point of view, the main difference between continuous and batch distillation is their different modes of operation. Continuous distillation plants are mostly operated at steady state, whereas batch processes are

at unsteady state (Diwekar, 1995). Although the latter is desirable to main-
tain flexibility of the plant, it makes control and optimization more complex.

As with most chemical processes, control strategies for batch distillation pro-
cesses often try to achieve *optimal* operation of the plant. Possible scenarios
for this *dynamic optimization* task are shown in figure 1.1.
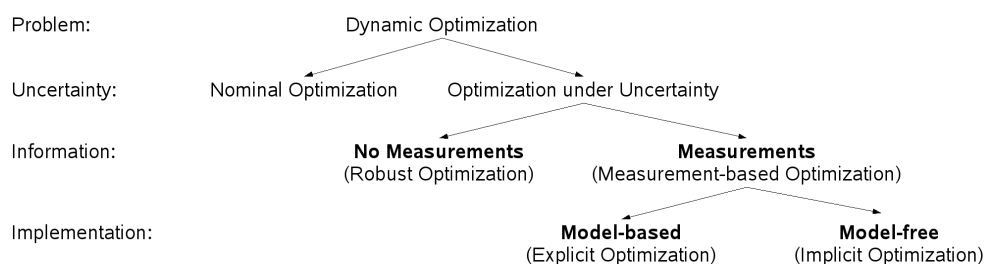


Figure 1.1: Dynamic optimization scenarios
adopted from Srinivasan et al. (2003)

This approach suggests three levels of classification. To classify a certain sce-
nario, it must be considered whether the optimization is carried out under
uncertainty, whether measurements are included and whether a model of the
process is used for implementation purposes.

Each branch of the illustrated classification tree has advantages and draw-
backs. On the first level, including uncertainty assures feasibility even in case
of disturbances or changes in operating parameters but might require solving
more complex equations than for nominal optimization. Level two distin-
guishes robust optimization from measurement-based optimization. Robust
optimization is used when no measurements are available. Possible distur-
bances must thus be taken into account explicitly, leading to a more con-
servative solution (Skogestad and Postlethwaite, 1996). This is caused by
the large back-off from the constraints, leading to a noticeable loss in perfor-
mance. Improvements in measurement technology and equipment during the
last years have enabled engineers to include measurements in process opti-
mization (Srinivasan et al., 2003). This allows for less conservative solutions
than with robust optimization. Furthermore, measurements can be used not
only within the batch, but also in a batch-to-batch manner to help improve
overall performance. Although this is a valuable feature of measurement-
based optimization, it will not be considered further in this thesis.

When a process model is used in the final control implementation as shown

on level three in figure 1.1, explicit optimizations can be carried out repeatedly with each new measurement. This is similar to model predictive control (MPC), a control strategy widely used in industry today (Qin and Badgewell, 1997). As commonly acknowledged, the huge computational burden caused by repeated online optimization, especially for models of large and very nonlinear systems, is the main drawback of model-based optimization (Srinivasan et al., 2003). In contrast, model-free control implementations do not suffer from these disadvantages. To obtain optimal operation, measurements need then be utilized directly.

Generally speaking, the idea behind this thesis is to develop a model-free control implementation for a batch distillation plant model. To achieve this, the so-called method of *self-optimizing control* seems to be both appropriate and promising. Self-optimizing control has emerged from the work of Morari et al. (1980) and Skogestad and Postlethwaite (1996). The original definition of self-optimizing control as given by Skogestad (2000) is

> **Self-optimizing control** *is when acceptable operation can be achieved using constant setpoints for the controlled variables, without the need to re-optimize when disturbances occur.*

However, this definition is intended for steady state processes. Thus, for non-steady state batch processes a slightly modified definition seems more appropriate and will be used throughout this thesis (Dahl-Olsen et al., 2007):

> **Self-optimizing control** *is when acceptable performance can be achieved using pre-computed references, without the need to re-optimize when disturbances occur.*

Several methods for finding a self-optimizing control structure for linear steady state processes have been found in recent years. These include the so-called *direct loss evaluation method* (Skogestad, 2004), the *local method / maximum gain rule* (Halvorsen et al., 2003) and the *nullspace method* (Alstad, 2005).

In contrast to steady state processes, batch processes usually contain a finite number of input jump discontinuities. For each interval in-between these discontinuities, one self-optimizing controller is sought. However, a robust strategy is needed to switch between the distinct controllers.

The aim of this thesis is to find a model-free control structure for a batch distillation process that delivers near-optimal performance even when disturbances are present. For switching from one controller to the next, robust feedback-based switching rules are studied. It is examined whether the nullspace method is suitable for this purpose.

## 1.2   Thesis Outline

This thesis consists of 6 chapters and is structured as follows:

**Chapter 2** describes the batch distillation process that has been studied. Assumptions about the plant configuration as well as about the process itself are stated. The system's equations and numerical parameters are given to reproduce the results. Furthermore, different control objectives are discussed.

**Chapter 3** deals with the open-loop solution of the optimization problem. Software that has been used for this thesis is introduced and briefly compared. Both optimal open-loop trajectories and minimal batch times have been computed.

**Chapter 4** is dedicated to the closed-loop system. The nullspace method is introduced mathematically and applied to the process. An alternative approach to handle the discrete switching decisions is presented. The chapter concludes with simulation results of the feedback-controlled system.

**Chapter 5** discusses both various methodical aspects as well as results from the previous chapters. Open-loop and closed-loop solutions are compared.

**Chapter 6** sums up and concludes the thesis. It also proposes some directions for further work.

# Chapter 2

# Process Description

## 2.1 Batch Distillation

Distillation in general is a thermal process to separate different substances from a liquid mixture. It makes use of the different boiling points of the chemicals present in the mixture.

A typical setup of a batch distillation column is shown in figure 2.1. It normally consists of a reboiler at the bottom, a cylindrical tower with multiple trays and a condenser with reflux drum on top. Although most industrial batch columns are packed, theoretical tray models can nevertheless be used. The number of theoretical trays is then related to the packing height.

Before operation, the reboiler is usually fed with the liquid mixture that is to be separated. During operation, the liquid inside the reboiler is heated and the resulting vapor rises through small holes in the bottom of the trays to the top of the column. There, the rising vapor is condensed and flows either to a tank or is fed back to the uppermost tray of the column. The descending liquid flows across weirs on each tray to the next tray below.

On each tray, descending liquid and rising vapor streams meet and are well mixed. While the vapor is enriched with the more volatile components through this process, the concentrations of the same components decrease in the liquid stream.

The enriched top products are then drained continuously from the reflux drum into the product tank, as can be seen in figure 2.1. This, together with the depletion of the reboiler contents, makes the operation of batch
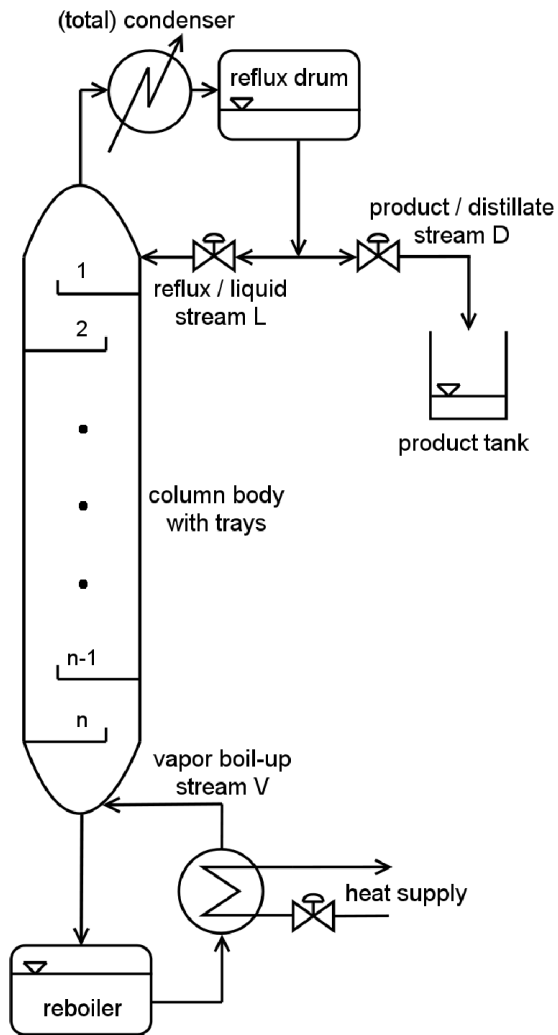
Figure 2.1: Setup of a batch distillation column

distillation plants an unsteady process.

## 2.2   Configuration and Assumptions

A simple model of a batch distillation column has been used for optimization, analysis and control. The following assumptions were made:

1. Binary mixture. The mixture consists of only two components.

2. Constant molar holdup. The liquid holdup on each tray is assumed constant during operation, dynamic effects are neglected.

3. Negligible vapor holdup.

4. Perfect mixing. This assumes that all physical properties do not have any spacial gradients on each tray, reboiler, reflux drum and tank.

5. Constant relative volatility. This is assumed to represent the vapor-liquid equilibrium.

6. Thermodynamic equilibrium on each tray.

7. Total condenser with no sub-cooling. All rising vapor is immediately condensed at its boiling point.

8. Constant vapor boil-up rate. Usually, a constant heat duty is supplied to the reboiler. This would lead to changes in the vapor boil-up rate as the reboiler contents deplete. This change is usually small and a constant boil-up rate is assumed.

For this work, both the reflux stream $L$ and the product stream $D$ as shown in figure 2.1 are considered as manipulated variables. Although the vapor boil-up stream is constant during the batch process, its deviation from the nominal value is regarded as the main disturbance to the system.

## 2.3   Model Equations

Using the assumptions above, material balances are sufficient to describe the batch distillation plant mathematically. In case of the reflux drum, the differential equations for the mole fraction of the more volatile component as well as for the holdup are as follows:

$$\frac{\mathrm{d}x_{\mathrm{RD}}}{\mathrm{d}t} = \frac{V}{N_{RD}}(y_1 - x_{RD}) \tag{2.1}$$

$$\frac{\mathrm{d}N_{\mathrm{RD}}}{\mathrm{d}t} = V - (L + D) \tag{2.2}$$

Here, $x_{RD}$ and $N_{RD}$ denote the mole fraction of the more volatile component and the holdup in the reflux drum, respectively. $V$ is the vapor boil-up rate, $L$ and $D$ are the liquid reflux and distillate streams as shown in figure 2.1. $y_1$ refers to the molar fraction of the more volatile component in the vapor phase on the uppermost tray.

Using the concept of a constant relative volatility $\alpha$, the equilibrium relationship between vapor composition $y$ and liquid composition $x$ on each tray and in the reboiler can be approximated as follows (Stichlmair and Fair, 1998):

$$y = \frac{\alpha x}{(\alpha - 1)x + 1} \tag{2.3}$$

This equation derives directly from the definition of the relative volatility. For a binary mixture of two components $A$ and $B$, $\alpha_{AB}$ is defined as follows:

$$\alpha_{AB} := \frac{y_A/x_A}{y_B/x_B}. \tag{2.4}$$

Finally, substituting $x_B = 1 - x_A$ and $y_B = 1 - y_A$ in equation 2.4 results in equation 2.3 above.

