Plant-wide Controllability and Structural Optimization of Plants with Recycles
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Plantwide Controllability and Structural Optimization of Plants with Recycles

Sander Groenendijk
Plantwide Controllability and Structural Optimization of Plants with Recycles

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Chapter 1

Introduction

1.1 Scope

The central question in this thesis is ‘How to design and optimize complex plants with superior dynamic behavior and controllability features’. The design of complex integrated plants is nowadays well established as far as the steady state operation is concerned. However, the analysis of plant dynamics during the conceptual design stage, which aims to produce better flowsheet alternatives from controllability point of view, is a recognized, but yet unresolved problem. The goal of this work is to develop an approach for the conceptual design of an optimal flowsheet structure of a complex chemical plant with good plantwide controllability properties.

The synthesis of complex processes with good controllability characteristics is a huge and challenging problem with many aspects. It requires the simultaneous optimization of flowsheet structure and equipment sizing while taking into account the dynamics of all units and all dynamic interactions. Special attention has to be paid to the recycle structure, since recycle interactions may have a strong effect on dynamic behavior, especially in complex plants. This may have a significant influence on the performance of individual units. Therefore, the behavior of a unit in an integrated plant may differ considerably from the behavior of the same unit as a stand-alone object. Consequently, the control system for a complex plant should not be designed by considering only stand-alone units. Effective plantwide control structures must be identified and implemented.

Several concepts are available to develop a plantwide control system for a given plant design (Luyben et al., 1999). However, constraints originating from the design may be limiting the
optimization of the control system. In such cases design modifications that relax the constraints will improve the controllability of the plant. Therefore, a real need exists to incorporate a controllability study early in the conceptual design, in order to evaluate several flowsheet structure alternatives on their dynamic behavior and controllability. One may then select the best alternative, not only regarding steady state economics, but also with respect to controllability.

It may also be interesting to include optimization techniques in the design procedure. The simultaneous optimization of flowsheet structure and equipment sizing may be seen as a large Mixed Integer Non-Linear Programming (MINLP) problem. A super-structure of flowsheet alternatives can be formulated, using integer variables and rigorous dynamic non-linear unit operation models. The objective is the minimization of a certain cost function. Plantwide controllability criteria can be added as additional constraints to assure a controllable plant design. Both the incorporation of controllability criteria and the use of optimization techniques in the conceptual design procedure will be covered in this thesis.

1.2 Motivation

The synthesis of complex processes with good controllability characteristics requires specific attention for the recycle structure. Convergence problems in steady state simulations may be caused by infeasible specifications in combination with recycle loops. Recycle interactions may also have a strong effect on dynamic behavior. Overall response times are much larger as a result of recycle loops and dead times may lead to resonant peaks in the frequency response. Two simple examples will demonstrate these effects.

![Figure 1.1; Simple flowsheet with reactor, separator and recycle loop](image)

The simulation will not converge if a purge flowrate is specified. A better specification is the ratio between purge and recycle or the recycle flowrate itself.
1—

**Figure 1.2; Plantwide control for make-up streams**

*A workable plantwide control structure is obtained if the make-up streams of both A and B are introduced in the recycle loops via a level control of the reflux drum, respectively the bottom of the separation columns, while recycle flowrates of A and B are fixed.*

### 1.2.1 Convergence problems in steady state modeling

Steady state simulations are confronted sometimes with very difficult convergence or non-convergence. These problems may originate from infeasible specifications at the flowsheet level, if the material balance is not respected, or strong interactions between recycle loops. It should be realized that flowsheeting problems might also reveal practical plantwide control problems. This is illustrated with a classical simple example.

Figure 1.1 shows a simple flowsheet. The reaction $A + B \rightarrow C$ is performed in a reactor R. The outlet mixture passes through a condenser, followed by the separation of the product from unconverted reactants being recycled. A purge is necessary because of impurities initially contained in reactants. The purge flowrate and the optimal A/B ratio in the reactor may be considered as specifications. A simulation exercise shows that it is difficult, if not impossible, to obtain convergence using these specifications. The situation improves when the purge flowrate is expressed as a ratio with respect to the recycle stream. Moreover, the convergence will be very easy when the recycle flowrate is fixed and the purge may vary freely.
Luyben (1993) therefore proposed an important generic rule for designing plants with recycle streams: 'fix some flowrate somewhere in the material balance recycle loop'. The make-up flow of reactants can then be 'regulated' with a controller to meet the reaction requirements and to compensate losses. This rule is illustrated by a plant where the reaction $A + B \rightarrow C$ takes place in a liquid phase reactor R (Figure 1.2). In S1 the unconverted reactant B is separated from the mixture A/C and recycled to the reactor. In S2 the product C is separated from the reactant A, which is also recycled. A workable plantwide control structure is obtained when the make-up streams of both A and B are fed into the recycle loops via a level control of the reflux drum, respectively the bottom of the separation columns, while recycle flowrates of A and B are fixed. Then changing the recycle flowrates can modify the throughput.

1.2.2 Recycle interaction effects on the dynamic behavior

The existence of a recycle may profoundly affect the dynamic behavior of a process. The overall plant response will have a longer characteristic time and a higher steady state gain than the individual elements (Denn and Lavie, 1982). This is illustrated by the following example.

Figure 1.3 shows the schematic representation of a closed loop system, where the forward process may be described by the second order transfer function:

$$G_f(s) = \frac{K_f}{\tau_f^2 s^2 + 2\xi_f \tau_f s + 1}$$  \hspace{1cm} (1.1)

while the recycle may be described by a first order transfer function with lag time:

$$G_r(s) = \frac{K_r e^{-T_d s}}{\tau_r s + 1}$$  \hspace{1cm} (1.2)

where $K_f$ forward process gain  
$\tau_f$ forward time constant  
$\xi_f$ forward damping factor  
$K_r$ recycle process gain  
$\tau_r$ recycle time constant  
$T_d$ recycle lag time

The closed loop process is then described by:

$$G(s) = \frac{G_f(s)}{1 - G_f(s)G_r(s)} = \frac{K_f (\tau_r s + 1)}{(\tau_f^2 s^2 + 2\xi_f \tau_f s + 1)(\tau_r s + 1) - K_r K_r e^{-T_d s}}$$  \hspace{1cm} (1.3)
Figure 1.3: Closed loop system with forward and recycle process

Figure 1.4 shows the response of this system for $K_f = 1$, $\tau_f = 1$, $\xi_f = 1$, $K_r = 0.5$ and several time constants ($\tau_r$) and lag times ($T_d$) of the recycle process. It can be seen that enlarging the recycle time constant considerably increases the global time constant and resonant peaks will appear if the recycle loop contains a long lag time.

Figure 1.4: Frequency responses of a closed loop system

When the recycle time constant is increased, the response starts to deviate from steady state at a lower frequency, which implies that the overall time constant is larger. When additionally the recycle lag time is increased, the overall time constant becomes even larger. The resonant peak around 0.31 rad/s is the result of interaction between the forward and the recycle processes. Around this frequency the recycle process oscillates in the same phase as the forward process. This enlarges the magnitude of the overall process. The peaks around 0.63 rad/s, 0.95 rad/s and higher frequencies are overtones. Their magnitudes decrease regularly by $1/e$. 
The examples given above suggest the idea that convergence difficulties in steady state flowsheeting, dynamic material balances and plantwide control problems are linked with each other. This has inspired us to get a deeper understanding of the controllability properties of a flowsheet, including the effect of recycles. It would be desirable to have quantitative tools to evaluate such effects. The use of rigorous simulation software would be also preferable, because this preserves the physical reality, particularly with respect to thermodynamics and details of design.

1.3 History

Gilliland et al. (1964) started in the early 60-ties the study of the basic couple in a flowsheet, the reactor/separato r system. They showed that the overall dynamics may strongly differ from the dynamic behavior of individual units. In general, it was found that a recycle increases the process response time as well as the sensitivity to disturbances (positive feedback). Later Verykios and Luyben (1978) considered the same problem with separation dynamics, demonstrating that the recycle may also exhibit an underdamped behavior. Denn and Lavie (1982) found that resonant peaks may occur in the frequency response when the recycle path contains a time delay, these peaks being of the same order of magnitude as the plant steady state gain. Papadurakis et al. (1987) also studied the simple reactor/separato r system and found that RGA for isolated units is insufficiently reliable to give a correct measure of interactions in the flowsheet.

Buckley (1974) has invented a first synthesis methodology for plantwide control systems based on the dynamics of the material balance, which proved to be fruitful in industry. Price has reported an improvement of this methodology with respect to throughput control (Price et al., 1994). Downs (1992) has demonstrated the importance of component inventory for plantwide control strategies. In this respect also the importance of purge placement (Joshi and Douglas, 1992) should be mentioned.

Luyben (1993) started a more systematic study on the rationale of recycle systems dynamics, demonstrating that recycle and reactant feed or make-up policies are interrelated. He proposed an important generic rule for designing plants with recycle streams: ‘fix some flowrate somewhere in the material balance recycle loop’. Consequently, new reactor feed procedures with superior operability properties may be considered. Luyben studied the application of these guidelines to more complex flowsheets (1995), finding that reaction steps and inventory regulation of intermediate species affect the operability. Some control
structures may have multiple steady states and produce closed-loop instability. All of these findings have recently been published in a first book about plantwide control (Luyben et al., 1999).


Although considerable progress has been reported in the sources mentioned, it is not obvious how to obtain profit from these tools in the design practice of complex plants. Not only analytical investigations using simplified models, but also industrial case studies with design and thermodynamic constraints should be employed as test cases in order to achieve a systematic methodology in integration of conceptual design and plantwide control. In addition it should be noticed that most of the work has been performed only on how to evaluate existing design alternatives, but little on how to design the plant in order to meet controllability and flexibility requirements. This remains a big challenge.

1.4 Outline of this thesis

In chapter 2 a description is given of a method where the traditional steady state design is combined with dynamic modeling and controllability analysis tools, both static and in the frequency domain. In addition to well-know controllability analysis tools as Relative Gain Array (RGA) and Singular Value Decomposition (SVD), new tools are introduced to analyze the performance of multivariable control structures in terms of controller errors. These tools are the Performance Relative Gain Array (PRGA), the Closed Loop Disturbance Gain (CLDG) and the Relative Disturbance Gain (RDG). They are applied in this thesis, for the first time, for plantwide control purposes. This is in contrast with previous studies, directed almost exclusively to individual units of equipment or academic exercises.

The systems approach renders simulations more profitable than the usual sensitivity studies do. Complex flowsheet structures and alternative control systems can be evaluated, controllability features can be improved by design modifications and finally the best flowsheet structure and control system alternative can be selected.
In chapter 3 the systems approach will be illustrated by a case study dealing with the dynamics of impurities in a complex Vinyl Chloride Monomer (VCM) plant. It is demonstrated how connectivity between units and interactions between recycles may be exploited to create flowsheet alternatives with plantwide control structures that would be infeasible in a stand-alone unit. The control structures may involve variables belonging to different parts of the plant. The controllability properties are determined by the competition between *positive feedback* effects, typically recycles, and *negative feedback* effects like exit streams and chemical reactors. In this example an extra reactor is introduced, where impurities that are difficult to handle are transformed into other components. Since these components are easily removed from the recycle, the closed loop performance of the system is improved with respect to disturbance rejection.

The introduction of the extra reactor in the VCM case study gives access to several alternative recycle structures. These structures and their controllability properties will be investigated in chapter 4. This will lead to a better understanding of the interaction between recycle loops and the effect of these interactions on the controllability of material balances. It will be shown that the recycle structure strongly affects the nominal operating point of the plant and how this will affect the controllability. Therefore, part of the discussion on recycle structures shifts to a discussion on nominal operating points, in particular the nominal values of the impurity levels.

The case studies show that through dynamic flowsheeting, with control features being incorporated, more essential design and operation knowledge is obtained. In addition, the large dynamic plant models give access to a whole class of controllability tools that usually are applied on small problems. Consequently, a large dynamic model requires an adequate *reduction* in size, which is not a trivial problem. This will be discussed in chapter 5.

Chapter 6 deals with a more rigorous approach to optimize complex flowsheet structures. Dynamic simulations may be combined with optimization techniques in order to find an optimal flowsheet structure, according to a certain objective function for a given set of design and control constraints. This objective function is most likely, but not necessary an economic function. The constraints will contain plantwide controllability criteria to ensure a controllable plant design. One option is to solve the dynamic model separately at each iteration of the optimization program. Another option is the direct approach, where the dynamic simulation problem is added to the optimization problem as a set of equality constraints. Dynamics are dealt with using discretization of the differential equations by a collocation technique. The discrete character of the problem is dealt with by formulating a
superstructure of flowsheet alternatives, expressed as models containing integer variables and rigorous dynamic nonlinear unit operation sub-models. This requires optimization techniques for discrete variables and thus finally the problem is reformulated as a dynamic MINLP problem. Both methods will be introduced and illustrated by some practical examples. Then a comparison is made and suggestions for improvement are given. Finally, the main results and conclusions from this thesis are collected in chapter 7.
Chapter 2

Systematic Approach of Plantwide Controllability

2.1 Introduction

Attempts to incorporate dynamics in the development of methods for process flowsheet synthesis are only scarce (Mohideen et al., 1996). Clearly, a systematic analysis of plantwide dynamics and controllability is difficult, in part due to the effect of recycles. As Luyben noted, ‘Processes with recycle streams are quite common but their dynamics poorly understood’ (Luyben, 1993). This is crucial in the context of zero discharge plants where even more material must be recycled. A complex plant may involve strong interactions between recycle loops that sometimes lead to a significant influence on the performance of individual units. Therefore, a real need exists to find a quantitative methodology for analyzing the effects of interactions. Flowsheeting is a well-established technique reflecting the complex system behavior by means of an accurate plant model (Dimian, 1994). The current practice in the analysis of large plants seems to be limited to the exploration of the operating window by extensive steady state flowsheeting. However, through dynamic flowsheeting and by incorporating control features, more and deeper design and operation knowledge is obtained. In addition, large dynamic plant models in principle give access to a whole class of controllability tools that usually are applied on small problems. This does require an adequate reduction of these models, which is not a trivial problem as will be discussed in chapter 5.

In this chapter a methodology will be presented where steady state and dynamic modeling are combined with controllability analysis tools. The objective of this approach is to have a quantitative measure of the performance of the plant according to reference tracking and
disturbance rejection in an early design stage. A better understanding of dynamic interactions between recycles is desired, which reveals design modifications with improved operability characteristics without using complex control strategies. The next chapter will demonstrate its use by means of a practical problem: the dynamics of the plant material balance, particularly of impurities.

2.2 Systems approach

Table 2.1 presents the systematic approach that we have developed for the combination of steady state flowsheeting with dynamic simulations and controllability analysis tools. This is applicable to both new design and revamp. Design freedom may be used to improve the controllability properties of the plant.

The approach starts with a definition of the objectives of the plant and identification of the inputs, outputs, targets and constraints. Subsequently, a rigorous steady state simulation model is developed. It is used to find a nominal operating point, where the system meets all targets and constraints. The input/output behavior is studied around this point by exploration of the operating window. At this stage a selection can be made of the variables that have to be controlled during operation and the variables that can be manipulated in a control structure. These variables are normally related to the design specifications and the design variables.

A very important aspect in the approach is scaling, as it makes model analysis and controller design much simpler. It also gives the possibility to compare different models (flowsheet and control alternatives). Thus, the engineer is obliged to make a judgement at the start of the design process about the required performance of the final system. Estimations have to be made of the expected magnitudes of disturbances and reference changes, of the allowed magnitude of each input signal, and of the allowed deviation of each output. The disturbances and reference values are scaled between their minimum and maximum expected values. The inputs and outputs are scaled on their minimum and maximum allowed values (Skogestad and Postlethwaite, 1996). Thus, all variables obtain values in the interval [-1,1]. This scaling simplifies the interpretation of controllability analysis tools. Apart from this, scaling is necessary for the tools that evaluate the performance of the closed loop dynamic system, as will be shown in section 2.4.4. A formal description of scaling will be given in section 2.3.3.

Extensive steady state simulations around the nominal operating point are performed to develop a static gain matrix. Steady state RGA and SVD analyses are used to evaluate the plantwide control structure alternatives. The Relative Gain Array (RGA) is a useful measure
Table 2.1: Systems Approach

1. Problem definition
   - Operating window
   - Inputs, Outputs, Targets, Constraints
2. Steady state flowsheeting
   - Rigorous modeling
   - Detailed material balance around nominal operating point
3. Plantwide control objectives
   - Control variables
   - Manipulated variables
   - Disturbances
   - Scaling
4. Steady state analysis
   - Static Gain calculations
   - Relative Gain Array (RGA) analysis
   - Singular Value Decomposition
     - Condition number
     - Morari Resiliency Index
   - Evaluation of control structure alternatives
5. Dynamic flowsheeting
   - Development of a reduced model, incorporating the
     main design and dynamic features of the complex
     plant detected by steady state analysis.
   - Dynamic responses of system on perturbations
6. Dynamic analysis
   - Development of a linear dynamic model as:
     set of transfer functions (identification method)
     state space description (model based)
   - Frequency analysis
     - Bode diagrams for stability and crossover frequencies
     - RGA and RGA number for control structure selection
     - PRGA, CLDG and RDG for controllability performance
   - Evaluation of control structure alternatives
   - Controller Design
7. Closed loop simulation
   - Implementation and (fine)tuning of controllers
   - Rigorous dynamic closed loop simulation
   - Evaluation of control structure alternatives
8. Design alternatives
   - Unit operations
   - Recycle structure alternatives
9. Conclusions
   - Flowsheet structure
   - Plantwide control strategy
of interactions between control loops. It may be used to select a combination of single-input-single-output controllers (multi-SISO structure) with minimal interaction. The Singular Value Decomposition (SVD) and related indices as the Condition Number (CN) and Morari Resiliency Index (MRI) give more information about the available control power and its directions. It can also be used to evaluate the power and direction of disturbances. An extensive description of these and other controllability tools will be given in section 2.4.

After exploration of the steady state plant model, the approach continues with the incorporation of dynamic features. To this end a rigorous dynamic simulation model has to be developed. Such a model should incorporate the main design and control features as detected by the steady state analysis. In addition, rigorous dynamic models also require information concerning equipment sizes and basic level and pressure controllers. Thus, certain extra decision variables are introduced, which are also available for optimization. The simulation model may be used to study the dynamic responses of the system on perturbations. One may detect time lags, inverse responses, overshoots and especially the different time scales at which the complex processes in a large plant are operating.

This preliminary study of the dynamic behavior will be followed by an extensive controllability analysis. Since dynamic models usually are too large and complex for a controllability analysis, they have to be simplified and linearized. A well-known method that is often used in practice is the curve fitting of experimental data with standard functions. Simple first and second order transfer functions often give already acceptable descriptions of the input-output behavior of complex systems, while high order polynomials can be used to give an accurate description. Extensive dynamic simulations can be used to generate the experimental data. The advantage of this method is that one can make small linear systems, which are easy to handle. However, the whole procedure can be very time consuming, especially when experimental data have to be generated by extensive dynamic simulations.

When a dynamic model is available, it is much easier to generate a linear state space description by performing a Taylor series expansion of the nonlinear functions around the nominal operating point, neglecting second and higher order terms. Modern dynamic simulation programs like SPEEDUP™ have such a feature. In a state space description the input and output variables are interconnected through the states.

An automatic linearization procedure will include all states from the complex nonlinear model and the linear state space realization may become very large and difficult to handle. Therefore a real need exists to reduce a state space realization to lower order. This topic will be discussed in chapter 5.
The controllability analysis starts with a study of the Bode diagrams, being representations of the dynamic responses of the linearized system to oscillatory perturbations as a function of its frequency. These plots show the locations where the dynamic behavior of the plant starts to differ from steady state as well as the crossover frequencies, up to which feedback control should be active. In order to study the closed loop behavior, a certain control structure has to be assumed. In this approach a decentralized control structure is selected, containing only control loops with one input and one output. Furthermore, the inputs and outputs are arranged such that the proportional gains in the corresponding controller matrix are on the diagonal, which explains the synonym 'diagonal' control. The RGA number is used to see whether the preferred diagonal control structure as inferred from the steady state analyses holds well over the whole frequency range of interest. The Performance Relative Gain Array (PRGA), Closed Loop Disturbance Gain (CLDG) and Relative Disturbance Gain (RDG) are used as indicators for the performance of the diagonal control structure according to reference (setpoint) tracking and disturbance rejection. They are also used to design the controllers and find appropriate settings (gains, integral times). Interactions between the controllers in a diagonal structure are also taken into account by these indicators. A detailed description of diagonal feedback control and the relevant controllability tools, based on Skogestad and Postlethwaite (1996) will be given in section 2.4.4.

The controllability analysis is supposed to produce an optimal control structure. This structure is implemented in the nonlinear dynamic model. The controller settings that are indicated by the controllability analysis are a good starting value. However, they are based on the linearized model and therefore need to be fine-tuned first. Then a closed loop simulation can be performed to check the conclusions of the controllability analysis.

Analyzing and understanding the dynamic behavior of a model generates suggestions for improvement. The basic plant design may be modified and several flowsheet alternatives may be generated. The procedure described can be applied on all these alternatives, finally yielding an optimal flowsheet design and plantwide control strategy.

### 2.3 Modeling

Models play a key role in the systems approach that is described in this chapter. Rigorous steady state and dynamic models are used for simulations and the controllability analysis is performed on their linearized versions. A brief description of models and linearization, including the scaling procedure, is given in this section. It is beyond the scope of this part to
give a complete description of each unit operation model, steady state or dynamic, and the thermodynamic equations that they use. The models are normally available in simulation software tools like Aspen Plus™ and Speedup™. The interested reader is referred to specialized books like ‘The Properties of Gases and Liquids’ from Reid, Prausnitz & Poling or the ‘Chemical Engineering’ series of Coulson & Richardson for more details.

2.3.1 Steady state models

A nonlinear steady state model can be represented by the following sets of equations:

\[
\begin{align*}
  f(x, u) &= 0, \\
  y &= g(x, u)
\end{align*}
\]  

(2.1)

where \( f \) and \( g \) are general nonlinear functions, \( x \) a vector containing \( n \) state variables, \( u \) a vector containing \( m \) input variables and \( y \) a vector containing \( l \) output variables. In general \( f \) contains the material and energy balances and \( g \) contains the output relations.

The static gain matrix \( G \) is a linear steady state input-output model around the nominal operating point. Each element \( g_{ij} \) in this matrix stands for the change in an output variable \( y_i \) after a unit step on an input variable \( u_j \).

\[
\begin{align*}
  g_{ij} &= \frac{\Delta y_i}{\Delta u_j}, \\
  \Delta y_i &= g_{ij} \Delta u_j
\end{align*}
\]  

(2.2)

where \( \Delta y_i = y_i - y_i^{\text{nominal}} \) and \( \Delta u_j = u_j - u_j^{\text{nominal}} \)

The static gain matrix does not contain state variables.

Usually, the static gain matrix is restricted to controlled variables as outputs and manipulated variables as inputs. Another group of input variables is formed by the disturbances. They may be stored in a vector \( d \) of length \( k \). The linear steady state model that connects these disturbances to the outputs is known as the static disturbance gain matrix \( G_d \). Its elements \( g_{dik} \) are given by:

\[
\begin{align*}
  g_{dik} &= \frac{\Delta y_i}{\Delta d_k}, \\
  \Delta y_i &= g_{dik} \Delta d_k
\end{align*}
\]  

(2.3)

where \( \Delta d_k = d_k - d_k^{\text{nominal}} \)
A complete steady state linear model will be given by:

\[ y = Gu + G_d d \]  
(2.4)

where \( y \) is a vector with the deviations of the controlled output variables \( \Delta y_i \), \( u \) a vector with the changes in manipulated variables \( \Delta u_j \) and \( d \) a vector containing the changes in disturbances \( \Delta d_k \). \( G \) and \( G_d \) are the static gain, respectively the static disturbance gain matrix. This model is expressed in absolute values, centered on the nominal operating point.

### 2.3.2 Dynamic models

A dynamic nonlinear model can be represented by the following sets of equations:

\[ \dot{x} = f(x, u), \quad y = g(x, u) \]  
(2.5)

where \( \dot{x} = dx/dt \), \( f \) and \( g \) are general nonlinear functions, \( x \) a vector containing \( n \) state-variables, \( u \) a vector containing \( m \) input variables and \( y \) a vector containing \( l \) output variables. In general \( f \) contains the material and energy balances and \( g \) contains the output relations. The only real difference between the models (2.1) and (2.5) is the time derivative of the state variables. In a steady state model this is zero by definition, while it may and normally will have a non-zero value in a dynamic model.

A linear representation of a dynamic model may be given by a state space description:

\[
\begin{align*}
\dot{x}(t) &= Ax(t) + Bu(t) \\
y(t) &= Cx(t) + Du(t)
\end{align*}
\]  
(2.6)

Here \( A, B, C \) and \( D \) are real matrices:

\[
A = \frac{\partial x}{\partial x}, \quad B = \frac{\partial x}{\partial u}, \quad C = \frac{\partial y}{\partial x}, \quad D = \frac{\partial y}{\partial u}
\]  
(2.7)

and \( x, u \) and \( y \) are deviations of a certain nominal value. A state space realization describes the input-output behavior through the states.

By Laplace transformation of the state space realization (2.6), a linear input-output model around the nominal operating point may be generated where the states are eliminated:

\[ y(s) = G(s)u(s) \]  
(2.8)
The transfer function model $G(s)$ in terms of $A$, $B$, $C$ and $D$ is given by:

$$G(s) = C(sI - A)^{-1}B + D \quad (2.9)$$

and $s$ is the Laplace operator. For $s = 0$, and therefore $t = 1/s = \infty$, the steady state transfer function model $G(0) = G$ is returned. With $s = j\omega$ ($j^2 = -1$), the dynamic response of the system may be calculated as function of the frequency $\omega$.

When the input variables are divided again into manipulated variables and disturbances, the state space realization (2.6) is extended to:

$$\begin{align*}
\dot{x}(t) &= Ax(t) + Bu(t) + Ed(t) \\
y(t) &= Cx(t) + Du(t) + Fd(t)
\end{align*} \quad (2.10)$$

Here the disturbance terms $E$ and $F$ are defined by:

$$\begin{align*}
E &= \frac{\partial \tilde{y}}{\partial \tilde{d}}, \\
F &= \frac{\partial \tilde{y}}{\partial \tilde{d}}
\end{align*} \quad (2.11)$$

The disturbance transfer function model $G_d(s)$ in terms of $A$, $C$, $E$ and $F$ is given by:

$$G_d(s) = C(sI - A)^{-1}E + F \quad (2.12)$$

A complete dynamic linear model in Laplace form follows as:

$$y(s) = G(s)u(s) + G_d(s)d(s) \quad (2.13)$$

Both the state space notation and the Laplace form will be used in the remainder of this thesis. They are related to each other by equations (2.9) and (2.12).

### 2.3.3 Scaling

A very important aspect of the approach is scaling, which simplifies model analysis and controller design and gives the possibility to compare different flowsheet and control alternatives. The scaling procedure is presented in this section, followed by a discussion on the controllability analysis tools in section 2.4.

Let the unscaled linear model of the process in deviation variables be

$$\begin{align*}
\tilde{y} &= \tilde{G}\tilde{u} + \tilde{G}_d\tilde{d}, \\
\dot{\tilde{e}} &= \tilde{y} - \tilde{r}
\end{align*} \quad (2.14)$$
where \( u \) are the inputs, \( d \) the disturbances, \( y \) the outputs, \( e \) the errors and \( r \) the reference values. \( G \) represents the input-output model and \( G_d \) the disturbance model. They may be either static gain matrices or dynamic transfer functions. The scaling procedure is indifferent to that. A hat (\(^\wedge\)) is used to show that the variables are in their unscaled units.

A useful approach for scaling is to make the variables less than one in magnitude by dividing each variable through its maximum allowed or expected change. For manipulated variables and disturbances, we use the scaled variables:

\[
\text{ud} = \frac{\text{u}}{\text{u}_{\text{max}}}, \quad \text{dd} = \frac{\text{d}}{\text{d}_{\text{max}}} \quad (2.15)
\]

where \( \text{u}_{\text{max}} \) is the largest allowed change of the manipulated variable and \( \text{d}_{\text{max}} \) is the largest expected change in disturbance. As the largest change allowed the smallest absolute value of the maximum increase and the maximum decrease relative to the nominal operating value is taken, while for the maximum expected change the largest value of the two is assumed.

The variables \( \text{y} \), \( \text{e} \) and \( \text{r} \) are in the same units, so the same scaling factor should be used. Two alternatives are possible: \( \text{e}_{\text{max}} \) is the largest allowed control error, \( \text{r}_{\text{max}} \) is the largest expected change in reference value (setpoint). Since a major objective of control is to minimize the control error \( \text{e} \), one usually chooses to scale with respect to the maximum control error:

\[
y = \frac{\text{y}}{\text{e}_{\text{max}}}, \quad \text{e} = \frac{\text{e}}{\text{e}_{\text{max}}}, \quad \text{r} = \frac{\text{r}}{\text{e}_{\text{max}}} \quad (2.16)
\]

To formalize the scaling procedure, the following scaling factors are introduced:

\[
\text{D}_u = \frac{\text{u}_{\text{max}}}{\text{u}}, \quad \text{D}_d = \frac{\text{d}_{\text{max}}}{\text{d}}, \quad \text{D}_e = \frac{\text{e}_{\text{max}}}{\text{e}}, \quad \text{D}_r = \frac{\text{r}_{\text{max}}}{\text{r}} \quad (2.17)
\]

For MIMO systems each variable in the vectors \( \text{u} \), \( \text{d} \), \( \text{e} \) and \( \text{r} \) may have different maximum values, in which case \( \text{D}_u \), \( \text{D}_d \), \( \text{D}_e \) and \( \text{D}_r \) become diagonal scaling matrices.

The corresponding scaled variables to use for control purposes are thus:

\[
d = \text{D}_d^{-1} \text{d}, \quad u = \text{D}_u^{-1} \text{u}, \quad y = \text{D}_e^{-1} \text{y} \quad \text{e} = \text{D}_e^{-1} \text{e} \quad \text{r} = \text{D}_r^{-1} \text{r} \quad (2.18)
\]

and introducing the scaled transfer functions
\[ G = D_e^{-1}D_u \quad \text{and} \quad G_d = D_e^{-1}D_d \]  

yields the following model in terms of scaled deviation variables:

\[ y = G u + G_d d, \quad e = y - r \]

Here, \( u \), \( d \) and \( e \) should be less than or equal to 1 in magnitude.

Use of the scaling factors from (2.17) and \( D_x \) as scaling factor of the states will result in the following scaling procedure for the state space matrixes:

\[
\begin{align*}
A &= D_x^{-1}D_x \\
B &= D_x^{-1}D_u \\
C &= D_e^{-1}C_D_x \\
D &= D_e^{-1}D_u \\
E &= D_x^{-1}D_d \\
F &= D_e^{-1}D_d
\end{align*}
\]  

Scaling of the state variables may improve the model, but normally this step will be omitted. Instead of \( D_e \) one might use \( D_r \) for scaling on reference values. Then \( r \) should be less than or equal to 1 in magnitude.

### 2.4 Controllability tools

Once the plant model, either steady state or dynamic, is linearized and scaled, a controllability analysis may be performed. The use of controllability measures as evaluation tools in Conceptual Design has been promoted by several authors (Barton et al., 1991, Mizsey and Fonyo, 1991, Lyman and Georgakis, 1995, Morud and Skogestad, 1993, Wolff and Skogestad, 1992). They may give valuable information of the (dynamic) behavior and controllability of a system that is hard to find with simulations only. The tools being used in the systems approach will be described in this section. It is mainly based on the book of Skogestad and Postlethwaite (1996), presenting an overview of multivariable feedback control and relevant controllability analysis tools.

#### 2.4.1 The Relative Gain Array

A useful measure of interaction between input and output is given by the relative gain. Consider the open loop static gain, the change \( \Delta y_i \) in output \( y_i \) relative to a change \( \Delta u_j \) in input \( u_j \) where all other inputs remain constant.
\[
\begin{pmatrix}
\Delta y_i \\
\Delta u_j
\end{pmatrix}
\bigg|_{u_{m\neq j} = 0}
\tag{2.22}
\]

In this case the other outputs may or may not change. Another open loop gain is defined as the change \(\Delta y_i\) in output \(y_i\) relative to a change \(\Delta u_j\) in input \(u_j\) where all other outputs remain constant. Again, the other inputs may or may not have to be changed.

\[
\begin{pmatrix}
\Delta y_i \\
\Delta u_j
\end{pmatrix}
\bigg|_{y_{\neq i} = 0}
\tag{2.23}
\]

The ratio between these two open loop gains defines the relative gain \(\lambda_{ij}\), between output \(y_i\) and input \(u_j\):

\[
\lambda_{ij} = \frac{\begin{pmatrix}
\Delta y_i \\
\Delta u_j
\end{pmatrix}
\bigg|_{u_{m\neq j} = 0}}{\begin{pmatrix}
\Delta y_i \\
\Delta u_j
\end{pmatrix}
\bigg|_{y_{\neq i} = 0}}
\tag{2.24}
\]

If \(\lambda_{ij} = 0\), then \(y_i\) does not respond to \(u_j\) and \(u_j\) should not be used to control \(y_i\). On the other hand, if \(\lambda_{ij} = 1\), then \(y_i\) does not respond to any other \(u_{m\neq j}\) and the loop between \(y_i\) and \(u_j\) is not affected by other loops. This is the preferred case. If \(0 < \lambda_{ij} < 1\) or \(\lambda_{ij} > 1\), then interaction is present between \(y_i\) and the other \(u_{m\neq j}\). The stronger \(\lambda_{ij}\) deviates from 1, the larger the interaction. If \(\lambda_{ij} < 0\), then \(y_i\) is strongly affected by the other \(u_{m\neq j}\) in opposite direction, caused by \(u_j\). This may give rise to instabilities and therefore one should avoid such pairing.

The Relative Gain Array (RGA) is a square matrix containing the relative gains between all inputs and outputs. It can be shown that the sum of the relative gains in any row or column of the array is equal to 1. From the RGA we select the control loops by pairing the controlled outputs \(y_i\) with the manipulated inputs \(u_j\) in such a way that the relative gains \(\lambda_{ij}\) are positive and as close as possible to unity.

\[
\Lambda = \begin{bmatrix}
u_1 & u_2 & \cdots & u_n \\
\lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n} \\
\lambda_{21} & \ddots & & \\
\vdots & & \ddots & \\
\lambda_{n1} & \cdots & \lambda_{nn}
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2 \\
\vdots \\
y_n
\end{bmatrix}
\tag{2.25}
\]
If we have the static gain matrix $G$ of a system, the relative gain array of this system, $\text{RGA}(G)$, can be calculated as:

$$ \text{RGA}(G) = \Lambda(G) \triangleq G \times (G^{-1})^T $$

(2.26)

where the operation $\times$ stand for element by element multiplication and $^T$ for the matrix transpose. The relative gain array is independent of scaling. For non-square systems, the system has to be split into a number of square subsystems each to be evaluated separately.

**2.4.1.1 RGA number**

Using the steady state relative gain array for selecting control loops does not warrant that the dynamic interaction between the loops is also minimal. Therefore the dynamic relative gains have to be examined, i.e. the relative gains as a function of frequency. Calculating relative gain elements as a function of frequency leads to complex numbers to be dealt with either by taking the absolute value of the complex relative gains or taking the real part only. Since the real parts of the relative gains in any row or column obey the summation equal to one, as it is in the steady state RGA, it seems logical to take the real parts as measure of the interaction between control loops and ignore the imaginary part. On the other hand, the magnitude of the gains is given by the absolute value. However, the sign is lost in that case meaning a loss of information about the direction of the interactions.

These problems are overcome when using the RGA number, defined as the sum norm (sum of the absolute values of all elements) of the RGA matrix minus the identity matrix:

$$ \| \text{RGA} - I \|_{\text{sum}} $$

(2.27)

The identity matrix is the ideal RGA matrix if the inputs and outputs are arranged such that the preferred parings are on the diagonal. The RGA number therefore gives a quantitative measure of non-ideality of the RGA matrix and can be used to check whether the steady state pairing holds well over that part of the frequency range where control is needed.

**2.4.2 Singular Value Decomposition**

Any complex $l \times m$ matrix $G$ may be factorized into a singular value decomposition:

$$ G = U \Sigma V^H $$

(2.28)
The \( l \times l \) unitary matrix \( U \) contains the output singular vectors \( u_j \), the \( m \times m \) unitary matrix \( V \) contains the singular input vectors \( v_i \), and the \( l \times m \) matrix \( \Sigma \) contains a diagonal matrix of \( k = \min\{l,m\} \) real non-negative singular values, \( \sigma_i \), arranged in a descending order. The other singular values are zero.

The singular values are the positive square roots of the eigenvalues of \( G^H G \), where \( G^H \) is the complex conjugate transpose (Hamiltonian) of \( G \).

\[
\sigma_i(G) = \sqrt{\lambda_i(G^H G)} \tag{2.29}
\]

The columns of \( U \), denoted \( u_i \), represent the output directions of the plant and the columns of \( V \), denoted \( v_i \), represent the input directions. These input and output directions are related through the singular values. Since \( V \) is unitary, we have \( V^H V = I \), so (2.28) may be written as \( GV = U \Sigma \), which for column \( i \) becomes

\[
Gv_i = \sigma_i u_i \tag{2.30}
\]

where \( v_i \) and \( u_i \) are vectors and \( \sigma_i \) is a scalar. That is, when considering an input in the direction \( v_i \), then the output is in the direction \( u_i \) and the gain of the matrix \( G \) in this direction is given by the singular value \( \sigma_i \).