Similar to equations 2.1 and 2.2, material balances for the reboiler (index $RB$) and tank (index $T$) yield the following equations:

$$\frac{\mathrm{d}x_{\mathrm{RB}}}{\mathrm{d}t} = \frac{L}{N_{RB}}(x_n - x_{RB}) + \frac{V}{N_{RB}}(x_{RB} - y_{RB}) \tag{2.5}$$

$$\frac{\mathrm{d}N_{\mathrm{RB}}}{\mathrm{d}t} = L - V \tag{2.6}$$

$$\frac{\mathrm{d}x_{\mathrm{T}}}{\mathrm{d}t} = \frac{D}{N_T}(x_{RD} - x_T) \tag{2.7}$$

$$\frac{\mathrm{d}N_{\mathrm{T}}}{\mathrm{d}t} = D \tag{2.8}$$

where $n$ denotes the lowest tray in the column.

In addition, equations for the mole fraction in the liquid phase of each tray are required. The index $k = 2, 3, \ldots, (n-1)$ indicates the position of the tray within the column, where 1 refers to the uppermost and $n$ to the lowest tray as shown in figure 2.1.

$$\frac{\mathrm{dx_1}}{\mathrm{dt}} = \frac{L}{H}(x_{RD} - x_1) + \frac{V}{H}(y_2 - y_1) \tag{2.9}$$

$$\frac{\mathrm{dx_k}}{\mathrm{dt}} = \frac{L}{H}(x_{k-1} - x_k) + \frac{V}{H}(y_{k+1} - y_k) \tag{2.10}$$

$$\frac{\mathrm{dx_n}}{\mathrm{dt}} = \frac{L}{H}(x_{n-1} - x_n) + \frac{V}{H}(y_{RB} - y_n) \tag{2.11}$$

## 2.4 Parameters, Initial Conditions and Constraints

Parameters and initial conditions are shown in table 2.1.

| Description | Symbol | Value | Unit |
|---|---|---|---|
| Holdup of each tray | $H$ | 1 | mol |
| Initial holdup of reboiler | $N_{RB,0}$ | 50 | mol |
| Initial holdup of tank | $N_{T,0}$ | 0.001 | mol |
| Initial liquid mole fraction on all trays, in reflux drum, reboiler and tank | $x_0$ | 0.5 | - |
| Nominal value of vapor boil-up rate | $V^{\mathrm{nom}}$ | 1 | mol / min |

Table 2.1: Parameters and initial conditions

The initial holdup of the tank has been set to 0.001 mol instead of setting it to 0 to avoid division by zero in equation 2.7.

The number of trays $n$ as well as the relative volatility $\alpha$ were set to distinct values in each of the two scenarios that have been examined.

For optimization and implementation, the inputs $L$ and $D$ have been constrained. Furthermore, natural constraints on the states apply. All constraints are shown in table 2.2.

| Description | Symbol(s) | Lower Bound | Upper Bound | Unit |
|---|---|---|---|---|
| Reflux stream | $L$ | 0.1 | 5 | mol / min |
| Product stream | $D$ | 0 | 5 | mol / min |
| Holdups | $N_{RD}, N_{RB}, N_T$ | 0 | - | mol |
| Mole fractions | $x, y$ | 0 | 1 | - |

Table 2.2: Constraints on states and inputs

The reflux stream has been assigned a lower bound of 0.1 mol / min to avoid flooding of the column. Although this effect is not modeled here, it can become a serious problem in industrial plants. Constraining the reflux flow rate ensures that the column contents are not blown out prematurely and that the constant molar holdup assumption remains valid.

Note that some additional parameter and initial conditions, as for example the number of trays, have been chosen according to the specific operating strategy and are provided later in section 2.6.

## 2.5   Choice of Control Objective

One of the steps involved in process optimization is the choice of a proper objective function. For batch distillation processes, several objective functions have been studied in the literature. Some of the most common choices include:

1. Maximization of the sharpness of separation, e.g. Houtman and Husain (1956),

2. Maximizing the profit when the reflux ratio can be varied, e.g. Diwekar et al. (1989),

3. Maximizing the amount of distillate in a fixed duration of time, e.g. Farhat et al. (1990) or

4. Minimizing the final batch time $t_f$ such that composition and amount of distillate meet the specified requirements, e.g. Mujtaba and Macchietto (1991).

This work adopts the 4th approach of minimizing the batch time. Thus, the problem is mathematically described as follows:

$$\min t_f \qquad \text{s.t.} \qquad \begin{aligned} \mathrm{x_T} &\geq x_T^{\mathrm{spec}} \\ N_T &\geq N_T^{\mathrm{spec}} \end{aligned} \qquad\qquad (2.12)$$

The numerical values for $x_T^{\mathrm{spec}}$ and $N_T^{\mathrm{spec}}$ are given in section 2.6. In addition, the differential equations of section 2.3 and the contraints given in section 2.4 apply.

The motivation for this minimum time problem is manifold. First of all, profit is important in industrial context. While this calls for objective 2, additional economical parameters would be required that are usually difficult to obtain. On the other hand, minimizing the time for each batch allows producing the maximum number of batches per time unit. Normally, this will also result in a maximized profit.

It should be noted here that minimum time problems might be harder to optimize numerically than problems with a fixed final time. To some extend, this also depends on the software and optimization algorithm used.

## 2.6   Operating Strategy

Prior to optimization, a operating strategy must be chosen. In this work, two different scenarios have been considered and are described in this section. The corresponding parameters can be found in table 2.3.

### 2.6.1   Scenario 1

In a first scenario, the plant is operated under total reflux until steady state is reached. During this phase, the vapor stream is assumed to be at its nominal value and the reflux stream at its upper bound. Since the constant relative volatility $\alpha$ has been set to 5, separation is relatively easy considering that $\alpha$ is around 1.1 to 2.5 in many real industrial processes (McCabe, 2005). Therefore, the time to reach steady state is much smaller than the actual production phase and can safely be neglected (Sørensen, 1994).

### 2.6.2 Scenario 2

In the second scenario, separation was made more difficult by setting $\alpha$ to 2. For such processes, the duration of the initial phase in which the column is operated under total reflux may contribute greatly to the total batch time (Sørensen, 1994). In contrast to the first scenario, switching from the total reflux to the normal operation phase has been considered important. Furthermore, the reflux drum holdup has been assumed to be constant, thus reducing the ordinary differential equation 2.2 to the following algebraic equation:

$$0 = V - (L + D) \tag{2.13}$$

| Description | Symbol | Scenario 1 | Scenario 2 | Unit |
|---|---|---|---|---|
| Constant relative volatility | $\alpha$ | 5 | 2 | - |
| Number of trays | $n$ | 5 | 10 | - |
| Reflux drum holdup | $N_{RD}$ | variable | constant | mol |
| Initial reflux drum holdup | $N_{RD,0}$ | 10 | 5 | mol |
| Minimum required terminal product composition in tank | $x_T^{spec}$ | 0.9 | 0.8 | - |
| Minimum required terminal amount of substance in tank | $N_T^{spec}$ | 32.5 | 32.5 | mol |

Table 2.3: Additional Parameters for the different scenarios

# Chapter 3

# Optimal Open-Loop Operation

## 3.1 Motivation

One of the advantages of self-optimizing control is to avoid computationally expensive online optimization. However, to find the self-optimizing control structure itself, offline open-loop optimization is required. The *optimal solution* is also needed to evaluate the performance of the applied process controller.

## 3.2 Software

Two proprietary software packages have been used to obtain the optimal open-loop solutions to the problems described in chapter 2: MATLAB[1] and gPROMS[2]. While the internal MATLAB optimizer *fmincon* was used to optimize the first scenario, gPROMS turned out to be the better choice for optimizing scenario two. Table 3.1 shows a rough comparison of the two programs based on personal experiences while working on this thesis.

Additionally, a commercial toolbox for MATLAB, called TOMLAB[3], has been used without any success for trying out various approaches (see section 3.3) to obtain an optimal solution for scenario 2.

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[1] vendor: The MathWorks, `http://www.mathworks.com/`
[2] vendor: Process Systems Enterprise Limited, `http://www.psenterprise.com/`
[3] vendor: Tomlab Optimization, `http://tomopt.com/tomlab/`

| Program | Advantages | Disadvantages |
|---------|-----------|---------------|
| MATLAB | <ul><li>flexible programming</li><li>detailed graphical figures</li><li>many opportunities for result analysis</li><li>useful debugging information</li></ul> | <ul><li>laborious implementation of ODE-integrations with varying duration</li><li>poor convergence and strange behavior of built-in optimizer *fmincon*</li></ul> |
| gPROMS | <ul><li>easy implementation of model equations, constraints etc.</li><li>optimization uses symbolic calculations and is much faster</li><li>handles varying time durations naturally</li></ul> | <ul><li>unfriendly user interface with buggy dialogs</li><li>external programs are needed to process and analyze results</li><li>incomprehensible error messages</li></ul> |

Table 3.1: Comparison of MATLAB and gPROMS

## 3.3  Optimal Open-Loop Solution

### 3.3.1  Scenario 1

As mentioned before in section 2.6, the plant is operated in total reflux mode prior to optimization. After steady state is reached, both inputs $L$ and $D$ are assumed to be piecewise constant until the objective composition and tank holdup terminal constraints are met.

In a first step, the time domain is split into 4 intervals. The lengths of the intervals as well as the values of $L$ and $D$ are then determined by the optimizer. This is not only done for the nominal value of the vapor boil-up rate $V$ but also for disturbed values $V = (1 \pm 0.1)V^{\text{nom}}$. The resulting op-