The largest gain for any input direction \( d \) is therefore equal to the maximum singular value:

\[
\sigma(G) = \sigma_1(G) = \max_{d \neq 0} \frac{\|Gd\|_2}{\|d\|_2} = \frac{\|Gv_1\|_2}{\|v_1\|_2} \tag{2.31}
\]

and the smallest gain for any input direction \( d \) is equal to the minimum singular value:

\[
\sigma(G) = \sigma_k(G) = \min_{d \neq 0} \frac{\|Gd\|_2}{\|d\|_2} = \frac{\|Gv_k\|_2}{\|v_k\|_2} \tag{2.32}
\]

where \( k = \min\{l,m\} \). Thus, for any input vector \( d \) we have:

\[
\sigma(G) \leq \frac{\|Gd\|_2}{\|d\|_2} \leq \sigma(G) \tag{2.33}
\]

Define \( u_1 = \bar{u} \), \( v_1 = \bar{v} \), \( u_k = u \) and \( v_k = v \). Then it follows that

\[
G \bar{v} = \bar{\sigma} \bar{u} \quad \text{and} \quad Gv = \sigma u \tag{2.34}
\]
The vector $\vec{v}$ corresponds to the input direction with the largest amplification, and $\vec{u}$ is the corresponding output direction in which the inputs are most effective. The directions involving $\vec{v}$ and $\vec{u}$ are sometimes referred to as the "strongest", "high-gain" or "most important" directions. The "least important", "weakest" or "low-gain" directions are associated with $\vec{y}$ and $\vec{u}$.

### 2.4.2.1 Condition Number

A system is said to be well-conditioned if all output directions can be realized with roughly the same effort of the inputs. This can be quantified by the condition number (CN); the ratio between the gains in the strong and weak directions.

$$CN = \frac{\sigma}{\sigma'}$$  \hspace{1cm} (2.35)

A high condition number means that the system is ill conditioned, that is, some combinations of the inputs have a strong effect on the outputs, whereas other combinations have a weak effect on the outputs. A condition number close to one is therefore preferable.

### 2.4.2.2 Morari Resiliency Index

The minimum singular value of the plant, $\sigma(G)$, is a useful measure for evaluating the feasibility of achieving acceptable control. If the inputs and outputs have been scaled between [-1,1] (SVD is scaling dependent), then with an input of unit magnitude an output magnitude of at least $\sigma(G)$ may be achieved in any output direction. In particular, if $\sigma(G) > 1$, the complete operating range of any output is covered within that of the operating range of any input. Preferably, $\sigma(G)$ is as large as possible. The quantity $\sigma(G)$ is known as the "Morari resiliency index".

### 2.4.2.3 Disturbances

The static disturbance gain matrix $G_d$ is defined as a linear model that connects the disturbances to the outputs. If $G_d$ is factorized into its singular values, a measure is obtained of the effect of the disturbances on the outputs. A large disturbance condition number means that some combinations of disturbances strongly affect the outputs whereas other combinations of disturbances only slightly affect the outputs. If all singular values of a properly scaled $G_d$ are below one, then not any combination of disturbances exists that will bring the outputs outside their upper and lower values and therefore no disturbance rejection control is needed.
2.4.2.4 Non-square systems

The SVD is also useful for non-square systems. If there are more outputs than inputs, the remaining output singular vectors indicate in which directions the system cannot be controlled or which output directions are not affected by the disturbances. If there are more inputs than outputs, the remaining input singular vectors show in which directions the input will have no effect.

2.4.2.5 Dynamic systems

For dynamic systems the singular values and their associated directions vary with frequency. The singular values are usually plotted as function of frequency in a Bode magnitude plot with a log-scale for magnitude and frequency.

2.4.3 Feedback control

Consider the linear dynamic plant model from (2.13):

\[ y(s) = G(s)u(s) + G_d(s)d(s) \quad (2.13) \]

where \( G(s) \) is the input-output system, \( u \) a vector with inputs, \( G_d(s) \) is the disturbance system, \( d \) a vector with disturbances and \( y \) a vector with outputs. Consider also a controller model \( K(s) \) with input \( r(s) - y(s) \), where \( r \) is the reference value (setpoint) and \( y \) is the measured output. The input to the plant is then given by:

\[ u(s) = K(s)(r(s) - y(s)) \quad (2.36) \]

Substitution of (2.36) in (2.13) and rearrangement gives the closed-loop model:

\[ y(s) = (I + G(s)K(s))^{-1}G(s)K(s)r(s) + (I + G(s)K(s))^{-1}G_d(s)d(s) \quad (2.37) \]

or, in shorter notation:

\[ y = Tr + SG_d \quad (2.38) \]

The error becomes then:

\[ e = y - r = -Sr + SG_d \quad (2.39) \]

where use is made of the following notation and terminology:

- \( L = GK \) loop transfer function
- \( S = (I + GK)^{-1} = (I + L)^{-1} \) sensitivity function
\[ T = (I + GK)^{-1}GK = (I + L)^{-1}L \]  
complementary sensitivity function

and the fact that \( S + T = I \). \( S \) can be identified as the closed loop transfer function from the disturbances to the outputs, while \( T \) is the closed loop transfer function from the reference signals to the outputs. By using controllers, the error \( e \) should become as small as possible and therefore the sensitivity function \( S \) should be small for feedback control to be effective.

### 2.4.3.1 Bandwidth

The frequency range \([\omega_1, \omega_2]\) over which feedback control will be effective is called the bandwidth. Normally, tight control at steady state is needed, so \( \omega_1 = 0 \) and then \( \omega_2 = \omega_b \) is simply called the bandwidth.

For reference tracking performance of a SISO system, the relative error is \( |e(j\omega)| / |r(j\omega)| = |S(j\omega)| \) (see 2.39), and the bandwidth is taken as the frequency where \( |S(j\omega)| \) first crosses \( 1/\sqrt{2} \approx 0.707 \) (\(-3\) dB) from below. A large bandwidth corresponds to a faster rise time, since high frequencies are more easily passed on to the outputs. With a small bandwidth, the time-response will be slow, but the system will usually be more robust.

For MIMO systems, the ratio \( ||e(j\omega)||_2 / ||r(j\omega)||_2 \) is considered, where \( r \) is a vector containing the reference values, \( e \) is a vector containing the control errors and \( || \cdot ||_2 \) is the vector 2-norm. The ratio depends on the direction of \( r(j\omega) \) and according to (2.33) it is bounded by the maximum and minimum singular values of \( S \),

\[
\sigma(S) \leq \frac{||e(j\omega)||_2}{||r(j\omega)||_2} \leq \sigma(S) \tag{2.40}
\]

In terms of performance, it is reasonable to require that the ratio is small for any direction of \( r(\omega) \), including the "worst-case" direction, which gives a ratio equal to the maximum singular value of \( S \). The bandwidth will depend on the directions and we have a bandwidth region between a lower frequency where the maximum singular value reaches 0.7, and a higher frequency where the lower singular value reaches 0.7.

### 2.4.3.2 Crossover frequency

Another important frequency is the phase crossover frequency, \( \omega_{180} \), defined as the first frequency where the phase lag of the response to an oscillatory input is half a period. This frequency is used in the definition of the gain margin:

\[
GM = 1/|L(j\omega_{180})| \tag{2.41}
\]
The gain margin is the factor by which the loop gain $|L(j\omega)|$ may be increased before the closed-loop system becomes unstable. Notice that $L = GK$, so the loop gain may be increased by increasing the controller gain $K$ and therefore the gain margin is the maximum controller gain. The question is whether this gain will be enough for reference tracking and disturbance rejection, keeping the error below its bounds. Therefore we need to know the minimum controller gain that is needed to keep the error below its bounds under reference changes and disturbances. This will be discussed next.

### 2.4.4 Decentralized feedback control

A special structure of feedback controllers is formed when each output is controlled with only one input and each input is used to control only one output. This combination of single-input single-output controllers is called a decentralized feedback control structure. Usually, the inputs and outputs are arranged such that the models in the corresponding controller matrix are on the diagonal, which explains the term *diagonal* control.

Consider again the $m \times m$ square plant $G(s)$ that has to be controlled using a diagonal controller structure:

$$K(s) = \text{diag}\{k_i(s)\} = \begin{bmatrix} k_1(s) & & \\ & k_2(s) & \\ & & \ddots \\ & & & k_m(s) \end{bmatrix}$$ \hfill (2.42)

If $G(s)$ is rearranged such that the paired elements are along the diagonal of $G(s)$, then:

$$\tilde{G}(s) = \text{diag}\{g_{ii}(s)\} = \begin{bmatrix} g_{11}(s) \\ g_{22}(s) \\ \vdots \\ g_{mm}(s) \end{bmatrix}$$ \hfill (2.43)

The loop transfer function in loop $i$ is denoted $L_i = g_{ii}k_i$, while $L = GK$.

The magnitude of the off-diagonal elements of $G(s)$ (the interactions) relative to its diagonal elements are given by the matrix

$$E = (G - \tilde{G})\tilde{G}^{-1}$$ \hfill (2.44)
A very important relationship for decentralized control is given by the following factorization of the return difference operator:

\[
(I + GK) = (I + \tilde{G}K) (I + E\tilde{T})
\tag{2.45}
\]

or, in terms of the sensitivity function \( S = (I + GK)^{-1} \),

\[
S = \tilde{S}(I + E\tilde{T})^{-1}
\tag{2.46}
\]

where

\[
\tilde{S} = (I + \tilde{G}K)^{-1} = \text{diag}\left\{ \frac{1}{1 + g_{ii}k_i} \right\}
\]

and

\[
\tilde{T} = I - \tilde{S}
\tag{2.47}
\]

are the sensitivity and complementary sensitivity functions for the individual loops. It is important to notice that the elements of these two matrices are different from the diagonal elements of the full sensitivity and complementary sensitivity functions \( S \) and \( T \) in themselves.

### 2.4.4.1 Performance Relative Gain Array

An alternative factorization is given by:

\[
S = (I + \tilde{S}(\Gamma - I))^{-1}\tilde{S}\Gamma
\tag{2.48}
\]

where \( \Gamma \) is the performance relative gain array (PRGA):

\[
\Gamma(s) = \tilde{G}(s)G^{-1}(s)
\tag{2.49}
\]

which is a scaled inverse of the plant. Notice that, in terms of the PRGA, \( E = \Gamma^{-1} - I \).

The diagonal elements of the PRGA are equal to the diagonal elements of the RGA, but the off-diagonal elements are dependent on the relative scaling of the outputs, whereas RGA is scaling independent. On the other hand, the PRGA measures also one-way interactions, whereas the RGA only measures two-way interactions.

### 2.4.4.2 Closed Loop Disturbance Gain

Related to the PRGA is the closed loop disturbance gain (CLDG) matrix, defined as:

\[
\tilde{G}_d(s) = \Gamma(s)G_d(s) = \tilde{G}(s)G^{-1}(s)G_d(s)
\tag{2.50}
\]

The CLDG depends on both output and disturbance scaling.
2.4.4.3 Closed loop error

At frequencies where feedback control is active, $S \approx 0$, and from (2.48) we have $S \approx \tilde{S}\Gamma$. The closed loop error (2.39) then becomes:

$$e = SG_d d - Sr \approx \tilde{S}G_d d - \tilde{S}\Gamma r$$

(2.51)

and the response on output $i$ to a single disturbance $d_k$ and a single reference input $r_j$ is

$$e_i = \tilde{s}_i \tilde{g}_{ dik} d_k - \tilde{s}_i \gamma_{ ik} r_k$$

(2.52)

where $\tilde{s}_i = 1/(1 + g_{ij} k_i)$ is the sensitivity function for loop $i$ by itself. For acceptable disturbance rejection, $|e_i|<1$ for $|d_k|=1$, so we must require $|\tilde{s}_i \tilde{g}_{ dik} d_k|<1$ and therefore:

$$|1 + L_i| > |\tilde{g}_{ dik}| \forall i$$

(2.53)

Similarly, to achieve reference tracking, $|e_i|<1$ for $|r_j|=|R_j|$, so we must require $|\tilde{s}_i \gamma_{ ik} R_j|<1$ and therefore:

$$|1 + L_i| > |\gamma_{ ik} | |R_j| \forall i$$

(2.54)

From these two inequality constraints, the minimum controller gains can directly be determined to achieve acceptable reference tracking and disturbance rejection, since $L=GK$. Meanwhile, it should be kept in mind that in the same time the gain margin has to be respected to assure that the closed loop system will be stable.

2.4.4.4 Relative Disturbance Gain

The relative disturbance gain (RDG) $\beta_i$ is the ratio between $\tilde{g}_{ di}$ (CLDG) and $g_{ di}$, where $g_{ di}$ is the effect of a disturbance $g_d$ on output $i$ with no control.

$$\beta_i = \frac{\tilde{g}_{ di}}{g_{ di}} = \left[ \frac{GG^{-1}g_d}{[g_d]} \right]_{ii}$$

(2.55)

Thus $\beta_i$, which is scaling independent, gives the change in the effect of the disturbance caused by decentralized feedback control. If $\beta_i$ is small, the interactions are such that they reduce the apparent effect of the disturbance in such a way that high gains in the individual loops are not required.
The discussion above shows that PRGA, CLDG and RDG are important indicators in analyzing the closed loop performance of decentralized control systems. A discussion about the interpretation of these indicators will be given in the next chapter, where their use is illustrated by an example.

2.5 Controllability analysis

When considering decentralized (diagonal) control of a plant, the first step is to compute the RGA-matrix as a function of frequency and to determine an adequate set of input-output pairs, while keeping in mind the following aspects:

- Prefer pairings yielding the RGA-matrix close to identity at frequencies around crossover to ensure that interactions from other loops do not cause instability.
- Avoid a pairing with a negative steady state relative gain to assure tight control at low frequencies.
- Prefer a pairing \( i,j \) where \( g_{ij} \) puts minimal restrictions on the achievable bandwidth. Specifically, the phase crossover frequency of \( g_{ij} \) should be as large as possible. This gives the largest possible gain margin on \( L_i \) and therefore more easily achieves acceptable disturbance rejection and reference tracking while in the same time realizing stability.

The transfer function matrix \( G \) should then be rearranged to have the pairings along the diagonal, so a controllability analysis can be performed.

1. Compute the PRGA and the CLDG, and plot these as function of frequency.

2. For systems with many loops, it is best to analyze one loop at a time. So, for each loop \( i \), plot \( |\tilde{g}_{dk}| \) (CLDG) for each disturbance \( k \) and plot \( |\gamma_{ij}| \) (PRGA) for each reference \( j \) (assuming here that each reference is of unit magnitude). For performance, \( |1 + L_i| \) needs to be larger than each of these.

\[
\text{Performance: } \quad |1 + L_i| > \max_{k,j} \left( \left| \tilde{g}_{dk} \right|, \left| \gamma_{ij} \right| \right) \tag{2.56}
\]
In order to achieve stability of each individual loop, the performance bandwidth must be feasible. The attainable bandwidth in each loop will be limited by the phase crossover frequency in the bode-plot of $g_{ii}(s)$ ($\angle g_{ii} = -180^\circ$).

3. In order to avoid input constraints, the input magnitude should be large enough to reject all disturbances and therefore

$$|g_{ii}| > |\tilde{g}_{di_k}| \forall k \quad (2.57)$$

at frequencies where control is needed ($|\tilde{g}_{di_k}|$ larger than 1).

If the plant is not controllable, then one may consider another choice of pairings and perform a controllability analysis of the new pairings.

4. If the pairing is controllable then (2.56) directly yields the required magnitude of $|L_i| = |g_{ii}k_i|$, which can be used as a basis for designing the controller $k_i(s)$ for loop $i$.

### 2.6 Conclusions

The simulation-based methodology that is presented in this chapter may be used during the conceptual design to develop an optimal flowsheet structure of a complex chemical plant with good plantwide controllability properties. The objective of this systems approach is to have a quantitative measure of the performance of the plant according to reference tracking and disturbance rejection in an early design stage. A better understanding of dynamic interactions between the units and recycle streams may lead to suggestions for design modifications with improved operability characteristics without using complex control strategies. This will be demonstrated in the next chapter by a practical problem: the dynamics of the plant material balance, particularly of impurities.
Chapter 3

Plantwide Controllability of Impurities in a Plant with Recycles

3.1 Introduction

Recycle loops strongly affect dynamics and control of a complex plant. The stability of control structures for component inventories may be influenced by recycle interactions and by connectivity, which leads to flowsheet alternatives possessing different control properties. The previous chapter presented a simulation-based methodology for evaluating these phenomena and finding the best flowsheet structure from controllability point of view. Steady state and dynamic simulations are combined with controllability analysis tools, both static and in the frequency domain, which enables to get more value from simulation than the usual sensitivity studies. The power of this approach will be demonstrated in this chapter by an industrial case study about the handling of impurities in a Vinyl Chloride Monomer plant.

3.2 Problem definition

The removal of impurities in a balanced Vinyl Chloride Monomer (VCM) process is known to be difficult. Significant market fluctuations require a wide operating window, while maintaining product purity under economical conditions. Higher reaction conversion or plant throughput typically yields more secondary products and impurities that may accumulate and cause unstable operation.
3.2.1 Reactions

A balanced VCM process contains three main reactions, which may be described as follows:

- **Chlorination**  
  \[ \text{C}_2\text{H}_4 + \text{Cl}_2 \rightarrow 1,2\text{-C}_2\text{H}_4\text{Cl}_2 (\text{DCE}) + \text{impurities} \]

- **Cracking**  
  \[ \text{DCE} \rightarrow \text{C}_2\text{H}_3\text{Cl} (\text{VCM}) + \text{HCl} + \text{impurities} \]

- **Oxychlorination**  
  \[ \text{C}_2\text{H}_4 + 2 \text{HCl} + \frac{1}{2} \text{O}_2 \rightarrow \text{DCE} + \text{H}_2\text{O} + \text{impurities} \]

The intermediate product 1,2-dichloroethane (DCE) is produced by the direct chlorination of ethylene with fresh chlorine. The cracking of this intermediate gives Vinyl Chloride (VCM). The Hydrogen Chloride that is produced as a byproduct of the cracking process will be used to chlorinate more ethylene in the oxychlorination process. Oxygen is added here to remove hydrogen. As a result all fresh chlorine that is added to the process will be used finally to produce VCM. There is no net production of HCl. Therefore the process is said to be in balance.

3.2.2 Impurities

The oxychlorination process may also use HCl waste streams from other plants as chlorine source. This will reduce the net consumption of fresh chlorine but may also introduce additional impurities in the process. In general, waste and impurities in the effluent of the three reactors may originate from (1) feed impurities, (2) secondary reactions with the main reactant(s) and (3) supplementary reactions with feed impurities.

Each reaction section may have its own separation system, but some of the impurities from different reactors may be collected and eliminated in a central separation system. Recycling of impurities over more than one reactor may generate even more waste material. Generally, the impurities lead to operation problems. Their upper limit concentration must be strictly controlled to prevent polymerization or fouling. However, in special cases some impurities may be useful catalyzing or inhibiting some reactions and their concentration has to be kept at an optimum value by balancing formation and elimination rates. Thus, impurity control and main component control are strongly coupled. A special feature of impurity dynamics is the fact that some of them are always in transient state, hence a simultaneous steady state optimization of both is impossible. However, an accurate steady state plant simulation model contributes to understand and to evaluate quantitatively formation and elimination mechanisms as well as interactions between them.
3.3 Plant structure

Figure 3.1 presents the flowsheet of the balanced VCM process. The reactions take place in the reactors R1 (Chlorination), R2 (Cracking) and R3 (Oxochlorination). The washing/drying section S0 removes unconverted reactants. A first amount of (light) impurities is removed by column S1. Three main recycle loops cross in the distillation column S2 whose main function is to purify fresh and recycled DCE. Three other distillation columns are involved in this operation: S3 for finishing DCE, S4 for ‘Lights’ and S5 for ‘Heavies’ removal. The column S2 will collect also impurities associated with the production and the recycling of DCE, which may contain lights, intermediates and heavies. Among the impurities three significant components are identified for this process: chloroprene (I1), trichloroethylene (I2) and CCl4 (I3). These components are lighter than the main component DCE. Both I1 and I2 are polymerizable and have concentration constraints in the bottom product of column S2. They can leave the plant as Lights via column S4 but significant amounts will remain in the recycle to reactor R1. There they are transformed to Heavies (C6Cl4), which are easily removed by column S5. They are also drawn as a side-stream from column S2, being directly recycled to reactor R1. This creates a fourth loop, also containing S2. They may also be destroyed in a supplementary reactor, R4, between the columns S2 and S4. This will decrease the impurities loading of S4, which will improve its performance. Therefore, this alternative design may have better control properties.

![Flowsheet of the balanced VCM process with optional reactor R4](image)

Figure 3.1; Flowsheet of the balanced VCM process with optional reactor R4
A major feature of the VCM process is the fact that impurity I$_3$ has a beneficial role since it enhances both conversion and yield of the cracking reaction. It can leave the system only via column S4 as Lights. Therefore, regarding the removal of I$_1$ and I$_2$, a compromise has to be found with an optimal concentration of I$_3$ in the bottom of the column S2. These considerations show that the design and operation of S2 are essential for the process as a whole. S2 is a large distillation column, operating at a very large reflux ratio. Its operation is constrained by specifications on the quality of the bottom product: $\text{spec}_1$ the maximum concentration of I$_1$, $\text{spec}_2$, the maximum concentration of I$_2$ and $\text{spec}_3$ the optimum concentration of I$_3$.

### 3.3.1 The nominal operating point

Rigorous steady state simulation models are used to find the nominal operating points of the basic plant structure and the alternative structure with additional reactor R4. Details of the models are given in an appendix at the end of this thesis. The nominal operating values of variables that are interesting from controllability point of view are given in Table 3.1.

Introduction of the extra reactor R4, between column S2 and S4 for the transformation of impurities I$_1$ and I$_2$ into Heavies leads to a different steady state behavior of the system. The Heavies that are produced by reactor R4 will leave column S4 through the bottom, while the impurities I$_1$ and I$_2$ left the basic system as Lights. Therefore, in this alternative design the concentration of impurity I$_3$ in the top distillate of column S4 is higher. To keep $\text{spec}_3$, the optimum concentration of I$_3$, the distillate flowrate of column S4 has been reduced with about 40%. Furthermore, the nominal values of I$_1$ and I$_2$ become significantly lower. The impact of these changes on the controllability of the system will be studied by a steady state analysis. But first the control problem has to be defined and a selection of input and output variables has to be made.

### 3.4 Plantwide control strategy

In a complex plant as the balanced VCM process, a large number of variables have to be controlled. Most of them - pressures, temperatures, levels - may be controlled locally. However, material balances in general and especially the material balances of impurities are established by interactions between the different operating units and recycles in a plant. Therefore, the control of all material balances requires a plantwide approach.
Consequently, the handling of impurities is dealt with as a multivariable control problem. Here the controlled variables (outputs) are maximum or optimum values of concentrations (flowrates) of impurities on selected streams or locations. They can be measured in an operating plant, but also set as ‘design specifications’. These specifications may be achieved by manipulating inputs as distillate flowrate, reflux ratio, reboiler duty, feed temperature, etc. These may also be seen as ‘design variables’ in a new design or revamp. It is obvious that one manipulated variable affects more than one controlled variable, so interaction between controller loops should be taken into account.

In this study we focus our attention on the material balances of the impurities I₁, I₂ and I₃. Since these have a slow dynamic behavior, the fast control loops are assumed to operate instantaneously. Therefore pressures, temperatures and levels are fixed in the simulation models while duties and flowrates are free (calculated). In the distillation columns S₂ and S₄ the reflux flow is much larger than the distillate flow, therefore we assume that the reflux flow is used to control the drum level and the bottom flow to control the reboiler level. The reboiler duties and distillate flowrates are used then to meet the specifications.

3.4.1 Inputs, outputs and disturbances

In this work we focus our attention on the slow dynamics of the material balances, therefore the concentrations of the impurities I₁, I₂ and I₃ in the bottom product of column S₂ are the outputs of the control problem. Normally the design variables of this column S₂, the distillate flowrate (D₂), side stream flowrate (SS₂) and reboiler duty (Q₂), will be used then as the input variables of the control problem. However, by trying to satisfy the specifications on the impurities I₁, I₂ and I₃ in the bottom product of column S₂ during the calibration of the plant steady state model, the important role of column S₄ as an exit of impurity I₃ became evident. Simulations did not converge with a too small distillate flowrate. Impurity I₃ is then built up in the plant (‘snowball effect’ on impurities concentration, see also Figure 3.4). Therefore, to resolve this problem, in addition to the column S₂ distillate flowrate (D₂), side stream flowrate (SS₂) and reboiler duty (Q₂), also the column S₄ distillate flowrate (D₄) and reboiler duty (Q₄) are taken into account as possible manipulated variables in a plantwide control structure (inputs). The main disturbance of the plant is the throughput, being modified by the flowrate of the external DCE feed (F_{DCE}). A second disturbance that will be taken into account is the fraction of impurity I₃ in this stream (X₁₃).
Table 3.1; Nominal operating values and scaling factors

<table>
<thead>
<tr>
<th></th>
<th>basic plant</th>
<th>alternative with R4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>spec</td>
<td>nominal value</td>
</tr>
<tr>
<td>Output</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>Wt-ppm</td>
<td>&lt;100</td>
</tr>
<tr>
<td>$I_2$</td>
<td>Wt-ppm</td>
<td>&lt;600</td>
</tr>
<tr>
<td>$I_3$</td>
<td>Wt-ppm</td>
<td>2000</td>
</tr>
<tr>
<td>Input</td>
<td></td>
<td></td>
</tr>
<tr>
<td>D2</td>
<td>Kmol/h</td>
<td>14.5</td>
</tr>
<tr>
<td>SS2</td>
<td>Kmol/h</td>
<td>35</td>
</tr>
<tr>
<td>Q2</td>
<td>GJ/h</td>
<td>34</td>
</tr>
<tr>
<td>D4</td>
<td>Kmol/h</td>
<td>5.59</td>
</tr>
<tr>
<td>Q4</td>
<td>GJ/h</td>
<td>1.0</td>
</tr>
<tr>
<td>Disturbance</td>
<td>F_DCE</td>
<td>Kmol/h</td>
</tr>
<tr>
<td>$X_{13}$</td>
<td>Mole-%</td>
<td>0.12</td>
</tr>
</tbody>
</table>

3.4.2 Scaling

Scaling of the input and output variables makes model analysis and controller design much simpler. A useful approach is to make the variables less than one in magnitude (see 2.3.3). The scaling factors of the impurities $I_1$ and $I_2$ are therefore based on their maximum allowed value while that of $I_3$ is based on the maximum expected change of its reference value. The inputs are scaled by 25% of their nominal value. Proper operation of the distillation columns should normally be guaranteed within this range, but problems may occur when the operating variables become outside this range. For each disturbance, the largest expected change is taken as scaling factor. The nominal values and scaling factors of the inputs, outputs and disturbances are given in Table 3.1. The nominal values of $I_1$ and $I_2$ become significantly lower when the extra reactor R4 is introduced. This lead to larger scaling factors. The impact of these differences on the controllability of the system will be studied next.

3.5 Steady state analysis

From extensive steady state simulations a scaled gain matrix $G$ can be generated according to the relation $c = Gm$, where $c$ are the scaled plantwide control variables and $m$ are the scaled manipulated variables (eq. 2.2). With the scaled disturbances $d$, a scaled disturbance gain matrix $G_d$ is generated, according to the relation $c = G_d d$ (eq. 2.3). The introduction of scaled variables allows reformulation of the plantwide control problem. To keep the impurities within their bounds under disturbances, control is necessary when the scaled disturbance gains are greater than one.
3.5.1 Basic flowsheet

3.5.1.1 Static gains

Table 3.2 shows the static gain matrices for the basic plant structure. Control is necessary, since the scaled disturbance gains are greater than one. When regarding the sign of the input/output gains, it is noticed that both D2 and SS2 have a negative effect on the impurities I1 and I2, while the effect on I3 is positive. Increasing these manipulated variables means recycling more material through reactor R1. Impurities I1 and I2 are transformed to Heavies here ('negative feedback'), but I3 is build up in the recycle ('positive feedback').

Increasing the reboiler duty Q2 will give rise to fewer impurities in the bottom product. This holds also for the distillate flowrate and reboiler duty of column S4 (D4 resp. Q4). The first is an exit for the impurities while the second will purify the recycle stream to R1, so both have a reverse effect on the controlled variables. The high gain values are in line with their important role in removing impurities, especially for I3.

Table 3.2; Static gain matrices of the basic VCM-plant

<table>
<thead>
<tr>
<th></th>
<th>G</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
<th>D4</th>
<th>Q4</th>
</tr>
</thead>
<tbody>
<tr>
<td>I1</td>
<td></td>
<td>-0.075</td>
<td>-0.261</td>
<td>-5.742</td>
<td>-0.376</td>
<td>-0.079</td>
</tr>
<tr>
<td>I2</td>
<td></td>
<td>-0.212</td>
<td>-0.527</td>
<td>-3.574</td>
<td>-0.437</td>
<td>-0.071</td>
</tr>
<tr>
<td>I3</td>
<td></td>
<td>0.411</td>
<td>0.030</td>
<td>-0.893</td>
<td>-2.829</td>
<td>-0.616</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Gd</th>
<th>F_DCE</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>I1</td>
<td>4.424</td>
<td>0.132</td>
<td></td>
</tr>
<tr>
<td>I2</td>
<td>3.193</td>
<td>0.192</td>
<td></td>
</tr>
<tr>
<td>I3</td>
<td>2.606</td>
<td>1.631</td>
<td></td>
</tr>
</tbody>
</table>

3.5.1.2 Controllability indices

Table 3.3 resumes the steady state controllability analysis with RGA and SVD. The manipulated variables are arranged such that the preferred pairings are on the main diagonal. The indices show a great difference between the possible combinations of manipulated variables. Notice first that the lower singular values, also known as the Morari Resiliency Index, are less than unity for all scaled systems. This demonstrates that the outputs cannot be set independently. This is also reflected by the large condition numbers, indicating that the plant may be drawn into some directions more easily than into others.

Notice that as long as the reboiler duty of column S2, denoted as Q2, is used as one of the manipulated variables, there is still some control power into the weakest direction. However, when Q2 is not used, the lower singular value becomes almost zero and the condition number is therefore also extremely high. So, Q2 should always be used in a control structure and furthermore it is preferably paired with I1. The high static gain is dominating here.
### Table 3.3: Controllability indices of the basic VCM-plant

<table>
<thead>
<tr>
<th>Paired with</th>
<th>RGA diagonal elements</th>
<th>Singular Values</th>
<th>Condition Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q2, SS2, D2</td>
<td>1.48, 1.56, 1.05</td>
<td>6.84, 0.50, 0.24</td>
<td>28.8</td>
</tr>
<tr>
<td>Q2, SS2, D4</td>
<td>1.47, 1.43, 1.01</td>
<td>6.91, 2.71, 0.31</td>
<td>22.0</td>
</tr>
<tr>
<td>Q2, SS2, Q4</td>
<td>1.47, 1.44, 1.01</td>
<td>6.84, 0.60, 0.31</td>
<td>22.3</td>
</tr>
<tr>
<td>Q2, D2, D4</td>
<td>1.43, 1.08, 0.86</td>
<td>6.89, 2.74, 0.17</td>
<td>41.8</td>
</tr>
<tr>
<td>Q2, D2, Q4</td>
<td>1.47, 1.17, 0.93</td>
<td>6.83, 0.74, 0.12</td>
<td>55.0</td>
</tr>
<tr>
<td>Q2, D4, Q4</td>
<td>1.10, 4.25, 2.01</td>
<td>6.90, 2.77, 0.02</td>
<td>370</td>
</tr>
<tr>
<td>Q4, D4, D2</td>
<td>9.30, 5.19, 0.48</td>
<td>2.98, 0.30, 0.008</td>
<td>397</td>
</tr>
<tr>
<td>Q4, D4, SS2</td>
<td>8.67, 5.17, 0.02</td>
<td>2.96, 0.58, 0.008</td>
<td>369</td>
</tr>
<tr>
<td>SS2, D2, D4</td>
<td>17.6, 13.7, 3.87</td>
<td>2.91, 0.65, 0.006</td>
<td>480</td>
</tr>
<tr>
<td>SS2, D2, Q4</td>
<td>71.3, 59.1, 16.6</td>
<td>0.75, 0.63, 0.001</td>
<td>605</td>
</tr>
</tbody>
</table>

The static gain matrix showed already that the effect of the distillate flowrate and reboiler duty of column S4 (D4 resp. Q4) on the control variables is comparable. When they are used both as manipulated variables, the lower singular value becomes very small and the condition number correspondingly high. So it is not useful to combine them in a control structure.

This will leave five possible combinations of manipulated variables that have acceptable properties. They all have RGA diagonal elements near unity, which suggest that diagonal control would be possible without too many interactions. The combinations where the distillate flowrate of column S2 (D2) is used to control I2 have a smaller Morari Resiliency Index and a higher condition number than the combinations where the side draw of this column (SS2) is used. Furthermore, the low static gains of D2 and Q4 result in two singular values below unity when they are used to control I3, while the use of D4 will give only one singular value below unity. Therefore the combination of controllers I1-Q2, I2-SS2 and I3-D4 seems to be preferable from a steady state point of view. However, the four other structures should not be discarded yet, because they might have better dynamic properties.

#### 3.5.1.3 Disturbances

A singular value decomposition of the static disturbance gain matrix gives the singular values 6.11 and 1.36, which are comparable with the magnitudes of the disturbance vectors themselves (6.05 and 1.65). The matrix with input directions is therefore almost equal to the identity matrix. This indicates that the two disturbances are almost independent of each other and their combined effect is not relevant. Therefore the rejection of the two disturbances may be treated separate.
3.5.2 Flowsheet with impurity destroying reactor R4

3.5.2.1 Static gains

The nominal values of the impurities $I_1$ and $I_2$ become significantly lower when introducing the extra reactor. Their scaling factors are therefore larger than in the basic flowsheet. This reduced the static gains of the inputs on $I_1$ and $I_2$ slightly, as can be seen in Table 3.4.

The impact of the distillate flowrate on impurity $I_3$ is almost doubled. Also the sensitivity of $I_3$ to the sidestream flowrate is increased by a factor 5. This is the result of recycle interactions. $I_3$ is built up in all four recycle streams originating in column S2 and the only exit is the distillate flow of column S4. By reducing this exit, the sensitivity of $I_3$ to the recycle interactions is increased. This increasing sensitivity to recycle interactions is a remarkable result, especially relevant in the context of waste minimization and zero discharge plants, where the impurities removal is even further reduced. It demonstrates that such design modifications meant to reduce waste have a strong impact on the performance of the system and may become detrimental in operation.

<table>
<thead>
<tr>
<th>G</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
<th>D4</th>
<th>Q4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$</td>
<td>-0.076</td>
<td>-0.184</td>
<td>-4.325</td>
<td>-0.154</td>
<td>-0.041</td>
</tr>
<tr>
<td>$I_2$</td>
<td>-0.140</td>
<td>-0.302</td>
<td>-2.298</td>
<td>-0.215</td>
<td>-0.061</td>
</tr>
<tr>
<td>$I_3$</td>
<td>0.737</td>
<td>0.156</td>
<td>-0.908</td>
<td>-2.136</td>
<td>-0.727</td>
</tr>
</tbody>
</table>

3.5.2.2 Controllability indices

Table 3.5 shows the steady state controllability indices for the alternative flowsheet. Only the five possible combinations of manipulated variables that have acceptable properties are shown here. The higher RGA diagonal elements indicate slightly more interaction and the lower singular values indicate a smaller operating window than in the basic plant, but the differences are very small. An SVD analysis of the static disturbance gain matrix confirms the conclusion that the two disturbances are almost independent of each other and their rejection may be treated separate. We may conclude that on the basis of the steady state analysis of both alternatives no clear preference can be assigned to the different design and control alternatives.
Table 3.5; Controllability indices of VCM-plant with reactor R4

<table>
<thead>
<tr>
<th>$I_1$, $I_2$, $I_3$ paired with</th>
<th>RGA diagonal elements</th>
<th>Singular values</th>
<th>Condition number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q2, SS2, D2</td>
<td>1.49, 1.69, 1.12</td>
<td>4.99, 0.79, 0.15</td>
<td>33.67</td>
</tr>
<tr>
<td>Q2, SS2, D4</td>
<td>1.49, 1.39, 0.96</td>
<td>5.03, 2.05, 0.19</td>
<td>26.36</td>
</tr>
<tr>
<td>Q2, SS2, Q4</td>
<td>1.48, 1.40, 0.96</td>
<td>4.99, 0.73, 0.18</td>
<td>27.32</td>
</tr>
<tr>
<td>Q2, D2, D4</td>
<td>1.48, 0.95, 0.68</td>
<td>5.03, 2.17, 0.12</td>
<td>41.08</td>
</tr>
<tr>
<td>Q2, D2, Q4</td>
<td>1.45, 0.99, 0.71</td>
<td>4.99, 1.03, 0.09</td>
<td>58.43</td>
</tr>
</tbody>
</table>

3.5.3 Column S2

The control problem concentrates on the impurities level in the bottom product of the large distillation column S2. Four recycle loops cross in this column, so its operation is strongly coupled to the rest of the plant by the effect of recycle interactions. Nevertheless it is interesting to study the column as a stand-alone object, without the interaction of recycles. Table 3.6 shows that the scaled static process gains of the stand-alone column are much smaller than in the studied flowsheet structures. There is only little control power available in the column itself. A singular value decomposition of this static gain matrix gives the singular values 2.0, 0.01 and 1.5e-5. This indicates that the system can in fact be drawn into one direction only. The lower two singular values are close to zero, so there is almost no control power into these directions. This means that the impurity levels cannot be varied independently. The interactions between the controllers are such that only one impurity can be controlled properly at a time. The high and negative RGA elements also are an indication of this. It is clear that the stand-alone column cannot be controlled properly. In general, the behavior of a stand-alone unit may differ considerably from its behavior when the unit is integrated in a flowsheet. This is mainly due to the effect of recycle interactions. A control structure for the whole plant can therefore not be developed unit by unit. Only a plantwide approach can solve the problem.

Table 3.6; Scaled static process gains

<table>
<thead>
<tr>
<th>G</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$</td>
<td>-0.0766</td>
<td>-0.1613</td>
<td>-2.0370</td>
</tr>
<tr>
<td>$I_2$</td>
<td>-0.0045</td>
<td>-0.0142</td>
<td>-0.0616</td>
</tr>
<tr>
<td>$I_3$</td>
<td>-0.0005</td>
<td>-0.0010</td>
<td>-0.0139</td>
</tr>
</tbody>
</table>

Table 3.7; RGA matrix

<table>
<thead>
<tr>
<th>$\Lambda$</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$</td>
<td>-35.3</td>
<td>17.0</td>
<td>19.3</td>
</tr>
<tr>
<td>$I_2$</td>
<td>3.25</td>
<td>-0.89</td>
<td>-1.36</td>
</tr>
<tr>
<td>$I_3$</td>
<td>33.0</td>
<td>-15.1</td>
<td>-16.9</td>
</tr>
</tbody>
</table>
3.6 Dynamic simulation

3.6.1 Identification of main dynamics

Prior to construction of the dynamic flowsheet, model decisions have to be made regarding the flowsheet elements of which the dynamics have to be taken into account. The steady state analysis showed the important role of the impurities destruction in reactor R1 and R4. Therefore the impact of these two liquid phase reactors on the plant dynamics is considered in this part, first for the basic flowsheet then for the flowsheet with impurity destroying reactor R4.

Reactors R2 and R3 are assumed to have no contribution to the plant dynamics, because as gas phase reactors they possess a negligible holdup and residence times with orders of magnitude of seconds or minutes only and hence they are supposed to act instantaneously.

The separation system is simulated dynamically with a reduced set of components. The reactants having zero flow in the reactor outlet streams are omitted. Since phenomena concerning the impurity material balances are taking place at long time scales, level and pressure controllers are assumed to operate instantaneously. Therefore condenser pressures are fixed and total material balances in drums and reboilers are modeled assuming steady state. So, condenser duties and reflux and bottom flowrates are free while reboiler duties and distillate flowrates are specified. Details of the dynamic model are given in Appendix 1.

3.6.2 Basic flowsheet

Dynamic simulations with step perturbations on the disturbances and manipulated variables show interesting responses (for the concentration of I₃ in the bottom of S2, see Figure 3.2). All impurities will finally reach steady state values, but in different times. For steps on distillate and side stream flowrates of column S2, the manipulated variables D₂ and SS₂ respectively, new steady states are reached in about 24 hours. The responses are influenced by the recycle interactions. In both cases a recycle through reactor R1 is increased. More impurities I₁ and I₂ are destroyed, while I₃ is being built up, on the contrary. After two hours the concentration of I₃ will reach a maximum and then decreases to the final value. This is so because this impurity I₃ finally leaves the plant via column S4. Increasing the reboiler duty Q₂ will boil out the impurities immediately. Recycles are responsible for a small increase after half an hour, but the steady state is reached within two hours, which is much faster than the responses on D₂ and SS₂.
Simulations of an increase in distillate flowrate (D4) or reboiler duty (Q4) of column S4 show a decrease in impurities with a dualistic character, since the response is initially fast but it continues more slowly later on. The slowest part of the response is the more significant one, but it takes about 30 hours to reach steady state. This is the time needed for all recycles to become in equilibrium. A similar dualistic response is observed from steps on disturbance variables (Figure 3.3): a long settling time of impurity I₃ after an increase of the same impurity in the external DCE feed (X₁₃) or in DCE feed flowrate (F_DCE). An increased flowrate of DCE will result in a higher production rate of both product and impurities. The impurities are build up in the DCE recycle and go to the top of column S₂ from where one part is recycled to R₁ (destruction of I₁ and I₂) and another will flow to column S₄, were the three impurities can leave the plant.

As shown in Figure 3.4, the operating window of the distillate flowrate of column S₄ has a lower limit of 80% relative to its nominal value. When the flowrate is lower, feed and produced impurity I₃ cannot be purged from the plant anymore, hence I₃ will build up in the recycles and its concentration increases to unacceptable high levels. This is a kind of ‘snowball effect’ occurring to the concentration of impurities rather than to the whole system.

![Figure 3.2](image_url)

**Figure 3.2;** Dynamic response of impurity I₃ in the bottom of S₂ after a scaled step perturbation of I on resp. D₂, Q₂ or D₄ in the basic VCM plant

*When D₂ is increased, I₃ increases fast in the beginning and later decreases slowly to its final value. Increasing Q₂ gives an almost instantaneous drop of I₃, followed by a fast increase. The final value is reached must faster than after a step on D₂. A step on D₄ gives the slowest response. This is due to the time needed for the recycles to become in equilibrium with each other.*
When the DCE flow is increased, more VCM will be produced and also more HCl, which is recycled and leads to a higher DCE production rate. The higher DCE production and cracking rates give rise to more production of impurities on the short term and more build up of these impurities in the recycles on the longer term. An increase of the impurity content $I_3$ in the external DCE flow also yields more build up in the recycles. The long settling time is due to the time needed for the recycles to become in equilibrium with each other.

The only exit for $I_3$ is the top distillate of column S4 (D4). When this flowrate is decreased to 90% of its nominal value, $I_3$ will rise and reaches a new steady state value after about 50 hours. When D4 is decreased to 70%, $I_3$ will rise continuously and a new steady state is never reached. The amount of $I_3$ that is feed to and produced in the plant is higher than the amount that can leave the plant and therefore $I_3$ is build up in the recycles (kind of 'snowball effect'). The limiting value for D4 is about 80% of its nominal value.
3.6.3 Flowsheet with impurity destroying reactor R4

Introduction of the reactor R4 has a strong influence on the dynamic behavior of the plant. Because the impurities I₁ and I₂ in the top distillate D₂ of column S₂ are transformed into heavies in R₄, increasing flowrate D₂ results in a fast drop of I₁ and I₂ in the bottom of S₂. In the same time, the feed of column S₄ contains less I₁ and I₂ and therefore more I₃ can leave the plant via the Lights directly, compensating the build-up in the recycle. It will not reach a maximum first (in contrast to the same response in the basic flowsheet, Figure 3.2) but goes in a dual fast-slow response to its steady state value (Figure 3.5). Now I₁ and I₂ show a minimum because their transformation in R₄ results in lower concentrations and therefore in less transformation in R₁ through which the side steam is recycled. The dynamic characteristics of the responses on steps in the other inputs are the same as in the basic flowsheet, but their final values are changed, as was already shown in the steady state analysis.

![Graph showing dynamic response of impurities I₁, I₂ and I₃ (bottom S₂) after a scaled step perturbation of 1 on the distillate flow D₂ of column S₂ in the VCM plant with extra reactor R₄.]

**Figure 3.5; Dynamic response of impurities I₁, I₂ and I₃ (bottom S₂) after a scaled step perturbation of 1 on the distillate flow D₂ of column S₂ in the VCM plant with extra reactor R₄.**

The impurities I₁ and I₂ are transformed into heavies in reactor R₄, located between column S₂ and column S₄, so their concentrations decrease fast when the distillate flow of S₂ is increased. On the longer term they increase slightly because their lower concentrations lead to less transformation in reactor R₁. Impurity I₃ is built up in the recycle and therefore increases.
3.7 Dynamic controllability analysis

From the dynamic Speedup™ plant model a scaled linear state space description has been generated as a basis for frequency responses to be calculated in Matlab®. In this case study full order state space descriptions are used. However, state space descriptions may become very large and difficult to handle. Chapter 5 will deal with this subject.

From Figure 3.6 it can be seen that the static gains appear to hold well for frequencies up to 0.02 h⁻¹. At frequencies above 10 h⁻¹ the system is not responding anymore to disturbances and feedback control is no longer needed. Besides, the system is neither responding anymore to the manipulated variables. For oscillations with a frequency in between, the system responses feature a delay and the magnitudes are lower. This clearly demonstrates why a steady state analysis of the plant behavior falls short. During operation of the plant there will always be oscillatory disturbances with frequencies in this range, hence impurity concentrations will always be in a transient.

![Figure 3.6; Frequency responses of impurity I₃ to D₂, Q₂ and D₄](image)

The response of I₃ to an oscillation on D₄ starts to deviate from steady state at a low frequency already. Column S₄ cannot follow these fluctuations. The response of I₃ to an oscillation on D₂ starts to increase at the same frequency. The removal of I₃ by column S₄ seems to compensate the build up effect of D₂ at low frequencies. The response of I₃ to an oscillation on Q₂ remains the same for the whole frequency range where feedback control is needed. At frequencies where the system is not responding anymore to D₂ and D₄ because the recycles cannot follow these fast fluctuations, the effect of Q₂ is not yet affected. Only at frequencies that are corresponding with the time constant of the column itself, the magnitude of Q₂ on I₃ first increases before it also goes to zero. The effect of Q₂ on I₃ is only reduced by the reflux over the top of the column and is hardly affected by recycle interactions.
Chapter 3

Taking a closer look at the frequency responses, a clear difference between D2, Q2, and D4 can be seen. The Lights removal by D4 affects the impurity concentrations in the bottom of column S2 through the recycles. At frequencies above \(0.02\ h^{-1}\) the large holdups in the main recycle paths are damping the effects and the response of I3 to D4 starts to deviate from steady state. This also affects the response of I3 to D2 (and SS2, not shown). The build up of I3 in the short recycle loop through reactor R1 can follow the intermediate frequencies, but the removal of I3 via D4 does not compensate this effect anymore. This leads to a higher magnitude for the response on D2 (and SS2) between \(0.1 - 1\ h^{-1}\). Its maximum around a frequency of \(0.3\ h^{-1}\) corresponds to the maximum in the step response (Figure 3.2). This recycle also becomes to have a delaying effect leading to damping of oscillations at frequencies around \(2\ h^{-1}\). For these values the residence time in reactor R1 corresponds to half a period and the recycle interactions are such that the responses to D2 (and also D4) are zero. At higher frequencies the direction of these inputs is opposite to steady state, which will complicate feedback control.

The response to the reboiler duty Q2 shows another behavior. It is mainly a result of the interaction between the reboiler and the column S2 itself and is hardly affected by recycle interactions. Therefore the system follows the input changes up to much higher frequencies. At frequencies between \(2 - 20\ h^{-1}\), where the period of the fluctuations is of the same order as the response time of the column, the magnitude of Q2 is increased because the opposite effect of the reflux over the top of the column is damped. The maximum gain around \(12\ h^{-1}\) corresponds to the minimum in the step response (6 min., Figure 3.2). At higher frequencies, also the reboiler does not affect the impurities anymore.

3.7.1 Relative Gain Array

In order to analyze the interaction behavior of the system an RGA analysis has been applied. The RGA number, defined by equation 2.27 as \(||RGA - I||_{\text{sum}}\), is used as indicator. Note that RGA numbers close to zero are preferred over the whole frequency range when diagonal feedback control is concerned, since such values would predict a minimum of interactions. The recycle interactions indicated above have a significant influence on the RGA elements. The direction of responses on inputs D2 and D4 at frequencies between 1 and \(10\ h^{-1}\) become opposite to that at steady state (Figure 3.6). Hence, more interactions between control loops at higher frequencies are expected. This is confirmed by high RGA numbers for the diagonal structures with I1-Q2, I2-SS2, I3-D2 or I1-Q2, I2-SS2, I3-D4 as control loops at these frequencies (Figure 3.7).
This figure shows that at low frequencies the control structure with D4 has fewer interactions than the one with D2. At higher frequencies, interaction between the different control loops increases fast for both structures.

### 3.7.2 Diagonal controller performance

The effects of loop closing by a diagonal pattern (input 1 - output 1, input 2 - output 2, etc.) is investigated now, realizing that any loop closing alters the interactions in a plant. The closed loop analysis follows ideas of Skogestad and Postlethwaite (1996), who utilized the Performance Relative Gain Array (PRGA) and the Closed Loop Disturbance Gain (CLDG) to tune MIMO systems with diagonal control. The closed loop analysis is based on an approximation of the closed loop error $e$ in response on disturbances $d$ and references $r$, containing PRGA ($\Gamma$) and CLDG ($\tilde{G}_d = \Gamma G_d$):

$$
e = SG_d d - Sr \approx \tilde{S}G_d d - \tilde{S} \Gamma r$$

(2.51)

The crucial assumption here is that the sensitivity matrix $S$, which in principle is a complex function of all the controller gains and the whole plant behavior, is decoupled and approximated by a product of two terms, $S \approx \tilde{S} \Gamma$. The diagonal sensitivity matrix $\tilde{S} = \text{diag}\{1/(1 + k_i g_i)\}$, $g_{ij}$ being the open loop gain and $k_i$ the controller gain, has only diagonal elements. Therefore, the two terms of the error expression also are diagonal matrices of which the elements may be evaluated loop-by-loop. Due to the approximation these responses have become split into the diagonal sensitivity and the plant transfer matrices, corrected for interaction, $\tilde{G}_d$ and $\Gamma$. The diagonal form of $\tilde{S}$ allows the evaluation of the individual controllers independent from the others, which is convenient for tuning.
addition, the PRGA and CLDG allow analyzing the impact of the diagonal control structure through interaction prior to tuning. In other words PRGA and CLDG measure the changed input-output behavior under diagonal closing, which helps to predict the impact of each diagonal controller, before it is actually implemented. Thus, PRGA and CLDG have some resemblance to RGA, which also describes the impact of loop closing on the input-output behavior, but in a different manner, as will be explained in the next section. As regards the physical interpretation of the PRGA and CLDG matrices, it will be explained how they represent real responses on setpoint changes and disturbances. Here, we will first explain the significance of PRGA in comparison with RGA in the context of setpoint tracking and illustrate this on the VCM example. Then along similar lines CLDG will be explained as serving disturbance rejection. After that, PRGA and CLDG will be applied to the tuning of the diagonal controller.

3.7.2.1 Performance Relative Gain Array

The performance relative gain array (PRGA) may be explained with the ordinary RGA as a reference. The RGA measures the interaction characteristics of a plant by comparing the open loop performance to the closed loop performance assuming ideal setpoint tracking of the outputs. It is used to identify the optimal input-output pairing in diagonal control, but not all elements are usable to analyze the performance of the controller. Only the elements corresponding to the selected input-output pairs - preferably being closest to 1 and positioned on the diagonal of the RGA - are relevant. The PRGA also measures plant interaction, but in a different way, allowing to analyze the controller performance. From the derivation of the PRGA \( \Gamma \) in chapter 2 (eq. 2.49) it may be realized that the diagonal elements of \( G \) follow as \( \bar{G} = \Gamma G \), in other words, \( \Gamma \) represents the inverse of the off-diagonal plant elements. Since these off-diagonal elements are responsible for the interaction, causing other outputs to change rather than changing the desired output, \( \Gamma \) is a certain measure for this interaction. More precisely stated, the closed loop response of any output \( i \) on a unit step change of the setpoint of one output \( r_j \) follows from \( \Gamma \) as element \( \gamma_{ij} \), be it under the following assumptions. Firstly, every loop is assumed to be closed according to a diagonal control structure, and secondly, the controller gain \( k_i \) is assumed to be zero. Hence, in equation 2.51 \( \bar{S} = I \) and the response becomes equal to \( \Gamma \) for a setpoint change of 1. Hence, these values have a clear, physical meaning in the performance analysis of the diagonal controller with unit setpoint changes. Exact setpoint tracking would imply values equal 1 for the diagonal elements of \( \Gamma \),
meaning absence of interaction. Since RGA and PRGA diagonal elements are equal, PRGA
does not give more information as regards the diagonal. However, the off-diagonal PRGA
elements are a measure of the interactions in the diagonally controlled plant. Zero values
mean no interactions. Non-zero values show quantitatively to which extent the setpoint
tracking of one particular output has impact on the other outputs. If control on boundaries
rather than setpoint tracking is acceptable for those other outputs, then the criterion is that
PRGA elements should not exceed one. This means that the setpoint tracking of one output
does not lead to violation of boundaries for the other outputs that evidently are automatically
kept under control. However, values larger than 1 indicate violations of boundaries indeed,
which means that the setpoint tracking of one output simultaneously requires additional
control action to keep other outputs within boundaries. The tuning of such a controller is
discussed in section 3.8.

As another interesting difference between RGA and PRGA it should be realized that PRGA is
also the more sensitive instrument, since it not only allows for 2-way interactions like RGA,
but also takes 1-way interactions into account. If an open loop input-output pair has a zero
gain, meaning no direct influence of the input on that output, the corresponding PRGA may
have a finite value > 0, indicating that this particular output is affected by the input indirectly
via the diagonal control structure, hence by pure interaction. Note that the PRGA is analyzed
in the frequency domain, which should represent physically realistic fluctuations in setpoint
tracking, supposed to take place for operational reasons.

We will perform now a PRGA analysis on the VCM plant. Figure 3.8 shows the effect of a
setpoint change of impurity $I_3$ between the bounds $[-1,1]$ as a function of frequency, assuming
that the diagonal control structure $I_1$-$Q_2$, $I_2$-$S_2$, $I_3$-$D_2$ is implemented in the basic flowsheet.
The setpoint tracking of $I_3$ in itself is effective at low frequencies, while the unwanted impact
on $I_1$ and $I_2$ is acceptable. The PRGA elements for these two impurities are close to zero, that
for $I_2$ being somewhat higher. At higher frequencies, where the interactions between the
control loops become significant, all impurities will exceed their bounds, so feedback control
is no longer effective. Figure 3.9 shows the performance of the alternative diagonal structure
$I_1$-$Q_2$, $I_2$-$S_2$, $I_3$-$D_4$ for the same setpoint tracking problem. Again, at low frequencies $I_3$ is
controlled effectively, while the impurities $I_1$ and $I_2$ are only slightly affected. However, $I_1$
will exceed bounds at somewhat lower frequency than before. Note that although both
structures show violations at high frequencies, this is not expected to be a problem in
operation since the setpoint of the initiator for the cracking process is not normally changed
at such high frequencies. In conclusion, the PRGA analysis shows both diagonal structures to be nearly equivalent: if only $I_3$ is controlled on setpoint, the other impurities are automatically kept between boundaries, so no additional control action is required.

Now, it is interesting to see the impact of a flowsheet change - the addition of an extra impurity-destroying reactor $R_4$ - on the setpoint tracking performance, when the same two control structures are implemented. Figure 3.10 shows the performance of the control structure $I_1-Q2$, $I_2-SS2$, $I_3-D2$ to be similar to that of the same structure in the base case flowsheet (Figure 3.8), although the unwanted impact on $I_1$ and $I_2$ is somewhat smaller. The same holds for the second diagonal control structure, $I_1-Q2$, $I_2-SS2$, $I_3-D4$ (Figure 3.11), which shows a similar performance as that structure in the base case. In conclusion, the introduction of the extra reactor $R_4$ in the alternative flowsheet has only a minor improving effect on the performance of the diagonal controller when setpoint tracking is concerned.

![Graph](image)

**Figure 3.8; Performance Relative Gain Array elements for the effect of a reference change of $I_3$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1-Q2$, $I_2-SS2$, $I_3-D2$ in the basic VCM plant**

The figure shows that $I_3$ is controlled close to its new reference value of 1 while $I_1$ will remain close to zero. $I_2$ is greatly affected as a result of the interaction between the control loops at low frequencies. At higher frequencies this effect is reduced. All PRGA elements show a fast increase at frequencies where the response of the system goes to zero. At these frequencies feedback control is no longer effective.
The control of $I_3$ with $D_4$ follows the fluctuation of the reference value of $I_3$ between −1 and 1, while $I_1$ and $I_2$ are hardly affected. The decreased magnitude of $D_4$ at intermediate frequencies is reflected by an increased effect of the reference change of $I_3$ on the control of $I_1$. However, reference values are seldom changed at these frequencies.

The magnitude of $D_2$ on $I_3$ is larger in the plant with reactor R4, relative to the base case (Figure 3.8), while the magnitude of $D_2$ on $I_2$ is lower. This is reflected by this figure of PRGA elements. The impurities $I_1$ and $I_2$ are less affected by a reference change of $I_3$ than in the base case.
Figure 3.11; Performance Relative Gain Array elements for the effect of a reference change of $I_3$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the alternative flowsheet with additional reactor R4

If this figure is compared to Figure 3.9, we see that the effect of a reference change of $I_3$ on $I_1$ and $I_2$ remains low for a larger frequency range. This is a result of the lower magnitude of D4 on $I_1$ and $I_2$, relative to the base case.

3.7.2.2 Closed Loop Disturbance Gain

The performance of diagonal feedback control with respect to disturbance rejection is studied by calculating the closed loop disturbance gains (CLDG), denoting the effect of a disturbance on the outputs when a diagonal control structure is implemented. This is another tool, also introduced by Skogestad and Postlethwaite (1996) to analyze the output sensitivity of the plant as changed by the diagonal control structure, before actually tuning it. In this respect the CLDG may be compared to the open loop disturbance gain of the outputs. When scaled open loop disturbance gains remain below 1 then, according to the acceptable control criterion, one would guess that control is not necessary at all for such outputs, since they would stay within bounds even without control. Applying the same reasoning to a diagonally closed plant, finding closed loop gains below 1 would imply that no control for the associated outputs is needed, since these stay within boundaries for any disturbance. This is reflected in the elements of CLDG that physically represent the closed loop responses on disturbances for a diagonal control structure and zero controller gains. According to equation 2.51 this means $\bar{S} = I$, so the response equals $\bar{G}_d$. When CLDG elements are below 1, the corresponding outputs are automatically under control due to the diagonal control structure and the
interactions invoked by this. Note that this is the result of the concerted action of all the manipulated variables acting on this output under the diagonal control structure. It might well be that not all of these manipulated variables do have an open loop effect on this output. In such a case disturbance rejection is realized only because of interaction. Now, if a CLDG element exceeds 1, then indeed extra control action is necessary to realize disturbance rejection and keep this output within boundaries. The tuning of such a controller is discussed in the next section.

The CLDG analysis has been applied on the VCM example for two disturbances, the feed stream $F_{DCE}$ and the concentration of impurity $I_3$ in this feed stream, $X_{i3}$, under the 2 diagonal control structures mentioned above, for both flowsheet alternatives. The results are shown in Figure 3.12 to Figure 3.19. Figure 3.12, showing all CLDG elements to be above one, indicates the necessity of extra control action to reject disturbances of the feed flow $F_{DCE}$ on any of the impurity levels for the structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D2$ in the base case. Figure 3.13 indicates for the other disturbance ($X_{i3}$), that impurity $I_1$ in this case automatically stays within acceptable bounds when only $I_2$ and $I_3$ are controlled, hence the system is almost indifferent to the presence or absence of the controller $I_1$-$Q2$.

Figure 3.14 shows the behavior of the alternative control structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D4$ to be improved with respect to disturbance $F_{DCE}$, since here impurity $I_2$ does not require control, while $I_1$ and $I_3$ still do. Figure 3.15 also shows improvement for the other disturbance, since under the alternative structure only $I_3$ needs control and $I_2$ and $I_1$ do not. Hence, in the base case flowsheet the structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D4$ performs best, since impurity $I_2$ never requires control. Figure 3.16 shows a result for the alternative flowsheet containing the reactor $R4$. Disturbance $F_{DCE}$ in structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D2$ requires impurities $I_1$ and $I_3$ to be controlled only, so the controllability of this flowsheet is slightly better than that of the base case. Figure 3.17 shows this situation even to be improved for the $X_{i3}$ disturbance, only requiring control for $I_3$. Figure 3.18 and Figure 3.19 indicate that the alternative control structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D4$ does not lead to further improvement in this flowsheet, like it did in the base case. For disturbance $F_{DCE}$ $I_1$ and $I_3$ and for $X_{i3}$ again only $I_3$ have to be controlled.

In conclusion, both the alternative control structure and the alternative flowsheet structure perform better than the base case. Choosing the best alternative, still always $I_3$ has to be controlled with $D4$, while for disturbance $F_{DCE}$ also $I_1$ has to be controlled with $Q2$. 


Figure 3.12; Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 in the basic VCM plant

The figure shows that all three impurities are affected by the feed disturbance in this closed loop system and therefore need to be controlled.

Figure 3.13; Closed Loop Disturbance Gains for the impurity disturbance $X_{I3}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 in the basic VCM plant

This figure shows that $I_1$ is hardly affected by the impurity disturbance with this control structure, while $I_2$ and $I_3$ need only to be controlled at low frequencies.
Figure 3.14: Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant

This figure shows that $I_2$ is hardly affected by the feed disturbance in this control structure with D4. This is in contrast with the base case, where $I_3$ is controlled with D2.

Figure 3.15: Closed Loop Disturbance Gains for the impurity disturbance $X_{I3}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant

The impurities $I_1$ and $I_2$ are hardly affected by the impurity disturbance, while $I_3$ is only affected at low frequencies.
The introduction of reactor R4 lowers the closed loop disturbance gains. As a result of the controller interactions, $I_2$ will be kept between its bounds and does not need to be controlled itself for this disturbance.

The Closed Loop Disturbance Gain of $I_3$ becomes larger with R4, but that of $I_2$ is lower.
Figure 3.18: Closed Loop Disturbance Gains for the feed disturbance $F_{DCE}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the alternative flowsheet with additional reactor R4.

The Closed Loop Disturbance Gains with reactor R4 are all lower than without this reactor.

Figure 3.19: Closed Loop Disturbance Gains for the impurity disturbance $X_{I3}$ on the outputs $I_1$, $I_2$ and $I_3$ with the diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the alternative flowsheet with additional reactor R4.

With reactor R4 included, both $I_1$ and $I_2$ are not affected by the impurity disturbance.
3.7.2.3 Relative Disturbance Gain

The ratio between the closed loop disturbance gain and the open loop disturbance gain, giving the change in input-output behavior due to diagonal feedback control, is called the relative disturbance gain (RDG). The elements of this matrix are preferably smaller than one, which would mean that the interactions between the controllers are such that they reduce the apparent effect of the disturbance. In such cases relatively small gains are sufficient for the individual loops. However, they may also be larger than 1, indicating that the apparent effect is enhanced instead, implying high gains for the loops concerned.

Assuming the structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the base case flowsheet and the concentration of impurity $I_3$ in the DCE feed ($X_{I3}$) as the disturbance this time, RDG values have been plotted in Figure 3.20 for all three impurities. At low frequencies they are below one, so the system can be controlled with small controller gains. At frequencies between 1 and 10 h$^{-1}$ the RDG elements rise to high values, indicating an opposite direction of the controller interactions, which complicates control of the impurities. At these frequencies control would not even be possible, but this is not a problem since according to the CLDG elements, the impurities are automatically kept between their bounds, hence control is also not required.

![Figure 3.20](image)

Figure 3.20; Relative Disturbance Gains of impurity $I_3$ in the external DCE feed $X_{I3}$ for the outputs $I_1$, $I_2$, and $I_3$ with diagonal control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D4 in the basic VCM plant

This figure shows that the apparent effect of the disturbance on $I_2$ with this control structure implemented is reduced enormously at low frequencies, so a low controller gain would be enough. At higher frequencies, the closed loop disturbance gains are higher than the open loop disturbance gains due to negative controller interactions. However, the absolute values are low in this frequency range and therefore no control is needed.
Figure 3.21: Relative Disturbance Gains of the external DCE feed flowrate $F_{DCE}$ for the outputs $I_1$, $I_2$, and $I_3$ with diagonal control structure $I_1$-$Q2$, $I_2$-$SS2$, $I_3$-$D4$ in the basic VCM plant

This figure shows that the apparent effect of the flow disturbance on $I_2$ with this control structure implemented is also reduced enormously at low frequencies, so a low controller gain would be enough. At higher frequencies, the closed loop disturbance gains are again higher than the open loop disturbance gains due to negative controller interactions.

Another disturbance, the step on the DCE feed ($F_{DCE}$), gives also rise to RDG elements less than one at low frequencies (Figure 3.21), but they are not so high at intermediate frequencies. So, for this disturbance the apparent effect of the controller interactions is such that the open loop behavior is less affected.

Especially the RDG values of $I_2$ at low frequencies are very small for both disturbances. The controller interactions are such that the apparent effect of the disturbances on $I_2$ is reduced enormously and only small controller gains are needed. This is in agreement with the conclusion from the CLDG analysis that $I_2$ does not need to be controlled because it is automatically kept between its bounds due to controller interactions.

### 3.8 Tuning the diagonal controller

The tuning of MIMO control systems with classical (SISO) tuning methods like Cohen-Coon and Ziegler-Nichols is frustrated by interaction, since tuning of one loop is influenced by tuning of the other ones. This problem is overcome using the controllability tools PRGA and CLDG that provide means to perform tuning of a diagonal control system loop-by-loop, by
capturing the interaction impact in one matrix, the PRGA matrix $\Gamma$. This may clearly be seen from equation 2.51, showing the error to be approximated by terms that each are products of the diagonal sensitivity matrix $\tilde{S}$ with $\tilde{G}_d$ and $\Gamma r$ for disturbance rejection and reference tracking, respectively. Evidently, small errors are realized by small $\tilde{S}$ or small $\tilde{G}_d$ and $\Gamma r$ values. The impact of the latter has been discussed in the previous section. Here, we are interested in tuning criteria, also derived from the mentioned error expression.

In chapter 2 it has been shown that for disturbance rejection in order to keep the outputs between their bounds [-1,1], the value of $(\tilde{S})^{-1} = \text{diag} \{(1 + k_ig_{ij})\}$ should be larger than the closed loop disturbance gain $\tilde{G}_d$ over the whole frequency range where control is needed (eq. 2.53). Since $\tilde{S}$ has diagonal elements only and so has the product of $\tilde{S}$ with $\tilde{G}_d$, this inequality may be tested for each loop individually by comparing the diagonal elements $(1 + k_ig_{ij})$ with $\tilde{g}_{ai}$. The proportional gains then are determined by plotting $(1 + k_ig_{ij})$ and $\tilde{g}_{ai}$ for all disturbances in one frequency graph and choosing $k_i$ in such a way that the former curve always lies above the latter ones in the required part of the frequency domain.

This has been carried out for the VCM case, resulting in Figure 3.22 to Figure 3.25. From the previous section it was concluded that for the base case flowsheet and control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 impurities $I_2$ and $I_3$ always would have to be controlled. Now, we will investigate whether this is possible indeed, first for $I_2$ then for $I_3$. Figure 3.22 shows the impact on impurity $I_2$ for changes in the two disturbances analyzed before: $F_{DCE}$ (dashed curve) and $X_{I3}$ (dotted curve), the former having a more serious impact. The figure shows the open loop gain of the manipulated variable to control $I_2$, in this structure being $g_{22} = SS2$. Since this gain is lower than the CLDG curves, there is not enough input magnitude to control $I_2$ on setpoint. On the other hand, the curve of $(1 + k_2g_{22})$ for a maximum (scaled) controller gain of 1 lies entirely above the CLDG of the $I_3$ disturbance of the DCE feed $\tilde{g}_{d2}$ ($d = X_{I3}$), so this disturbance can be rejected and control of $I_2$ within bounds for this disturbance is possible. However, at low frequencies $(1 + k_2g_{22})$ is smaller than $\tilde{g}_{d2}$ ($d = F_{DCE}$), so there is lack of control power for the feed disturbance and $I_2$ will become outside its bounds.
This figure shows that the effect of the disturbances in a closed loop system is higher than the available control power (input magnitude). Therefore $I_2$ cannot be controlled on setpoint with $SS2$ in this control structure. It also shows that $SS2$ has not enough magnitude to keep $I_2$ between its bounds. The closed loop transfer function with the maximum controller gain of 1 has still a lower value than the closed loop disturbance gain of the feed step.

This figure shows that $D2$ has not enough input magnitude and $I_3$ can not be controlled between its bounds in this control structure at low frequencies.
Figure 3.24; Input magnitude of SS2 and loop transfer function of I2-SS2 with the Closed Loop Disturbance Gains for the diagonal control structure I1-Q2, I2-SS2, I3-D4 in the basic VCM plant

This figure shows that the apparent effect of the disturbances in this control structure is such that the impurity I2 remains between its bounds and therefore does not have to be controlled (controller gain zero). However, there is enough input magnitude to control I2 on setpoint.

Figure 3.25; Input magnitude of D4 and loop transfer function of I3-D4 with the Closed Loop Disturbance Gains for the diagonal control structure I1-Q2, I2-SS2, I3-D4 in the basic VCM plant

From this figure it is seen that D4 has enough input magnitude to control I3 on setpoint. To keep I3 only between its bounds, the control capacity available is not even fully required. A scaled controller gain of 0.36 is sufficient.
Figure 3.23 shows a similar plot for impurity I₃, in this control structure to be controlled with D2. It shows that D2 lacks control power to control either of the two disturbances on setpoint or within bounds. In conclusion, where the previous analysis indicated the necessity to control I₂ and I₃ indeed, finally it turns out from the tuning procedure, that control within bounds is not possible in this case.

Regarding the alternative control structure I₁-Q2, I₂-SS₂, I₃-D₄, in the previous section it has been concluded that never control was required for I₂, while control is needed always for I₃ and sometimes for I₁. Figure 3.24 confirms this conclusion for I₂, showing \((1 + k₂g₂₂)\) always to be larger than \(g_{d₂}\), even with zero gain. In contrast, impurity I₃ needs control and from Figure 3.25 it indeed appears to be possible for a controller gain even below the maximum.

In conclusion, the closed loop controllability tools indeed are able to discriminate between various control and flowsheet alternatives, proving that the two flowsheets are controllable with the alternative control structure, while they are not with the basic control structure. The closed loop tuning technique proved to confirm this conclusion and was successfully used to tune the alternative controller with respect to the control of I₃ with D₄.

### 3.9 Closed loop simulations

Closed loop simulations with the full nonlinear dynamic model have been carried out to compare with the results of the controllability analysis. Figure 3.26 and Figure 3.27 show the response of impurities I₂ and I₃, respectively, on a feed disturbance \(F_{DCE}\) for the base case flowsheet and several control structures. Implementing only one controller, I₁ with Q₂, automatically yields effective control of I₂, but that is not so for I₃, although the response is suppressed to some extent. Again assuming a 1-controller system but this time controlling I₂ with SS₂ gives surprisingly bad results for I₂ itself and the result for I₃ is even worse. Another 1-controller system that is evaluated, I₃ with D₂, produces bad performance for both impurities. However, controlling I₃ with D₄ works out very well for I₃, but only poorly for I₂. Hence, none of the 1-controller systems works satisfactorily for both impurities, which is in agreement with the controllability analysis.

Two 2-controller systems have been implemented. The system I₁-Q₂, I₂-SS₂ performs very well for I₂ but does not keep I₃ within bounds, even when a 3rd controller is added, I₃-D₂, which is in agreement with the controllability results, predicting bad performance for all
impurities in case of control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_2$. The 2-controller system $I_1$-$Q_2$, $I_3$-$D_4$ works well for all impurities, which also fits with the controllability analysis, indicating a better performance for the alternative control structure $I_1$-$Q_2$, $I_2$-$SS_2$, $I_3$-$D_4$. Hence, it is also confirmed that a 3rd controller, to control $I_2$, is not necessary.

Closed loop simulations with the controller structure $I_1$-$Q_2$ and $I_3$-$D_4$ implemented in the flowsheet with reactor R4 showed that the disturbances are reduced with about the same amount. Since the nominal values of impurities $I_1$ and $I_2$ are lower in this flowsheet structure, their values stay lower in the closed loop simulations with disturbances. Impurity $I_3$ follows the same pattern. However, all impurities show a small oscillation on their main pattern with a period of about 10 minutes. A closer examination shows that this is caused by $Q_2$. The step response has an overshoot on all disturbances in the first 10 minutes. In the closed loop simulations, the controllers are continuously correcting this overshoot on a short time period, while on the longer term they also control the disturbance. Although this oscillatory behavior is a disadvantage, the lower values of $I_1$ and $I_2$ make this alternative flowsheet preferable above the base case, which again confirms the controllability conclusions.

![Diagram](image)

**Figure 3.26; Closed Loop Dynamic responses of $I_2$ to a step disturbance on $F_{DCE}$**

*When only the controller $I_1$-$Q_2$ is implemented, $I_2$ is kept between its bounds, while only implementing the controller $I_2$-$SS_2$ this is not the case. $SS_2$ will reach its bound in that situation. When both controllers are combined ($I_1$-$Q_2$ and $I_2$-$SS_2$) $I_2$ is kept between its bounds. When the controller $I_3$-$D_2$ is the only active one, $I_2$ is increased relative to the open loop response, while the controller $I_3$-$D_4$ has a reducing effect on $I_2$.***
Control of $I_1$ with $Q2$ reduces the effect of the disturbance on $I_3$ more than when $I_3$ itself is controlled with $D2$. In this case $D2$ reaches its bound and $I_3$ cannot be controlled further. This is still the case when all three controllers $I_1$-$Q2$, $I_2$-$S2$ and $I_3$-$D2$ are implemented. However, $I_3$ can be controlled with $D4$. Because this also reduced the disturbance effect on impurity $I_1$, the closed loop response of $I_3$ with both controllers $I_1$-$Q2$ and $I_3$-$D4$ is slightly higher, but the impurity is kept well between its bounds $[-1,1]$.

### 3.10 Conclusions

In chapter 2 we have presented a simulation based methodology for evaluating flowsheet design and control alternatives on their controllability and closed loop behavior. In this chapter the systems approach is illustrated with an industrial case study concerning the removal of impurities in a balanced VCM process. It is shown that the combination of steady state and dynamic simulations, together with a linear controllability analysis in the frequency domain improves understanding of the behavior of a large plant with complex recycle structure to a greater extent than extensive steady state simulations only.

It is furthermore shown that the material balance of impurities in the VCM plant is a plantwide problem. It is demonstrated how the interaction between recycles may be exploited to create flowsheet and control alternatives with feasible plantwide control properties that cannot be reached with the stand-alone column. Using the positive feedback effects of the recycle streams and the negative feedback effects of chemical reactors and exit streams gives a flowsheet design and control structure alternative with acceptable control properties. In this
structure the manipulated variables belong to different units, as already could be expected from the steady state analysis. The interaction between the controllers is such that all three impurities can be kept between their bounds with only two controllers implemented. This was predicted by the controllability analysis and confirmed by the closed loop simulations, but a steady state analysis alone turned out to be insufficient to obtain this result. This proves that a linear controllability analysis in the frequency domain with tools like PRGA and CLDG is useful and is capable to discriminate between flowsheet and control alternatives in an effective way. Especially, using the controllability analysis it appeared that the problems mainly originate from the interaction between the different units in the flowsheet. This also illustrates the difference in nature between the controllability characteristics of a plant as compared to those of a single column. Column dynamics may be complex as well, but they do not offer such a wide variety of problem causes distributed in unknown ways over the system and consequently do not possess so many unexpected ways to solve those problems. These solutions also are less well detectable by intuitive means, and stress the importance of controllability tools even more.

The case study was devoted to a large complex plant, the Vinyl Chloride Monomer plant. It showed that the material balance of impurities is always in a transient with time constants in the order of days, making a dynamic analysis unavoidable. The steady state analysis suggested to use the side stream SS2 as a manipulated variable to control one of the impurities (I2). However, dynamic simulations showed that this gives a serious inverse response. Controllability analysis tools indicated the shortcoming of input magnitude and closed loop simulations showed that a new steady state could not even be achieved. Changing the control loop for another impurity, using D4 instead of D2 to control I3, reduces the apparent effect of the disturbance such that control of I2 is no longer needed. The improved performance of this control alternative could never have been predicted by intuition.