timal trajectories as calculated with MATLAB are shown in figure 3.1 and 3.2. For both mole fractions and holdup plots, only the nominal case is presented here. The trajectories of the disturbed cases look qualitatively very similar and are not of further interest. The second column of table 3.2 shows the value of the objective function, that is, the total batch time for each case.
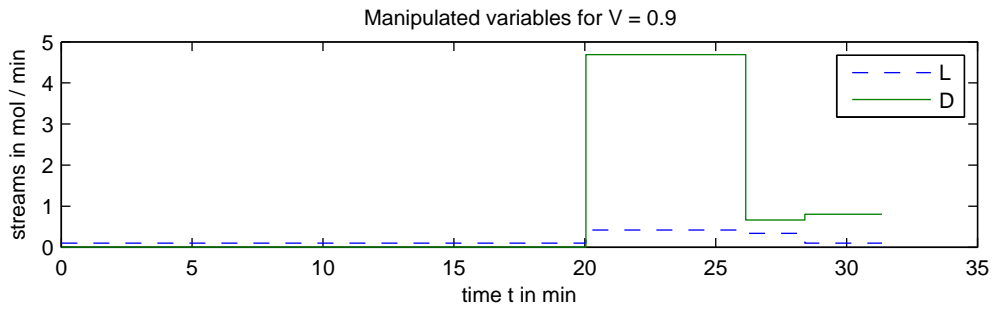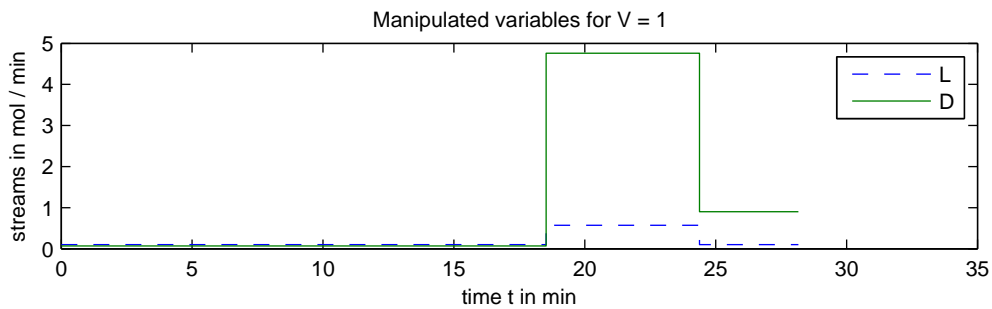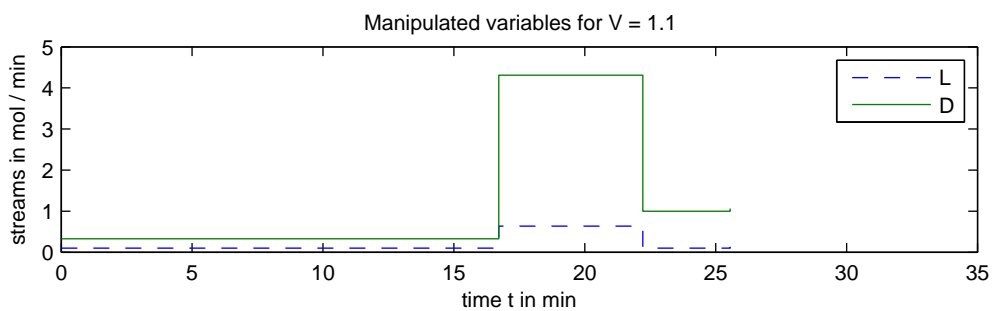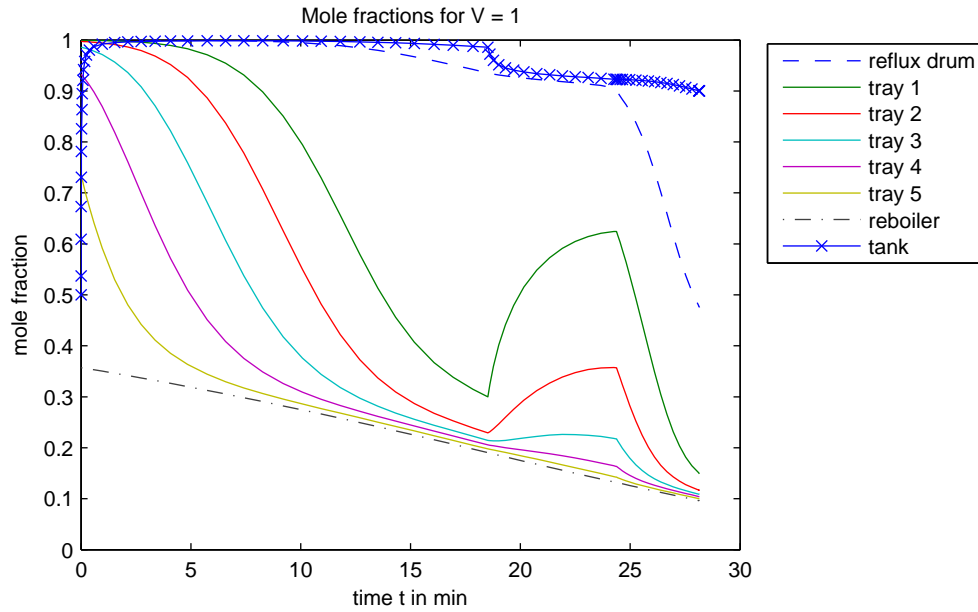


(a) Disturbed case: $V = 0.9$



(b) Nominal case: $V = 1.0$



(c) Disturbed case: $V = 1.1$

Figure 3.1: Optimal open-loop input trajectories for 4 intervals

It can be seen from figure 3.1 that the optimal input trajectories for each value of $V$ are quite similar. However, there are two major differences be-

(a) Optimal mole fraction profiles. Concentration is highest on the first tray and decreases to the fifth tray
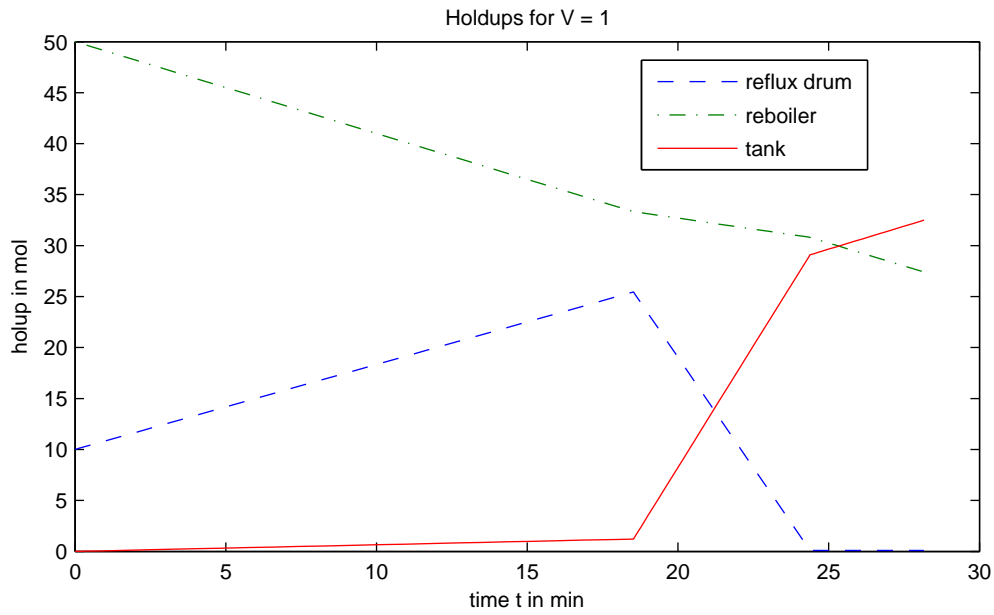


(b) Optimal holdup profiles

Figure 3.2: Optimal open-loop mole fraction and holdup trajectories for the nominal case with 4 intervals

tween them. First, the set of active constraints changes with the disturbance. For example, for $V = 0.9$, $D$ hits its lower bound in the first interval unlike in the disturbed cases. Second, for $V = 1$ and $V = 1.1$, the last interval has a duration of nearly zero in contrast to the case where $V = 0.9$.

While these issues might be related to numerics, it is important for the verification of the nullspace method that the qualitative behavior is as similar as possible and that the set of active constraints does not change with possible disturbances. This will be discussed in more detail in section 4.2 together with an introduction to the nullspace method itself.

For those reasons, the operating policy has been modified in a second step: Instead of 4 intervals, the batch time is now only divided in 3 intervals with variable length. Furthermore, the inputs of the first and the last phase have been fixed: $L$ has been set to its lower bounds in both intervals while $D$ has been set to zero in the first and to $D = L - V$ in the final phase, so that the holdup of the reflux drum remains constant at the end of the batch process. Again, the optimal input trajectories were calculated by *fmincon*. They are plotted in figure 3.3 and the total batch time is shown in the third column of table 3.2.

| Vapor boil-up rate $V$ in mol / min | Original operating policy (4 phases) | Modified operating policy (3 phases) |
|---|---|---|
| 0.9 | 31.35 min | 31.36 min |
| 1.0 | 28.12 min | 28.16 min |
| 1.1 | 25.55 min | 25.55 min |

Table 3.2: Final batch time $t_f$ for different disturbances and operating policies

It becomes clear from table 3.2 that the total batch time obtained with the modified operating policy is nearly the same as for the optimized original operating policy, even though the latter has more degrees of freedom.
Finally, the same set of constraints is active in each phase for all disturbances. This can be seen in figure 3.3 and figure 3.4. The same qualitative behavior of all cases has been achieved and the gathered data can now be used to analyze whether the nullspace method can be applied to unsteady state processes.

### 3.3.2   Scenario 2

In the second scenario, the initial phase in which the column is operated under total reflux is not neglected anymore. This is because the constant relative volatility $\alpha$ is now set to 2, making the separation much harder. The following strategies were tried to obtain an optimal open-loop solution to this problem:

- Using the same approach as for scenario 1. That is, the total batch
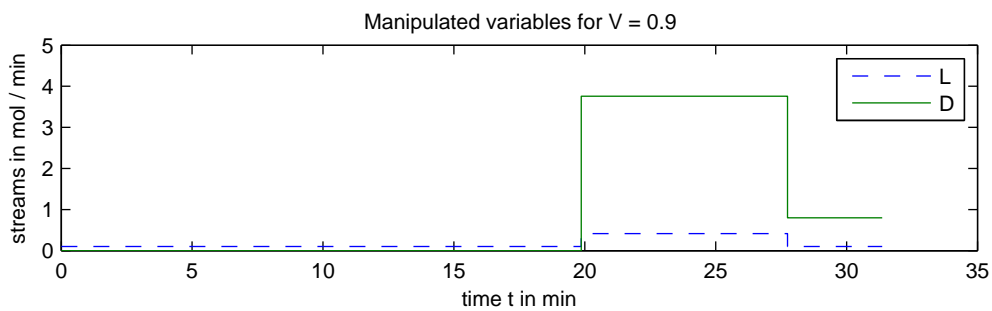