The introduction of an additional reactor to destroy impurities that are difficult to remove was expected to give an improved performance. We have seen that the behavior of the alternative flowsheet structure, both steady state and dynamic, is different, especially with respect to D2. It was shown that control of I2 is not needed even with the basic control structure. However, also this design alternative does not have enough control power to keep I1 and I3 between its bounds under disturbances with this control structure. Again the alternative control structure should be used. So, the control structure turned out to be more important than the design.
However, the design alternative has lower levels of impurities, resulting in larger scaling factors. In fact this implies more operational freedom and therefore this design alternative, in combination with the alternative control structure, is preferable.

The introduction of the extra reactor gives access to alternative flowsheets with different recycle structures. The effect of these design modifications on the performance of the system will be studied in the next chapter.
Chapter 4

Recycle Interaction effects on Plantwide Controllability

4.1 Introduction

The synthesis of complex processes with good controllability characteristics requires specific attention for the recycle structure, since recycle interactions may have a strong effect on the dynamic behavior. Two simple examples in chapter 1 have demonstrated this point in essence. Convergence problems in steady state simulations may be caused by infeasible specifications in combination with recycle loops. Overall response times are much larger as a result of recycle loops and dead times may lead to resonant peaks in the frequency response. The systems approach that is presented in chapter 2 may be used to get a better understanding of dynamic interactions between the units and recycle streams. This has been demonstrated in the previous chapter by a practical problem: the removal of impurities in a balanced VCM process. It was shown how the interaction between recycles might be exploited to create flowsheet and control alternatives with feasible plantwide control properties. Furthermore it was shown how the introduction of an extra reactor for the transformation of some light impurities into heavies improved the controllability of the plant's material balance.

In this chapter, the attention is focused on the effect of the recycle structure of this plant. Several alternative recycle structures are possible when the extra reactor is introduced. These structures will be studied and compared with the basic flowsheet. This will lead to a better understanding of the interaction between the recycle loops and the effect of these interactions on the controllability of the material balance.
4.2 Process description

An extensive description of the balanced Vinyl Chloride Monomer (VCM) process is already given in chapter 3. Here, only the main aspects are resumed. The reactions are described by:

- **Chlorination**: \( C_2H_4 + Cl_2 \rightarrow 1,2-C_2H_4Cl_2 \) (DCE) + impurities
- **Cracking**: DCE \( \rightarrow C_2H_3Cl \) (VCM) + HCl + impurities
- **Oxychlorination**: \( C_2H_4 + 2 \text{HCl} + \frac{1}{2} \text{O}_2 \rightarrow \text{DCE} + \text{H}_2\text{O} \) + impurities

The intermediate product 1,2-dichloroethane (DCE) is produced by the direct chlorination of ethylene with fresh chlorine. The cracking of this intermediate gives Vinyl Chloride (VCM) and HCl, which is reused in the oxychlorination process. Waste and impurities in the effluent of the three reactors may originate from (1) feed impurities, (2) secondary reactions with the main reactant(s) and (3) supplementary reactions with feed impurities.

Figure 4.1 shows the basic flowsheet. The reactions take place in the reactors R1 (Chlorination), R2 (Cracking) and R3 (Oxychlorination). Three recycle loops cross in the distillation column S2 whose main function is to purify fresh and recycled DCE. Three other distillation columns are involved in this operation: S3 for ‘finishing’ DCE, S4 for ‘Lights’ and S5 for ‘Heavies’ removal.

![Flowsheet of the balanced VCM process with additional reactor R4](image-url)
Column S2 will collect also a great variety of impurities associated with the production and the recycling of DCE. Among the impurities three significant components are identified for this process: chloroprene (I1), trichloroethylene (I2) and CCl4 (I3). Both I1 and I2 are polymerizable and have concentration constraints in the bottom product of the column S2. They can leave the plant as Lights via column S4 but they can also be transformed into Heavies in reactor R1, which are easily removed by column S5. Therefore they are drawn as a side stream of column S2, recycled back to reactor R1. This operation creates a fourth loop, as well originated in S2.

A major feature of this process is the fact that impurity I3 has a beneficial role since it enhances both conversion and yield of the cracking reaction. It can leave the system only via the top of column S4. Therefore the removal of I1 and I2 has to find a compromise with an optimal concentration of I3 in the bottom of the column S2. Its operation is constrained by specifications on the quality of the bottom product: spec1 the maximum concentration of I1, spec2 the maximum concentration of I2 and spec3 the optimum concentration of I3.

In the previous chapter it has been shown how column S4 may be used to improve performance. S4 is a small distillation column that not only controls the exit of Lights, but also the amount of impurities in the recycle loops crossing the column S2. Improving the separation characteristics of the column S2 would be useless without the simultaneous revamp of column S4. Both are linked through the overall material balance. It was also shown how the introduction of a supplementary reactor R4, between the columns S2 and S4, for the transformation of I1 and I2 into Heavies improved the performance of the whole system. This extra reactor gives access to alternative recycle structures.

![Flowsheet alternatives](image-url)

**Figure 4.2; Flowsheet alternatives**
Since substantial parts of $I_1$ and $I_2$ are transformed into Heavies in R4, it is no longer needed to send the bottom product of column S4 back to reactor R1. Instead, it can be drawn to column S5, where the heavies are removed directly. This is shown in Figure 4.2 as alternative A. The top distillate of S5 should then be sent to column S2. This creates a Lights removal loop S2-R4-S4-S5-S2 that crosses the Heavies removal loop S2-S3-S5-S2. This modification has the advantage to reduce the Heavies in S2 and to increase the robustness in operation by eliminating the loop S2-R4-S4-R1-S2.

In alternative B the bottom of S4 returns directly to S2. This creates a small Lights removal loop S2-R4-S4-S2, while the Heavies leave the plant via S2-S3-S5. The increased amount of Heavies in S2 may have a danger for more fouling as compared to the previous alternative.

In alternative C the bottom of S4 goes to the finishing column S3, which is now subject to more fouling. A failure of S4 may also affect immediately the quality of DCE. It may be expected that each recycle structure alternative will have distinct control properties. The final selection for one of the alternatives should take this into account.

### 4.3 Control strategy

In a complex plant like the one described here, many variables have to be controlled. Most of them – pressures, temperatures, levels – may be controlled locally. However, material balances in general and especially the material balances of impurities are established by interactions between the different operating units and recycle loops in a plant. Therefore, the control of all material balances requires a plantwide approach.

In this case study we focus our attention on the material balances of the impurities $I_1$, $I_2$ and $I_3$ (the outputs of the control problem). The objective is to control their concentration in the bottom product of column S2, for which stream the three specifications are given. This may be achieved by manipulating the column S2 distillate flowrate ($D_2$), side stream flowrate ($SS_2$) and reboiler duty ($Q_2$). Since the columns S2 and S4 are strongly coupled to each other by the recycle loops, we may also make a combination with the column S4 distillate flowrate ($D_4$) and reboiler duty ($Q_4$). These five variables are the inputs of the control problem.

The main disturbance of the material balance in a plant is associated with a change of the production rate. Its influence on the impurities material balances will be studied by modifying the flowrate of the external DCE feed ($F_{DCE}$). A second disturbance is the amount of impurities in the feed streams. For this reason also the fraction of impurity $I_3$ in the DCE feed ($X_{I3}$) is taken into account.
Because the material balances of impurities are characterized by long settling times, it is assumed that pressures, temperatures and levels are well controlled within the time scale of interest. Therefore their values are fixed and the corresponding heat duties and flow rates are calculated directly instead of using real controllers. This considerably simplifies the modeling without affecting the heart of the case study, being the effect of recycle interactions on the dynamics and control of the material balance of impurities.

4.4 Steady state analysis

A steady state simulation model of the basic flowsheet with the additional reactor R4 included is used to find the nominal operating point. This is the point where the specifications on the impurities \( I_1 \), \( I_2 \), and \( I_3 \) in the bottom product of column S2 are satisfied. These specifications are maximum concentrations of \( I_1 \) and \( I_2 \) and an optimal concentration for \( I_3 \). The nominal operating points of the alternatives A, B and C, which have a different recycle structure, are found in the same way. The values of the control system inputs and outputs are given in Table 4.1.

Although the nominal values of the impurities \( I_1 \) and \( I_2 \) are below their maximally allowed values, they are different for each alternative. This is a consequence of our comparison strategy to select the nominal operating points of the alternatives as close as possible to the operating point of the base case. This implies that the optimal value for \( I_3 \) is maintained in the alternatives, while the fractions of impurities \( I_1 \) and \( I_2 \) in the bottom product of column S2 are left free as long as they are below their maximum. This yields some additional operational freedom, being the range between the nominal point and their maximum acceptable value. Hence, these alternatives here already show some advantage over the base case as regards controllability of impurities \( I_1 \) and \( I_2 \).

### Table 4.1: Nominal operating points

<table>
<thead>
<tr>
<th></th>
<th>spec</th>
<th>base</th>
<th>alt A</th>
<th>alt B</th>
<th>alt C</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Output</strong></td>
<td>( I_1 )</td>
<td>Wt-ppm</td>
<td>&lt;100</td>
<td>81.7</td>
<td>69.4</td>
</tr>
<tr>
<td></td>
<td>( I_2 )</td>
<td>Wt-ppm</td>
<td>&lt;600</td>
<td>547</td>
<td>567</td>
</tr>
<tr>
<td><strong>Input</strong></td>
<td>D2</td>
<td>Kmol/h</td>
<td>14.5</td>
<td>14.5</td>
<td>14.5</td>
</tr>
<tr>
<td></td>
<td>SS2</td>
<td>Kmol/h</td>
<td>35</td>
<td>39</td>
<td>45</td>
</tr>
<tr>
<td></td>
<td>Q2</td>
<td>GJ/h</td>
<td>34</td>
<td>37.5</td>
<td>34</td>
</tr>
<tr>
<td></td>
<td>D4</td>
<td>Kmol/h</td>
<td>3.53</td>
<td>3.48</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>Q4</td>
<td>GJ/h</td>
<td>0.9</td>
<td>0.85</td>
<td>0.96</td>
</tr>
<tr>
<td><strong>Disturbance</strong></td>
<td>( F_{DCE} )</td>
<td>Kmol/h</td>
<td>175</td>
<td>175</td>
<td>175</td>
</tr>
<tr>
<td></td>
<td>( X_{13} )</td>
<td>Mol-%</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
</tr>
</tbody>
</table>
During the attempts to satisfy the specifications on the steady state plant models of the flowsheet alternatives, it turned out to be extremely difficult to get an acceptable value for $I_2$, while maintaining a constant, optimal value for $I_3$. Keeping the manipulated variables on their base case nominal values when changing the recycle structure leads to a drop of the $I_3$ concentration while the concentration of $I_2$ in the system is rising. The supplementary reactor R4 has a short residence time, which is enough to realize a high conversion of $I_1$, but the conversion of $I_2$ is too low. To compensate this, one may increase the Lights removal via column S4 (D4), but then the amount of impurity $I_3$ will drop further. In fact, D4 should be decreased to keep $I_3$ in the system, but then the concentration of $I_2$ will further rise. On the other hand, when the side draw from column S2 (SS2) is increased, more impurities are recycled to reactor R1 where $I_2$ is transformed into Heavies. $I_3$ is then kept in the system. To achieve both specifications, a compromise has to be found between increasing the side draw and decreasing the Lights removal. However, these modifications also affect the impurity $I_1$, yielding additional constraints.

Notice that in alternative A the distillate flow of column S5 is returned to column S2. This stream still contains a large amount of impurity $I_2$. A larger reboiler duty and a slightly increased side draw will bring its amount on an acceptable value. Small changes to the column S4 variables are enough to keep $I_3$ on its optimal value, but the nominal value of $I_1$ becomes much lower as compared with the base case.

This is in contrast with the alternative B, where the reboiler duty of column S2 is the same as in the base case. Therefore the side draw has to be increased much more to remove $I_2$, while the Lights removal has to be decreased to keep $I_3$ on its optimal value. The nominal value of $I_1$ becomes much higher as compared with the base case.

Alternative C is a special case. Because the bottom of column S4 is sent directly to the finishing column S3, the amount of light impurities should be much lower than in the previous cases. This requires a higher Lights removal and a very high side draw. Although this is unfavorable for the operation of R1, we will keep this alternative in our case study because it may have special controllability properties.

In conclusion we can say that only small changes of the input variables are needed to keep the nominal operating point close to that of the base case while the recycle structure is changed. The fact that it was difficult to find these new settings suggests that the outputs are very sensitive to the inputs, so let us look now to the static gains.
4.4.1 Static gains

For each alternative we have developed a static gain matrix around the nominal operating point by extensive steady state simulations. All gains in this analysis are scaled. The scale factors are the maximum allowed (inputs/outputs) or expected (disturbances) variation, so the expected values of all variables are between $-1$ and $1$ (see also Chapter 2). Table 4.2 resumes the static gains for the base case. We have already seen in the previous chapter that there are indeed some high gains, in particular for the reboiler duty (Q2) and the flowrate of the external DCE feed ($F_{DCE}$). Hence the system is very sensitive to disturbances.

Table 4.2; Static gain matrices of the base case

<table>
<thead>
<tr>
<th>G</th>
<th>D2</th>
<th>SS2</th>
<th>Q2</th>
<th>D4</th>
<th>Q4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$</td>
<td>-0.076</td>
<td>-0.184</td>
<td>-4.325</td>
<td>-0.154</td>
<td>-0.041</td>
</tr>
<tr>
<td>$I_2$</td>
<td>-0.140</td>
<td>-0.302</td>
<td>-2.298</td>
<td>-0.215</td>
<td>-0.061</td>
</tr>
<tr>
<td>$I_3$</td>
<td>0.737</td>
<td>0.156</td>
<td>-0.908</td>
<td>-2.136</td>
<td>-0.727</td>
</tr>
</tbody>
</table>

The development of the static gain matrices drew our attention to an important difference between the base case and the alternatives, concerning the effect of the distillate flowrate of column S2 (D2) on the impurities $I_1$ and $I_2$ (Table 4.3). When D2 is increased, the throughput of reactor R4 is also increased, which decreases the residence time. This leads to a lower conversion of impurities $I_1$ and $I_2$ and an increase of their concentration in the bottom product of column S4. In the base case, this product is recycled to reactor R1, where more of the impurities $I_1$ and $I_2$ are converted into Heavies. Finally, the concentrations of impurities $I_1$ and $I_2$ in the bottom product of S2 will decrease. However, in the alternatives the bottom product of column S4 will not pass the reactor R1 and therefore the increased amount of impurities will come back in column S2. In alternative B this only means a recycling of impurities in the short loop S2-R4-S4-S2 and the effect of D2 on $I_1$ and $I_2$ is only slightly positive. In alternative A the impurities are recycled through the loop S2-R4-S4-S5-S2 and their amount in the bottom product of S2 considerably increases. This effect becomes even worse in alternative C, where the impurities will come directly in the top product of S3, which requires a cleaner bottom product of S2.

Table 4.3; Steady state magnitudes of D2

<table>
<thead>
<tr>
<th>G</th>
<th>base</th>
<th>alt A</th>
<th>Alt B</th>
<th>alt C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$</td>
<td>-0.076</td>
<td>0.226</td>
<td>0.007</td>
<td>0.378</td>
</tr>
<tr>
<td>$I_2$</td>
<td>-0.140</td>
<td>0.672</td>
<td>0.080</td>
<td>0.726</td>
</tr>
<tr>
<td>$I_3$</td>
<td>0.737</td>
<td>0.800</td>
<td>0.500</td>
<td>0.369</td>
</tr>
</tbody>
</table>
The effect of D2 on I3 is positive and of comparable magnitude in all cases. This impurity is mainly built up in the large DCE recycle loop S2-S3-R2-S6-S7-S2 that all cases contain. Most gains of the other manipulated variables are comparable, although small changes may have a great impact on the interactions between control loops. Therefore it is interesting to perform an RGA analysis.

4.4.2 RGA analysis

We have calculated relative gain arrays (RGA) for all square control systems. The results for the three most promising combinations are given in Table 4.4. It can be seen that strong interactions exist between the control loops I1-Q2 and I2-SS2 in all alternative design and control structures, while the control loop of I3 with either D2, D4 or Q4 is less affected by interactions with the other loops. Especially the loops I3-D4 and I3-Q4 in the base case and I3-D4 in alternative C are hardly affected, as can be seen from their RGA elements being close to one.

Table 4.4; RGA diagonal elements

<table>
<thead>
<tr>
<th>I1, I2, I3</th>
<th>Base</th>
<th>alt A</th>
<th>alt B</th>
<th>alt C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q2, SS2, D2</td>
<td>1.47, 2.01, 1.34</td>
<td>1.58, 1.27, 1.10</td>
<td>1.37, 1.27, 0.89</td>
<td>1.63, 0.96, 0.83</td>
</tr>
<tr>
<td>Q2, SS2, D4</td>
<td>1.43, 1.35, 0.96</td>
<td>1.51, 1.38, 1.13</td>
<td>1.43, 1.29, 0.92</td>
<td>1.61, 1.43, 1.06</td>
</tr>
<tr>
<td>Q2, SS2, Q4</td>
<td>1.43, 1.36, 0.97</td>
<td>1.65, 1.48, 1.25</td>
<td>1.43, 1.30, 0.93</td>
<td>1.74, 1.57, 1.19</td>
</tr>
</tbody>
</table>

Notice that the RGA elements of the loops with I1 and I2 are always greater than one, while the RGA elements of the loops with I3 are in some cases less than one. An RGA element greater than one means that the open loop gain exceeds the closed loop gain, so the interactions are in an opposite direction. When the interactions are in the same direction as the single loop, the closed loop gain will be greater than the open loop gain and the RGA element will be smaller than one. Thus it is concluded that the magnitudes of Q2 and SS2 are reduced by interactions.

We can also see that the effect of the controller interactions on the control loop of I3 depends on the recycle structure. When the column S4 is connected to the column S2, either via reactor R1 (base case) or directly (alternative B), the effect of the S4 variables on I3 is enhanced by closing the other loops. This effect is reduced in the alternatives A and C, where the Heavies that are produced in R4 are not passing S2, but directly removed by S5.
The above steady state analysis showed that systems with alternative recycle structures could be operated close to the base case nominal operating point by minor changes in manipulated variables. The system is very sensitive to disturbances and there are strong interactions between control loops. However, what is the dynamic consequence?

4.5 Dynamic simulations

The steady state analysis showed the important role of the impurities destruction in reactor R1 and R4. Therefore the impact of these liquid phase reactors on the plant dynamics is considered. The gas phase reactors R2 and R3 have a negligible holdup and are assumed to operate instantaneously. The separation system is simulated dynamically with a reduced set of components. The reactants having zero flow in the reactor outlet streams are left out. Since phenomena of the impurities material balances are taking place at long time scales, level and pressure controllers are assumed to operate instantaneously as well. Therefore condenser pressures are fixed and total material balances in drums and reboilers are modeled in a steady state manner.

4.5.1 Step responses

Dynamic simulations with step perturbations on the manipulated variables and disturbances showed interesting responses of the outputs. All impurities will finally reach steady state values, but in different lengths of time. The responses on the perturbations will be discussed in detail.

Increasing the distillate flowrate of column S2 (D2) in the base case flowsheet will increase the throughput of reactor R4, which slightly reduces the conversion of impurities. The increased load of column S4, right after R4, will lead to the removal of more light impurities, including impurity I1, while the intermediate impurities I2 and I3 are forced to go to the bottom. This bottom flow is recycled to reactor R1 where more I1 and I2 are transformed into Heavies. The conversion of impurities in this large reactor is hardly affected by the increased recycle, which is only a small part of the total throughput that is dominated by the fresh feed. An increased recycle through reactor R1 therefore leads to more transformation of impurities I1 and I2 into Heavies. The Heavies are easily removed by column S5 and the concentration of impurities I1 and I2 in column S2 are decreasing (Figure 4.3). After 1½ hours the concentration of impurities I1 and I2 in the top distillate of column S2 are at a value where
Figure 4.3: Concentration of impurities $I_1$, $I_2$ and $I_3$ in the bottom of column S2 versus time after a step on D2 in the base case

More impurities $I_1$ and $I_2$ are transformed into Heavies in reactor R1 and their concentration decreases. On the contrary, $I_3$ is built up in the recycles in the first hours. When the concentration of $I_3$ in the top of column S4 also increases, more $I_3$ is removed from the system and its concentration in the bottom of S2 increases more slowly. Later, the high concentration of $I_3$ in the top of column S4 forces $I_1$ and $I_2$ to go to the bottom, so their concentrations in the system and therefore also in the bottom of S2 increase. After about 50 hours the recycle loops are in equilibrium and the system reaches a new steady state.

their partial flows are equal to the partial flows before the step change of D2. This implies a breakpoint in the operation of column S4, which starts to remove more $I_3$ while the concentrations of light impurities in the top distillate of column S4 are decreasing.

This effect is reflected by the concentration of $I_3$ in the bottom of column S2, which still increases, but with a much slower rate. Since the distillate flow of column S4 contains more $I_3$, the amount of $I_1$ and $I_2$ that leave the plant as Lights decreases. Therefore, after 8 hours, the concentrations of $I_1$ and $I_2$ in the bottom of column S4 start to rise again, which leads to an increase of their concentrations in all recycle loops as well. It will finally take about 50 hours to reach steady state values of the impurities concentrations.

Increasing the side stream flowrate of column S2 (SS2) in the base case flowsheet also increases the recycle flow through R1. The impurities $I_1$ and $I_2$ are transformed into Heavies and their concentration in the system decreases (Figure 4.4). The increase of SS2 leads to a fast drop of the concentration of $I_3$ in the top distillate D2, while the concentration of $I_3$ in the bottom product rises. The lower concentration of impurities in the top distillate also affects the removal of Lights in column S4. The amount of $I_3$ being removed by the top distillate D4
More impurities $I_1$ and $I_2$ are transformed into Heavies in reactor $R_1$ and their concentration decreases. This is in contrast with $I_3$, which is built up in the recycles in the first hours. When the concentration of $I_3$ in the top of column $S_4$ also increases, more $I_3$ is removed from the system and its concentration in the bottom of $S_2$ decreases. After about 50 hours the recycle loops are in equilibrium and the system reaches a steady state.

shows a decrease in the first 1½ hours. Then it rises again because the recycling of $I_3$ has increased its concentration. This yields a lower concentration of $I_3$ in the recycle loops that slowly become steady state after 50 hours. At 8 hours the removal of $I_3$ by $D_4$ shows a maximum and then it drops to its steady state value. The impurities $I_1$ and $I_2$ are less affected by the operation of column $S_4$ now and they become almost steady state after 10 hours.

The responses described above are a result of the interaction between the units and the recycle loops. This is in contrast with the effect of the reboiler duty of column $S_2$ ($Q_2$). Now, the responses of the impurities show a fast drop in a few minutes followed by a slow rise to reach the new steady state values in about two hours (Figure 4.5). The fast drop originates from the direct effect of the reboiler duty, which boils out the light impurities. The impurity concentrations rise again since the vapor is recycled over the top of the column. The effect of the recycle structure is negligible here. The column response itself is dominating.

The column $S_4$ variables $D_4$ and $Q_4$ are using the recycle structure of the base case flowsheet to affect the impurity concentrations in the bottom product of column $S_2$. The Lights removal is an exit for all three impurities and an increase of either $D_4$ or $Q_4$ will result in a decrease of their concentrations in the bottom of column $S_4$. This stream is recycled through reactor $R_1$ and column $S_2$. So, the impurity concentrations in the bottom product of column $S_2$ will also decrease. The impurities that are recycled through all loops have to become in
Figure 4.5; Concentration of impurities $I_1$, $I_2$ and $I_3$ in the bottom of column S2 versus time after a step on Q2 in the base case

The light impurities are boiled out of the bottom product by increasing the reboiler duty, which lead to a fast drop of the impurity levels. The recycle over the top of the column leads to an increase after 20 minutes. After two hours the system is almost steady state. The column effect in itself is dominant here and the effects of the recycle interactions are negligible.

equilibrium. Therefore it takes also 50 hours before a steady state value of the impurities concentrations is reached. This time is also required for the system to reach steady state after a disturbance, either the flowrate of the external DCE feed ($F_{DCE}$) or its impurity $I_3$ fraction ($X_{I3}$). This time seems to be characteristic for the recycle structure of the base case.

4.5.2 Alternative flowsheets

The alternative flowsheet structures differ in the location where the bottom product of column S4 is recycled. This has an influence on the steady state values that the outputs reach but the profiles are comparable. The response of $I_3$ to D2 in the base case was already discussed. In the alternatives A and B, $I_3$ shows the same profile with a different magnitude, but in alternative C it is different (Figure 4.6). In the beginning the removal of $I_3$ by column S4 is decreased and therefore its amount in the recycle loops starts to rise, as it did in the other alternatives. After 1½ hours this removal of $I_3$ increases again, which leads to a slower increase of $I_3$ in the base case. In alternative C, where the impurities material balances are more strongly affected by the operation of column S4, $I_3$ goes through a maximum and then drops to become steady state. The mechanism is the same, but the different magnitudes lead to a different profile. We can conclude that all alternatives show the same mixture of dynamic elements. However, the relative magnitudes of these elements are different, so they sum up to different overall dynamic responses.
The recycle structure strongly affects the time profile of $I_3$ after a step on D2. However, a close examination shows that the same phenomena are responsible and the differences are only caused by the different magnitudes. In the beginning, $I_3$ is forced to go to the bottom of column S4 and its concentration in all recycle loops starts to increase. After 1½ hours more $I_3$ may leave the plant via the top distillate of column S4, resulting in a slower increase of $I_3$ in the base case but a decrease in alternative C, where the impact is larger.

The only real structural difference between the base case and the alternatives is the recycle of the bottom product of column S4. Raising D2 in the base case increases this recycle flow through reactor R1, which leads to more transformation of impurities $I_1$ and $I_2$ into Heavies and a decrease of their concentration in the bottom product of column S2 (Figure 4.7). In the alternatives, the increased flow is recycled over a different path, not passing reactor R1. Instead of transforming the impurities into Heavies, they are only recycled and their concentrations in the bottom product of column S2 are increased. After a while their concentrations in the side draw to reactor R1 also increase, leading to more transformation into Heavies. The concentrations of $I_1$ and $I_2$ in the alternatives A and C therefore go through a maximum at 1½ hours followed by a decrease.

In alternative B the bottom product of column S4 is directly send to column S2, where it enters at a stage near the side draw. Therefore, the concentrations of impurities $I_1$ and $I_2$ in this side draw to reactor R1 increase almost instantaneously, leading to a decrease of $I_1$ and $I_2$ in the bottom of column S2. Finally, the buildup of impurity $I_3$ in the system leads to a competition with $I_1$ and $I_2$ in column S4. A higher concentration of $I_3$ in the Lights removal implies less removal of $I_1$ and $I_2$, so that these impurities will go to the bottom of this column and remain in the system. In the base case this leads to a small increase after 8 hours. The
The recycle structure strongly affects the time profile of $I_1$ after a step on D2. In the base case raising D2 increases the recycle through reactor R1, resulting in additional transformation of $I_1$ and therefore a lower concentration in the bottom of column S2. In the alternatives, reactor R1 is not passed and $I_1$ is recycled. Therefore in alternative A and C the concentration of $I_1$ in the bottom of column S2 rises. In alternative B, the concentration of $I_1$ in the side draw also rises in the short term, which leads to extra transformation of $I_1$ in reactor R1 by another mechanism as in the base case, but with the same result: a lower concentration in the bottom of column S2. The competition between $I_1$ and $I_3$ in column S4 finally leads to an increase again on the long term so the final response becomes almost zero.

alternatives A and C also show this small increase. In alternative B, however, this increase is larger and almost equal to the decrease in the first hours. Therefore the new steady state values are almost equal to the old ones and the magnitudes of D2 on $I_1$ and $I_2$ in alternative B are almost zero.

Hence, the most remarkable dynamic effect of changing the recycle structure is concentrated in the response of the system to a change of the top distillate of column S2 (D2). This is associated to the change of effect in the static gain matrices (Table 4.3).

### 4.6 Frequency analysis

A scaled linearized state space realization around the nominal operating point of the dynamic model has been generated as a basis for the calculation of frequency responses. The frequency analysis is expected to show the static gain impact of changing the recycle structure (in particular the effect of D2) as well as the dynamic impact at the higher frequencies.
In the previous chapter it was already shown that the static gains appear to be representative for frequencies up to 0.02 h\(^{-1}\). At frequencies above 10 h\(^{-1}\) the system is not responding anymore to disturbances and feedback control is no longer needed. Besides, the system is neither responding anymore to the manipulated variables. For oscillations with a frequency between 0.02 and 10 h\(^{-1}\) the system responses feature a delay and the magnitudes are lower. This clearly demonstrated why a steady state analysis of the plant behavior falls short. During operation of the plant there will always be oscillatory disturbances with frequencies in this range, hence impurity concentrations will always be in a transient.

Taking a closer look at the frequency responses of the base case, a clear difference between D2, Q2 and D4 can be seen (Figure 4.8). The response of I3 to an oscillation of D4 starts to deviate from steady state at a low frequency already. The Lights removal by D4 cannot follow these fluctuations and its effect is damped. The response of I3 to an oscillation of D2 also decreases at this frequency. In the analysis of the step responses it is already explained how the recycle effect of column S4 is playing an important role in the response of I3 to D2.

![Frequency response for D2, Q2 and D4](image)

**Figure 4.8; Frequency responses of impurity I3 for D2, Q2 and D4 in the base case**

The response of I3 to an oscillation of D4 starts to deviate from steady state at a low frequency already. The Lights removal by D4 cannot follow these fluctuations. The response of I3 to an oscillation of D2 also decreases at this frequency because of the recycle effect of column S4, playing an important role in the response of I3 to D2. At higher frequencies, where the oscillations are faster than the response time of column S2 itself, the magnitude of D2 drops fast. At these frequencies the magnitude of Q2 is increased because there is no counteracting effect of the recycle over the top (reflux).
When the Lights removal by D4 cannot follow the fluctuations anymore, the response of I₃ to D2 is also affected. At higher frequencies, where the fluctuations are faster than the response time of column S2 itself, the magnitude of D2 completely breaks down. At these frequencies the magnitude of Q2 is increased because there is no counteracting effect of the recycle over the top. The frequency where the response to Q2 shows a maximum corresponds to the time where the step response of I₃ to Q2 shows a maximum (Figure 4.5). Both the step and frequency responses show that the magnitude of the reboiler duty is large and mainly affected by the recycle over the top of the column. The response of the impurities to Q2 in the flowsheet alternatives is almost equal in profile and magnitude of the base case. Therefore, the effect of the recycle loops in the flowsheet is negligible in the case of Q2.

The effect of the recycle structure on the response of the outputs for the other inputs is mainly related to the magnitude. This was already shown by the step responses. The frequency where the response starts to differ from steady state in the alternatives is equal to that in the base case. The most important contribution to the recycle effects at low frequencies is originating from the Lights removal by column S4. Although the bottom product of this column is recycled to different places, the column effect is damped at the same frequency. This yields a damped magnitude for all outputs in all alternatives at this frequency. Hence, new differences between the alternatives are not detected with the frequency analysis.

4.7 Controllability study

Previously, the high sensitivity of the plant to changes has been revealed. The recycle interaction effects in the alternative flowsheet structures are comparable with the base case. They only differ in magnitude. However, this may have a strong effect on the controllability of the system. Therefore, let us analyze the sensitivity of the flowsheet alternatives in a systematic manner using closed loop controllability tools in the frequency domain.

4.7.1 Relative Gain Array

The steady state RGA analysis already showed that a control structure with D2-I₃ is more severely affected by interaction with the control loops for I₁ and I₂ than for the case of I₃ being controlled by either D4 or Q4. This is confirmed by an RGA analysis in the frequency domain (Table 4.4). The RGA number is defined as \( \| \text{RGA} - 1 \|_{\text{sum}} \) and gives a quantitative measure of the interactions in a diagonal control structure. All structures show an increased RGA number at the frequency range where the effects of the recycle interactions are
decreasing (Figure 4.9). This is caused by the reboiler duty that has an amplifying effect on all outputs, while the magnitude of the other manipulated variables are decreasing. This strongly affects the relative gains in negative direction, resulting in an increased RGA number. This effect is independent of the recycle structure and the alternatives therefore show the same behavior in this respect.

Figure 4.9; RGA numbers versus frequency of three control structures in the base case

The control structure with $D2-I3$ has more interactions than the structures where $I3$ is controlled with either $D4$ or $Q4$. All structures show an increased RGA number at the frequency range where the effects of the recycle interactions are decreasing. This is caused by the reboiler duty, having an amplifying effect on all outputs, while the magnitude of the other manipulated variables are decreasing. This strongly affects the relative gains in negative sense, resulting in an increased RGA number.

4.7.2 Closed loop performance

At the frequencies where interaction between the control loops increases, the effect of the disturbances is decreasing, but feedback control might still be needed. Therefore we will take a look at the closed loop disturbance gains. These parameters give the performance of a diagonal control system with respect to disturbance rejection. A description of the performance of decentralized control is given in chapter 2. In order to keep the control error between acceptable bounds, the closed loop disturbance gain should be smaller than the loop transfer function $(1+g_{ii}(s)k_i(s))$, for each disturbance. Here $g_{ii}(s)$ is the open loop input-output model and $k_i(s)$ is the controller model.
Figure 4.10; Closed loop disturbance gain and loop transfer function for $I_3$, controlled with $D_2$, and an impurity disturbance $X_{13}$ in the base case, while $I_1$ is controlled with $Q_2$ and $I_2$ with $SS_2$

The loop transfer function is drawn with a proportional controller with gain 1, which is not enough to come on top of the CLDG line at low frequencies. This means that the input magnitude of $D_2$ is too small to keep $I_3$ between its bounds when the disturbance $X_{13}$ is maximal at low frequencies in this control structure.

Figure 4.10 shows the closed loop disturbance gain and loop transfer function for the control of $I_3$ with $D_2$ and the impurity concentration in the DCE feed $X_{13}$ as disturbance in the base case, while $I_1$ is controlled with $Q_2$ and $I_2$ with $SS_2$. The loop transfer function is drawn with a proportional controller with gain 1, which is insufficient to become larger than the CLDG at low frequencies. To keep $I_3$ between its bounds, the loop transfer function should be larger. This may be achieved by increasing the controller gain. However, a scaled controller gain above 1 is not possible, because the input will become outside its bounds with an output error below 1. This implies that the input magnitude of $D_2$ is too small to keep $I_3$ between its bounds when the disturbance $X_{13}$ is maximal at low frequencies in this control structure. The problem is even worse in the alternative recycle structures, where the input magnitude of $D_2$ is much smaller.

Figure 4.11 shows the closed loop disturbance gains of $I_2$ to $F_{DCE}$ and $X_{13}$ in the base case with the controllers $I_1$-$Q_2$, $I_2$-$SS_2$ and $I_3$-$D_4$. Both closed loop disturbance gains are below 1 over the whole frequency range. This means that $I_2$ does not exceed its bounds when the controlled system is disturbed with either $F_{DCE}$ or $X_{13}$. Therefore it is not necessary to control $I_2$ between its bounds. The open loop magnitude of $F_{DCE}$ on $I_2$ is around 2 at low frequencies,
which indicates that a controller is required indeed. However, in the closed loop disturbance gain the interactions between the controllers are also taken into account. Then it is seen that the control of I₁ by Q₂ and I₃ by D₄ are interacting in such a way that I₂ is automatically kept between its bounds. The disturbances affect the outputs in the same direction. The reboiler duty and the side draw also affect the impurities I₁ and I₂ in the same direction. So both controllers are assisting each other in rejecting the disturbance. Because the magnitude of Q₂ is much larger than the magnitude of SS₂, the controller I₁-Q₂ is dominating and the controller I₂-SS₂ is not needed. Closed loop simulations with only the controller I₁-Q₂ implemented show that the effect of the disturbance F₇DCE on I₂ is reduced by 80% (Figure 4.14). I₂ is then below its maximum and further reduction is not needed. Still, a controller is required if I₂ has to be kept on setpoint, but the objective in this case study is to keep I₂ below its maximum. This may be achieved by control of I₁ by Q₂ and I₃ by D₄.

In the alternative flowsheet structures I₂ is also kept between its bounds with the controllers I₁-Q₂ and I₃-D₄. The CLDG values for I₂ are somewhat higher as a result of the recycle interactions, but they are below 1 over the whole frequency range so boundary control is not needed.

![Figure 4.11](image)

Figure 4.11; Closed loop disturbance gains for I₂ in the base case with the controllers I₁-Q₂, I₂-SS₂ and I₃-D₄

The CLDG for I₂ is below 1 for both disturbances over the whole frequency range of interest, which means that I₂ will never become outside its bounds under these disturbances and therefore does not need to be controlled between its bounds. The high CLDG value for the feed flowrate disturbance F₇DCE is around a frequency of 8 cycles per hour, which is an unrealistic fast fluctuation for this feed with this amplitude (75 kmol/h). Only small fluctuations may occur at these high frequencies and these will not cause problems.
If Q4 is used to control I3, I2 does not need control either, but the input magnitude of Q4 is too small to keep I3 between its bounds over the whole frequency range. Therefore, the only possible control structure is the control of I1 with Q2 and I3 with D4, keeping I2 free to vary between its bounds.

If we calculate the RGA number for this control system in the base case (Figure 4.12), we see that the interaction is much lower than the control systems with the loop SS2-I2 included (Figure 4.9). In fact, at low frequencies, the control loops Q2-I1 and D4-I3 are almost decoupled. The higher RGA numbers in the 3x3 control system are a result of the interaction between Q2-I1 and SS2-I2, which is in fact a positive interaction in this case study because we can keep I2 between its bounds with the control of I1 only. Furthermore it is seen that the controller interactions in alternative B are also very low, but they increase rapidly at intermediate frequencies. At these frequencies the magnitude of D4 drops fast. Because of the recycle structure this affects the controller interactions in alternative B to a larger extent than in the base case. The controllers in alternatives A and C have already more interactions at low frequencies, so the base case seems to be the better one.