(a) Disturbed case: $V = 0.9$
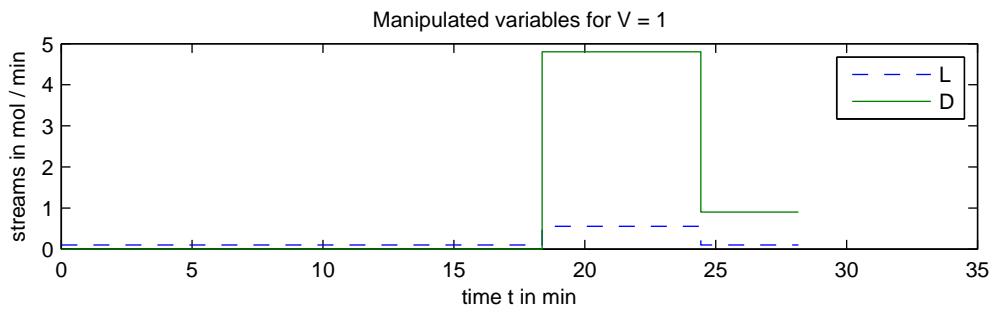


(b) Nominal case: $V = 1.0$
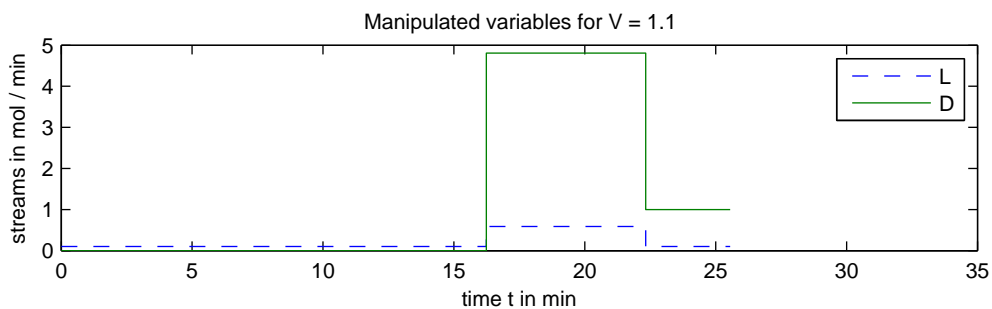


(c) Disturbed case: $V = 1.1$

Figure 3.3: Optimal open-loop input trajectories for 3 intervals
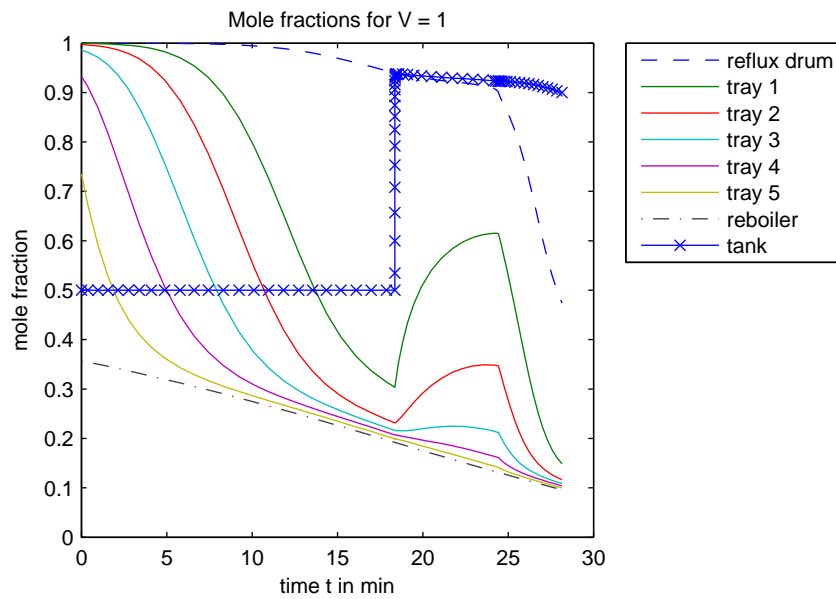
(a) Optimal mole fraction profiles. Concentration is highest on the first tray and decreases to the fifth tray



(b) Optimal holdup profiles

Figure 3.4: Optimal open-loop mole fraction and holdup trajectories for the nominal case with 3 intervals

time was first split in several intervals. Afterwards, *fmincon* was used to optimize both the lengths of the intervals and the optimal value for $L$ which has been considered to be piecewise constant. Remember that due to equation 2.13 $D$ depends on $L$ as only one manipulated variable is left. However, *fmincon* did not converge to any result.
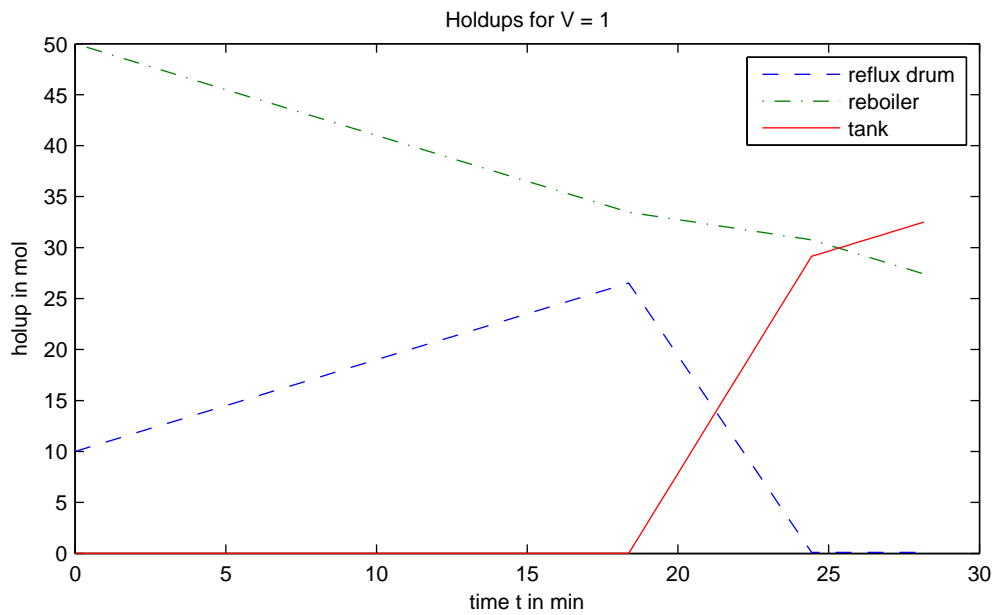
- For the second approach, concentration thresholds were introduced to act as optimization parameters. The ideas was that if a certain concentration exceeds the specified threshold, integration is stopped for the current interval and the next interval is calculated. Direct optimization of the very sensitive time duration can thus be avoided. This strategy did also not converge. Moreover, not all events have been detected by the *Event Location Property* functionality provided by the MATLAB ODE-solvers, especially if the threshold is approached too slowly.

- Next, a different objective function was chosen. Instead of minimizing the total batch time, the derivation between the final states $x_f$ and their required values was minimized. Again, convergence could not be achieved.

- Finally, a simple proportional controller for $L$ has been implemented before the optimization was carried out. This way, not $L$ but a set point for the mole fraction $x_2$ on the second tray was optimized. The control law is given below in equation 3.1.

$$L = 5(x_{2,sp} - x_2) \tag{3.1}$$

where $x_{2,sp}$ denotes the set point for the mole fraction on tray 2. Although this approach did not work with MATLAB, convergence could be achieved in gPROMS.

| Vapor boil-up rate $V$ | Total batch time $t_f$ |
| --- | --- |
| 0.9 mol / min | 100.48 min |
| 1.0 mol / min | 86.75 min |
| 1.1 mol / min | 78.82 min |

Table 3.3: Final batch time $t_f$ for different disturbances in scenario 2

The last approach has been successfully optimized with gPROMS. The time following the initial, total reflux phase has been divided into two intervals. Equivalently to scenario 1, the length of both intervals as well as the value of

$x_{2,sp}$ were determined by the optimizer, in this case, by the multiple shooting algorithm $CVP\_MS$ inherent in gPROMS. The optimal trajectories look similar for all considered disturbances. The resulting trajectories for the nominal case are shown in figures 3.5 and 3.6. Table 3.3 contains the final batch time for different disturbances.

An interesting question remains, though. Why is optimizing and controlling a mole fraction in the column more promising than directly optimizing the reflux stream $L$? This question will be discussed in section 5.2.
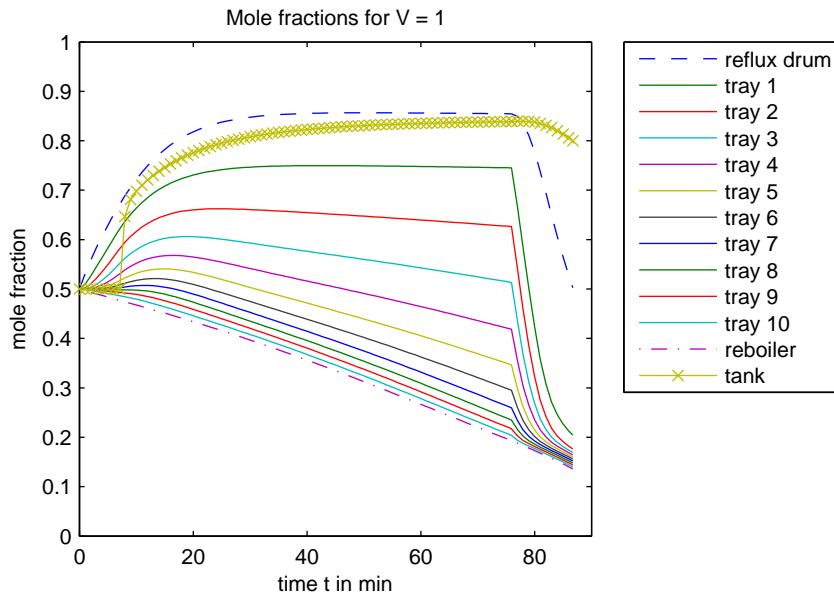
(a) Optimal mole fraction profiles. Concentration is highest on the first tray and decreases to the tenth tray
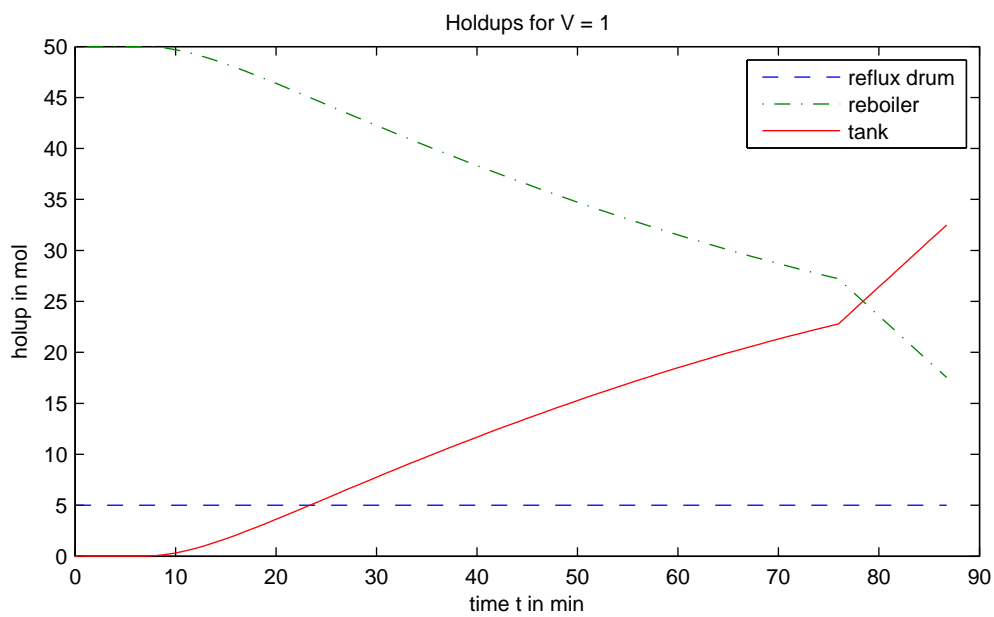


(b) Optimal holdup profiles

Figure 3.5: Optimal open-loop mole fraction and holdup trajectories for scenario 2

(a) Optimized reference and actual values of $x_2$



(b) Resulting optimal trajectories for L and D

Figure 3.6: Controlling L by tracking the optimal reference for $x_2$ in scenario 2
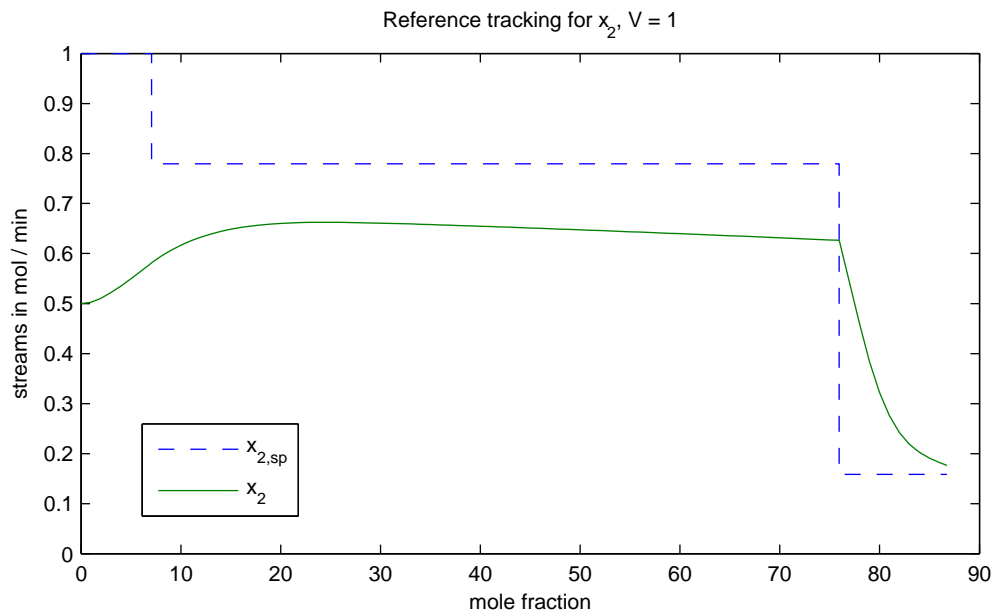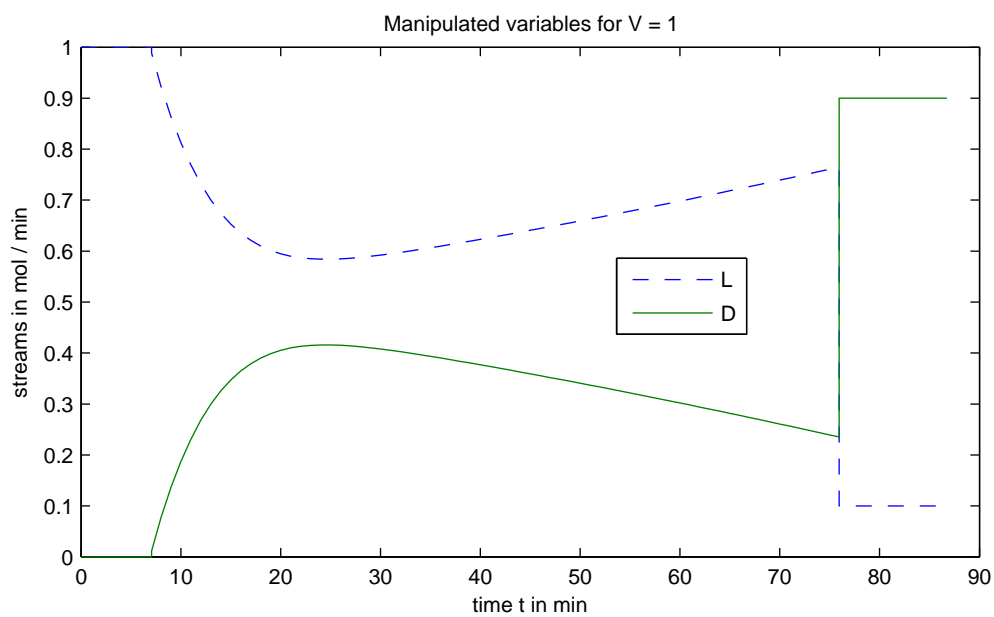
# Chapter 4

# Closed-Loop Control

## 4.1  Motivation

In the previous chapter, optimal open-loop or feedforward control laws for batch distillation processes have been calculated. If the value of the disturbance $V$ is known, the appropriate control can be directly applied to the plant. However, measurements of disturbances are often not available. A robust feedback control structure is therefore desirable.

In this chapter, such a feedback structure is derived. The perfect control structure would for all expected disturbances deliver near-optimal performance compared to the feedforward solution without using a plant model for implementation. Having these objectives in mind, several approaches were examined. The *nullspace method*, originally developed for steady state processes, looks promising and serves as a starting point.

## 4.2  Discrete Switching Decisions

As shown in the previous chapter, discrete decisions are required that determine when to switch between the different continuous controllers. These decisions should be based on feedback. To find such an applicable switching strategy is the focus of this work.

### 4.2.1  The Nullspace Method

The nullspace method has been developed to select optimal measurement combinations as controlled variables in steady state processes (Alstad, 2005). Since this idea might also work for batch processes, it is briefly introduced

here in its traditional form for continuous processes.

Consider a dynamic system with a vector $\mathbf{y}_0$ that contains all measureable variables of the system. Linear combinations $\mathbf{c}$ of a subset $\mathbf{y}$ of those measurements are described as follows:

$$\mathbf{c} = \mathbf{Hy} \tag{4.1}$$

where $\mathbf{H}$ is a constant coefficient matrix.

In steady state, the optimal value of $\mathbf{y}$, $\mathbf{y}_{\mathrm{opt}}$, *depends* on the disturbance $\mathbf{d}$. The idea is to find a matrix $\mathbf{H}$ such that the optimal value of $\mathbf{c}$ is however *independent* of $\mathbf{d}$:

$$\mathrm{d}\mathbf{c}_{\mathrm{opt}}(\mathbf{d}) = \mathbf{0} \tag{4.2}$$

When equation 4.2 holds, $\mathbf{c}$ can be controlled at a constant set point to achieve optimal performance despite disturbances.

Next, consider a constant sensitivity matrix $\mathbf{F}$ for small disturbances $\mathbf{d}$, evaluated at the nominal optimal point:

$$\mathbf{F} = \left( \frac{\mathrm{d}\mathbf{y}_{\mathrm{opt}}}{\mathrm{d}\mathbf{d}} \right)^T \tag{4.3}$$

This gradient can be calculated numerically by repeated optimization of the process for small perturbations of the disturbances. Note that the set of active constraints must not change with the perturbed disturbances. Otherwise, $\mathbf{F}$ is not well defined.

Using equation 4.3 to substitute $\mathbf{y}$ in equation 4.1 and inserting the result in equation 4.2 finally leads to

$$\mathbf{HF} = \mathbf{0} \tag{4.4}$$

This equation can be verbalized as "$\mathbf{H}$ must lie in the left nullspace of $\mathbf{F}$", which is the reason why this method is called *nullspace method*.

Now how can this method be used for determining the switching instants $t_s$ in batch distillation control? Analogous to the continuous case, the optimal switching instants depend on the disturbances:

$$t_{s,\mathrm{opt}} = f(\mathbf{d}) \tag{4.5}$$

Switching at nominal time might not only lead to non-optimal results as in
the continuous case but even to infeasibility. The idea is to find a combination
of measurements that results in a scalar and steady function $c$ which is either
monotonously in- or decreasing. For example, consider a constant coefficient
matrix $\mathbf{H}$, such that

$$c = \mathbf{Hy} \tag{4.6}$$

If then at the optimal switching instant $t_{s,\mathrm{opt}}$ the value of $c$, denoted $c_{\mathrm{opt}} = c\,(t = t_{s,\mathrm{opt}})$, was independent of the disturbances $\mathbf{d}$, it could be used to trig-
ger switching to the next continuous controller. Thus, equation 4.2 should
hold again, leading in turn to equation 4.4 that could be used to determine
$\mathbf{H}$. Using the data from scenario 1, section 3.3, this idea is examined for the
first switching instant (occurring at $t_{s,opt} = 18.36$ min in the nominal case).
For several disturbances, the optimal switching time $t_{s,\mathrm{opt}}$ is shown in table
4.1.

| Vapor boil-up rate $V$ | Switching time $t_{s,\mathrm{opt}}$ |
|---|---|
| 0.90 mol / min | 19.373 min |
| 0.99 mol / min | 18.310 min |
| 1.00 mol / min | 18.364 min |
| 1.01 mol / min | 18.080 min |
| 1.10 mol / min | 16.265 min |

Table 4.1: First optimal switching instants for scenario 1

Since all states are assumed to be measurable, table 4.2 shows the states in
scenario 1 at the optimal switching time for several values of $V$.

In this scenario $V$ is the only disturbance, so $d = V$ is scalar. Thus, both $\mathbf{F}$
and $\mathbf{H}$ are vectors, not matrices, and will be written $\mathbf{f}$ and $\mathbf{h}^T$ respectively.
In a first step, $\mathbf{f}$ has been calculated numerically using a finite difference
approximation:

$$\mathbf{f} = \frac{1}{V^+ - V^-}\left(\mathbf{y}^+ - \mathbf{y}^-\right) \tag{4.7}$$

where $V^+ = 1.01$, $V^+ = 0.99$ and $\mathbf{y}^+$ and $\mathbf{y}^-$ correspond to the states at
the optimal switching time $t_{s,\mathrm{opt}}$ for each value of V. The elements of the
sensitivity vector $\mathbf{f}$ can also be found in table 4.2.

| State $\mathbf{y}_i$ | Vapor boil-up rate $V$ in mol / min | | | | | Sensitivity $\mathbf{f}_i$ |
|---|---|---|---|---|---|---|
| | 0.90 | 0.99 | 1.00 | 1.01 | 1.10 | |
| $N_{RD}$ | 25.499 | 26.296 | 26.528 | 26.453 | 26.265 | 7.865 |
| $N_{RB}$ | 34.501 | 33.704 | 33.472 | 33.547 | 33.735 | -7.865 |
| $N_T$ | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.000 |
| $x_{RD}$ | 0.952 | 0.942 | 0.939 | 0.940 | 0.940 | -0.100 |
| $x_{RB}$ | 0.202 | 0.195 | 0.192 | 0.193 | 0.196 | -0.075 |
| $x_T$ | 0.500 | 0.500 | 0.500 | 0.500 | 0.500 | 0.000 |
| $x_1$ | 0.340 | 0.310 | 0.303 | 0.304 | 0.303 | -0.260 |
| $x_2$ | 0.249 | 0.235 | 0.231 | 0.233 | 0.236 | -0.120 |
| $x_3$ | 0.229 | 0.219 | 0.216 | 0.217 | 0.221 | -0.090 |
| $x_4$ | 0.219 | 0.210 | 0.207 | 0.208 | 0.212 | -0.085 |
| $x_5$ | 0.210 | 0.202 | 0.199 | 0.200 | 0.204 | -0.075 |

Table 4.2: Further data from scenario 1 to examine whether the nullspace method is applicable for the first switching instant

In a second step, all coefficients in $\mathbf{h}^T$ have been set to 1 with the exception of the first component $\mathbf{h}_1$ which was calculated such that equation 4.4 is satisfied. Although there are an infinite number of solutions vectors $\mathbf{h}$, the above solution was chosen for simplicity. In general, other solutions might be more appropriate to reduce the effect of measurement errors or to achieve a certain control structure (Alstad, 2005). However, these issues are not within the scope of this thesis.