![Graph showing RGA number for different control structures](image)

**Figure 4.12;** RGA number of the control structure I1-Q2 and I3-D4 versus frequency for all flowsheet structures

*Hardly any interaction exists between the controllers I1-Q2 and I3-D4 in the base case and alternative B at low frequencies. At intermediate frequencies the interactions in alternative B increase fast while the interactions in the base case remain low till frequencies where control is no longer needed. In the alternatives A and C there is more interaction at low frequencies, but this is still low compared to the interactions with the control loop I2-SS2 included.*
4.7.3 Controller gains

Table 4.5 shows the minimal controller gains that are required to keep the outputs between their bounds under the disturbances $F_{DCE}$ and $X_{13}$ with the proportional controllers $I_1$-Q2 and $I_3$-D4. The controller gain for $I_1$ in alternative A is small compared to the others, but in this alternative the nominal value of $I_1$ is considerably lower and therefore it may vary more before it exceeds its bounds. Because of this difference in nominal value, alternative B has a higher gain.

<table>
<thead>
<tr>
<th></th>
<th>base</th>
<th>alt A</th>
<th>alt B</th>
<th>alt C</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$-Q2</td>
<td>0.46</td>
<td>0.13</td>
<td>0.53</td>
<td>0.46</td>
</tr>
<tr>
<td>$I_3$-D4</td>
<td>0.40</td>
<td>0.47</td>
<td>0.56</td>
<td>0.38</td>
</tr>
</tbody>
</table>

The controller gain for $I_3$-D4 in alternative B is also larger. While in the other alternatives the impurity disturbance $X_{13}$ is the most difficult to reject, in alternative B it is the flow disturbance $F_{DCE}$. The open loop disturbance gain of $F_{DCE}$ to $I_3$ in alternative B is already larger than in the base case, while for alternative C this is lower. On the other hand, the nominal value of D4 in alternative B is lower than in the base case, while for alternative C it is larger (Table 4.1). We have seen before that the impurity removal by column S4 and the impurity buildup in the recycle loops are strongly related to each other. A higher nominal value of D4 means more effective removal of impurities and less buildup in the recycle loops. This leads to the result that the impurity level of $I_3$ is less sensitive to disturbances and hence less control action is required to keep $I_3$ between its bounds during a disturbance. So, the controller gain for $I_3$-D4 in alternative C may be lower than in the base case and in alternative B it should be higher. We can conclude that the controller gains in the alternative flowsheet structures differ mainly because of the different nominal operating points, but it must be realized that these are a result of the recycle interactions.

4.8 Closed loop simulations

Dynamic simulations of the full order nonlinear disturbed system with the control structure $I_1$-Q2, $I_2$-SS2, $I_3$-D2 implemented show that $I_3$ becomes outside its bounds when D2 is clipped on its bounds (Figure 4.13). The input magnitude of D2 is indeed too small to control $I_3$, as was indicated by the analysis of the closed loop performance.
Figure 4.13; Closed loop response of I3 in the base case with controllers I1-Q2, I2-SS2 and I3-D2 for the step disturbance F_{DCE}

$I_3$ becomes outside its bounds because the magnitude of D2 is too small.

We already referred to the simulation with only the controller I1-Q2 implemented. The effect of the flow disturbance F_{DCE} on I2 is then reduced with 80% (Figure 4.14). We also implemented the controllers I1-Q2 and I3-D4 with the controller gains from Table 4.5. This affects impurity I2 in such a way that it never exceeds its bounds and control of I2 is not needed. We also see that the impurities I1 and I3 (Figure 4.15) are well controlled and do not exceed their bounds. The nonlinear behavior on the dynamic model affect the control system in such a way that the bounds are even not reached with the most difficult disturbance, although the controller gains that are calculated with the linearized model are based on these bounds.

Figure 4.14; Time response of I2 after a step on F_{DCE} in the base case

If the control loop I1-Q2 is closed, also the effect of F_{DCE} on I2 is reduced (by 80%). If the loop I3-D4 is also closed, I2 is well below its maximum and no further control is needed.
In other cases the nonlinear behavior may lead to a slightly increased effect, so the bounds may be exceeded. However, when the linear model gives an acceptable description of the dynamic system, the controller settings from the linear model are a good starting guess. They may be fine-tuned in the dynamic system but that is beyond the scope of this case study.

![Graph showing the closed loop response of I3 in the base case with controllers I1-Q2 and I3-D4 for a step on the disturbances F_{DCE} and X_{I3}.]

4.9 Conclusions

This thesis started with two simple examples to demonstrate that recycle interactions strongly affect the material balance and its controllability. As a more complex case study the balanced VCM-plant with all its recycle loops and alternative flowsheet structures has been introduced. We described the problem of controlling the impurities material balances and analyzed the dynamic behavior and controllability properties in a systematical way. We may conclude that this case study clearly demonstrates that recycle interactions are affecting the dynamics and controllability properties of the material balance indeed. Moreover, the case study allows analyzing in detail how and on which part of the plant these effects are realized!

We have seen that the interaction of recycle loops leads to an increase of response times. This was demonstrated by an example in chapter 1, but it is also reflected by the case study. The system is almost at steady state in two hours after a step on the reboiler duty of column S2, while it takes about 50 hours to reach a steady state when one of the other inputs is changed. The reboiler duty has a strong effect on the impurities material balance in the column itself and recycle interaction effects are negligible. On the other hand, the effect of the other inputs
is mainly a result of the interactions between columns S2 and S4 being connected by the recycle loops. Therefore, these inputs affect the system on a complete different time scale than the reboiler duty does.

In this chapter it was specifically shown that the recycle structure strongly affects the nominal operating point of the plant and how this affects the controllability. Therefore, part of the discussion on recycle structures shifts to a discussion on nominal operating points, in particular the nominal values of the impurity levels. The lower nominal value of I1 in alternative A widens its operating range considerably and therefore less control action (lower gain) is required to keep its value below the maximum. From this point of few alternative A would be preferable. However, it requires a higher nominal value of the reboiler duty Q2, which is unfavorable in respect with operating costs.

We have seen that the removal of lights by column S4 has a great influence on the material balance of the impurities and how its nominal value affects the sensitivity of the impurities to disturbances. Alternative B has a relative low nominal value of D4 as compared to the other alternatives, but I3 is more sensitive to disturbances and a higher controller gain is needed to keep it between bounds. Hence, alternative B is not recommendable from this respect.

In conclusion we can say that low nominal values of impurity levels are preferable since they enlarge the operating range. However, this is unavoidable counteracted by the related phenomena that the nominal values of the manipulated variables are required to be larger. Hence, the lower nominal values of impurity levels have to be balanced with the higher operating costs associated with the higher levels of the manipulated variables, being energy consumption, reflux ratios and recycle flowrates. This conclusion may be generalized to other plants with impurity problems. Low impurity levels are more easily controllable, but require high basic recycle loads.

It was also demonstrated that control of the impurities I1, I2 and I3 is not possible only using the input variables on column S2 itself (D2, SS2 and Q2). The input magnitude of D2 is too small to keep I3 between its bounds. On the other hand, when the Lights removal D4 is used to control I3, together with the controller Q2-I1, I2 does not require control. The interaction between the controllers and recycle loops is such that all three impurities are kept between their bounds with only these two controllers. Closed loop simulations have confirmed these conclusions.
Comparing the different flowsheet structures, we may state that the high nominal value of SS2 in alternative C is unfavorable for the operation of reactor R1, while the controllability is not improved as compared to the base case. In alternative B, the low value of D4 increases the system’s sensitivity to disturbances and a high controller gain for D4-I3 is needed for compensation. This results in a fast increase of interactions between the controllers Q2-I1 and D4-I3 at intermediate frequencies, which makes this alternative also unfavorable. In alternative A the higher nominal value of Q2 is compensated by a lower nominal value of I1 and therefore a lower controller gain for Q2-I1, as compared to the base case. The higher interaction between the controllers Q2-I1 and D4-I3 at low frequencies does not affect the controllability. Therefore alternative A is a good alternative flowsheet structure for the base case.
Chapter 5

Large Scale Model Reduction

5.1 Introduction

Waste minimization and flexibility are key issues in the design of a new chemical plant. The development of a 'zero discharge' plant often leads to a complex structure with many recycle loops included. Flowsheeting is a well-established technique reflecting the complexity of these systems by means of an accurate steady state simulation model. Through dynamic flowsheeting even more design and operation knowledge is obtained. In addition, large dynamic plant models give access to a whole class of controllability tools. A method for the combination of steady state and dynamic modeling with linear controllability analysis tools was described in chapter 2.

By applying this systems approach on a case study about the handling of impurities in a balanced VCM process, as described in chapter 3 and 4, we observed that the derivation of a linear model for a large, nonlinear dynamic plant is far from trivial. When a dynamic model is available, it is easy to generate a linear state space description by performing a Taylor series expansion of the nonlinear functions around the nominal point, neglecting second and higher order terms. Dynamic simulation programs like SPEEDUPTM posses such features. However, an automatic linearization procedure will inevitably include all states from the complex nonlinear model and the linear state space realization may become very large and difficult to handle. Therefore there is a real need to reduce a state space realization to lower order, which is the subject of this chapter.
5.2 Dynamic modeling

A description of dynamic models and linearization was already given in chapter 2. Let’s recall this for a better understanding of the remainder of this chapter.

5.2.1 Dynamic model

A dynamic plant model contains material and energy balances (including reactions), phase equilibrium relations and volume equations. It is a combination of differential equations for the material and energy holdup relations and additional algebraic equations. In general, the model can be described as:

\[
\begin{align*}
\dot{x}(t) &= f(x(t), u(t)) \\
y(t) &= g(x(t), u(t))
\end{align*}
\]  

(5.1)

where \( \dot{x} = dx/dt \), \( x \) denotes a vector of \( n \) state variables, \( u \) a vector of \( m \) input variables and \( y \) a vector of \( l \) output variables, while \( f \) and \( g \) are general nonlinear functions.

The first stage of model reduction already takes place during the development of the dynamic model. An important issue is the number of components to be included, since component balances have to be solved for all trays in every column. By including only components being important for the dynamic behavior and, in addition, lumping impurities and trace components, the number of state variables can be reduced considerably. Another issue is the separation of equipment into units determining the overall dynamic behavior of the plant and units with minor influence on this behavior, to be omitted. Describing the fast responding units with instantaneous models reduces the number of state variables further, while the overall dynamic behavior is almost not affected. However, doing this the final dynamic model will normally still left with a large number of state variables, all being included in the linear state space realization.

5.2.2 Linearization

A well-known method for the development of a linear model is the curve fitting of experimental data with standard functions. Simple first and second order transfer functions often give already acceptable descriptions of the input-output behavior of complex systems, while high order polynomials can be used to give an accurate description. Extensive dynamic simulations can be used to generate the input-output data. As an advantage, this method leads
to small linear systems being easy to deal with. However, this procedure may be very time consuming, especially when experimental data have to be generated by extensive dynamic simulations.

More conveniently a linear state space realization is derived from a dynamic model. Performing a Taylor series expansion of the nonlinear functions around the nominal operating point and neglecting second and higher order terms gives:

\[
\frac{dx(t)}{dt} = \frac{\partial f}{\partial x} dx(t) + \frac{\partial f}{\partial u} du(t)
\]

or \( x(t) = Ax(t) + Bu(t) \)  \( y(t) = Cx(t) + Du(t) \)  \( (5.2) \)

Now \( x, u \) and \( y \) are deviations from the nominal point and \( A, B, C \) and \( D \) are real matrices.

With a dynamic process simulator like SPEEDUP™, the user may specify the input and output variables to be included in the linear model. The program will carry out a linearization around the nominal point and generates the matrices \( A, B, C \) and \( D \). Such a state space realization contains only input and output variables of interest to the user, but the model inevitably contains all state variables. For control studies of complex plants, typically only 10 to 20 input and output variables are concerned, but the number of states easily amounts to thousands. Thus, the state space description has a large size and is difficult to handle. In addition, the matrix \( A \) may be numerically ill conditioned. However, realizing that states are not equally important, the possibility exists to reduce the size of the state space realization while retaining sufficient accuracy in the description of the dynamic input-output behavior. This requires special model reduction techniques.

### 5.3 Reducing a state space realization

A number of algorithmic procedures exist to reduce a linear state space realization to lower order. The simplest method is to discard part of the states from the model, called truncation. Another method is residualization, where part of the model is simulated steady state. A description of these methods will be given below and demonstrated on a case. The first step is to select states to be truncated or residualized. This may be performed manually for small models, but this is not feasible for models containing over a thousand states. For this reason a certain ordering of the states is required before the realization can be reduced.
5.3.1 Jordan form

A well-known method for the ordering of a state space realization is based on its corresponding time constants. To this end the A-matrix is transformed into its Jordan form, where the eigenvalues of the system are put on the main diagonal in descending order. Consider the transformation matrix $T$ with the eigenvectors $t_i$ of the $n \times n$ matrix $A$ as its columns and the corresponding eigenmatrix $\Lambda$:

$T = [t_1 \ t_2 \ \cdots \ t_n], \quad \Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \lambda_n \end{bmatrix}$

Now, introduce the new states $z$:

$z = T^{-1}x \leftrightarrow x = Tz \tag{5.4}$

Substituting these in the state space description (5.2) will give the ordered realization:

$Tz = ATz + Bu \Leftrightarrow \dot{z} = \Lambda z + T^{-1}Bu$

$y = CTz + Du \tag{5.5}$

where $\Lambda = T^{-1}AT$ is the A-matrix in Jordan form. Note that this also produces a new B-matrix $T^{-1}B$ and a new C-matrix $CT$. The D-matrices are identical. The variables $x$, $y$, $z$ and $u$ are still time dependent, but for simplicity the notation $(t)$ is omitted here.

5.3.2 Splitting

If the A-matrix is in Jordan form, the states are ordered such that the first state is connected to the fastest process and the last state to the slowest one. The states are then readily partitioned into two groups, the first containing fast and the second slow modes.

$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

The corresponding state space description becomes:

$\dot{x}_1 = A_{11}x_1 + A_{12}x_2 + B_1u$

$\dot{x}_2 = A_{21}x_1 + A_{22}x_2 + B_2u \tag{5.7}$

$y = C_1x_1 + C_2x_2 + Du$
where the matrices $A, B$ and $C$ are split up as follows:

$$
A = \begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}, \quad B = \begin{bmatrix}
B_1 \\
B_2
\end{bmatrix}, \quad C = \begin{bmatrix}
C_1 & C_2
\end{bmatrix}
$$

(5.8)

### 5.3.3 Truncation

When regarding fast dynamics the slow part of the system can be discarded, yielding the state space description:

$$
\begin{align*}
\dot{x}_T &= A_T x_T + B_T u \\
y &= C_T x_T + D_T u
\end{align*}
$$

(5.9)

where

$$
x_T = x_1, \quad A_T = A_{11}, \quad B_T = B_1, \quad C_T = C_1, \quad D_T = D
$$

(5.10)

Discarding states from a system that is ordered by its eigenvalues (Jordan form) is called modal truncation.

### 5.3.4 Residualization

Regarding slow processes, it should be realized that the fast processes are almost instantaneous as relative to the slow ones and therefore the states associated with the fast part of the system may be modeled as steady state:

$$
\begin{align*}
0 &= A_{11} x_1 + A_{12} x_2 + B_1 u \\
\dot{x}_2 &= A_{21} x_1 + A_{22} x_2 + B_2 u \\
y &= C_1 x_1 + C_2 x_2 + D u
\end{align*}
$$

(5.11)

From the above system $x_1$ can be solved, resulting in

$$
\begin{align*}
\dot{x}_R &= A_R x_R + B_R u \\
y &= C_R x_R + D_R u
\end{align*}
$$

(5.12)

where

$$
\begin{align*}
\dot{x}_R &= \dot{x}_2 \\
A_R &= A_{22} - A_{21} A_{11}^{-1} A_{12} \\
B_R &= B_2 - A_{21} A_{11}^{-1} B_1 \\
C_R &= C_2 - C_1 A_{11}^{-1} A_{12} \\
D_R &= D - C_1 A_{11}^{-1} B_1
\end{align*}
$$

(5.13)

Residualization of a system in Jordan form is called modal residualization.
A typical and important property of residualization is that it retains the steady state gain of the system by putting derivatives to zero, which obviously represents steady state. This is in sharp contrast to modal truncation that on the contrary retains the system's behavior at infinite frequency. For this reason modal truncation should be used when accuracy is required at high frequencies, whereas modal residualization is preferred for low frequency modeling.

**Example 5.1; Modal Truncation**

Consider a dynamic vapor-liquid flash drum with pressure and level control, where a 3-component mixture is separated into a vapor and a liquid. The feed flowrate and composition may fluctuate and therefore the partial component flowrates are selected as input variables of the linear model. The purity of the top and bottom products have to be controlled and therefore the fraction of component 1 in the outlet streams are selected as the output variables of the linear model. The pressure and temperature of the flash are manipulated to control the output variables so they also serve as input variables.

The state space realization, generated with the CDI interface from SPEEDUP™, contains 5 input variables, two output variables and 10 state variables; the material holdup of each of the three component, the total energy holdup and three states for each PID controller. The states in this realization can be ordered by transforming the A-matrix into its Jordan form, where the eigenvalues are put on the diagonal in descending order. These eigenvalues are:

\[
\text{eig}(A) = [-3215, -62.0, -18.9, -10.5, -10.0, -10.0, -5.0, -1.0, -1.0, -0.001]
\]

Since the last eigenvalue is much smaller than the other ones, this state might be truncated when considering fast dynamics. Regarding slow dynamics only, the first state might be residualized.

Unfortunately, little is known a priori about the effect of these reductions on the quality of the description of the overall input-output behavior. In a large and complex plant the input-output behavior is often determined by a combination of fast and slow processes, so the Jordan form is not optimal in ordering states. Apparently, it is more appropriate to order the states according to their contribution to the input-output behavior. This is the outline of the balanced realization to be described next.
5.4 Balanced realizations

A balanced realization is an asymptotically stable minimal realization with controllability and observability Gramians being equal and diagonal [Skogestad and Postlethwaite, 1996]. This is to be explained as follows. Firstly, a system is stable if it reaches a new steady state within finite time after a disturbance. This occurs when the A-matrix of the state space realization only contains negative eigenvalues, as was the case in the flash drum introduced above. Then, a minimal realization only contains states that do contribute to the input-output behavior. Non-controllable and/or non-observable states are omitted. Following this line of thought is seems proper to introduce the concepts of state controllability and state observability now.

5.4.1 State controllability

The dynamic system \( \dot{x}(t) = Ax(t) + Bu(t) \), or equivalently the pair \((A,B)\), is said to be state controllable if, for any initial state \( x(0) = x_0 \) any time \( t_1 > 0 \) and any final state \( x_1 \), an input \( u(t) \) exists such that \( x(t_1) = x_1 \). Otherwise the system is state uncontrollable.

In other words, if a system is state controllable it can be moved from any initial state to any final state within a given finite time by using its inputs.

Many ways exist for checking whether a system is state controllable. One option is based on the controllability matrix \( C \) for the system pair \((A,B)\), being defined as:

\[
C^A = \begin{bmatrix} B & AB & A^2B & \cdots & A^{n-1}B \end{bmatrix}
\] (5.14)

The system \((A,B)\) is state controllable if and only if the controllability matrix has rank \( n \) (full row rank), where \( n \) is the number of states.

According to an alternative method of checking controllability, the input profile \( u(t) \) is considered moving a state from its initial value \( x_0 \) to a value \( x_1 \) in time \( t_1 \), given by:

\[
u(t) = -B^T e^{A^T (t_1 - t)} W_c(t_1)^{-1} \left( e^{At_1} x_0 - x_1 \right)
\] (5.15)

where \( W_c(t) \) represents the Gramian matrix at time \( t \),

\[
W_c(t) = \int_0^t e^{At}BB^Te^{A^T \tau}d\tau
\] (5.16)
and $^T$ is used to specify the transpose of a matrix. The system $(A,B)$ is state controllable if and only if the Gramian matrix has full rank for any $t > 0$.

As regards stable systems only the Gramian matrix at infinite time needs to be considered,

$$W_c(\infty) \equiv P = \int_0^\infty e^{At}BB^Te^{A^Tt}dt$$

(5.17)

$P$ is called the controllability Gramian and plays an important role in the balancing of a state space realization. Matrix $P$ may also be obtained as solution to the following Lyapunov equation:

$$AP + PA^T + BB^T = 0$$

(5.18)

Solving this Lyapunov equation is not always a trivial task. Standard algorithms may fail for large systems, so special techniques are required. This will be discussed in section 5.5.

5.4.2 State observability

The dynamic system $\dot{x}(t) = Ax(t) + Bu(t)$, $y(t) = Cx(t) + Du(t)$ or the pair $(A,C)$, is said to be state observable if, for any time $t_i > 0$, the initial state $x(0) = x_0$ can be determined from the time history of the input $u(t)$ and the output $y(t)$ in the interval $[0,t_i]$. Otherwise the system is state unobservable.

Hence, a system is state observable if the value of all individual states can be obtained by measuring the output $y(t)$ over a period of time.

In order to check whether a system is state observable, the observability matrix $O$ for the system pair $(A,C)$ has to be considered:

$$O = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix}$$

(5.19)

The system $(A,C)$ is state observable if and only if the observability matrix has rank $n$ (full column rank), where $n$ is the number of states.
On the other hand, analogously to state controllability it is found that the Gramian matrix $W_0(t)$ at time $t$ is equal to,

$$W_0(t) = \int_0^t e^{A^T \tau} C^T Ce^{A\tau} d\tau$$  \hspace{1cm} (5.20)

The system $(A,C)$ is state observable if and only if the Gramian matrix has full rank in the interval $[0,t]$.

Again regarding stable systems one should consider:

$$W_0(\infty) = Q = \int_0^\infty e^{A^T \tau} C^T Ce^{A\tau} d\tau$$  \hspace{1cm} (5.21)

$Q$ is called the observability Gramian and may also be obtained as solution to the following Lyapunov equation:

$$A^T Q + QA + C^T C = 0$$  \hspace{1cm} (5.22)

### 5.4.3 Minimal realization

It should be noted that only controllable and observable states contribute to the input-output behavior of the system. If a state is uncontrollable, it is not affected by the inputs $u$. If a state is unobservable, is does not affect any output $y$. This leads to the statement that a state space realization is minimal if and only if $(A,B)$ is state controllable and $(A,C)$ is state observable. This means that $A$ has the smallest possible dimension (i.e. the fewest number of states).

#### Example 5.2; Minimal realization

Consider the state space realization of the flash problem from above. Since the eigenvalues of the $A$-matrix are all negative, the realization is stable and only the controllability and observability Gramians have to be considered. These are obtained by solving the Lyapunov equations 5.18 and 5.22. Both, the controllability Gramian $P$ and the observability Gramian $Q$ are of full rank, so the state space realization is minimal.

### 5.4.4 Hankel norm

Before describing the balanced realization in a more formal way, one additional concept has to be introduced, the Hankel norm and the associated Hankel singular values.
The Hankel norm of a stable system $G(s)$ is obtained when an input $u(t)$ is applied up to $t = 0$ and the output $y(t)$ is measured for $t > 0$. Furthermore $u(t)$ is selected to maximize the ratio of the 2-norms of the output- and input-signal:

$$
\|G(s)\|_H = \max_{u(t)} \frac{\sqrt{\int_0^\infty y(\tau)^2 d\tau}}{\sqrt{\int_0^\infty u(\tau)^2 d\tau}}
$$

The Hankel norm may be interpreted as an induced norm from past inputs to future outputs and is defined as the maximum Hankel singular value $\sigma_1$

$$
\|G(s)\|_H = \sigma_1
$$

It may be shown (Skogestad and Postlethwiate, 1996) that the Hankel norm is equal to

$$
\|G(s)\|_H = \sqrt{\rho(PQ)}
$$

where $\rho$ is the spectral radius (maximum eigenvalue), $P$ is the controllability Gramian and $Q$ the observability Gramian. The corresponding Hankel singular values are the positive square roots of the eigenvalues of the product $PQ$, so one obtains:

$$
\sigma_i = \sqrt{\lambda_i(PQ)}
$$

The name “Hankel” is used because the matrix $PQ$ has the special structure of a Hankel matrix (which has identical elements along the “wrong-way” diagonals).

The Hankel norm has a special property; it is less than or equal to twice the sum of the Hankel singular values:

$$
\|G(s)\|_H \leq 2 \sum_{i=1}^n \sigma_i
$$

This property can be used as error criterion for model reduction of a balanced realization.

### 5.4.5 Balanced realization

Now, the definition of a balanced realization is revisited in a more formal way. Let $(A,B,C,D)$ be a minimal realization of a stable, rational transfer function $G(s)$, then $(A,B,C,D)$ is called a balanced realization if the solutions to the related Lyapunov equations 5.18 and 5.22 are equal and therefore diagonal, so
with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

P and Q are the controllability and observability Gramians respectively, while $\sigma_i$ are the ordered Hankel singular values, given by 5.26. Since the controllability and observability Gramians of a balanced system are equal, we simply refer to the Gramian of the system by $\Sigma$.

Typically, in a balanced realization each state is just as observable as controllable. Furthermore, $\sigma_i$ is a relative measure for the contribution of the related state $x_i$ of the balanced realization to the input-output behavior of the system. States corresponding to small singular values have a small contribution and may be discarded by truncation.

Since the Hankel norm is always less than or equal to twice the sum of the singular values, this may be used as a measure of the error introduced by discarding states. The Hankel norm of the difference between the full and the reduced model is less than or equal to twice the sum of the Hankel singular values that correspond to the discarded states.

$$\|F_n(s) - F_m(s)\|_H \leq 2 \sum_{i=m+1}^{n} \sigma_i$$

(5.29)

### 5.4.6 Balancing

Next, the balancing of a state space realization is discussed. Normally the controllability Gramian $P$ and observability Gramian $Q$ of a stable minimal realization $(A,B,C,D)$ are not equal. It is known that the joint controllability and observability Gramian of the balanced system should be a special matrix with the Hankel singular values on the main diagonal and with its non-diagonal entries being all zero. Now, if $P$ and $Q$ are the solutions to the corresponding Lyapunov equations 5.18 and 5.22, they may be decomposed into their Cholesky factors $R$ and $S$, defined as:

$$P = R^T R \quad \text{and} \quad Q = S^T S$$

(5.30)

Then equation 5.26 can be written as:
\[
\sqrt{\lambda_{PQ}} = \sqrt{\lambda_{R^T R S^T S}} = \sqrt{\lambda_{R S^T S R^T}} = \sigma_{SR^T} \tag{5.31}
\]

where \(\sigma_{SR^T}\) are the singular values of \(SR^T\). These values may be obtained by Singular Value Decomposition:

\[
SR^T = u_{SR^T} \sigma_{SR^T} v_{SR^T}^T \tag{5.32}
\]

Now, the following operations will balance the system:

\[
A_{bal} = u_{SR^T}^T S A R^T v_{SR^T}
\]

\[
B_{bal} = u_{SR^T}^T S B \tag{5.33}
\]

\[
C_{bal} = C R^T v_{SR^T}
\]

\[
D_{bal} = D
\]

**Example 5.3; Balanced truncation**

The balanced truncation is demonstrated on the flash drum example. Since the controllability and observability Gramians of the minimal realization are known, the system may be balanced. Table 5.1 shows the Hankel singular values that are positioned on the main diagonal of the joint controllability and observability Gramian of the balanced realization. They form a measure of the contribution of the corresponding states to the input-output behavior. The table also shows the maximum error if the system is truncated after the state concerned. According to equation 5.29 this is equal to twice the sum of the discarded Hankel singular values.

**Table 5.1; Hankel singular values and error bound for the balanced state space realization of the 3-component flash with level and pressure control.**

<table>
<thead>
<tr>
<th>State</th>
<th>Hankel singular value</th>
<th>Max. modeling error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.03e+01</td>
<td>8.32e+00</td>
</tr>
<tr>
<td>2</td>
<td>2.80e+00</td>
<td>2.71e+00</td>
</tr>
<tr>
<td>3</td>
<td>1.35e+00</td>
<td>3.58e-03</td>
</tr>
<tr>
<td>4</td>
<td>1.45e-03</td>
<td>6.74e-04</td>
</tr>
<tr>
<td>5</td>
<td>3.37e-04</td>
<td>3.88e-14</td>
</tr>
<tr>
<td>6</td>
<td>1.71e-14</td>
<td>4.60e-15</td>
</tr>
<tr>
<td>7</td>
<td>1.68e-15</td>
<td>1.23e-15</td>
</tr>
<tr>
<td>8</td>
<td>5.49e-16</td>
<td>1.31e-16</td>
</tr>
<tr>
<td>9</td>
<td>6.45e-17</td>
<td>2.05e-18</td>
</tr>
<tr>
<td>10</td>
<td>1.03e-18</td>
<td>0</td>
</tr>
</tbody>
</table>
It is clearly seen that the last five states have hardly any contribution and may be discarded without affecting the quality of the input-output description significantly. If less accuracy is required, the balanced system might even be truncated after the third state.

This example clearly illustrates that balancing is a more elegant way of ordering the states than the Jordan form. Especially for large and complex systems, where the input-output behavior depends on processes operating at different time scales, the Jordan form is not useable while discarding states from a balanced system proceeds in a straightforward manner.

5.5 Solving Lyapunov equations

It should be recalled that the solution to the Gramians might be obtained by solving the Lyapunov equations. In case of low dimensional problems ($n \leq 50$) numerous solution techniques are available. One of the most efficient and widely used procedures is the Bartles-Steward algorithm (Bartles and Steward, 1972). In this algorithm the A-matrix is transformed into a real Schur form $H = U^T A U$ in which $U$ is orthogonal and $H$ is quasi upper triangular. This gives the modified Lyapunov equation:

$$H\tilde{P} + \tilde{P}H + U^T B B^T U = 0 \quad (5.34)$$

in which $\tilde{P} = U^T P U$, and this equation is easily solved by back substitution.

Unfortunately, this method is unsuitable for solving large Lyapunov equations, since the computation time and storage requirements become prohibitive, while the method suffers from numerical instability too. In order to resolve this problem, Jaimoukha [Jaimoukha et al., 1992; Jaimoukha and Kasenally, 1994] presented an algorithm to compute low rank approximate solutions to the Lyapunov equations for large systems using classical Krylov subspace methods.

5.5.1 Low rank approximations

The solutions of the Lyapunov equations are normally used to balance the state space realization in order to select the states to be discarded from the model. This does not require an exact solution. Since the dominant eigenspace of $P$ is known to be associated with the dominant modes of the system, only the dominant eigenspace of the solution $P$ is of interest,
rather than P itself. Therefore, in practice, solutions to large Lyapunov equations frequently admit good low rank approximations.

The idea is to approximate the solution to the Lyapunov equation (5.18) by projecting the state space matrices A and B on an orthogonal matrix \( V_m \in \mathbb{R}^{nxm} \) of low rank (Oblique projection) and calculating the exact solution \( X_m \) to the reduced order Lyapunov equation:

\[
(V_m^TAV_m)X_m + X_m(V_m^TA^TV_m) + V_m^TBB^TV_m = 0 \tag{5.35}
\]

The estimate of \( P \) is then given by \( P_m = V_mX_mV_m^T \).

In the same manner, the approximate solution to the Lyapunov equation (5.22) can be found by projecting \( A^T \) and \( C^T \) on an orthogonal basis \( W_m \in \mathbb{R}^{nxm} \) and solving the reduced order Lyapunov equation:

\[
(W_m^TA^TW_m)Y_m + Y_m(W_m^TAW_m) + W_m^TC^TCW_m = 0 \tag{5.36}
\]

The estimate of \( Q \) is then given by \( Q_m = W_mY_mW_m^T \).

The remainder of this section is focussed on the approximation \( P_m \) and the basis \( V_m \), but this also is a valid procedure for the approximation \( Q_m \) and the basis \( W_m \).

### 5.5.1.1 The basis

The problem of obtaining a good approximate solution \( P_m \) to the full order Lyapunov equation 5.18 is focussed on the selection of the orthogonal matrix \( V_m \) serving as a basis for the projection of the state space matrices A and B. In order to obtain the dominant modes of the system, this basis should contain at least the dominant eigenspace of \( P \).

To this end the \( mp \)-dimensional Krylov space \( K_m \) is defined as a subspace of the controllability matrix \( \mathcal{C} \) for the system pair (A,B):

\[
K_m = \text{span}\{[B \ AB \ A^2B \ ... \ A^{m-1}B]\} \tag{5.37}
\]

The matrix \( V_m \) may be selected then to be an orthonormal basis of this subspace.

### 5.5.1.2 Arnoldi process

The orthonormal basis \( V_m \) for the Krylov subspace \( K_m \) may be calculated with the well-established Arnoldi algorithm. This algorithm starts with the orthogonalization of the state
space matrix $B$ by a standard QR factorization and then adds directions that are associated with $AB$, $A^2B$, ... $A^{m-1}B$. It is basically outlined as follows:

- Compute $B = Q_1R_1$ and set $p_1 := \text{number of columns of } Q_1$. (QR factorization)
- Do $j = 1, ..., m$
  
  (a) Set $V_j = [Q_1 \ Q_2 \ ... \ Q_j]$
  
  (b) Compute
  
  $\begin{bmatrix}
  A_{1j} \\
  A_{2j} \\
  \vdots \\
  A_{jj}
  \end{bmatrix} = V_j^T AQ_j$

  (c) $Q_{j+1}A_{j+1,j} = AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$, (QR factorization) and
  
  $p_{j+1} := \text{number of columns of } Q_{j+1}$.

- End Do.

The QR factorization in the Arnoldi algorithm may be performed, for example, according to the modified Gram-Smidt orthogonalization process.

5.5.1.3 Rank deficiency

The QR factorization of $B \in \mathbb{R}^{nxp}$ will normally produce a unitary matrix $Q \in \mathbb{R}^{nxp}$ and an upper triangular matrix $R \in \mathbb{R}^{n \times n}$. Problems might occur when $B$ does not have full column rank. In that case, let the QR factorization be given by:

$$BI = \begin{bmatrix} \tilde{Q}_1 & \tilde{Q}_2 \end{bmatrix} \begin{bmatrix} \tilde{R}_{11} & \tilde{R}_{12} \\ 0 & 0 \end{bmatrix}$$ (5.38)

where $\Pi$ is a permutation matrix so that $\tilde{R}_{11}$ is upper triangular. Now set $Q_1 := \tilde{Q}_1$ and $R_1 := \begin{bmatrix} \tilde{R}_{11} & \tilde{R}_{12} \end{bmatrix} \Pi^T$. Then $p_1 = \text{rank}(Q_1) = \text{rank}(B)$ and $V_1$ has only $p_1$ columns. The upper-triangular structure of $R_1$ is lost because of the permutation with $\Pi$, but this does not affect the Arnoldi process. In the same manner a rank drop of $AQ_j - \sum_{k=1}^{j} Q_k A_{kj}$ in the main loop of the Arnoldi process is resolved.
Values on the main diagonal of $R$ being lower than a certain tolerance may also be treated as zero. This may prevent the Arnoldi process from adding vectors to the basis $V_m$ that do not correspond to directions of the Krylov subspace, but rather to directions of the residue being a result of numerical errors.

### 5.5.1.4 Residual error

After $m$ steps of the Arnoldi process associated with $Z_m(A,B)$, an orthonormal basis $V_m$ is produced. Then the exact solution $X_m$ of the reduced order Lyapunov equation (5.35) can be computed and an approximate solution $P_m$ to the original Lyapunov equation (5.18) can be found. The question then rises whether this low rank approximation is acceptable.

This regards the residual error of the full order Lyapunov equation (5.18) in terms of the orthonormal basis $V_m$ and the exact solution $X_m$ of the reduced order Lyapunov equation (5.35), given by:

$$R_m(X_m) = A(V_m^T X_m V_m^T) + (V_m^T X_m V_m^T)A^T + V_mB_mB_m^T V_m^T$$  \hspace{1cm} (5.39)

where $B_m = \begin{bmatrix} R_1 \\ 0_{kxl} \end{bmatrix}$, $l$ is the number of inputs and $k = \sum_{j=2}^{m} p_j$, so $B = V_mB_m$.

Now, with the $mpxmp$ block upper Hessenberg matrix $A_m$, defined as:

$$A_m = \begin{bmatrix} A_{11} & A_{12} & \cdots & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & \cdots & \vdots \\ 0 & A_{32} & A_{33} & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 0 & \cdots & 0 & A_{m,m-1} & A_{mm} \end{bmatrix}$$  \hspace{1cm} (5.40)

where $A_{11}, \ldots, A_{mm}$ originate form step b of the Arnoldi Process, it is easy to verify that

$$AV_m = V_{m+1}A_{m+1,m} = V_mA_m + Q_{m+1}A_{m+1,m}E_m^T$$  \hspace{1cm} (5.41)

and

$$A_m = V_m^T A V_m$$  \hspace{1cm} (5.42)

where $E_m$ is a matrix of the last $p$ columns of an identity matrix with the same size as $V_m$ and $V_{m+1} = [V_m \: Q_{m+1}]$. Substituting (5.41) into (5.39) gives:

$$R_m(X_m) = V_{m+1} \begin{bmatrix} A_mX_m + X_mA_m^T + B_mB_m^T & X_mE_mE_m^T \\ A_{m+1,m}E_m^T X_m & 0 \end{bmatrix} V_{m+1}^T$$  \hspace{1cm} (5.43)
Large Scale Model Reduction

With \( A_m = V_m^T A V_m \) and \( B_m = V_m^T B \), it is verified that the upper left element between the brackets equals zero, since \( X_m \) is the exact solution to the reduced order Lyapunov equation (5.35).

Now it is interesting to take the Frobenius norm of this residue, defined as:

\[
\|R_m\|_F = \sqrt{\text{tr}(R_m R_m^T)}
\]  

(5.44)

Since \( V_{m+1} \) is part of an orthonormal basis, the Frobenius norm of the residual error becomes:

\[
\|R_m (X_m)\|_F := \sqrt{\frac{1}{2}} \|A_{m+1,m} E_m^T X_m\|_F
\]  

(5.45)

This residual error norm does not require the computation of the approximate solution \( P_m \) at each iteration, but it is computable using low dimensional matrix products. This provides a useful stopping criterion in a practical implementation of the algorithm. It allows evaluating the quality of the low rank approximation in an economic way.

The key points of the above method are summarized as follows. Firstly, that the Lyapunov equation 5.35 is of low dimension and can be solved accurately using the Bartels-Steward algorithm. Secondly \( P_m \) may be efficiently stored as the product of low matrices. Thirdly, the residual error norm is calculated via low dimensional matrix products. However, a drawback of the method is that manipulations with \( V_m \) become expensive and storage requirements excessive with increasing \( m \).

**Example 5.4; Approximating Gramians**

In the previous example, the Bartels-Steward algorithm is used to solve the Lyapunov equations of the flash system, which yield \( P \) and \( Q \). They may also be approximated with the Oblique projection method yielding \( P_m \) and \( Q_m \). In this example the reduced order Gramians and residual errors have been calculated after each Arnoldi step to show the progress of the approximations (Table 5.2 and Table 5.3). For large systems several Arnoldi steps (typically 3 or 4) may be executed before calculating the reduced order Gramian and residual error.

Five input variables are to be selected for the flash problem, but the B-matrix does not have full column rank. This rank drop is tackled in the way described above, so the approximation of the controllability Gramian starts in iteration 1 with an order 4. In the second Arnoldi step, another rank drop occurs while the residual error already becomes small. In the third step two
more directions are added to the basis \( V_m \) and the residual error is now sufficiently small to ensure a good approximation of the controllability Gramian.

The approximation of the observability Gramian starts with an order 2, which is the rank of matrix \( C \) that contains two output directions. Again, in the second Arnoldi step a rank drop occurs. The residual error is already small this time. Adding another direction (the third step), the residual error norm is almost zero implying that the approximated solution to the observability Gramian has been found.

Now the approximated Gramians \( P_m \) and \( Q_m \) may be compared with the exact solutions \( P \) and \( Q \), calculated with the Bartels-Steward algorithm. Taking the 2-norm of the differences yields \( \|P-P_m\|_2 = 1.77e-6 \) and \( \|Q-Q_m\|_2 = 2.76e-11 \), which proves that the low rank approximations are acceptable solutions to the full order Lyapunov equations.

**Table 5.2; Progress of the controllability Gramian approximation**

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Order of the approximation</th>
<th>Residual error norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>2.97e-01</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>1.34e-04</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>2.42e-06</td>
</tr>
</tbody>
</table>

**Table 5.3; Progress of the observability Gramian approximation**

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Order of the approximation</th>
<th>Residual error norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>3.46e-01</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>1.38e-04</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>1.61e-11</td>
</tr>
</tbody>
</table>

### 5.6 Krylov Space Model Reduction

The Oblique projection method described in the previous section is used to find approximate solutions to the Lyapunov equations. These solutions are needed to generate a balanced realization of a state space description, which can then be reduced to lower order. For large systems this procedure may be rather expensive. Although low rank approximate solutions to the Lyapunov equations are realized, the balancing procedure is performed on the full order model. More conveniently it seems to directly use Krylov subspace techniques providing computationally efficient model reduction schemes for large-scale state space systems. Jaimoukha described such a method (Jaimoukha and Kasenally, 1995) to be discussed next.
When considering the transfer function $G(s)$ in terms of the state space matrices $(A,B,C,D)$:

$$G(s) = C(sI - A)^{-1}B + D = \begin{bmatrix} A & B \\ C & D \end{bmatrix} s$$  \hspace{1cm} (5.46)

Equation 5.46 may be rewritten as $G(s) = CG_B(s) + D = G_C(s)B + D$, where $G_B(s) = (sI - A)^{-1}B$ and $G_C(s) = C(sI - A)^{-1}$. Consequently, $G_B(s)$ and $G_C(s)$ can be considered as solutions to the coupled linear systems:

$$(sI - A)G_B(s) = B \quad \text{and} \quad G_C(s)(sI - A) = C$$  \hspace{1cm} (5.47)

Now $G(s)$ is approximated by obtaining approximate solutions $G_{B,m}(s)$ and $G_{C,m}(s)$ to these linear systems leading to two different realizations:

$$G_{m,1}(s) = CG_{B,m}(s) + D, \quad G_{m,2}(s) = G_{C,m}(s)B + D$$  \hspace{1cm} (5.48)

Good approximations of $G(s)$ should contain states contributing to the input-output behavior. These states should be both controllable and observable. In order to select controllable states, the approximate solution $G_{B,m}(s)$ of $G_B(s)$ should be a part of the Krylov subspace $\mathcal{K}_m(A,B)$ of the controllability Gramian $\mathcal{G}$. In the same manner, the approximation $G_{C,m}(s)$ should be part of the Krylov subspace $\mathcal{L}_m(A^T, C^T)$ of the observability Gramian $\mathcal{G}$.

In order to include all states contributing to the input-output behavior, the residue of the approximation $G_{B,m}(s)$, given by $(sI - A)G_{B,m}(s) - B$, should not contain observable states and therefore should not be a part of the Krylov subspace $\mathcal{L}_m(A^T, C^T)$, so

$$\mathcal{L}_m(A^T, C^T) \perp (sI - A)G_{B,m}(s) - B$$  \hspace{1cm} (5.49)

For the same reason, the residue $G_{C,m}(s)(sI - A) - C$ should not contain controllable states and therefore should not be a part of the Krylov subspace $\mathcal{K}_m(A,B)$, so

$$\mathcal{K}_m(A,B) \perp G_{C,m}(s)(sI - A) - C$$  \hspace{1cm} (5.50)

The Arnoldi process may be used to find the orthogonal basis $V_m$ for the Krylov subspace $\mathcal{K}_m(A,B)$ and the orthogonal basis $W_m$ for the Krylov subspace $\mathcal{L}_m(A^T, C^T)$. Then the problem is to find approximate solutions $G_{B,m}(s) = V_m H_m(s)$ and $G_{C,m}(s) = F_m(s)W_m^T$ that satisfy the Galerkin-type conditions:
\[ W_m^T (sI - A)V_m H_m (s) - B) = 0 \quad \forall s \]  
\( \text{and} \)
\[ \{ F_m (s) W_m^T (sI - A) - C \} V_m = 0 \quad \forall s \]

It has been observed before that from the Arnoldi process associated with \( \mathcal{A}_m(A, B) \) an upper Hessenberg matrix \( H_m \) can be produced and that:

\[ B = V_m B_m \quad \text{and} \quad AV_m = V_m H_m + \tilde{V}_m \tilde{H}_m \]  
\( \text{in which} \)
\[ B_m := \begin{bmatrix} R_i \\ 0_{k \times i} \end{bmatrix}, \]  
where \( i \) is the number of inputs, \( k = \sum_{j=2}^m p_j \), \( \tilde{V}_m = Q_{m+1} \) and
\[ \tilde{H}_m = H_{m+1, m} E_m^T, \]  
where \( E_m^T \) are the last \( p \) columns of the identity matrix.

Similarly, associated with \( \mathcal{L}_m(A^T, C^T) \), the Arnoldi process produces a lower Hessenberg matrix \( F_m \) and

\[ C^T = W_m C_m \quad \text{and} \quad A^T W_m = W_m F_m + \tilde{W}_m \tilde{F}_m \]

\( \text{in which} \)
\[ C_m := \begin{bmatrix} S_i & 0_{o \times k} \end{bmatrix}, \]  
where \( o \) is the number of outputs, \( k = \sum_{j=2}^m q_j \), \( \tilde{W}_m = O_{m+1} \) and
\[ \tilde{F}_m = F_{m+1, m} E_m^T. \]

With these results the following matrices can be defined:

\[ \hat{H}_m := T_m^{-1} W_m T \quad \text{and} \quad \hat{V}_m := H_m + T_m^{-1} W_m \tilde{V}_m \tilde{H}_m \]

\( \text{and} \)
\[ \hat{F}_m := W_m T \quad \text{and} \quad \hat{F}_m := F_m + \tilde{W}_m \tilde{F}_m V_m T^{-1} \]

for nonsingular \( T_m = W_m T \) while noticing that \( \hat{H}_m \) and \( \hat{F}_m \) are upper and lower Hessenberg, respectively.

Now it is readily verified that the Galerkin-type conditions 5.51 and 5.52 are satisfied if and only if \( H_m(s) = (sI - \hat{H}_m)^{-1} B_m \) and \( F_m(s) = C_m(sI - \hat{F}_m)^{-1} \). Under these conditions the residual error norms are:
and the approximations, given by:

\[
G_{m,1}(s) = CV_m H_m(s) + D = \begin{bmatrix} T_m^{-1} W_m^T A V_m & T_m^{-1} W_m^T B \\ C V_m & D \end{bmatrix} \begin{bmatrix} \hat{H}_m \\ \hat{B}_m \end{bmatrix}
\]

(5.59)

\[
G_{m,2}(s) = F_m(s) W_m^T B + D = \begin{bmatrix} W_m^T A V_m T_m^{-1} & W_m^T B \\ C V_m T_m^{-1} & D \end{bmatrix} \begin{bmatrix} \hat{F}_m \\ T_m B_m \end{bmatrix}
\]

(5.60)

are different low order realizations of the transfer function \(G(s)\).

### 5.6.1 Minimal realization

When \(m\) steps of the Arnoldi process have been taken and \(H_{m+1,m} = 0\), then the matrix \(V_m\) forms an orthogonal basis for the controllable space. This implies that the low order realizations \(G_{m,1}(s)\) and \(G_{m,2}(s)\) are equivalent to the high order model \(G(s)\). This holds also if \(F_{m+1,m} = 0\) and \(W_m\) forms an orthogonal basis for the observable space or when both \(H_{m+1,m} = 0\) and \(F_{m+1,m} = 0\). An important implication of these types of breakdowns of the model reduction schemes is that the reduced order realizations turn out to be just minimal realizations of the high order model \(G(s)\).

### 5.6.2 Breakdown

Suppose that after \(m\) steps of the Arnoldi process a basis \(V_m\) of order \(mp\) and a basis \(W_m\) of order \(mq\) are produced, such that \(mp \neq mq\). This means that the number of observable directions is not equal to the number of controllable directions. Then the matrix \(T_m = W_m^T V_m\) is non-square and \(T_m^{-1}\) is undefined. This type of breakdown will occur after a partial breakdown of the block Arnoldi process, or when \(p \neq q\). In that case the smaller base should be expanded executing some extra Arnoldi steps such that \(V_m\) and \(W_m\) will become equal in size.
Another breakdown of the reduction algorithm occurs if $T_m$ becomes singular. In this case there are observable directions that are uncontrollable and controllable directions that are unobservable. Expanding both $V_m$ and $W_m$ with some additional Arnoldi steps may resolve this problem.

A practical solution to deal with the above problems is replacing $T_m^{-1}$ in the equations 5.57 to 5.60 by the pseudo-inverse $T_m^* = \text{pinv}(T_m)$. The computation is based on a Singular Value Decomposition of $T_m$ and any singular value less than a certain tolerance is treated as zero. $T_m^*$ will have the dimension of $T_m^T$, $T_m^*T_mT_m^* = T_m^*$, $T_mT_m^*T_m = T_m$ and $T_m^*T_m$ and $T_m^*T_m$ are Hermitian. We have found such realizations to be good low order approximations to the full order model $G(s)$. However, $G_{m,1}(s)$ and $G_{m,2}(s)$ are not automatically minimal realizations. If the number of non-zero singular values of $T_m$ is less then $mp$ then $G_{m,1}(s)$ will contain redundant states, and if this number is less than $mq$, $G_{m,2}(s)$ is not minimal. However, since both approximations are only different realizations of the same transfer function, the smaller one may be considered as the reduced system. Moreover, since the reduced systems are much smaller than the original set, it is often possible to use a standard method to transform the larger one into a minimal realization.

**Example 5.5; Krylov space model reduction**

The flash problem is reconsidered to demonstrate the Krylov model reduction scheme. Previously, it was shown that the controllability Gramian $P$ could be approximated with the orthogonal basis $V_m$ for the Krylov space $\mathcal{K}_m(A,B)$ of order eight, while the orthogonal basis $W_m$ for the Krylov space $\mathcal{K}_m(A^T,C^T)$ of order five was used to approximate the observability Gramian $Q$. The Krylov model reduction scheme uses the same Arnoldi process, so identical bases are developed. Table 5.4 shows these bases $V_m$ to be of order eight and $W_m$ of order five, as developed after three Arnoldi steps, and to give an approximate realization $G_{m,2}$ of order five with a residual error norm close to zero. This is comparable to the result of the balanced realization being truncated after five states.

Notice that the approximate realization $G_{m,1}$, which should be just another realization of the same transfer function, is yet of higher order than $G_{m,2}$ as a result of the different order of the bases $V_m$ and $W_m$. This implies that the realization $G_{m,1}$ contains redundant states not contributing to the input-output behavior of the system. However, the basis $V_m$ should be
developed to an order 8 before it contains all observable directions needed for a good approximate solution $G_{m,2}$. Certain controllable directions being added in the first Arnoldi steps could be omitted, as they are not observable but that option does not exist in the Arnoldi process. Therefore, in this example, $G_{m,2}$ is the realization that should be used as reduced model, although the redundant states that $G_{m,1}$ contains can be removed by transforming this approximation to a minimal realization.

Table 5.4: Progress of the Krylov model reduction of the flash system

<table>
<thead>
<tr>
<th>Iteration</th>
<th>Order of $V_m$</th>
<th>Order of $W_m$</th>
<th>Residual error norm of $G_{m,1}$</th>
<th>Residual error norm of $G_{m,2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4</td>
<td>2</td>
<td>1.92e+03</td>
<td>2.39e-01</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>4</td>
<td>2.24e-03</td>
<td>2.97e-04</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
<td>5</td>
<td>3.38e-03</td>
<td>5.68e-11</td>
</tr>
</tbody>
</table>

5.7 Decomposition

Usually, only the dominant modes of a system are of interest and since the dominant eigenspace of $P$ is known to be associated with the dominant modes of the system, $V_m$ is selected to be the orthogonal basis of the Krylov subspace $K_m(A,B)$ and $W_m$ the orthogonal basis of the Krylov subspace $L_m(A^T,C^T)$. However, situations might exist where the input-output behavior cannot be described by dominant modes only. Suppose that the state space realization describes a system with many processes, operating at different time scales. The dominant modes are related to the fast processes and they are included in the reduced model first. Processes operating on longer time scales only are included in the reduced system if the bases $V_m$ and $W_m$ are developed to further extent. However, due to numeric problems the Arnoldi scheme is probably unable to find the required directions.

Yet another situation exists where this problem could rise. If the most controllable states are hardly observable and the most observable states are hardly controllable, the bases $V_m$ and $W_m$ should be developed almost to completeness before obtaining common directions. If such directions cannot be found, matrix $T_m := W_m^T V_m$ becomes singular and it is concluded that not any state exist contributing to the input-output behavior, although in fact this is only caused by an improper Arnoldi scheme.
In order to resolve the problems mentioned, the system should be separated into smaller fragments. Each of the subsystem should contain a group of states associated to processes operating at similar time scales. The Arnoldi process may subsequently be used to develop orthogonal bases and reduce each subsystem separately. Combining the reduced subsystems will give a reduced system that describes the complete input-output behavior. In other words, the system is decomposed into a number of subsystems with similar eigenvalues.

In order to decompose the system into two parts, the stable/anti-stable decomposition algorithm will be used. The A-matrix has to be transformed to its ordered real Schur form first, so the states are grouped according to their eigenvalues. This procedure will return a transformation matrix with which new B and C matrices can be generated:

\[
\begin{bmatrix}
A_{11} & A_{12} \\
0 & A_{22}
\end{bmatrix}
= U^T A U \\
\begin{bmatrix}
B_1 \\
B_2
\end{bmatrix}
= U^T B \\
\begin{bmatrix}
C_1 \\
C_2
\end{bmatrix}
= U^T C
\]

(5.61)

As regards the decomposition in itself, the Sylvester equation \( A_{11}X - XA_{22} + A_{12} = 0 \) is solved using Kronecker products. Subsequently, two subsystems can be formed.

\[
\begin{align*}
A_{s1} &= A_{11} & A_{s2} &= A_{22} \\
B_{s1} &= B_1 - XB_2 & B_{s2} &= B_2 \\
C_{s1} &= C_1 & C_{s2} &= C_1X + C_2
\end{align*}
\]

(5.62)

If states are grouped in such a way that \( A_{11} \) contains all negative eigenvalues of \( A \) and \( A_{22} \) the non-negative ones, then the subsystem formed by \( (A_{s1}, B_{s1}, C_{s1}, D) \) will contain the stable modes, while the subsystem formed by \( (A_{s2}, B_{s2}, C_{s2}, D) \) will be the unstable part. Now, when \( A_{11} \) is selected to contain the large eigenvalues of \( A_{s1} \) and \( A_{22} \) to contain the smaller, the stable part may be decomposed to further extent. By repeating this procedure several times a number of smaller subsystems are created.

The Arnoldi algorithm more easily deals with the subsystems and they may be reduced separately. However, apart form the additional time required to create subsystems, a drawback of this method is that reduced subsystems might contain common directions. In that case the reduced model is not a minimal realization and still contains redundant states.
Example 5.6; Krylov space model reduction with decomposition

The eigenvalues of the state space realization from the flash system of example 1 are: -3215, -62.0, -18.9, -10.5, -10.0, -5.0, -1.0, -1.0 and -0.001. A very large number appears, a very small one and an intermediate part exists, so it is beforehand to decompose the system into three subsystems that are reduced separately using the Krylov model reduction scheme. This leads to a first subsystem containing the mode with eigenvalue -0.001. The Krylov model reduction scheme did not find any common directions for this subsystem, so this part can be omitted completely. The second subsystem, containing the states corresponding to the intermediate eigenvalues, between -1 and -62, are reduced to a realization with four states. The last subsystem, containing the state corresponding to the large eigenvalue and consequently describing the fastest process in the system, cannot be reduced according to the Krylov model reduction scheme. Hence combining the reduced subsystems again yield a reduced state space realization of order five. This demonstrates that the decomposition may be used in combination with the Krylov model reduction scheme without affecting results.

5.8 Reduction of a large scale model

The described concepts of model reduction are applied now on a large system, the dynamic model of the balanced VCM process. The model that is used in chapter 3 is a simplified version of the complete system. The plant contains a liquid phase reactor that is modeled rigorously, including dynamics, while the two gas phase reactors are modeled as simple steady state conversion reactors, assumed to act instantaneous. Five important distillation columns are present, described by rigorous dynamic models considering individual sieve trays. The other units are combined to three simplified separation blocks. We have selected six important components to be taken into account in the rigorous dynamic distillation column models and another seven components only regarded in reactors and simplified separation blocks. The simplified dynamic model still contains 4384 equations.

In order to perform a controllability analysis, a linear state space description has been generated with the CDI interface from SPEEDUP™. The control problem involves three impurities to be controlled and five variables are identified to be useful as manipulated variables. These variables are from different units. The linear model contains 668 states. Performing a controllability analysis with this model is expensive and storage requirements are excessive. Therefore it is an obvious need to reduce the system to lower order.
Table 5.5; VCM plant state space model reduction

<table>
<thead>
<tr>
<th>Subsystem</th>
<th>Range of eigenvalues</th>
<th>Full order</th>
<th>Reduced order</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0 : -1</td>
<td>9</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>-1 : -10</td>
<td>30</td>
<td>13</td>
</tr>
<tr>
<td>4</td>
<td>-10 : -50</td>
<td>64</td>
<td>21</td>
</tr>
<tr>
<td>5</td>
<td>-50 : -100</td>
<td>45</td>
<td>15</td>
</tr>
<tr>
<td>6</td>
<td>-100 : -500</td>
<td>206</td>
<td>33</td>
</tr>
<tr>
<td>7</td>
<td>-500 : -1000</td>
<td>156</td>
<td>21</td>
</tr>
<tr>
<td>8</td>
<td>-1e3 : -5e3</td>
<td>56</td>
<td>9</td>
</tr>
<tr>
<td>9</td>
<td>-5e3 : -1e4</td>
<td>29</td>
<td>0</td>
</tr>
<tr>
<td>10</td>
<td>-1e4 : -∞</td>
<td>68</td>
<td>0</td>
</tr>
<tr>
<td><strong>Full system</strong></td>
<td><strong>668</strong></td>
<td><strong>115</strong></td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.2; Frequency responses of full (-) and reduced (...) order models.

The state space realization of the dynamic VCM model with 668 states is reduced to a realization with 115 states using the Krylov space model reduction scheme on subsystems. The magnitudes of the input-output responses of both models as function of frequency are comparable.
Dynamic simulations showed that a broad range of time constants exist in the system, ranging from a few minutes to several days. Therefore the system will be decomposed into a number of subsystems, 10 in total, while each subsystem will be reduced separately by applying the Krylov subspace model reduction technique. The results are given in Table 5.5.

Most subsystems can be reduced considerably, while the subsystems with the highest eigenvalues, corresponding to the fastest processes, can be even skipped completely. This is not surprising since control of impurities in a large and complex plant is a slow process. The complete reduced state space realization only contains 115 states, being less than 20% of the original system, while the description of the input-output behavior is sufficiently accurate across the whole frequency range of interest (Figure 5.2). So the order of the state space description of this problem can be reduced significantly.

5.9 Conclusions

As an essential part of designing chemical plants with complex structures and intricate dynamic characteristics the performing of controllability analyses on linearized models is required. The linearization of full dynamic plant models often leads to large state space descriptions, being difficult to use as such. In order to examine the dynamic behavior in an efficient way, linear dynamic models of a reduced order have to be generated. In this chapter it is explained how a state space description may be reduced to lower order without affecting the quality in describing the input-output behavior by truncation of a balanced realization.

In order to balance a state space realization, the Lyapunov equations have to be solved first. There are several techniques available for this, like the Bartles-Steward algorithm. However, they cannot be used to solve large order Lyapunov equations ($n>50$). For these systems, another method is more appropriate to find low order approximate solutions to the Lyapunov equations. An Arnoldi algorithm is used to develop low rank orthogonal bases for certain Krylov subspaces, which are subsystems of the controllability and observability matrices. The state space matrices $(A,B)$ respectively $(A^T,C^T)$ are projected on these bases to reduce the order of the corresponding Lyapunov equations. The low order Lyapunov equations may subsequently be solved by a standard algorithm and the solutions are transformed back to yield approximate solutions of the full order controllability and observability Gramians. With a dynamic flash drum example is has been shown that the approximate solutions are nearly identical to the solutions of the original system.
The orthogonal bases for the Krylov subspaces can also be used to generate low order approximate state space realizations without solving Lyapunov equations and balancing state space systems. This Krylov model reduction scheme works properly for most systems. A possible problem arising from large systems is the fact that the Arnoldi process is not able to find all directions of the Krylov subspaces needed to give a good approximation. This problem especially occurs if only weak relations exist between inputs and outputs of a state space description. Decomposition of such systems into small subsystems with similar eigenvalues is a simple way to resolve these problems. The reduction of each subsystem may be performed then with the Krylov model reduction scheme and the reduced subsystems can be combined again to form a complete state space realization of low order. Although the decomposition is relatively time-consuming, the overall process is still an economic procedure. As an extensive case study, the dynamic model of the VCM problem from chapter 3 is reduced by this approach from 668 states to 115 states, while the description of the input-output behavior is preserved with an acceptable accuracy. Calculations with this reduced realization are about 25 times faster than with the full order linear system. This proves that model reduction might be useful before a controllability analysis is applied.
Chapter 6

Dynamic Optimization of Flowsheet and Control Structures

6.1 Introduction

This thesis started with the question 'How to design and optimize complex plants with superior dynamic behavior and controllability features'. The simulation-based methodology that is presented in chapter 2 might be used for this purpose. By combination of the traditional steady state flowsheeting with dynamic flowsheeting and linear controllability analyses, more essential design and operation knowledge is obtained than with the exploration of the operating window only. This was demonstrated in chapter 3 by a case study about the handling of impurities in a balanced VCM process. Alternative recycle structures for this plant were investigated in chapter 4. This has lead to a better understanding of the interaction between recycle loops and the effect of these interactions on the controllability of material balances. In this respect, the systems approach has an added value. Unfortunately, optimization of complex flowsheet structures is not covered by the approach. One might evaluate several design and control alternatives in order to compare their performance with respect to some objective. However, it is not clear at all how to translate results from a linear controllability analysis in the frequency domain to modifications in the flowsheet structure and units design that improve this performance. Optimization of complex flowsheet structures proceeds in a more straightforward manner using an approach that stays close to physical reality. Such an approach will be introduced in this chapter, using optimization techniques in combination with nonlinear dynamic models. Flowsheet structure and unit design parameters are potential degrees of freedom for optimization. Plantwide controllability criteria, necessary for a controllable plant design, can be added as additional constraints.
The issue of addressing controllability aspects in early design stages has only scarcely been considered before, for example in the work of Luyben and Floudas (1994a,b), who suggest a multi-objective optimization framework. Control structure selection issues are considered in the work of Narraway and Perkins (1993a,b), while Bahri et al. (1996a,b) considered aspects of parametric uncertainty and disturbances in control optimization. Finally, Mohideen et al. (1996) have described a framework for the optimal design of dynamic systems under uncertainties. The approach is illustrated by an example where the objective is to design a ternary distillation column and the required control scheme at minimum total annualized cost, while being able to maintain feasible operation in the presence of variability. The number of trays, the location of the feed tray and the control structure are also taken as degrees of freedom. To this end a superstructure tray-by-tray model is constructed, using binary variables. Furthermore, the time-varying variables are parameterized according to the method of Cuthrell and Biegler (1987). This rather small-scale problem results in a mixed-integer nonlinear programming model of considerable size, which nevertheless can be solved. However, applying this method on complete flowsheet structures has not yet been realized. Hence, this remains highly challenging.

In this chapter, we will start with a description of two different methods for the optimization of dynamic systems. The first method deals with the dynamics using integration, the second one employs collocation in time. These methods are illustrated with examples and compared. Next, the optimization of mixed-integer problems in itself is discussed. Then the mixed-integer character is incorporated in the problem and a solution procedure is proposed in combination with both the integration and the collocation method. Thus, we finally arrive at a method to optimize complete flowsheet structures and control systems in the time-domain.

6.2 Optimization of differential-algebraic systems

Optimization in combination with dynamic flowsheeting cannot be performed with standard techniques, since direct optimization with a model containing differential equations is not possible. Therefore, dynamic simulation (integration) and optimization techniques must be combined according to newly to be developed algorithms mostly involving a two step iterative approach.

One alternative is to first integrate the dynamic model with fixed values for the optimization variables, subsequently find new values and repeat the integration. The usual trial and error
method, where the engineer just tries some values for the free variables, is in fact such a method. In this approach the optimization is based on experience and heuristics. In a systematic approach a certain algorithm will calculate new values for the optimization variables. An advantage of this approach is that well-known dynamic simulation tools can be used. Fast integration routines are available that can handle large dynamic problems. It is possible to build in some conditional equations to check whether the solution is still feasible and interesting with respect to the optimization function. If this is not the case, the integrator can be stopped and new optimization variables can be calculated. A disadvantage is that the breakdown described might happen very frequently. So, the optimization variables need to be bounded in a convenient way in order to find feasible solutions without bounding the optimization space.

This issue leads to a second alternative, the direct method. According to this the dynamic model is included in the optimization problem as a set of equality constraints. Thus, solving and optimization of the dynamic system is performed in one step. However, optimization algorithms cannot integrate, so the differential and algebraic equations have to discretized to be able to optimize over a certain time interval. Due to this discretization, which increases the number of equations considerably, the problem size might become very large. Another disadvantage stems from the highly nonlinear nature of the problem, mostly due to thermodynamics, which strongly complicates optimization. However, an advantage might be that some optimization algorithms are able to directly deal with binary variables, so direct optimization of flowsheet and control structures is possible. In the remainder of this chapter both the iterative and the direct method will be discussed and illustrated with examples.

Table 6.1; Iterative and Direct approach

<table>
<thead>
<tr>
<th>Iterative approach</th>
<th>Direct approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set starting point</td>
<td>Set starting point</td>
</tr>
<tr>
<td><strong>Repeat</strong></td>
<td></td>
</tr>
<tr>
<td>Integrate DAE system</td>
<td>Discretize DAE system and add to optimization problem as equality constraints</td>
</tr>
<tr>
<td>Calculate new values for optimization variables</td>
<td>Solve constrained nonlinear optimization problem</td>
</tr>
<tr>
<td>Until convergence</td>
<td></td>
</tr>
</tbody>
</table>
6.3 Iterative approach

According to the iterative approach, the dynamic model is solved with fixed values for the optimization variables in an inner loop, while new values for these optimization variables are calculated in an outer loop. Table 6.2 gives a schematic overview of the iterative approach as it can be implemented in MATLAB®.

The MATLAB® routine `constr` finds the constrained minimum of a scalar function of several variables, starting at an initial estimate. This is generally referred to as constrained nonlinear optimization, and is mathematically stated as

\[
\text{minimize } f(X) \quad \text{subject to: } G(X) \leq 0
\]

where bold uppercase characters indicate that $X$ and $G(X)$ are matrices, and plain lowercase characters indicate that $f(X)$ is a scalar function.

The routine `constr` uses a Sequential Quadratic Programming (SQP) method. In this method, a Quadratic Programming (QP) sub-problem is solved at each iteration. A positive-definite quasi-Newton approximation of the Hessian of the Langrangian is calculated at each iteration using the formula of Broyden, Fletcher, Goldfarb and Shanno (BFGS).

A line search is performed using a merit function similar to that proposed by Han and Powell. The QP sub-problem is solved using an active set strategy similar to that described in Gill, Murray, and Wright.

**Table 6.2; Iterative approach in MATLAB**

<table>
<thead>
<tr>
<th>Problem setup</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>constr(...)</code></td>
</tr>
<tr>
<td><code>eval( object function )</code></td>
</tr>
<tr>
<td><code>Solve Model</code></td>
</tr>
<tr>
<td><code>Calc. Objective</code></td>
</tr>
<tr>
<td><code>Calc. Constraints</code></td>
</tr>
<tr>
<td><code>return</code></td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\text{rk45( Simulink Model )} \\
\text{or} \\
\text{dea(Model, Jacobian)} \quad \text{modification of ode45}
\end{align*}
\]

| return |
| display results |
The solver behind dae is a modification of ode45, to solve additional algebraic equations simultaneously. dae in itself is a controlling routine that calls the DAE solver for a number of time intervals and can perform additional calculations between the intervals. In this way, the DAE solver can handle discontinuities in the time profiles.

Following this strategy, first the dynamic model is solved; then the results are used to calculate a value for the objective and additional constraints that are not included in the dynamic model. The optimization problem contains only the variables of the objective and the additional constraints. It does not 'know' the dynamic model. The two problems are separated and solved sequentially. Therefore the gradient of the objective and constraints to the design variables has to be developed numerically. Expanding the dynamic model with additional sets of equations containing analytical gradient information might be interesting, but is not implemented in this work.

In principle it should also be possible to take the structure of a flowsheet as a degree of freedom during the design. This may require the use of integer variables, or at least of binary variables, in the problem formulation. The constraint optimization routine in MATLAB® can not handle discrete variables, but MINLP routines are available that can be used in another environment. However, such an environment is not available and it might be interesting to develop one.

Next, the iterative approach will be demonstrated with some examples about the optimal operation of a reactor with a Trambouze reaction scheme (Trambouze and Piret, 1959). The dynamic reactor model, with discontinuities in the operation, will be solved with the DAE-solver dae, which is implemented in MATLAB®. The actual optimization is performed with the constraint optimization routine constr from the MATLAB® optimization toolbox.

**Example 6.1; Trambouze reaction in a batch reactor**

Consider the Trambouze reaction in a batch reactor:

\[ A \xrightarrow{k_1} B, \quad A \xrightarrow{k_2} C, \quad A \xrightarrow{k_3} D \]

with

- \( k_1 = 0.025 \) mole/l min (zero-order reaction)
- \( k_2 = 0.2 \) /min (first-order reaction)
- \( k_3 = 0.4 \) l/mole min (second-order reaction)

The feed concentration is 1 mole/l pure A, the reactor volume is 100 l and the desired product is component C.
In this reaction scheme the production of unwanted component B will dominate for low concentrations of component A (Ca < 0.125). On the other hand, for high concentrations of the reactant (Ca > 0.5) the production of unwanted component D dominates. Between these values, the production rate of component C will be the highest. Furthermore, when Ca=0.25, the production rate of component B is equal to the production rate of component D, while that of component C is twice this rate. For lower concentrations of A, relatively more B is produced, for higher concentrations of A relatively more D is produced. So, for a maximum production rate of component C, Ca=0.25 will be the optimal value of the reactant concentration. Now, when the total amount of feed is added in several steps instead of filling the total reactor at once, the concentration of component A can be kept around this optimal value. In this case the production of component C will be higher than in a batch reactor that is filled at once.

In the example, two different objective functions will be maximized separately, namely the overall fractional yield of C over A and the overall product yield of C in moles, $\Phi$ and $\gamma$, respectively defined as:

$$\Phi = \frac{(Cc(tf) - Cc0)}{(Ca0 - Ca(tf))}$$

$$\gamma = \frac{Cc(tf) \cdot V(tf)}{V(tf)}$$

where $V(tf)$ is the final volume of the reactor.

It is expected that the sole difference between optimal operation for a maximal overall fractional yield and optimal operation for a maximal overall product yield is the reaction time after the last discrete feed charge. When the production of B starts to dominate, the overall fractional yield of C over A will decrease. So, to maximize this yield, the process should be stopped when Ca=0.125. However, as long as component A is available, part of it will be transformed into component C. So, to maximize the overall product yield of C the process should continue till all A has been depleted.

The optimization problem is formulated as follows: The reactor is initially filled with a first amount of pure component A. Further amounts of fresh feed may be added instantaneously during the reaction. The discrete charges and the duration of each time interval are treated as optimization variables. The final volume of the reactor has to be 100 l as an equality constraint. The studied numbers of intervals are 2, 5 and 10.
The discrete charges are initially equally distributed and are bounded between 0 and 100 l, the duration of the intervals are bounded between 1 and 10 min., initialized at 3 min. The problem is solved with the two step method in MATLAB®. Every time the constraint optimization routine evaluates objective and constraints, a dynamic model, containing material balances, is solved by integration.

The results are given in Table 6.3. As expected, in both cases the yield becomes higher when the total amount of fresh feed is divided over more intervals. The total duration of the process also increases when more intervals are used. Adding small amounts of fresh feed with long time intervals in the beginning and larger amounts with shorter time intervals when the reactor volume becomes larger seems to be the best way to operate the reactor.

As expected, the optimal operation schemes for both objectives are almost equal. Maximizing the overall fractional yield of C over A is also important when the overall product yield of C is maximized. The same amount of fresh feed should be added at the same time. The only difference is the duration of the last interval. When the overall fractional yield of C over A is maximized, the reaction is stopped at a certain time, while the reaction still continues for a while when the overall product yield of C is maximized.

The reason for this difference can be seen clearly from Figure 6.1 to Figure 6.3, showing the concentration profiles of component A and C during operation of a process that maximizes the overall fractional yield (left) or the overall product yield (right). It can be seen that fresh feed is added when the concentration of A becomes below 0.125, so when the production of B starts to dominate. After the charge the concentration of A is about 0.5, so that the production of D does not dominate.

If the overall fractional yield of C over A is maximized, the reaction is stopped when the concentration of A becomes 0.125, otherwise the production of B will be dominating and the overall fractional yield of C over A will decrease. On the other hand, the reaction continues until all A has been converted if the overall product yield is maximized. Although relatively more B has been produced, also the production of C has increased. Therefore the duration of the last element is different.
Table 6.3; Trambouze reaction in a batch reactor with discrete charges

<table>
<thead>
<tr>
<th>( \phi )</th>
<th>0.448</th>
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<th>( \gamma )</th>
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<td>9</td>
<td>1.60</td>
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<td>25.21</td>
<td>total</td>
<td>12.22</td>
<td>20.65</td>
<td>31.01</td>
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</tbody>
</table>

Figure 6.1; Concentration profiles for 2 charges

In both cases fresh feed is added when \( Ca \) becomes low and the production of unwanted component \( B \) becomes dominating. When the overall fractional yield is maximized the process is stopped at a certain time, while the reaction continues till all \( A \) is converted in case the overall product yield is maximized.
When more intervals are used, the fluctuation of the concentrations becomes smaller.

By adding many small amounts of fresh feed, the concentration of reactant A is kept best around its optimal value.

Example 6.2; Trambouze reaction with continuous feed

An improved way of operating the reactor is to establish a continuous feed instead of discrete charges. Then the concentration of reactant A can be kept closer to its optimal value. In this example, the feed rate $u(t)$ will be treated as a control variable. Piecewise constant sections are used over 5 elements to approximate the control. The initial volume of the reactor is set to $10^5$ l. The control element sizes are bounded between 0 and 20 min, initialized at 3 min each. The control profile is bounded by 0 and 50 l/min, initially set to a uniform value of 5 l/min.

Table 6.4 shows the optimal feed flowrate and duration of each interval. The flowrate is increased at each next interval while its duration is shorter, which was also the case with the...
discrete charges. As expected, both yields are increased relative to the operation with discrete charges. In fact they become close to the absolute maximum values that can be reached, which is 0.5 for the overall fractional yield and 47.16 for the overall product yield. With a constant feed, the concentration of A can be kept much better around the optimal value of 0.25, as can be seen from Figure 6.4.

Table 6.4; Trambouze reaction in a batch reactor with piecewise constant feed

<table>
<thead>
<tr>
<th>Feed Flow Rate</th>
<th>Duration</th>
<th>Feed Flow Rate</th>
<th>Duration</th>
</tr>
</thead>
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<td>1</td>
<td>0.24</td>
</tr>
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<td>2</td>
<td>0.56</td>
<td>2</td>
<td>1.23</td>
</tr>
<tr>
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<td>1.82</td>
<td>3</td>
<td>3.82</td>
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<tr>
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<td>4.65</td>
<td>4</td>
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</tr>
<tr>
<td>5</td>
<td>9.88</td>
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<td>0.00</td>
</tr>
</tbody>
</table>

Figure 6.4; Concentration profiles for piecewise constant feed over 5 elements

By a continuous feed of fresh reactant A, its concentration can be kept better around an optimal value.

As one can see the feed flowrates and time intervals are different for the two objectives, while they where comparable in the example with discrete charges. However, notice that in case the overall product yield is maximized, the last element is used to complete the reaction and therefore the feed is added during the first four elements only, while five elements are used in the other case.
In fact, to compare both objectives, we should use an additional element for the maximization of the overall product yield. The results are given in Table 6.5. Now we find indeed almost the same values for the feed flow rate and duration of the first five elements, while no fresh feed is added anymore during the last interval. The overall product yield is almost equal to the value that is reached with five elements, which is not surprisingly, since it is already close to the absolute maximum value that can be reached.