It should also be noted here that with this choice of $\mathbf{h}^T$, scaling down the much larger holdups to the dimension of the mole fractions would not qualitatively change the result. Instead, by weighting both holdups with the same coefficient, and because $N_T = 0$ in the first phase, they cancel each other out when calculating $\mathbf{h}_1$. This can also be seen in the last column of table 4.2.

For the nullspace method to work, $c_{\mathrm{opt}} = \mathbf{h}^T \mathbf{y}$ must be constant for all possible disturbances. Indeed, table 4.3 shows that $c_{\mathrm{opt}}$ does not vary too much for the different values of $V$. However, $c$ cannot be used for triggering the switching: Although $c$ is steady and decreases monotonously, switching at a value of $c$ that differs only slightly from the optimal value $c_{\mathrm{opt}}$ means switching up to 2 minutes too early or too late. This is demonstrated in figure 4.1 for the case $V = 1.1$. According to table 4.1, the optimal switching time is

16.26 minutes. If switching was triggered by $c$ reaching the optimal value for the nominal case ($V = 1.0$) then it would take place at time $t = 18.3\,\mathrm{min}$ – more than 2 minutes later than optimal.

| Vapor boil-up rate $V$ | Optimal $c$-value $c_{\mathrm{opt}}$ |
|---|---|
| 0.90 mol / min | 55.2383 |
| 0.95 mol / min | 55.2235 |
| 0.99 mol / min | 55.2308 |
| 1.00 mol / min | 55.2284 |
| 1.01 mol / min | 55.2308 |
| 1.05 mol / min | 55.2352 |
| 1.10 mol / min | 55.2428 |

Table 4.3: Optimal values of $c$ for different disturbances

## 4.2.2   Indirect Information about Disturbances

In order to find an applicable, model-free switching strategy, another approach to control the system is needed. The key idea of the following method is to get some *indirect information* about the disturbance as it was assumed earlier that it is not *directly* measureable.

**Scenario 1**

Consider again the optimal open-loop solution for scenario 1 as shown in section 3.3. With $L$ and $D$ fixed at their lower limits during the first phase, the reflux drum holdup now only depends on the value of $V$. Equation 2.2 shows this mathematically. Therefore, the reflux drum holdup $N_{RD}$ can be used to indirectly gain information about the disturbance.

As stated in the context of the nullspace method, the variable that is used for switching must in- or decrease monotonously in each controller interval. The reflux drum holdup $N_{RD}$ satisfies this requirement. Together with a set of continuous controllers which is described in the following section 4.3, a control structure has been implemented where $N_{RD}$ is used to determine the switching to the next controller.
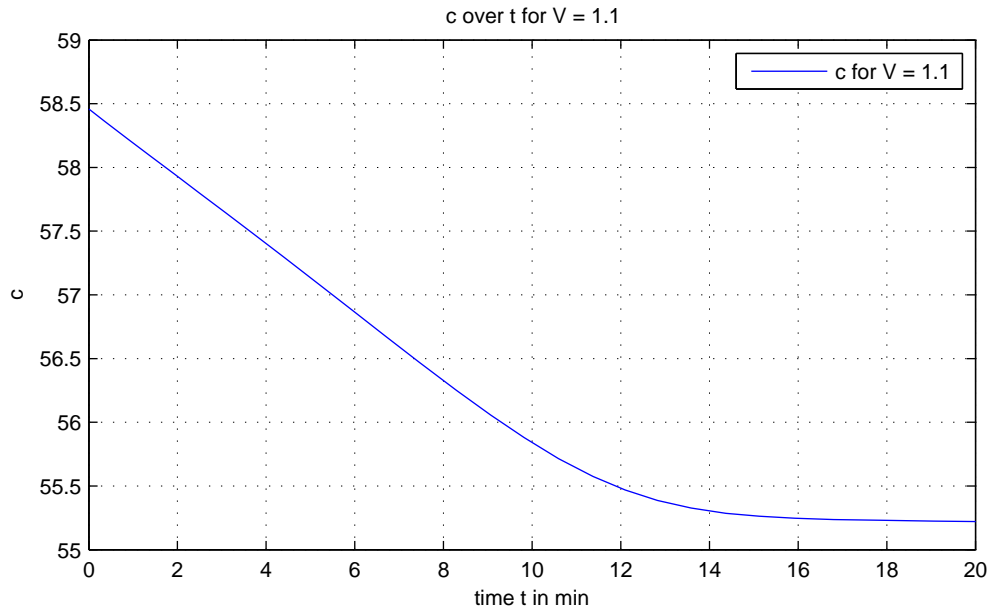
(a) Graph of $c$ over time for scenario 1, $V = 1.1$
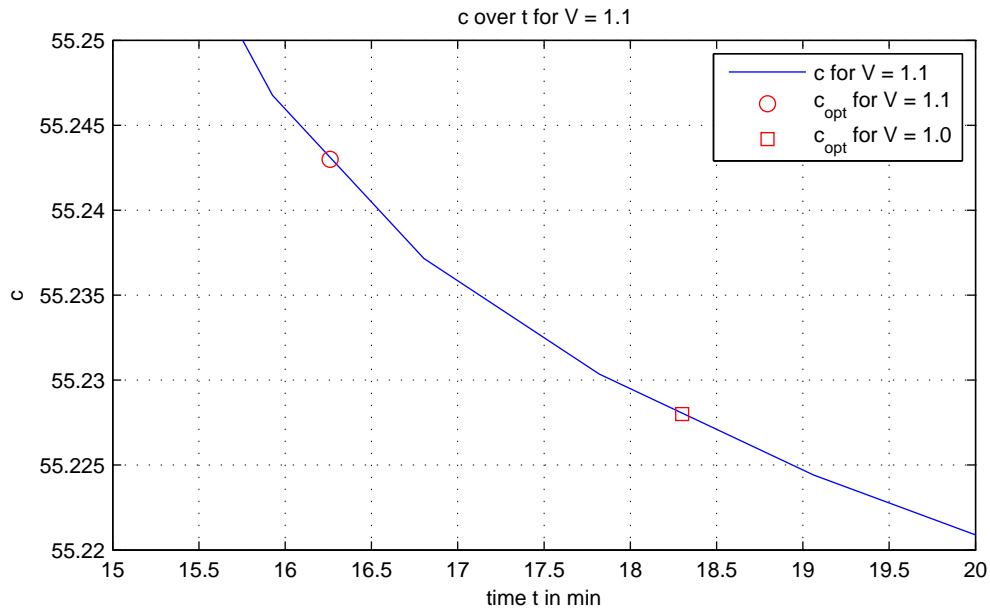


(b) Optimal and nominal switching

Figure 4.1: $c$ over time for $V = 1.1$. Switching at optimal *nominal* value of $c$ would be 2 minutes too late

The first continuous controller is used until $N_{RD}$ exceeds a value of 26. Then,

the second controller is activated until $N_{RD}$ falls below 0.2. Until the terminal constraints are met, the third and final controller takes over the system.

**Scenario 2**

In the second scenario, the reflux drum holdup has been fixed by setting equation 2.2 equal to zero and thus cannot be used as a decision variable. However, in the first phase the plant is operated in total reflux mode. Equation 2.1 shows that in this case $x_{RD}$ gives a good variable that fulfills all requirements as stated above. Thus, it will be used to activate the controller of phase 2 when a threshold of 0.7 is exceeded.

In the intermediate phase 2, the tank holdup $N_T$ has been chosen as the variable to decide about controller switching. Contrary to scenario 1, none of the model equations depends exclusively on $V$. However, $V$ has great influence on the reboiler holdup $N_{RB}$ as can be seen in equation 2.6. With equation 2.13, $V$ also effects $N_T$ as $N_T + N_{RB} = \text{const}$. Therefore, using $N_T$ is equivalent to using $N_{RB}$. Thus, when $N_T$ exceeds a threshold value of 20.4, the last phase is started.

# 4.3   Continuous Controllers

In addition to discrete switching decisions, continuous controllers must be present to operate the closed-loop system. While the basic idea behind the controlled variables and controller types was to mimic the open-loop behavior, it should be noted that the final controller tuning, including the thresholds for the switching variables in the previous section, was mostly done empirically as this was not the focus of this thesis.

## 4.3.1   Scenario 1

Table 4.4 summarizes the controller configuration for each phase. In phase 1 the reflux drum is filled. This is simply achieved by keeping $L$ and $D$ at their lower bounds like in the open-loop solution. In the second phase, a PI-type controller manipulates $L$ using a set point for the mole fraction on the second tray, $x_2$. $D$ is at its maximum to fill the tank as fast as possible. Finally, in the third phase, $L$ is controlled at its lower bound while $D$ is controlled by a P-type controller. Again, a set point for $x_2$ is used until the terminal constraints are satisfied.

| Phase | Continuous controller | Switching condition |
|---|---|---|
| initial phase | $D = 0$ <br> $L = 1$ | Steady state is reached |
| 1 | $D = 0$ <br> $L = 0.1$ | $N_{RD} > 26$ |
| 2 | $D = 5$ <br> $L = 5\,e + \int e\,\mathrm{dt}$ <br> $e = 0.45 - x_2$ | $N_{RD} < 0.2$ |
| 3 | $D = -20\,e$ <br> $e = (0.1 - x_2)$ <br> $L = 0.1$ | Terminal constraints are satisfied |

Table 4.4: Summary of the control structure for scenario 1

### 4.3.2 Scenario 2

Because of equation 2.13, only one degree of freedom is available in scenario 2. In the initial phase the column is operated at total reflux. Therefore, $L$ has been fixed at its maximum, that is at the value of $V$. This can be achieved by keeping the tank valve closed. $D$ is then zero and because of the constant reflux drum holdup, $L = V$. Afterwards in phase 2, a PI-type controller is used to control $L$ depending on the mole fraction $x_2$. Until the terminal requirements are satisfied, $L$ is set to its lower bound in the final phase. The complete control configuration can be found in table 4.5. Note that phase 1 is not strictly necessary. If the controller of phase 2 is used from the beginning, $L$ will become saturated at its upper bound automatically. Thus, an even simpler control structure consisting only of phase 2 and 3 leads to the same results.

| Phase | Continuous controller | Switching condition |
|---|---|---|
| 1 | $L = V$ | $x_T > 0.7$ |
| 2 | $L = 20\,e + 0.5 \int e\,\mathrm{dt}$ <br> $e = 0.7 - x_2$ | $N_T > 10.4$ |
| 3 | $L = 0.1$ | Terminal constraints are satisfied |

Table 4.5: Summary of the control structure for scenario 2

## 4.4   Simulation Results

The closed-loop control structure and controller parameters mentioned in the previous sections have been implemented in MATLAB. Simulations were run and the results are shown here.