Example 6.3; Trambouze reaction in a continuous stirred tank reactor

We may also consider the Trambouze reaction with operation in a continuous stirred tank reactor. With a feed flow rate of 100 l/min pure A, the objective is the overall fractional yield. The optimization variable will be the reactor volume, initialized at 250 l and bounded between 0 and 1000 l. The results are listed in Table 6.6. With the optimal reactor volume, the concentration of component A is exactly 0.25. Then, an overall fractional yield of 0.5 is reached, which is the maximum value for this Trambouze reaction.

The above examples demonstrate that the two step iterative approach can be used for optimization of dynamic problems. The DAE-solver that is implemented in MATLAB® can be used to solve the dynamic models with discrete changes. However, the number of iterations may become very large and the time to solve the problem therefore rather long. To improve this, the use of other solvers in another environment may be investigated. This will be a subject for further research. In this thesis, we continue with the direct approach.
6.4 An NLP formulation for differential-algebraic optimization problems

Another way to solve dynamic optimization problems is to include the dynamic model in the optimization problem as a set of additional equality constraints. A differential-algebraic optimization problem (DAOP) that includes an ODE model can be posed as:

$$\begin{align*}
\min_{d,C(t),X(t)} & \Phi[d,C(t),X(t)] \\
\text{s.t.} & \quad c[d,C(t),X(t)] = 0 \\
& \quad g[d,C(t),X(t)] \leq 0 \\
& \quad f[\dot{X}(t),d,C(t),X(t)] = 0 \\
& \quad X(0) = X_0 \quad \text{(DAOP)} \\
& \quad d^L \leq d \leq d^U \\
& \quad C^L \leq C \leq C^U \\
& \quad X^L \leq X \leq X^U 
\end{align*}$$

(6.1)

where
- $\Phi$ = object function
- $c$ = equality constraints
- $g$ = inequality constraints
- $f$ = differential equation constraints
- $d$ = decision (optimization) variable vector
- $X(t)$ = state profile vector
- $C(t)$ = control profile vector
- $d^L, d^U$ = bounds on decision variables
- $C^L, C^U$ = bounds on control variables
- $X^L, X^U$ = bounds on state variables

6.4.1 Discretization of the state and control profiles

To be able to solve this problem with optimization routines, the differential equations need to be transferred into algebraic equations. First, we have to write the time profiles as sum of known time functions. The state and control profiles will therefore be written as Lagrange form polynomials (Cuthrell and Biegler, 1987):

$$x_{K+1}(t) = \sum_{i=0}^{K} \gamma_i \phi_i(t) \quad \text{where} \quad \phi_i(t) = \prod_{k=0,i}^{K} \frac{(t-t_k)}{(t_i-t_k)}$$

(6.2)
where $x_{K+1}(t)$ denotes a $(K+1)$-th order (degree $\leq K+1$) polynomial and $c_K(t)$ a polynomial of degree $K$. The difference in the orders is due to the existence of the initial condition for $X(t)$.

The notation $k = 0, i$ indicates that $k = 0, \ldots, i-1, i+1, \ldots, K$.

The Lagrange form polynomials have the desirable property that $x_{K+1}(t_i) = \gamma_i$ and $c_K(t_i) = \mu_i$, because of the Lagrange condition $\phi_i(t_j) = \delta_{ij}$ ($\delta_{ij}$ = kronecker delta). The coefficients in the Lagrange form polynomials are therefore physically meaningful quantities. This becomes useful when providing variable bounds, initializing profiles or interpreting results.

Revisiting the ODE model as presented in the DAOP (6.1), this time written as an initial value problem with $t$ between 0 and 1, one has:

$$\dot{X}(t) = F[d, C(t), X(t)] \quad t \in [0,1]$$
$$X(0) = X_0$$

Substitution of the polynomial approximations gives the residual equation:

$$R(t) = \sum_{i=0}^{K} \left( \gamma_i \phi_i(t) - F[d, c_i(t), x_{K+1}(t)] \right)$$

with $\gamma_0 = X_0$, which remains still a function of time. Discretization of the residuals is next done through use of the method of collocation, which requires

$$\int_0^1 R(t) \delta(t-t_i)dt = 0 \quad i = 1, \ldots, K$$

($\delta$ = Dirac delta)

so,

$$R(t_i) = \sum_{j=0}^{K} \left( \gamma_j \phi_j(t_i) - F[d, c_K(t_i), x_{K+1}(t_i)] \right) = 0 \quad i = 1, \ldots, K$$

with $\gamma_0 = X_0$.

With the Lagrange condition, the polynomials evaluated at a discrete point reduce to the coefficients at that point, and thus:

$$R(t_i) = \sum_{j=0}^{K} \gamma_j \phi_j(t_i) - F(d, \mu_i, \gamma_i) = 0 \quad i = 1, \ldots, K$$

with $\gamma_0 = X_0$. 

$$c_K(t) = \sum_{i=1}^{K} \mu_i \psi_i(t) \quad \text{where} \quad \psi_i(t) = \prod_{k=i}^{K} \frac{(t-t_k)}{(t_i-t_k)}$$

(6.3)
Similarly the polynomial approximations when substituted into the DAOP (6.1) and evaluated at some \( t_i \) become just the corresponding coefficients. Using this, the DAOP becomes:

\[
\min_{d, \mu_i, \gamma_i} \Phi[d, \mu_i, \gamma_i] \\
\text{s.t.} \\
c[d, \mu_i, \gamma_i] = 0 \\
g[d, \mu_i, \gamma_i] \leq 0 \\
\sum_{j=0}^{K} \gamma_j \phi_j(t_i) - F[d, \mu_i, \gamma_i] = 0 \\
\gamma_0 = X_0 \quad i = 1, ..., K \quad \text{(NLP1)} \quad (6.9)
\]

\( \text{d}^L \leq d \leq \text{d}^U \)

\( C^L \leq \mu_i \leq C^U \)

\( X^L \leq \gamma_i \leq X^U \)

which is a nonlinear programming problem.

The locations of the points \( t_i, i = 1, ..., K \) are chosen to correspond to the shifted roots of an orthogonal Legendre polynomial of degree \( K \) (hence the term orthogonal collocation):

\[
P_K(t) = \sum_{i=0}^{K} (-1)^{K-i} y_i t^i \quad t \in [0,1] \quad (6.10)
\]

The coefficients \( y_i \) are chosen so, that \( M \cdot Y = 0 \), where

\[
m_{ji} = \frac{(-1)^{K-i}}{i + j + 1} \quad i = 0, 1, ..., K \quad j = 0, 1, ..., K-1
\]

and \( y_0 \) is 1.

\textbf{Table 6.7; Shifted roots of Legendre polynomials of order 2,3,4 and 5}

<table>
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<tr>
<th>Order</th>
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<th>( t_2 )</th>
<th>( t_3 )</th>
<th>( t_4 )</th>
<th>( t_5 )</th>
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<td></td>
<td></td>
</tr>
<tr>
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<td>0.67</td>
<td>0.93</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.05</td>
<td>0.23</td>
<td>0.50</td>
<td>0.77</td>
<td>0.95</td>
</tr>
</tbody>
</table>
At each collocation point there is one polynomial with a value of 1 and the other polynomials are zero. States have an initial value and therefore zero is also a collocation point for state profiles while control profiles are only colocated on the shifted Legendre roots.

For poorly behaving functions (rapidly changing in some small region) the global collocation method would require high order polynomials for an accurate approximation of the state and control profiles. The steep region could then be approximated well at the expense of over-approximating the rest of the function. An alternative to global collocation uses piecewise polynomial approximations. Here a set of \((K+1)\)-th order state polynomials and \(K\)-th order control polynomials is defined on finite elements. Each finite element \(\Delta \alpha_i\) is bounded by two knots, \(\alpha_i\) and \(\alpha_{i+1}\). The distribution of the elements can now be chosen so that the approximations are done both efficiently and accurately.
The orthogonal properties obtained with global collocation are preserved by mapping the domain \( t \in [0,1] \) to each finite element and the locations of the orthogonal Legendre roots are mapped to the points:

\[
t_{ij} = \alpha_i + t_j(\alpha_{i+1} - \alpha_i) \quad i = 1, ..., \text{NE} \quad j = 0, ..., K
\]

where \([ij]\) denotes \((i-1)(K+1)+j\). \text{NE} is the number of finite elements.

The Lagrange polynomials can now be expressed as:

\[
x_{ij}^k(t) = \sum_{i=0}^{K} y_{ij}^k \phi_{ij}(t) \quad \text{where} \quad \phi_{ij}(t) = \prod_{k=0,j}^{K} \frac{t - t_{ik}}{t_{ij} - t_{ik}}
\]

\[
c_{ij}^k(t) = \sum_{j=1}^{K} \mu_{ij} \psi_{ij}(t) \quad \text{where} \quad \psi_{ij}(t) = \prod_{k=1,i}^{K} \frac{t - t_{ik}}{t_{ij} - t_{ik}}
\]

for \( i = 1, ..., \text{NE} \).

The discretized residuals can be written as:

\[
R(t_{ik}, \Delta \alpha_i) = \sum_{j=0}^{K} y_{ij}^k \dot{\phi}_{ij}(t_{ik}) - F(d, \mu_{ik}, \gamma_{ik}) = 0
\]

\( i = 1, ..., \text{NE} \quad k = 1, ..., K \)

with \( y_{[10]} = X_0 \).

The calculation of the term \( \dot{\phi}_{ij}(t_{ik}) \) can be simplified by chain ruling derivatives to obtain:

\[
\dot{\phi}_{ij}(t_{ik}) = \frac{\dot{\phi}_j(t_k)}{\Delta \alpha_i} \quad i = 1, ..., \text{NE} \quad j = 0, ..., K \quad k = 1, ..., K
\]

So the residuals become:

\[
R(t_{ik}, \Delta \alpha_i) = \sum_{j=0}^{K} y_{ij}^k \frac{\dot{\phi}_j(t_k)}{\Delta \alpha_i} - F(d, \mu_{ik}, \gamma_{ik}) = 0
\]

\( i = 1, ..., \text{NE} \quad k = 1, ..., K \)

with \( y_{[10]} = X_0 \).

To complete the set of equations, each polynomial is extrapolated to the endpoint of its element to provide an initial condition for the next element (continuity equations)

\[
\gamma_{[i0]} = \sum_{j=0}^{K} y_{[i-1]j} \phi_j(t = 1) \quad i = 2, ..., \text{NE}
\]

Each overall approximation to the state profile is therefore a continuous and piecewise polynomial function of order \( K+1 \). Control profiles might be discontinuous at the knots.
Including the ODE model, discretized on finite elements, and the continuity equations at the knots, the NLP formulations becomes:

\[
\begin{align*}
\min_{d, \mu_{[ik]}, \gamma_{[ik]}} & \quad \Phi[d, \mu_{[ik]}, \gamma_{[ik]}] \\
\text{s.t.} & \quad c[d, \mu_{[ik]}, \gamma_{[ik]}] = 0 \\
& \quad g[d, \mu_{[ik]}, \gamma_{[ik]}] \leq 0 \\
& \quad \sum_{j=0}^{K} \frac{\phi_j(t_k)}{\Delta \alpha_i} - F[d, \mu_{[ik]}, \gamma_{[ik]}] = 0 \quad i = 1, \ldots, \text{NE} \quad k = 1, \ldots, K \\
& \quad \gamma_{[i0]} = X_0 \\
& \quad \gamma_{[i0]} = \sum_{j=0}^{K} \gamma_{[i-j]}\phi_j(t = 1) \quad i = 2, \ldots, \text{NE} \\
& \quad d^L \leq d \leq d^U \\
& \quad C^L \leq \mu_{[ik]} \leq C^U \\
& \quad X^L \leq \gamma_{[ik]} \leq X^U
\end{align*}
\]

(NLP2) (6.18)

6.4.3 Derivatives and integrals of Lagrange polynomials

As shown before, the derivative of a state variable when written in Lagrange polynomial formulation and discretized on finite elements reduces to:

\[
\dot{X}_{K+1}(t_{ik}) = \sum_{j=0}^{K} \gamma_{[ij]} \frac{\phi_j(t_k)}{\Delta \alpha_i} \quad i = 1, \ldots, \text{NE} \quad k = 1, \ldots, K
\]

(6.19)

where the term \( \phi_j(t_k) \) only depends on the degree of the polynomial and can be calculated before the NLP problem is solved.

Integration of a continuous variable will also be reduced when Lagrange polynomial formulation and discretization on finite elements are used. Chain ruling an integral results in multiplication by the size of the element, so

\[
\int_{t_{ik}}^{t_{ik+1}} \dot{X}_{K+1}(t) \, dt = \Delta \alpha_i \sum_{j=0}^{K} \gamma_{[ij]} \int_{t_k}^{t_{k+1}} \phi_j(t) \, dt \quad i = 1, \ldots, \text{NE} \quad k = 1, \ldots, K
\]

(6.20)

Gauss-Jacobi quadrates can be used for integration over a whole element.

\[
\int_{t_i}^{t_{i+1}} \dot{X}_{K+1}(t) \, dt = \sum_{j=0}^{K} \gamma_{[ij]} w_j \quad i = 1, \ldots, \text{NE}-1
\]

(6.21)
6.4.4 Knot placement

Instead of using equally spaced finite elements, one can consider an error minimization strategy by optimal knot placement (Cutrell and Biegler, 1987). A theoretical bound on the approximation error is given by:

\[ E_{K+1} \{ X(t); [\alpha_i, \alpha_{i+1}] \} \leq C \Delta \alpha_i^{K+1} \| X^{(K+1)}(t) \|_i \]  \hfill (6.22)

- \( E_{K+1} \{ X(t); [\alpha_i, \alpha_{i+1}] \} \) represents the local error between an optimal approximation polynomial of \((K+1)\)-th order and the function \(X(t)\) over some region \([\alpha_i, \alpha_{i+1}]\)
- \( C \) is a calculable constant dependent only upon \(K\)
- \( \Delta \alpha_i^{K+1} \) is the \((K+1)\)-th power of the \(i\)-th finite element length
- \( \| X^{(K+1)}(t) \|_i \) is the max-norm of the \((K+1)\)-th derivative of \(X(t)\) in the interval \([\alpha_i, \alpha_{i+1}]\)

To minimize the approximation error, the following NLP can be formulated:

\[
\begin{align*}
\text{Min} & \quad \text{Max} \Delta \alpha_i \left\| X^{(K+1)}(t) \right\|_{i}^{1/(K+1)} & \quad i = 2, \ldots, NE \\
\text{s. t.} & \quad \Delta \alpha_i \geq \varepsilon & \quad i = 1, \ldots, NE \\
& \quad \Delta \alpha_i = 0, \alpha_{NE+1} = 1, \varepsilon = \text{a small positive number.} & \quad (\text{NLP3}) \quad (6.23)
\end{align*}
\]

This problem can be simplified by noting that, as long as \( \Delta \alpha_i \geq \varepsilon \), the necessary and sufficient optimality condition for NLP3 becomes:

\[ \Delta \alpha_i \left\| X^{(K+1)}(t) \right\|_{i}^{1/(K+1)} = \text{constant} \quad i = 1, \ldots, NE \] \hfill (6.24)

As an approximation \( s_i \) for the unknown term \( \left\| X^{(K+1)}(t) \right\|_{i} \) is introduced:

\[
s_i = \begin{cases} 
\frac{2 \Delta \theta(\alpha_{3/2})}{\alpha_3 - \alpha_1} & \text{on } (\alpha_1, \alpha_2) \\
\frac{\Delta \theta(\alpha_{i-1/2})}{\alpha_{i-1} - \alpha_{i-1}} + \frac{\Delta \theta(\alpha_{i+1/2})}{\alpha_{i+2} - \alpha_i} & \text{on } [\alpha_i, \alpha_{i+1}]; \quad i = 2, \ldots, \text{NE-1} \quad (6.25) \\
\frac{2 \Delta \theta(\alpha_{NE-1/2})}{\alpha_{NE+1} - \alpha_{NE-1}} & \text{on } [\alpha_{\text{NE}}, \alpha_{\text{NE+1}}]
\end{cases}
\]
where \[ \Delta \theta(\alpha_{i+1/2}) = \theta(\alpha_{i+1/2}) - \theta(\alpha_{i-1/2}) \]

\[ \theta(\alpha_{i+1/2}) = x_{k+1}^{(i)} \quad i = 1, \ldots, NE \]

is the highest nonzero derivative of \( x_{k+1}^{(i)}(t) \) in \( \Delta \alpha \).

Then the knot placement equations become:

\[ h_i = \left( \sum_{m=1}^{M} (s_{i}^{2/(K+1)})_m \right)^{1/2} \Delta \alpha_i - \left( \sum_{m=1}^{M} (s_{i+1}^{2/(K+1)})_m \right)^{1/2} \Delta \alpha_{i+1} = 0 \quad (6.26) \]

This can be included in the NLP formulation of the DAOP (6.18), which becomes:

\[
\begin{align*}
\min_{d, \mu_{ik}, \gamma_{ik}} & \Phi[d, \mu_{ik}, \gamma_{ik}] \\
\text{s.t.} & \quad c[d, \mu_{ik}, \gamma_{ik}] = 0 \\
& \quad g[d, \mu_{ik}, \gamma_{ik}] \leq 0 \\
& \quad \sum_{j=0}^{K} \gamma_{(i,j)}(t_k) \Delta \alpha_i - F[d, \mu_{ik}, \gamma_{ik}] = 0 \quad i = 1, \ldots, NE \quad k = 1, \ldots, K \\
& \quad \gamma_{(i,0)} = X_0 \\
& \quad \gamma_{(i,10)} = \sum_{j=0}^{K} \gamma_{(i-1,j)} \phi_j(t=1) \quad i = 2, \ldots, NE \quad (NLP4) \quad (6.27) \\
& \quad h_i = 0 \quad i = 1, \ldots, NE-1 \\
& \quad \alpha_{i+1} \geq \alpha_i + \varepsilon \quad i = 1, \ldots, NE \\
& \quad d^L \leq d \leq d^U \\
& \quad C^L \leq \mu_{ik} \leq C^U \\
& \quad X^L \leq \gamma_{ik} \leq X^U 
\end{align*}
\]

This type of dynamic optimization is illustrated with an example next.

**Example 6.4: The car problem**

Consider the problem of a car that has to move from point A to point B, 300 m further, in the shortest time. It starts with zero speed and it also has to end with zero speed. Furthermore the maximum acceleration is 1 m/s\(^2\) and the maximum break power is 2 m/s\(^2\).
The problem can be formulated as:

\[
\begin{align*}
\min \ (t_{\text{end}}) \\
\text{s.t.} \\
\frac{dx}{dt} &= v \\
\frac{dv}{dt} &= u \\
x(t_0) &= 0 \\
x(t_{\text{end}}) &= 300 \\
u_{\min} &= -2 \\
u_{\max} &= 1
\end{align*}
\]

The optimal solution will be maximum acceleration till a certain time and then maximum break. The question is when to change? The mathematical proof is very complex, but the answer is easily found when the problem is formulated as an NLP problem with optimal knot placement. We have done that in MATLAB®.

The problem contains two differential equations, the initial and final conditions for distance \( x \) and speed \( v \) are fixed and there are constraints on the acceleration \( u \). We expect one discontinuity, so we need two elements. For both elements, the acceleration will be constant, the speed linear and the distance quadratic, so two interior collocation points per element will be enough. Figure 6.7 shows the result. At 20 s, the speed is 20 m/s, the driven way 200 m, still 100 m to go and with a break of 2 m/s\(^2\) the speed will be zero at 300 m, reached at 30 s.

![Figure 6.7; Car problem with two elements and two collocation points](image-url)
When we introduce a speed limit of 15 m/s, full acceleration is only possible for 15 s., then the second element will have no full break. Final time is 40 s. (Figure 6.8).

Figure 6.8; Car problem with speed limit, two elements and two collocation points

With three elements, one may have an intermediate part with full speed and zero acceleration, till 24 s. Final time will be 31.3 s. (Figure 6.9).

Figure 6.9; Car problem with speed limit, three elements and two collocation points
6.5 Comparing the dynamic optimization methods

The example with the car demonstrates that dynamic optimization problems can be easily solved if the dynamic model is included in the optimization problem formulation as a set of equality constraints, collocated on finite elements. Then the optimal solution of the dynamic profile can be found directly without the use of integration programs. To compare this direct approach with the two step iterative method, the Trambouze reaction from Example 6.1 is solved using this direct method.

The objective is to maximize the overall fractional yield of component C over component A. There are five discrete feed charges, so the total operation time is divided into five reaction intervals. Therefore, collocation of this problem should be done on five finite elements. Furthermore, since the highest order in the dynamic model is two (component D is produced by a reaction that is second order in reactant A), three collocation points per finite element are required. Additionally, the continuity equations have to take the effect of the discrete charges on the concentrations of the different components into account.

The result of this optimization problem compares well to the result found using the two step approach. However, there are major differences in the number of iterations and in simulation time.

Table 6.8; Problem characteristics of Trambouze reaction with 5 discrete charges

<table>
<thead>
<tr>
<th>Two step iterative method</th>
<th>Direct method with collocation</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 discrete charges</td>
<td>5 discrete charges</td>
</tr>
<tr>
<td>5 reaction intervals</td>
<td>5 reaction intervals</td>
</tr>
<tr>
<td>1 Objective</td>
<td>1 Objective</td>
</tr>
<tr>
<td>1 Constraint on Final volume</td>
<td>1 Constraint on Final volume</td>
</tr>
<tr>
<td>Separate Dynamic model</td>
<td>Collocated Dynamic model</td>
</tr>
<tr>
<td>Initialization</td>
<td>5 elements, 3 collocation points</td>
</tr>
<tr>
<td>4 component balances</td>
<td>60 Residual equations (4 x 5 x 3)</td>
</tr>
<tr>
<td>1 volume balances</td>
<td>16 Continuity equations (4 x (5-1))</td>
</tr>
<tr>
<td>Integration</td>
<td>4 End condition equations (4 x 1)</td>
</tr>
<tr>
<td>4 component balances</td>
<td>5 Volume balance equations (1 x 5)</td>
</tr>
<tr>
<td>Re-initialization after each discrete charge</td>
<td>85 additional equality constraints</td>
</tr>
<tr>
<td></td>
<td>85 additional variables</td>
</tr>
<tr>
<td>1 equality constraint</td>
<td>86 equality constraints</td>
</tr>
<tr>
<td>10 optimization variables</td>
<td>95 optimization variables</td>
</tr>
<tr>
<td>1692 function evaluations</td>
<td>438 function evaluations</td>
</tr>
<tr>
<td>142 gradient evaluations</td>
<td>184 gradient evaluations</td>
</tr>
<tr>
<td>201 s used for total problem *</td>
<td>104 s used for total problem *</td>
</tr>
<tr>
<td>194 s used for dynamic model *</td>
<td></td>
</tr>
<tr>
<td>on a Pentium II 400 MHz PC.</td>
<td></td>
</tr>
</tbody>
</table>
A great advantage of the direct method is that an analytical gradient function can be derived from the optimization model. This is in contrast with the two step method, where the gradient function has to be developed numerically. This requires a lot of additional function evaluations, including integration of the dynamic model. For this specific example, Table 6.8 shows that with the two step method most function evaluations are used for updating the numerical gradient (142 gradient evaluations x 10 optimization variables requires 1420 function evaluations). Furthermore, most of the simulation time is used to solve the dynamic problem. Therefore, although the optimization problem for the direct method contains many more variables, the optimal solution is found faster than with the two step iterative method.

In conclusion, when the dynamic optimization problem can be collocated on a restricted number of elements and collocation points, like the car and Trambouze problems, then the direct method is preferable. Whether this conclusion holds for large and complex problems to be collocated on many finite elements as well, will be discussed in section 6.8.

6.6 Mixed Integer Programming

A mixed integer optimization problem can be formulated as:

$$\begin{align*}
\text{min} & \quad f(x,y) \\
\text{s.t.} & \quad h(x,y) = 0 \\
& \quad g(x,y) \leq 0 \\
& \quad x \in X \subseteq \mathbb{R}^n \\
& \quad y \in Y \text{ integer}
\end{align*}$$

where $x$ is a vector of $n$ continuous variables and $y$ is a vector of $m$ integer variables, $f$ is the object function, $h$ are the equality constraints and $g$ are the inequality constraints.

Often one reduces the problem to 0-1 integer variables: $y \in Y = \{0,1\}$.

$$\begin{align*}
\text{min} & \quad f(x,y) \\
\text{s.t} & \quad h(x,y) = 0 \\
& \quad g(x,y) \leq 0 \\
& \quad x \in X \subseteq \mathbb{R}^n \\
& \quad y \in Y = \{0,1\}
\end{align*}$$
The simple minded approach of solving the (non)linear optimization problem for all combinations of 0-1 variables is normally not an option, since the number of combinations increases exponentially with the number of binary variables \(2^m\). Another simple approach is relaxation of the binary variables between 0 and 1. However, only special cases will yield an integer optimum. Non-integer solutions can be rounded to nearest integer bounds, but this may give infeasible or sub-optimal solutions. So another approach is required.

6.6.1 Branch and Bound

The most widely used method to solve a mixed integer linear problem is the branch and bound approach. The basic idea is to partition successively the integer space and solve relaxed linear problems to determine whether subregions can be eliminated. First the binary variables are relaxed between 0 and 1 and a linear problem is solved. This relaxed LP gives a lower bound to the MILP problem. Then, at subsequent iterations, more and more integer variables are fixed on 0 or 1 and the remaining relaxed problem is solved. If this remaining problem is infeasible, the sub-region can be eliminated. If the solution is feasible, the node can be further exploited. A special case is formed when the remaining problem has an integer solution. Then the solution forms an upper bound.

The first question is which variable to partition at each node. One may use a fixed priority or select the binary variable that is closest to 0.5. A better branching rule is the cost penalty, introduced by Driebeek (1966). If a relaxed binary variable is set on 0, the objective will increase. This is called the down penalty. Setting the relaxed binary variable on 1 gives the up penalty. Both penalties can be calculated with one dual simplex iteration. The smallest degradation for this binary variable is the minimum of these two. The rule is now to partition the variable for which the degradation is largest.

Another question is which node to enumerate next. When a variable is partitioned and the relaxed LP is solved, then a new subproblem should be selected. One can go into depth first. The most recent node is expanded until the remaining problem becomes infeasible or an integer solution is found. Then the path is backtracked. This method is simple, only little memory is needed and it is cheap to update the LP. When one goes into breadth first, all nodes are expanded at each level and the one with the lowest bound is selected. This method is expected to examine fewer nodes, but it requires more memory and the optimal basis for the relaxed LP must be recreated at each node. Therefore, most common in practice is a combination of both. Consider both branches at a node and proceed as depth first.
Example 6.5; MILP problem

Consider the following minimization problem:

\[
\begin{align*}
\text{min} & \quad z = x + y_1 + 2y_2 + 3y_3 \\
\text{s.t.} & \quad -x + 3y_1 + 2y_2 + y_3 \leq 0 \\
& \quad -5y_1 - 8y_2 - 3y_3 \leq -9 \\
& \quad x \geq 0 \quad y_1, y_2, y_3 = 0, 1
\end{align*}
\]

Solving the relaxed LP gives:

1. \( z = 5.8 \), \( x = 2.6 \), \( y_1 = 0.2 \), \( y_2 = 1 \), \( y_3 = 0 \)

It is clear that \( y_1 \) should be partitioned first, since this is the only relaxed binary variable with a non-integer solution. This results in:

2. \( z = 6 \), \( x = 2.33 \), \( y_1 = 0 \), \( y_2 = 1 \), \( y_3 = 0.33 \)
3. \( z = 6.5 \), \( x = 4 \), \( y_1 = 1 \), \( y_2 = 0.5 \), \( y_3 = 0 \)

Node 2 has the lower bound, so this should be enumerated next. On this node, \( y_3 \) should be partitioned further.

4. infeasible \( y_1 = 0 \), \( y_3 = 0 \)
5. \( z = 6.75 \), \( x = 2.5 \), \( y_1 = 0 \), \( y_2 = 0.75 \), \( y_3 = 1 \)

When \( y_1 \) and \( y_3 \) are both fixed on 0, the remaining problem becomes infeasible. Since \( y_2 \) is bounded between 0 and 1, the second constraint cannot be reached. When \( y_3 \) is fixed on 1, we get a feasible solution. In case of depth first, we should proceed with this node, but now we will proceed with node 3, since this node provided the lowest bound. On this node, \( y_2 \) should be partitioned further.

6. infeasible \( y_1 = 1 \), \( y_2 = 0 \)
7. \( z = 9 \), \( x = 5 \), \( y_1 = 1 \), \( y_2 = 1 \), \( y_3 = 0 \)

Node 6 is infeasible again and node 7 has an integer solution, providing an upper bound. Now node 5 is the only one that is left. Partitioning this node gives:

8. infeasible \( y_1 = 0 \), \( y_2 = 1 \), \( y_3 = 0 \)
9. \( z = 8 \), \( x = 3 \), \( y_1 = 0 \), \( y_2 = 1 \), \( y_3 = 1 \)

Node 8 is infeasible but node 9 is feasible and in this case also the optimal solution since it is an integer solution and the objective is lower than the upper bound provided by node 7.
6.6.2 Mixed Integer Nonlinear Programming

The majority of optimization problems in chemical engineering will contain equations that are nonlinear in their continuous variables. The branch and bound method can also be used to solve these problems. If the relaxed problem gives an integer solution, only one NLP has to be solved but in general large numbers of NLP’s may have to be solved. Because this is expensive in terms of computation time, there are algorithms developed that subsequently solve an NLP subproblem with fixed binary variables that provides an upper bound and an MILP master problem that gives a lower bound. One of these methods is the outer approximation method (Duran and Grossmann, 1986). The nonlinear equations in the MINLP problem are simply expanded in a Taylor series, neglecting second and higher order terms. This works fine for convex problems, but with non-convexities, the master problem can cut off the global optimum. Therefore Viswanathan and Grossmann (1990) introduced slack variables to allow for violations in linearizations. A weighted sum of the slacks is added to the objective as a penalty function. This method has been tested with many problems and three to five major iterations are normally enough to find the optimal solution of the MINLP problem.

6.7 Optimal design of flowsheet structures and control systems

The ultimate goal of this work is to develop an approach for the simultaneous design and optimization of flowsheet structures, while taking dynamic behavior and controllability features into account. To deal with dynamic variables in an optimization problem, the method of orthogonal collocation on finite elements can be used, while superstructures of flowsheets and control systems can be constructed by using binary variables. In fact, this means that the direct optimization method described before will be combined with a technique to deal with the discrete character of the optimization problem. Thus, one obtains a mixed-integer nonlinear programming model of considerable size, which can be solved using the outer approximation method with the branch and bound algorithm for the MILP master problems and an SQP type solver for the NLP subproblems. A combination of these solvers is available in the programming environment GAMS, which will be used henceforth to solve dynamic optimization problems of flowsheet structures and control systems.

Unfortunately, GAMS does not contain a library with unit operation models, neither an automatic collocation method. Hence, dynamic models for unit operations, collocated on finite elements, should be developed first, before a flowsheet superstructure can be built.
Since the overall convergence behavior is very sensitive to the quality of these models, it is relevant to address some aspects of "good modeling" first. Then, also quite unexpectedly, special attention has to be paid to the vapor-liquid equilibrium model. The usual equilibrium model is only valid in the two-phase region, which might cause problems when used in dynamic models for optimization. This particular integer-like problem requires a modification of the common two-phase equilibrium model to be implemented in the model describing the dynamics of a flash drum with controllers. Using GAMS these steps have to be taken first, before the overall optimization model can be constructed and run. The following description contains all the relevant steps.

6.7.1 Good modeling

Solving optimization problems can be very difficult. Writing a "good" model can help the solver. Some tips for "good" modeling:

- **Simple expression**
  - Avoid nonlinear functions of expressions, divisions by expressions and products of expressions
  - Define intermediate variables that are equal to the expressions. The model becomes larger, but the complexity is reduced, especially when the intermediate expressions are linear.
  - Make equalities of binding constraints

- **Initial values**
  - Select reasonable values for some variables that are important
  - Use the equations to derive values for the other variables

- **Bounds**
  - Model bounds, representing constraints on the reality; e.g. a variable must be positive
  - Algorithmic bounds, preventing the algorithm to move away from any optimal solution and into regions with singularities in the nonlinear functions or unreasonable large function or derivative values.
  - Use variable bounds instead of simple inequalities
  - Bounds can slow the solution process down
Scaling

- Basic variables have expected solutions around 1, e.g. between 0.01 and 100
- Non basic variables are at a bound, not larger than say 100
- Dual variables of active constraints are expected to be around 1, from 0.01, to 100
- Dual variables of non-binding constraints are of course zero
- Derivatives (or Jacobian elements) are expected to be around 1, between .01 and 100
- Scaling starts with the choice of the units of measurement; e.g. pressure in bar
- Next step is to use scaling factors for variables; e.g. 300 for the temperature in Kelvin
- Scale also equations if needed

6.7.2 Vapor-liquid equilibrium model

The mostly used technique for separation in large chemical plants is distillation, which is based on the equilibrium between components in the vapor and the liquid. To construct a model describing this piece of equipment the first step is to develop a vapor-liquid equilibrium model that can be used in these models.

A vapor-liquid equilibrium is generally described by:

\[ y_i = K_i(P,T)x_i \]
\[ \sum_{i=1}^{NC} (y_i - x_i) = 0 \]  
(6.30)

where \( x_i \) is the liquid mole fraction and \( y_i \) the vapor mole fraction of component i, \( K_i(P,T) \) the equilibrium constant of component i as function of pressure and temperature and NC the total number of components.

Raoult’s Law gives a simple expression for the equilibrium constant:

\[ K_i(P,T) = \frac{p_i(T)}{P} \]  
(6.31)

The partial pressure \( p_i \) as function of \( T \) can be calculated with the Antoine equation:

\[ p_i(T) = A_i + \frac{B_i}{C_i + T} \]  
(6.32)

A, B and C are component specific constants.
This simple, but already nonlinear model can be used to describe the vapor-liquid equilibrium in a two-phase system. However, problems will occur if just one phase exists, either vapor or liquid. The equilibrium may still be calculated, but the component mole fractions of the non-existing phase do not sum up to one anymore and therefore the sum-equation becomes infeasible. Hence, a special provision has to be made to render this equation feasible in the case of one-phase situations.

In our technique to deal with this problem, first the bubble and dew point temperatures of the mixture have to be calculated. The bubble point temperature is the temperature where, at the given pressure, the mixture is at the liquid bound. Above this temperature only vapor exists. The dew point temperature indicates the vapor bound, below which only liquid exists. Between these temperatures the system is in two-phase equilibrium and the sum equation is valid. Outside these bounds, the sum equation should be reduced to a summation of the component mole fractions of the existing phase only, which should be equal to 1. This results into the sum equation:

\[
\left(\sum_{i=1}^{NC}(y_i) - 1\right) \cdot \text{phase}_v = \left(\sum_{i=1}^{NC}(x_i) - 1\right) \cdot \text{phase}_l \quad (6.33)
\]

where \(\text{phase}_v\) and \(\text{phase}_l\) indicate whether the vapor respectively the liquid phase either (1) or not (0) exists. If both phases exist, this equation reduced to the original equation. If only one phase exists, the sum of the mole fractions should be equal to 1.

What remains is an expression for \(\text{phase}_v\) and \(\text{phase}_l\). This can be related to the temperature. If the temperature is above the bubble point temperature, \(\text{phase}_v\) is 1, otherwise \(\text{phase}_v\) is 0. If the temperature is below the dew point temperature, \(\text{phase}_l\) is 1, otherwise \(\text{phase}_l\) is 0. Unfortunately, simple ‘if then else’ statements cannot be implemented in a collocation model. Therefore, we use an arctan function to switch from 0 to 1. The following expressions are used:

\[
\text{phase}_v = \arctan\left(\frac{T - T_{\text{bub}}}{C}\right) / \pi + 0.5 \quad (6.34)
\]

\[
\text{phase}_l = \arctan\left(\frac{T_{\text{dew}} - T}{C}\right) / \pi + 0.5 \quad (6.35)
\]

For large constants \(C\) the arctan function switches from -\(\pi\) to \(\pi\) within a small temperature interval around the bubble respectively dew point temperature. These continuous functions can therefore be used to calculate the existence or non-existence of the vapor and liquid phases. This is illustrated by the following example.
Example 6.6; Vapor-liquid equilibrium of a benzene-toluene mixture

To demonstrate the vapor-liquid equilibrium model, consider the vapor-liquid equilibrium of a 50/50 mole-% Benzene/Toluene mixture at 1 bar to move through a rising temperature profile, starting in the liquid phase and passing the two-phase region to the vapor phase. The results are given in Table 6.9 and Figure 6.10.

Table 6.9; Vapor-liquid equilibrium of a benzene-toluene mixture

<table>
<thead>
<tr>
<th>Bubble temperature</th>
<th>364.8 K</th>
<th>Y Benzene</th>
<th>0.71</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dew temperature</td>
<td>371.5 K</td>
<td>X Benzene</td>
<td>0.29</td>
</tr>
</tbody>
</table>

![Figure 6.10; Vapor-liquid equilibrium of a benzene-toluene mixture at 1 bar.](image)

At temperatures below the bubble point there is only liquid and above the dew point there is only vapor. At temperatures between the bubble and dew point, the material is distributed over two phases being in equilibrium.

This example shows that the modified vapor-liquid equilibrium model applies to situations where vapor and liquid are in equilibrium, but also to one-phase systems, either liquid or vapor. The accuracy of the phase transition modeling lies within a temperature range of 0.1 K, which is practically sufficient for most problems. To increase the accuracy and reduce this range, the constant used in the model is only to be increased. We have implemented this vapor-liquid equilibrium model in a dynamic unit operation model.
6.7.3 Dynamic optimization problems

In addition to the vapor-liquid equilibrium model, a dynamic unit operation model contains material balances for each component, a total energy balance, enthalpy relations and additional models for vapor and liquid volumes. All of these equations have to be discretized, for which the technique of collocation on finite elements can be used. Subsequently, the model can be used in an optimization problem, after formulating an object function and addition of constraints.