Tables 4.6 and 4.7 contain the total batch times for scenario 1 and 2 respectively. Figures 4.2 - 4.5 illustrate the system's behavior in closed-loop operation, again for both scenarios. Only the nominal profiles are shown as the qualitative behavior is the same for all considered disturbances.

| Vapor boil-up rate $V$ | Total batch time $t_f$ |
| --- | --- |
| 0.9 mol / min | 31.56 min |
| 1.0 mol / min | 28.34 min |
| 1.1 mol / min | 25.75 min |

Table 4.6: Final batch time $t_f$ for scenario 1, closed-loop

| Vapor boil-up rate $V$ | Total batch time $t_f$ |
| --- | --- |
| 0.9 mol / min | 97.90 min |
| 1.0 mol / min | 87.40 min |
| 1.1 mol / min | 78.83 min |

Table 4.7: Final batch time $t_f$ for scenario 2, closed-loop
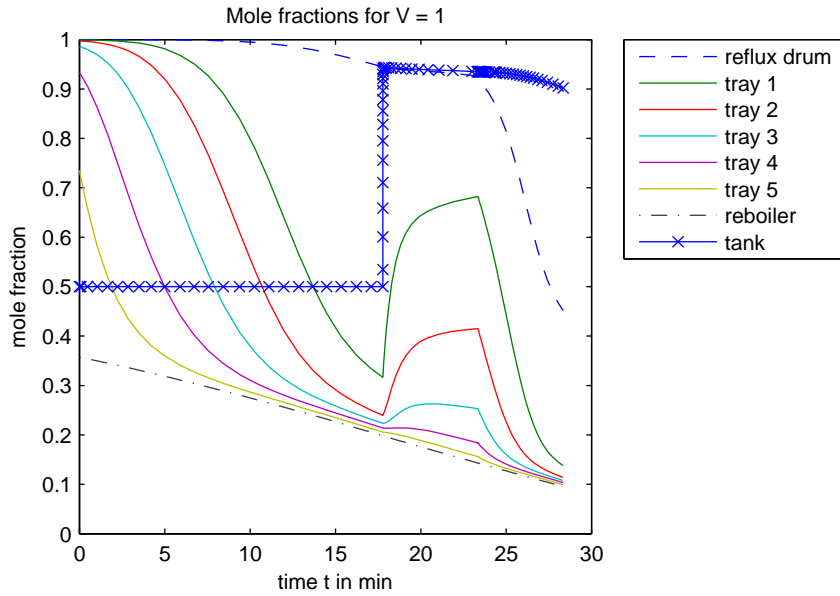
(a) Mole fraction profiles. Concentration is highest on the first tray and decreases to the fifth tray
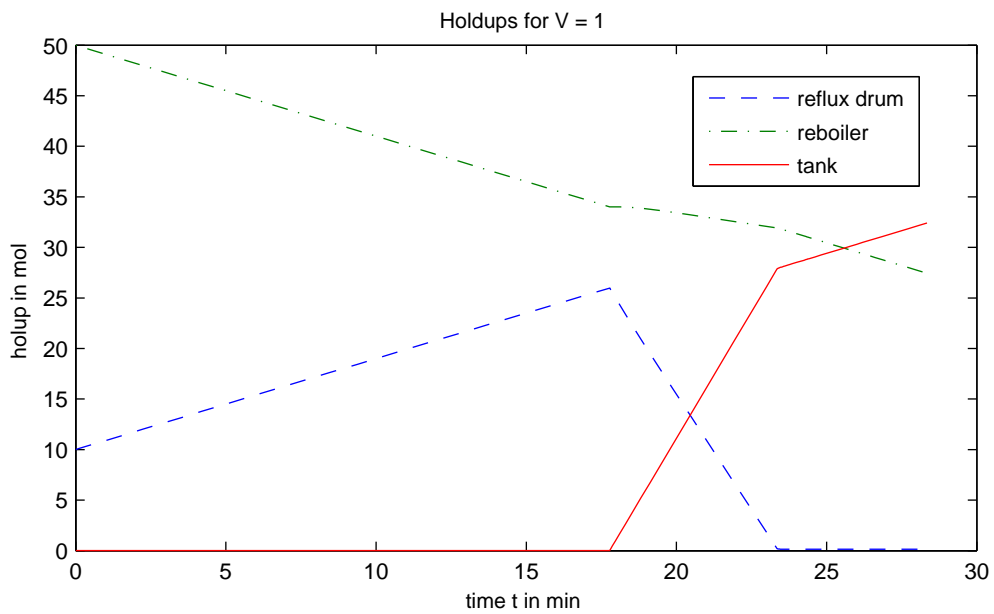


(b) Holdup profiles

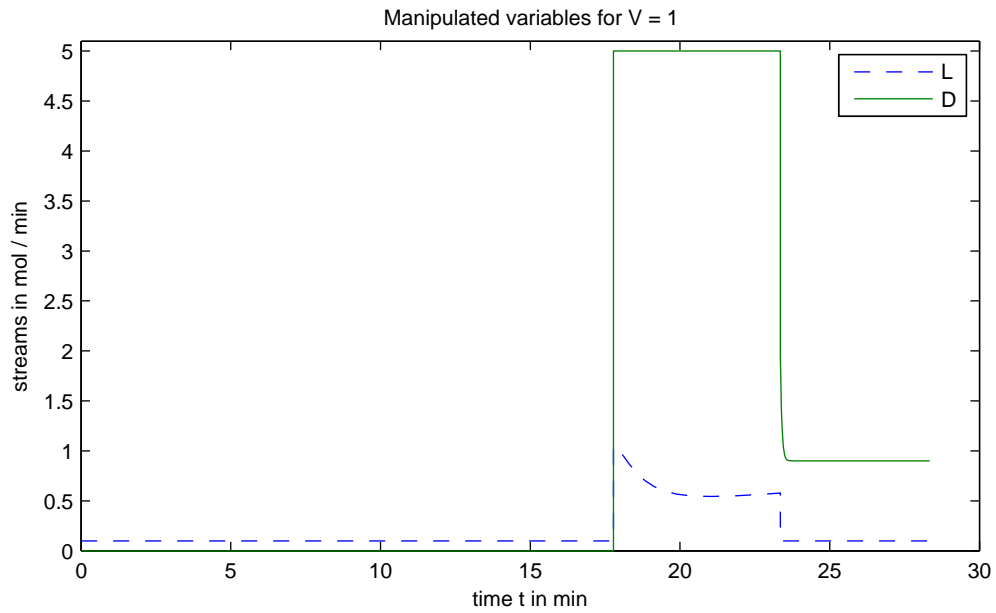Figure 4.2: Nominal closed-loop mole fraction and holdup profiles for scenario 1

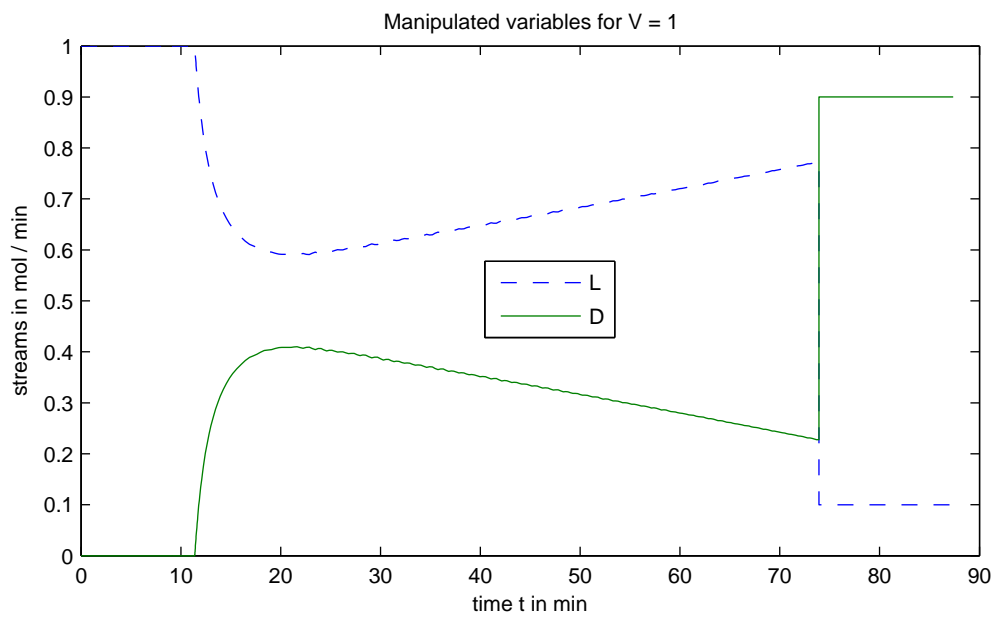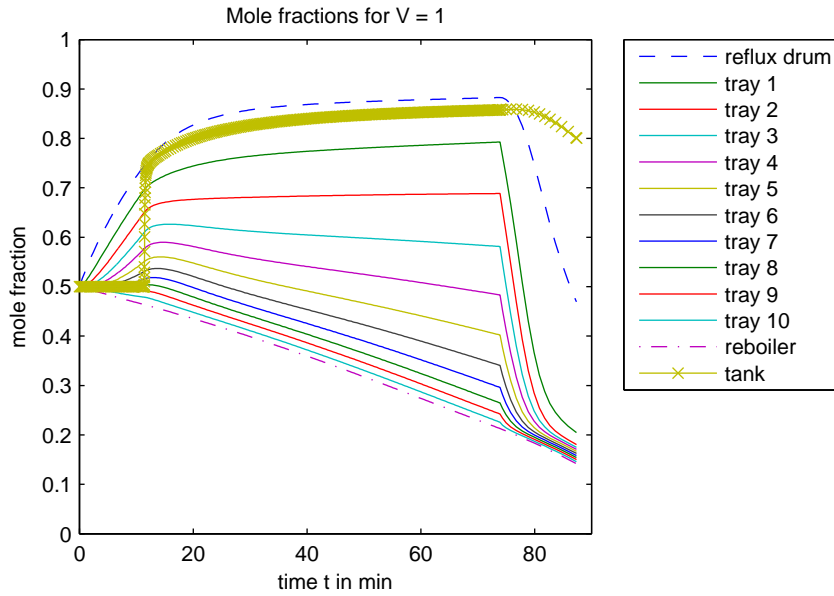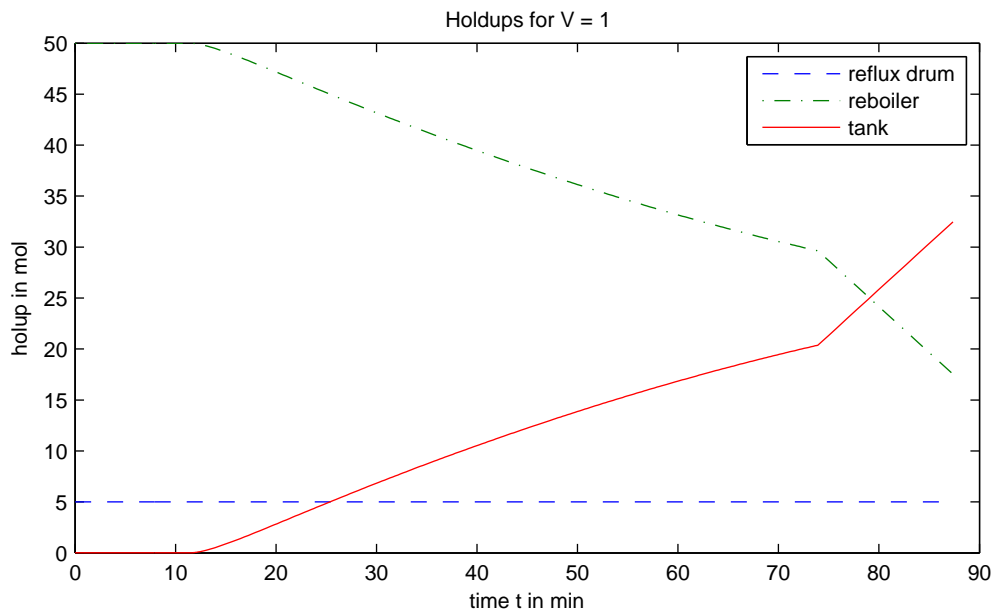Figure 4.3: Nominal closed-loop input profiles for scenario 1



Figure 4.4: Nominal closed-loop input profiles for scenario 2

(a) Mole fraction profiles. Concentration is highest on the first tray and decreases to the tenth tray



(b) Holdup profiles

Figure 4.5: Nominal closed-loop mole fraction and holdup profiles for scenario 2

# Chapter 5

# Discussion

## 5.1    Classification of the Optimal Control Task

It has already been denoted in chapter 3 that dynamic optimization of this batch distillation process is very difficult. Various software packages have been used to deal with this problem with varying success.

Reasons for these difficulties are manifold. The model contains strong nonlinearities as in equation 2.3 and the structure of the column leads to internally coupled states, as can be seen in equation 2.10. Some optimization algorithms might have additional problems with the minimum time objective. Even in a simple model with a very limited number of trays these effects prevent analytical solutions and complicate numerical optimization.

One of the most often used numerical solution strategies is the so-called control vector parameterization which is, for example, implemented in the gPROMS software. However, this strategy requires laborious and time-consuming manual adjustments of initial guesses and other parameters to make the algorithm converge. Moreover, the resulting solution is usually not easy to analyse as a meaningful physical interpretation of the solution can rarely be given.

Another optimization issue encountered in this thesis were multiple solutions that had close-to-optimal values of their objective function although their qualitative behavior was totally different. In cases like this, it is very hard to distinguish whether qualitative changes in the optimal solution for small disturbances are caused by the numerical optimization algorithm or if they are an inherent feature of the system itself. To avoid these qualitative

changes, some parameters have been fixed to allow only a certain solution structure in section 3.3.

In control strategies like MPC that require repeated optimization, the aforementioned problems would not only be encountered once before the batch but at every time step during the process. This once again emphasizes the need for a model-free, robust feedback control structure without the need for online optimization as has been developed in this thesis.

Another note should be made at this point: While a flat optimum implies a more difficult optimization as described above, it also means easier controller tuning since many control configurations lead to acceptable, near-optimal results.

## 5.2   Why Control $x$, not $L$?

In section 3.3 the question was raised why controlling a mole fraction like $x_2$ inside the column leads to a better convergence of the dynamic optimization than optimizing the input $L$ directly.

Traditionally, two strategies are used in control of batch distillation columns: operation with constant reflux and operation where a constant distillate composition is maintained (Diwekar, 1995). The first strategy is relatively easy to calculate and implement. For this reason, it is the most often used strategy in industry. However, the batch process can take a very long time when it is operated using this policy.

The second strategy tries to keep the reflux drum composition constant. This leads to a much faster solution but also to rapid changes in the reflux ratio that are hard to control.

The optimal reflux ratio is situated somewhere between those two strategies; changes in the reflux ratio are not as rapid as with the constant distillate composition policy. Thus, instead of controlling $L$ directly, a controlled variable that changes more slowly than the mole fraction of the reflux drum is sought. The mole fractions of the trays inside the column fulfill this requirement and have therefore been used successfully for optimization and control.

## 5.3    Remarks about the Nullspace Method

As has been examined in section 4.2, the nullspace method cannot simply be generalized to dynamic models as in batch distillation control. Although this method looked very promising in the beginning, this is not so much of a surprise since it was originally developed for linear processes that are operated in steady state and was now applied to a nonlinear dynamic system.

However, these results do not mean that the nullspace method is not able to handle nonlinear dynamic problems in general. If more variables are included in the available measurements, like state derivatives or the switching time itself, it might work. Nonlinear combinations of measurements could be another promising approach to account for nonlinearities present in many systems.

## 5.4    Remarks about the Implemented Control Structure

Instead of the nullspace method, an alternative method has been used to find an appropriate control structure. The key point with this method is to find variables that are preferably only affected by the present disturbance directly and not coupled with other states. Identification of those variables is easier if the system is rather small and physically explainable.

In this thesis, the variables have been found in a two-step procedure: First, some candidate variables have been identified that are more influenced by the disturbances than others. Both physical insight into the process and simulations can be used for this decision. Second, the corresponding model equations have been examined. Variables, whose differential equations then depended to the highest degree only on the disturbance were chosen.

After deciding for the switching variables, switching thresholds and continuous controllers still need to be found. Again, simulations were run to decide for the controller type and to check constraint satisfaction. Simple continuous controllers were preferred to make implementation and tuning as easy as possible. Especially for tuning, the optimal open-loop profiles were of great help. Optimizing the closed-loop system with respect to controller parameters might be another option. However, this was not done in this thesis.

## 5.5   Comparison of Open-Loop and Closed-Loop Performance

Besides examining whether the nullspace method provides an appropriate mechanism to switch between different continuous controllers, finding a model-free control structure was the main focus of this thesis. It was also required that the closed-loop control ensures near-optimal performance even in case of disturbances. In chapter 3, the minimal batch times have been calculated for different disturbances. They are shown in tables 3.2 and 3.3.

In chapter 4, a controller has been designed for each scenario. It fulfills all requirements stated in the introduction: It is model-free and thus does not need online-optimization, it consists of continuous sub-controllers and discrete switching decisions are made. For all considered disturbances, both path and terminal constraints are satisfied. The resulting batch times are found in tables 4.6 and 4.7, respectively.

These values indicate near-optimal performance of the closed-loop systems. The difference between open- and closed-loop performance is less than 12 seconds in scenario 1, corresponding to 0.6% of the optimal time. In scenario 2, the difference is less than 40 seconds or approximately 0.7%. For the scope of this work, this result is satisfactory.

As can also be seen in the tables mentioned above, the open-loop system performs a little better than the closed-loop system in most cases. However, this is not true for $V = 0.9$ mol / min in scenario 2. Here, the closed-loop system outperforms the open-loop one. The explanation for this is that in contrast to the open-loop optimization, the inputs are not piecewise constant when the process is feedback-controlled. This gives additional degrees of freedom which may either lead to better results than in the open-loop case or, if not properly designed, to infeasibility. Thorough simulations should be run to ensure feasibility.

Finally, only standard PI-type controllers are needed. Relatively easy implementation and tuning are the main reasons why those controllers are still predominant in many industries. Therefore, the small loss in performance compared to optimal open-loop behavior is acceptable and does not compromise the overall benefits of the control structure presented in this thesis.

# Chapter 6

# Conclusion

The overall aim of this thesis was to find a model-free feedback control structure for a batch distillation process that leads to near-optimal performance for a certain range of disturbances. Such a control structure has been developed in this thesis. Negligibly longer batch durations as compared to open-loop simulations are more than compensated by the simple feedback structure. At the same time, the necessary manual process interventions are reduced to a minimum.

In addition, it was found that the optimal open-loop input trajectories contain a finite number of jump discontinuities that are typical for dynamic control problems. The nullspace method which was originally developed for linear steady state processes looked promising to handle these discontinuities. Unfortunately, this method failed if only a linear combination of states was used. Future investigations might address this by including more process information, for example derivatives of the states, in the measurements or combining measurements in a nonlinear way.

As an alternative approach, physical insight into the process can be used to identify variables that provide indirect information about the disturbance. While it is unclear if this strategy would work for more complex process models as well, it has been successfully used in this thesis. It would also be interesting to see if this approach can be generalized to cases with more than one disturbance.

Finally, this thesis shows that application of self-optimizing control is not limited to continuous processes. Instead, with robust switching laws, batch processes are equally receptive for its benefits.

# Bibliography

Alstad, V. (2005). *Studies on selection of controlled variables.* Ph.D. thesis. Norwegian University of Science and Technology, Trondheim.

Bausa, J. and Tsatsaronis, G. (2001). *Reducing the energy demand of continuous distillation processes by optimal controlled forced periodic operation.* Computers & Chemical Engineering. 25(2-3):359–370.

Dahl-Olsen, H., Narasimhan, S. and Skogestad, S. (2007). *Optimal operation by measurements.* Nordic Process Control Workshop, Helsinki.

Diwekar, U. M. (1995). *Batch Distillation: Simulation, Optional Design and Control.* Taylor & Francis.

Diwekar, U. M., Madhavan, K. P. and Swaney, R. E. (1989). *Optimization of multicomponent batch distillation column.* Industrial & Engineering Chemistry Research. 28:1011ff.

Farhat, S., Czernicki, M., Pibouleau, L. and Domench, S. (1990). *Optimization of multiple-fraction batch distillation by nonlinear programming.* AIChe Journal. 36:1349ff.

Halvorsen, I., Skogestad, S., Morud, J. and Alstad, V. (2003). *Optimal selection of controlled variables.* Industrial & Engineering Chemistry Research. 42(14):3273–3284.

Houtman, J. P. W. and Husain, A. (1956). *Design calculations for batch distillation column.* Chemical Engineering Science. 5:178ff.

Humphrey, J. L. (1995). *Separation processes: Playing a critical role.* Chemical Engineering Progress. 91(10).

McCabe, W. L. (2005). *Unit operations of chemical engineering / Warren L. McCabe, Julian C. Smith, Peter Harriott.* McGraw-Hill/Higher Education, Boston, Mass. 7th ed ed.. ISBN 0072848235; 978007284823. URL `http://millenium.itesm.mx/record=i2605182&searchscope=0`.

Morari, M., Stephanopoulos, G. and Arkun, Y. (1980). *Studies in the synthesis of control structures for chemical processes. Part I: Formulation of the problem. Process decomposition and the classification of the control tasks. Analysis of the optimizing control structures.* AIChE Journal. 26(2):220–232.

Mujtaba, I. and Macchietto, S. (1991). *The role of holdup on the performance of binary batch distillation.* Proceedings PSE '91. pp. 1.19.1–1.19.15.

Qin, S. and Badgewell, T. (1997). *An overview of industrial model predictive control technology.* URL `citeseer.ist.psu.edu/qin97overview.html`.

Skogestad, S. (2000). *Plantwide control: The search for the self-optimizing control structure.* Journal of Process Control. 10(5):487–507.

Skogestad, S. (2004). *Near-optimal operation by self-optimizing control: from process control to marathon running and business systems.* Computers & Chemical Engineering. 29(1):127–137.

Skogestad, S. and Postlethwaite, I. (1996). *Multivariable Feedback Control.* John Wiley & Sons.

Srinivasan, B., Bonvin, D., Visser, E. and Palanki, S. (2003). *Dynamic optimization of batch processes II. Role of measurements in handling uncertainty.* Computers & Chemical Engineering. 27(1):27–44.

Stichlmair, J. G. and Fair, J. R. (1998). *Distillation: principles and practice.* Wiley-VCH.

Sørensen, E. (1994). *Studies on optimal operation and control of batch distillation columns.* Ph.D. thesis. University of Trondheim, Norwegian Institute of Technology.