Now, a number of dynamic optimization sub-problems around the model of a boiler will be considered. The first example concerns an open vessel containing a liquid mixture that is heated. There is no feed and the vapor produced will leave the system immediately, so a vapor holdup does not exist. The model contains the modified vapor-liquid equilibrium relations, material and energy balances and Rackett liquid volume relations to be able to calculate the liquid height in the vessel. Collocation is on finite elements and the solution procedure runs with fixed settings first. Subsequently, a number of optimization exercises will be explored using this system. The Conopt2 routine of GAMS is used to solve the optimization problems.

Example 6.7; Dynamic simulation of a liquid Boiler

Consider an open vessel containing 1 m$^3$ of a 50/50 mole-% Benzene/Toluene liquid mixture at 1 bar and a temperature that lies 5 K below the bubble point. The mixture is heated with a constant duty of 0.1 GJ/h.

The model is discretized on four elements and two collocation points per element. The first knot is initially placed such that the temperature is on the bubble point. The last knot is placed such that the vessel is empty and the other two are placed in between so that the same amount of material is vaporized during each of the latter three intervals. Each element is initialized separately. The last element cannot be initialized if the knot is placed exactly on the empty vessel. For this reason a small amount of material at the end is allowed during the initialization of this element. During solution of the model, the amount of material in the vessel on the last knot is minimized.

The boiler model contains 639 equations/variables, the Jacobian contains 1792 non-zero elements, of which 756 are nonlinear. The problem is solved in 18 iterations, taking a few seconds on a Pentium 133 MHz PC. This is so mainly since the initialization is close to the optimal solution. Without initialization the solver will not find a feasible solution at all.
Since control variables might be discontinuous at the knot points, they are not solved on the bounds of an element. Instead, their values at these points are extrapolated from the values at the intermediate collocation points, according to the Lagrange function. However, even if no discontinuities occur, the value of a control variable at the end of an element may slightly differ from its value at the beginning of the next element. This is due to the inaccuracy of the collocation method, but the differences can be minimized by optimal knot placement. The results of this example, described below, show that these differences are small compared to the absolute values and are therefore within acceptable limits.

Table 6.10; Time intervals (h)

<table>
<thead>
<tr>
<th>Alpha(I)</th>
<th>Initial</th>
<th>Final</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha(I1)</td>
<td>0.078</td>
<td>0.078</td>
</tr>
<tr>
<td>Alpha(I2)</td>
<td>1.022</td>
<td>1.682</td>
</tr>
<tr>
<td>Alpha(I3)</td>
<td>1.037</td>
<td>0.905</td>
</tr>
<tr>
<td>Alpha(I4)</td>
<td>0.504</td>
<td>0.515</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>2.641</strong></td>
<td><strong>3.180</strong></td>
</tr>
</tbody>
</table>

Figure 6.11; Holdup profiles

*The markers are placed on the collocation points.*

The first knot is kept on its initial value. The temperature in the first time interval is below the bubble point, so no vapor is produced and the holdup profiles are constant. At the first knot the temperature of the liquid is equal to the bubble point temperature. In the next intervals vapor is produced to keep the pressure constant. The time intervals are slightly changed, such that all material is vaporized at the last knot. Since Benzene is more volatile
than Toluene, its vapor fraction at the first knot is higher and its holdup initially decreases faster. For this reason the fraction of toluene in the vessel increases and both bubble and dew point temperatures rise. Because the vapor holdup is neglected, the temperature will be equal to the bubble point temperature. The Toluene fraction in the vapor also increases. The enthalpy of vaporization increases accordingly and the vapor production decreases, but only slightly. At the last knot, almost pure Toluene is removed. Bubble and dew point become nearly equal and close to the boiling point of Toluene at 1 bar (383.78K).

![Graph showing vapor and liquid mole fractions](image)

Figure 6.12; Vapor and Liquid mole fractions

Table 6.11; Temperatures and vapor production

<table>
<thead>
<tr>
<th></th>
<th>T</th>
<th>T bub</th>
<th>T dew</th>
<th>Vapor out</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>K</td>
<td>K</td>
<td>K</td>
<td>kmol/hr</td>
</tr>
<tr>
<td>I1J0</td>
<td>359.84</td>
<td>364.83</td>
<td>371.46</td>
<td>0.00</td>
</tr>
<tr>
<td>I1J1</td>
<td>360.89</td>
<td>364.83</td>
<td>371.46</td>
<td>0.00</td>
</tr>
<tr>
<td>I1J2</td>
<td>363.78</td>
<td>364.83</td>
<td>371.46</td>
<td>0.00</td>
</tr>
<tr>
<td>I1JE</td>
<td>364.84</td>
<td>364.83</td>
<td>371.46</td>
<td>0.00</td>
</tr>
<tr>
<td>I2J0</td>
<td>364.55</td>
<td>364.55</td>
<td>371.29</td>
<td>3.10</td>
</tr>
<tr>
<td>I2J1</td>
<td>365.63</td>
<td>365.63</td>
<td>372.21</td>
<td>3.09</td>
</tr>
<tr>
<td>I2J2</td>
<td>368.57</td>
<td>368.57</td>
<td>374.74</td>
<td>3.05</td>
</tr>
<tr>
<td>I2JE</td>
<td>369.64</td>
<td>369.64</td>
<td>375.66</td>
<td>3.04</td>
</tr>
<tr>
<td>I3J0</td>
<td>369.97</td>
<td>369.97</td>
<td>375.92</td>
<td>3.03</td>
</tr>
<tr>
<td>I3J1</td>
<td>371.34</td>
<td>371.34</td>
<td>376.79</td>
<td>3.02</td>
</tr>
<tr>
<td>I3J2</td>
<td>375.09</td>
<td>375.09</td>
<td>379.17</td>
<td>2.99</td>
</tr>
<tr>
<td>I3JE</td>
<td>376.45</td>
<td>376.45</td>
<td>380.04</td>
<td>2.98</td>
</tr>
<tr>
<td>I4J0</td>
<td>377.09</td>
<td>377.09</td>
<td>380.36</td>
<td>2.98</td>
</tr>
<tr>
<td>I4J1</td>
<td>378.41</td>
<td>378.41</td>
<td>380.99</td>
<td>2.97</td>
</tr>
<tr>
<td>I4J2</td>
<td>382.01</td>
<td>382.01</td>
<td>382.71</td>
<td>2.97</td>
</tr>
<tr>
<td>I4JE</td>
<td>383.33</td>
<td>383.33</td>
<td>383.34</td>
<td>2.96</td>
</tr>
</tbody>
</table>
Example 6.8; Boiler with constraints on vapor purity

Now, two additional constraints are added to the boiler model from the previous example. During the second interval, the Benzene fraction of the vapor should be at least 0.6 kmol/kmol and during the fourth interval the Toluene fraction of the vapor should be at least 0.7 kmol/kmol. The amount of vapor being produced during these two elements is maximized.

In the optimal solution, the second knot is placed in such a way that the benzene fraction in the vapor is exactly 0.6 kmol/kmol and at the third knot the Toluene fraction in the vapor is exactly 0.7 kmol/kmol. During the first interval, no vapor is produced and at the last knot the vessel is empty, so the vapor production in the second and fourth intervals are maximal with respect to the two constraints on the component fractions.

<table>
<thead>
<tr>
<th>Table 6.12; Time intervals (h)</th>
<th>Table 6.13; Vapor produced (kmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha(I1)</td>
<td>0.078</td>
</tr>
<tr>
<td>Alpha(I2)</td>
<td>1.393</td>
</tr>
<tr>
<td>Alpha(I3)</td>
<td>1.182</td>
</tr>
<tr>
<td>Alpha(I4)</td>
<td>0.527</td>
</tr>
<tr>
<td>Total</td>
<td>3.180</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Example 6.9; Boiler with vapor collection

Now, it is assumed that the vapor produced during the second interval is collected in a vessel and that produced during the fourth interval in another vessel. Constraints are put on the fraction of Benzene in the first vessel (min. 0.7 kmol/kmol) and the fraction of Toluene in the other vessel (min. 0.9 kmol/kmol). The total amount of material in the two vessels is maximized.

In the optimal solution the second knot is placed in such a way that the benzene fraction in the vessel is exactly 0.7 kmol/kmol and the third knot is placed such that the Toluene fraction in the other vessel becomes exactly 0.9 kmol/kmol, while all material is vaporized at the last knot. Thus, the vapor production in the second and fourth interval becomes maximal with respect to the two constraints on the component fractions.
**Table 6.14; Time intervals (h)**

<table>
<thead>
<tr>
<th>Alpha(I1)</th>
<th>0.078</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alpha(I2)</td>
<td>0.423</td>
</tr>
<tr>
<td>Alpha(I3)</td>
<td>2.204</td>
</tr>
<tr>
<td>Alpha(I4)</td>
<td>0.475</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>3.180</strong></td>
</tr>
</tbody>
</table>

**Table 6.15; Vapor produced (kmol)**

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total</strong></td>
<td>2.68</td>
<td></td>
</tr>
<tr>
<td>Vessel 1</td>
<td>1.30</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>0.91</td>
<td></td>
</tr>
<tr>
<td>Toluene</td>
<td>0.39</td>
<td></td>
</tr>
<tr>
<td>Xbenzene</td>
<td>0.7</td>
<td></td>
</tr>
<tr>
<td>Vessel 2</td>
<td>1.38</td>
<td></td>
</tr>
<tr>
<td>Benzene</td>
<td>0.14</td>
<td></td>
</tr>
<tr>
<td>Toluene</td>
<td>1.24</td>
<td></td>
</tr>
<tr>
<td>Xtoluene</td>
<td>0.9</td>
<td></td>
</tr>
</tbody>
</table>

### 6.7.4 Dynamic system with control

The examples concerning the boiler system show that the vapor-liquid equilibrium model can be incorporated in a dynamic model where material and energy balances are collocated on finite elements. The transition from one (liquid) phase stage to a two-phase stage, during which vapor is generated, is positioned at one knot. The other knots are placed such that the objective function is maximal (or minimal) with respect to the constraints.

A next step towards the simultaneous optimization of flowsheet and control structures is the introduction of a continuous dynamic flash model with controllers on temperature, pressure and liquid level. This in fact is already a simple flowsheet, although the structure still is fixed. The flash model is quite similar to the boiler model with as a major difference that the vapor holdup is taken into account now. There is a continuous feed and vapor and liquid in equilibrium will leave the system separately.

The controller model contains an error equation, which is a collocated differential equation to calculate the integral error, and a relation to determine the action. An additional equation is added to keep the action between a minimum and a maximum value. This relation again employs the arctan function:

\[
\text{Out} = \text{Min} + (\text{Action} - \text{Min}) \times \frac{\arctan((\text{Action} - \text{Min}) \times C) / \pi + 0.5}{(\text{Action} - \text{Max}) \times \frac{\arctan((\text{Action} - \text{Min}) \times C) / \pi + 0.5}}
\]

Bounding the controller output might be useful, especially when flowrates are manipulated. They cannot assume negative values, but Action might be negative and using this relation the output can be bounded on zero in this situation.
Example 6.10; Dynamic flash with control

A 50/50 mole-% Benzene/Toluene liquid mixture at 2 bar and 350 K is fed to a flash, operating at 1 bar and 367 K. The liquid level is controlled with the liquid outlet, the pressure with the vapor outlet and the temperature with the duty. To change the product quality, the temperature setpoint is changed to 370 K. The objective of this optimization problem is fast setpoint tracking, while keeping the pressure to its original setpoint. Therefore, the sum of the integral square errors of the pressure and temperature controllers is minimized by modifying controller gain and integral time. The level controller is not taken into account since it has another objective, namely keeping the level within bounds instead of on setpoint.

Table 6.16; Steady state operating points

<table>
<thead>
<tr>
<th>Initial steady state</th>
<th>Final steady state</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Temperature</strong> 367.0 °C</td>
<td><strong>Temperature</strong> 370.0 °C</td>
</tr>
<tr>
<td><strong>Pressure</strong> 1.00 bar</td>
<td><strong>Pressure</strong> 1.00 bar</td>
</tr>
<tr>
<td><strong>Pressure drop</strong> 1.00 bar</td>
<td><strong>Pressure drop</strong> 1.00 bar</td>
</tr>
<tr>
<td><strong>Duty</strong> 0.13 GJ/h</td>
<td><strong>Duty</strong> 0.28 GJ/h</td>
</tr>
<tr>
<td><strong>Vapor/Feed</strong> 0.33</td>
<td><strong>Vapor/Feed</strong> 0.77</td>
</tr>
<tr>
<td><strong>Benzene</strong> 0.43</td>
<td><strong>Benzene</strong> 0.84</td>
</tr>
<tr>
<td><strong>Toluene</strong> 0.23</td>
<td><strong>Toluene</strong> 0.69</td>
</tr>
<tr>
<td><strong>F (kmol/h)</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Benzene</strong> 5.00</td>
<td></td>
</tr>
<tr>
<td><strong>Toluene</strong> 5.00</td>
<td></td>
</tr>
<tr>
<td><strong>Z Benzene</strong> 0.50</td>
<td></td>
</tr>
<tr>
<td><strong>Toluene</strong> 0.50</td>
<td></td>
</tr>
<tr>
<td><strong>LIQ</strong></td>
<td></td>
</tr>
<tr>
<td><strong>F (kmol/h)</strong></td>
<td><strong>IN</strong> 10.00</td>
</tr>
<tr>
<td><strong>Benzene</strong> 5.00</td>
<td><strong>VAP</strong> 7.66</td>
</tr>
<tr>
<td><strong>Toluene</strong> 5.00</td>
<td><strong>LIQ</strong> 2.34</td>
</tr>
<tr>
<td><strong>Z Benzene</strong> 0.50</td>
<td><strong>IN</strong> 3.29</td>
</tr>
<tr>
<td><strong>Toluene</strong> 0.50</td>
<td><strong>VAP</strong> 2.13</td>
</tr>
<tr>
<td><strong>LIQ</strong></td>
<td><strong>LIQ</strong> 6.71</td>
</tr>
<tr>
<td><strong>T (C)</strong></td>
<td><strong>IN</strong> 367.0</td>
</tr>
<tr>
<td><strong>P (bar)</strong></td>
<td><strong>T (C)</strong> 367.0</td>
</tr>
<tr>
<td><strong>H (MJ/kmol)</strong></td>
<td><strong>IN</strong> 350.0</td>
</tr>
<tr>
<td><strong>F (kmol/h)</strong></td>
<td><strong>P (bar)</strong> 1.00</td>
</tr>
<tr>
<td><strong>Benzene</strong> 5.00</td>
<td></td>
</tr>
<tr>
<td><strong>Toluene</strong> 5.00</td>
<td><strong>H (MJ/kmol)</strong> 31.16</td>
</tr>
<tr>
<td><strong>Z Benzene</strong> 0.50</td>
<td><strong>LIQ</strong> 0.00</td>
</tr>
<tr>
<td><strong>Toluene</strong> 0.50</td>
<td><strong>IN</strong> 1.00</td>
</tr>
<tr>
<td><strong>LIQ</strong></td>
<td><strong>VAP</strong> 1.00</td>
</tr>
<tr>
<td><strong>F (kmol/h)</strong></td>
<td><strong>LIQ</strong> 367.0</td>
</tr>
<tr>
<td><strong>Benzene</strong> 5.00</td>
<td><strong>IN</strong> 350.0</td>
</tr>
<tr>
<td><strong>Toluene</strong> 5.00</td>
<td><strong>T (C)</strong> 370.0</td>
</tr>
<tr>
<td><strong>Z Benzene</strong> 0.50</td>
<td><strong>IN</strong> 367.0</td>
</tr>
<tr>
<td><strong>Toluene</strong> 0.50</td>
<td><strong>T (C)</strong> 370.0</td>
</tr>
<tr>
<td><strong>LIQ</strong></td>
<td></td>
</tr>
</tbody>
</table>
| Before the dynamic optimization problem can be solved, a number of initialization calculations have to be done. First the two steady state operating points are calculated with a steady state flash model. At given feed stream and operating pressure and temperature the steady state flash model is completely fixed (71 fixed equations / free variables). Some pre-calculation for the vapor-liquid equilibrium and enthalpy relations are performed and then the model can be solved quite easily. The results are given in Table 6.16.

Next, a dynamic problem is formulated where the flash is operated at the first steady state. The model is discretized on an arbitrary number of 100 elements of 0.04 hours with 3 internal collocation points each. This time it contains over 40000 equations/variables. By assigning
values to the controller settings, this system is completely fixed. It can be initialized with the results of the first steady state calculation and solved. Since the problem is initialized now at the solution, it is solved in one iteration.

Now the setpoint of the temperature is modified and the problem can be solved again, still with fixed controller settings. Unfortunately, the solver will not find a solution in this case. The first steady state is not a good initial guess of the solution to this dynamic problem. So, we have to develop the dynamic profile over the time domain.

Starting with the first element, it can be initialized at the initial steady state if the element length is close to zero, hence for a short time interval. Then the length of this element can be maximized, taking into account the error bound constraints on the collocated differential equations. The continuity equations can be used to initialize the next element and the complete time profile can be developed.

Applying this initialization method to the flash problem yields an initially feasible solution within a few minutes. Furthermore, it turned out that the final time of four hours is reached in element 35. The other elements are initialized on zero but they can as well be discarded from the model. Hence, this initialization method also determines the minimum number of elements required for collocation of the dynamic model. In this case, instead of selecting an arbitrary number of 100 elements, a minimum number of 35 elements can be used. This has reduced the size of the problem from 40000 to 15000 equations / variables.

Starting at the feasible solution allows the problem to be optimized. The objective is to minimize the sum of the integral square errors of the temperature and pressure controllers by modifying the controller gains and integral times. The system is modeled for a period of four hours total, hence sufficient time is available to reach the new steady state.

After 366 iterations, taking about 90 minutes on a Pentium 133 MHz computer, an optimal solution is found. Unfortunately, this solution is just a local optimum, restricted by the collocation scheme. After re-arranging the knots, the objective function can be further reduced. It sometimes occurs that the optimizer also stops at an infeasible solution. Then re-initialization using the most recent controller setting usually helps continuation. Repeating this procedure several times finally yields a solution that is no longer improvable, although this still might not be the global optimum. Starting from a completely different set of initial values probably leads to another local optimum. However, analyzing the area around the optimum by fixing the pressure controller settings and varying the temperature controller gain and integral time shows that there is a large area where the value of the objective is low (Figure 6.13). Zooming in at this area a real minimum is found.
Figure 6.13; Optimization area in dynamic flash problem

Table 6.17; Optimal controller setting for the Dynamic flash problem

<table>
<thead>
<tr>
<th>Initial settings</th>
<th>Pressure Controller (Vapor flow out)</th>
<th>Temperature Controller (Duty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Level Controller (Liquid flow out)</td>
<td>Setpoint</td>
<td>Bias</td>
</tr>
<tr>
<td>Setpoint</td>
<td>0.50</td>
<td>6.71</td>
</tr>
<tr>
<td>Bias</td>
<td>-25.00</td>
<td>3.29</td>
</tr>
<tr>
<td>Gain</td>
<td>0.75</td>
<td>0.00</td>
</tr>
<tr>
<td>Tau</td>
<td>0.00</td>
<td>20.00</td>
</tr>
<tr>
<td>ISE</td>
<td>6.36</td>
<td>ISE</td>
</tr>
</tbody>
</table>

Sum of integral square errors: 168.9

Optimal settings

<table>
<thead>
<tr>
<th>Level Controller (Liquid flow out)</th>
<th>Pressure Controller (Vapor flow out)</th>
<th>Temperature Controller (Duty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Setpoint</td>
<td>0.50</td>
<td>370.00</td>
</tr>
<tr>
<td>Bias</td>
<td>6.71</td>
<td>3.29</td>
</tr>
<tr>
<td>Gain</td>
<td>-25.00</td>
<td>-150.00</td>
</tr>
<tr>
<td>Tau</td>
<td>0.75</td>
<td>0.35</td>
</tr>
<tr>
<td>Min</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Max</td>
<td>20.00</td>
<td>20.00</td>
</tr>
<tr>
<td>ISE</td>
<td>5.87</td>
<td>ISE 4.51</td>
</tr>
</tbody>
</table>

Sum of integral square errors: 13.87
Figure 6.14; Level profile in dynamic flash problem

Figure 6.15; Pressure profile in dynamic flash problem

Figure 6.16; Temperature profile in dynamic flash problem
For this example, it is shown that the optimal settings are a major improvement as compared to the initial settings. The sum of the integral errors is reduced from 170 to 14. Figure 6.14 to Figure 6.16 show the dynamic profiles of the controlled variables. The markers in the following plots are placed on the collocation points. It is clear that the new steady state is also reached much faster. The temperature rises almost instantaneously to its new setpoint, while the pressure has only a slightly higher offset.

6.8 Revisiting the comparison between the dynamic optimization methods

The comparison between the two step and the direct method as applied to the Trambouze reaction problem (section 6.5) demonstrated that the latter one is preferable. In this direct method, the dynamic model is discretized and added to the optimization problem as equality constraints, which enlarges the problem size. However, since the gradient function can be developed analytically, the optimum is found much faster than with the two step method. In this two step method, the dynamic model is solved separately and the gradient function can only be developed numerically, requiring many additional function evaluations. So, if a dynamic optimization problem contains many optimization variables while the dynamic model can be collocated on a reduced number of finite elements, the direct method is preferable.

With these results in mind it was decided to use the discretization method of orthogonal collocation on finite elements in the approach for optimization of flowsheet structures and control systems. The first examples with this method, concerning a boiler, collocated on four finite elements, indeed turned out to be easily solvable. However, many difficulties arose with the dynamic flash problem. Collocation of this model required an extremely large number of finite elements, resulting in a very large optimization problem. On the other hand, in fact only four real optimization variables are present: the gains and integral times of the pressure and temperature controller. Therefore, before continuing with the introduction of integer variables, it seems relevant to re-compare the dynamic optimization methods, this time for the flash drum problem with controllers.

Table 6.18 shows the characteristics of both methods for the dynamic flash problem. While the direct method requires many elements to collocate the dynamic model, in the two step method, the integration routine simply takes many small steps. This requires a large number of dynamic model evaluations which is time consuming indeed, but it does not enlarge the size of the optimization problem. There are only four optimization variables. Each numerical
update of the gradient function therefore only requires four function evaluations. On the whole a moderate number of iterations is needed to find the optimum controller settings using the two step method.

In conclusion, dynamic optimization problems with complex dynamic models and only few free optimization variables are preferably solved using the two step iterative method, since it takes advantage of the small size of the optimization problem in combination with the fast integration routine. If on the contrary the number of optimization variables is large and the dynamic model can be collocated on a reduced number of finite elements, it may be more appropriate to use the direct method. Adding the collocated dynamic model as equality constrains enlarges the size of the optimization problem. However, the gradient function can be developed analytically, which considerably reduces the number of function evaluations. For this reason, this alternative might be faster than the two step method.

Table 6.18; Problem characteristics of dynamic flash with control

<table>
<thead>
<tr>
<th>Two step iterative method</th>
<th>Direct method with collocation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Objective</td>
<td>1 Objective</td>
</tr>
<tr>
<td>Separate Dynamic model</td>
<td>Collocated Dynamic model</td>
</tr>
<tr>
<td>9 differential equations</td>
<td>35 elements</td>
</tr>
<tr>
<td>67 algebraic equations</td>
<td>3 collocation points</td>
</tr>
<tr>
<td>No constraint</td>
<td>8916 equality equations</td>
</tr>
<tr>
<td>4 optimization variables</td>
<td>630 inequality equations</td>
</tr>
<tr>
<td></td>
<td>8920 optimization variables</td>
</tr>
<tr>
<td>373 function evaluations</td>
<td>19284 iterations</td>
</tr>
<tr>
<td>42 gradient evaluations</td>
<td>35 re-arrangements of elements</td>
</tr>
<tr>
<td>701952 dynamic model evals</td>
<td>3 re-initializations</td>
</tr>
<tr>
<td>9098 s used for total problem</td>
<td>59301 s used for total problem**</td>
</tr>
</tbody>
</table>

MATLAB 5 on a Pentium II 400 MHz PC **GAMS 2.50 on a Pentium 133 MHz PC

6.9 Conclusions

The simultaneous design and optimization of complex flowsheets, taking dynamic behavior and controllability features into account, requires the solution of a dynamic optimization problem. In this chapter two different techniques have been developed to solve this type of problems. In the first approach, a dynamic model is solved by standard integration at each iteration of the optimization routine, placed in an outer loop. The optimization problem in itself contains the object function and additional constraint to ensure a controllable plant design. This two step approach has the advantage that the optimization problem is small,
while fast integration routines can be used to solve the dynamic model. However, a disadvantage is that the gradient function of the optimization problem can only be developed numerically. This requires many additional function evaluations, including the integration of the dynamic model. Therefore, in some cases it might be better to add the dynamic model directly to the optimization problem as additional constraints. This requires the discretization of the model equations for which the method of orthogonal collocation on finite elements can be used. A disadvantage of this method is that the size of the optimization problem is enlarged considerably. However, since the gradient function can be developed analytically, the number of function evaluations is reduced and therefore the optimal solution might be found more efficiently.

Applying both methods on several examples clearly showed that this direct method is indeed more appropriate for problems with many optimization variables, while the dynamic model can be collocated on a reduced number of finite elements. Optimizing the operation of a Trambouze reaction system in a batch reactor with the total feed divided over several discrete charges by the two step method requires many function evaluations to update the gradient function. Using the direct method to solve this problem, collocated on a few elements, less iterations are needed and the optimal solution is found much faster. On the other hand, collocation of the flash model with its complex dynamic behavior requires many finite elements, resulting in a very large optimization problem. The solver stopped at intermediate infeasible or non-optimal solutions and a lot of restarts were required before the optimal controller settings were found. In this case, the two step method is the better alternative. The integration routine simply takes many small steps to solve the complex dynamic model. The solution might still be infeasible with respect to the optimization problem constraints for controllability, but since the optimization problem is much smaller, the optimization routine is better able to find a feasible solution and finally an optimal one.

In conclusion, a method for the simultaneous design and optimization of complex flowsheet structures that takes dynamic behavior and controllability features into account can be based on a two step iterative or a direct method. When the dynamic model can be collocated on a reduced number of finite elements, it is more beforehand to try the direct method. For systems with a complex dynamic behavior it is better to use the two step method. What has not yet been investigated in this chapter is the effect of using integer variables in flowsheet superstructures on the performance of both methods. That is a subject for further research.
The objective of this work was to develop an approach for the simultaneous design and optimization of complex flowsheet structures while explicitly taking dynamic behavior and controllability features into account. We have shown that there are many interactions between the structure of a flowsheet and its control system. We especially saw that recycles greatly affect dynamic behavior and controllability. In view of these considerations it is relevant to include controllability features in the conceptual design stage.

In this project we have developed a systematic approach to evaluate dynamic behavior and controllability of complex flowsheet structures. It consists of a combination of steady state and dynamic simulations with a linear controllability analysis, both static and in the frequency domain. In addition to the standard controllability tools (RGA, SVD), a number of more sophisticated tools applicable to MIMO systems (PRGA, CLDG, RDG) are employed to study the closed loop behavior of decentralized feedback control structures, before actually implementing them in a dynamic model. It is demonstrated that this approach improves understanding the behavior of a large plant with complex recycle structures as illustrated by a case study handling the impurities material balances in a balanced VCM plant.

Concerning the VCM case study, it is shown that the material balance of impurities is a plantwide problem. It is shown how the interaction between recycles may be exploited to create flowsheet and control alternatives with feasible plantwide control properties that cannot be achieved with a stand-alone column. Using the positive feedback effects of the recycle streams and the negative feedback effects of chemical reactors and exit streams yields a flowsheet design and control structure alternative with acceptable control properties. The
really plantwide nature of the problem clearly evolves from the fact that in the optimal structure the manipulated variables belong to different units.

It is furthermore shown that the introduction of an additional reactor to destroy hardly removable impurities improves the performance of the control system. However, by using manipulated variables from one column only (column S2) it is still not possible to keep all three impurities within their bounds under disturbances. Also the amount of impurities that is removed from the system (distillate of column S4) should be used in a control structure. In this situation only two controllers are required to control all three impurities.

The introduction of the extra reactor also gives access to alternative flowsheets with different recycle structures. Closer examination of these alternatives shows that the recycle structure strongly affects the nominal operating point of the plant and furthermore the way in which it influences the controllability. Therefore, part of the discussion on recycle structures shifts to a discussion on nominal operating points, in particular the nominal values of the impurity levels.

The case study also demonstrates that the application of controllability analysis tools on large dynamic models is not a trivial task. The linear state space realizations that are derived from nonlinear dynamic models of complex flowsheets might become very large and difficult to handle. Such state space realizations need to be reduced before a controllability analysis can be performed. A proper method for this reduction is truncation of a balanced realization. However, balancing large systems is not possible with standard tools. Therefore, we have introduced a method to find approximate solutions to the Lyapunov equations, required for balancing. This method is based on Oblique projections of the state space matrices on Krylov subspaces of the controllability and observability matrices. Based on the same approach, a low rank approximate state space realization can be developed directly, without the formation of a balanced realization first. Since this method might fail if there is only a weak relation between the inputs and the outputs of the state space realization, a decomposition step is introduced. The Krylov model reduction scheme is more appropriate to solve small subsystem with similar eigenvalues than large systems with a broad range of eigenvalues. Combining the reduced subsystems finally yields a state space realization of low order that still provides an accurate description of the input-output behavior of the corresponding system. Hence, when a controllability analysis cannot be performed on the complete state space realization, a reduced realization can be used yielding fast and accurate results.

In view of the objective as formulated in the beginning, optimization as a key issue had not been explicitly addressed until this stage of the work. The obvious reason is that it is not
trivial to incorporate optimization into a systems approach. In other words, the optimization of dynamic problems requires a special approach and we have tried several options. One option is to solve the dynamic model with an integration routine at each iteration of the optimization routine, that is placed in an outer loop. This separation of dynamic model and optimization problem has the advantages of keeping the optimization problem small while fast and robust dynamic solvers can be used. However, a disadvantage might be that the gradient function of the optimization problem has to be developed numerically. This requires many additional function evaluations, including integration of the dynamic model. Therefore it might be relevant to add the dynamic model to the optimization problem as equality constraints. Doing this the gradient function can be developed analytically, which reduces the number of function evaluations considerably. However, this requires discretization of the dynamic model, for which the method of orthogonal collocation on finite elements is used. Examples showed that if a moderate number of elements suffices to collocate the dynamic model, this approach is worthwhile. On the contrary, if many elements are required, the optimization problem becomes very large and difficult to solve, resulting in intermediate infeasible or non-optimal solutions. Therefore, for such systems the two step method is preferable.

Another advantage of the direct approach is the fact that it conveniently allows to formulate flowsheet and control superstructures with integer variables. Thus, the problem of finding an optimal flowsheet and control structure with respect to a certain objective function (e.g. an economic potential) can be formulated as a large Mixed Integer Nonlinear Optimization Problem. Additional constraints on design and control, including plantwide controllability criteria, can be added to this formulation. However, since it turns out to be difficult to find solutions for these large problems, the use of the two step method to solve such a problem still seems preferable. In principle, the same flowsheet and control superstructure can be formulated. In the dynamic model, 0-1 splitters can be used to put the streams in the right directions. On the other hand, it might be preferable to select only a few relevant basic flowsheet structures using heuristics and experience. Then subsequently each structure can be optimized with a reduced number of optimization variables and the final result can be compared. It cannot be said on beforehand which approach will be superior. To this end further research in this area will be needed.
References


SPEEDUP, Release 5.5-6, Aspen Technology Inc., (1998)


Publications


A.J. Groenendijk, A.C. Dimian and P.D. Iedema, “Recycle interaction effects on the controllability of a complex plant”

A.J. Groenendijk, A.C. Dimian and P.D. Iedema, “Large Scale Model Reduction”


Appendix

1

The VCM models

Flowsheet of the balanced VCM plant with optional reactor R4

Recycle structure alternatives
Components

<table>
<thead>
<tr>
<th>Name</th>
<th>Formula</th>
<th>ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylene</td>
<td>C₂H₄</td>
<td>C₂H₄</td>
</tr>
<tr>
<td>Chlorine</td>
<td>Cl₂</td>
<td>Cl₂</td>
</tr>
<tr>
<td>Vinyl Chloride</td>
<td>C₂H₃Cl</td>
<td>VCM</td>
</tr>
<tr>
<td>Hydrogen Chloride</td>
<td>HCl</td>
<td>HCl</td>
</tr>
<tr>
<td>1,2-Dichloroethane</td>
<td>C₂H₄Cl₂</td>
<td>DCE</td>
</tr>
<tr>
<td>Ethyl Chloride</td>
<td>C₂H₂Cl₂</td>
<td>Lt</td>
</tr>
<tr>
<td>Chloroprene</td>
<td>C₄H₅Cl</td>
<td>Clp</td>
</tr>
<tr>
<td>Carbon tetrachloride</td>
<td>CCl₄</td>
<td>RCl</td>
</tr>
<tr>
<td>Trichloroethylene</td>
<td>C₂HCl₃</td>
<td>Tri</td>
</tr>
<tr>
<td>Hexachloroethane</td>
<td>C₄Cl₆</td>
<td>Hv</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>H₂</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>O₂</td>
</tr>
<tr>
<td>Water</td>
<td>H₂O</td>
<td>H₂O</td>
</tr>
</tbody>
</table>

Thermodynamics

The vapor is assumed to behave ideal. UNIQUAC is used to calculate liquid activity coefficients. The binary parameters $a_{ij}$, $b_{ij}$, $c_{ij}$, and $d_{ij}$ are zero by default. The non-zero values are listed below.

<table>
<thead>
<tr>
<th>$i$</th>
<th>$j$</th>
<th>$a_{ij}$</th>
<th>$b_{ij}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCL</td>
<td>VCM</td>
<td>-2.3804000000</td>
<td>364.04770000</td>
</tr>
<tr>
<td>VCM</td>
<td>HCL</td>
<td>-16.4700000000</td>
<td>3237.72680000</td>
</tr>
<tr>
<td>RCL</td>
<td>DCE</td>
<td>0.053100000000</td>
<td>-52.53260000</td>
</tr>
<tr>
<td>DCE</td>
<td>RCL</td>
<td>0.156700000000</td>
<td>-85.80500000</td>
</tr>
<tr>
<td>LT</td>
<td>TRI</td>
<td>0</td>
<td>251.09120000</td>
</tr>
<tr>
<td>TRI</td>
<td>LT</td>
<td>0</td>
<td>-405.92020000</td>
</tr>
<tr>
<td>RCL</td>
<td>TRI</td>
<td>0</td>
<td>-83.58010000</td>
</tr>
<tr>
<td>TRI</td>
<td>RCL</td>
<td>0</td>
<td>79.07200000</td>
</tr>
<tr>
<td>DCE</td>
<td>TRI</td>
<td>0</td>
<td>10.46470000</td>
</tr>
<tr>
<td>TRI</td>
<td>DCE</td>
<td>0</td>
<td>-63.12270000</td>
</tr>
<tr>
<td>VCM</td>
<td>DCE</td>
<td>0</td>
<td>31.58320000</td>
</tr>
<tr>
<td>DCE</td>
<td>VCM</td>
<td>0</td>
<td>-8.84150000</td>
</tr>
<tr>
<td>CLP</td>
<td>H₂O</td>
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</tr>
<tr>
<td>H₂O</td>
<td>CLP</td>
<td>0</td>
<td>-336.950000</td>
</tr>
<tr>
<td>RCL</td>
<td>H₂O</td>
<td>0</td>
<td>-1204.800000</td>
</tr>
<tr>
<td>H₂O</td>
<td>RCL</td>
<td>0</td>
<td>-502.850000</td>
</tr>
<tr>
<td>DCE</td>
<td>H₂O</td>
<td>0</td>
<td>-164.179300</td>
</tr>
<tr>
<td>H₂O</td>
<td>DCE</td>
<td>0</td>
<td>-513.391000</td>
</tr>
<tr>
<td>TRI</td>
<td>H₂O</td>
<td>0</td>
<td>-1018.700000</td>
</tr>
<tr>
<td>H₂O</td>
<td>TRI</td>
<td>0</td>
<td>-762.960000</td>
</tr>
</tbody>
</table>
Reactions

**Chlorination Reactor (R1)**

Temperature: 80 °C  
Pressure: 3 bar  
Volume: 10 m³

Main reaction:

1) \( \text{C}_2\text{H}_4 + \text{Cl}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2 \)

Side Reactions:

a) \( \text{C}_2\text{H}_4 + 6 \text{Cl}_2 \rightarrow 2 \text{CCl}_4 + 4 \text{HCl} \)

b) \( \text{C}_2\text{H}_4 + 3\frac{1}{2} \text{Cl}_2 \rightarrow \frac{1}{2} \text{C}_4\text{Cl}_6 + 4 \text{HCl} \)

Conversion: 100% \( \text{C}_2\text{H}_4 \)

Selectivity to \( \text{C}_2\text{H}_4 \): 1) 0.9968965  
   a) 0.0000895  
   b) 0.0030140

Impurities destruction:

2) \( \text{C}_4\text{H}_5\text{Cl} + 5 \text{Cl}_2 \rightarrow \text{C}_4\text{Cl}_6 + 5 \text{HCl} \)

Conversion: 98% \( \text{C}_4\text{H}_5\text{Cl} \)

Kinetic constant: 196 H⁻¹

3) \( \text{C}_2\text{H}_2\text{Cl}_2 + 1\frac{1}{2} \text{Cl}_2 \rightarrow \frac{1}{2} \text{C}_4\text{Cl}_6 + 2 \text{HCl} \)

Conversion: 94% \( \text{C}_2\text{H}_2\text{Cl}_2 \)

Kinetic constant: 58 H⁻¹

4) \( \text{C}_2\text{HCl}_3 + \frac{1}{2} \text{Cl}_2 \rightarrow \frac{1}{2} \text{C}_4\text{Cl}_6 + \text{HCl} \)

Conversion: 91% \( \text{C}_2\text{HCl}_3 \)

Kinetic constant: 39 H⁻¹
**Cracking Reactor (R2)**

Temperature: 650 °C  
Pressure: 3 bar

Main reaction:
1) \( \text{C}_2\text{H}_4\text{Cl}_2 \rightarrow \text{C}_2\text{H}_3\text{Cl} + \text{HCl} \)

Side Reactions:
- a) \( \text{C}_2\text{H}_4\text{Cl}_2 \rightarrow \frac{1}{2} \text{C}_4\text{H}_5\text{Cl} + 1\frac{1}{2} \text{HCl} \)
- b) \( \text{C}_2\text{H}_4\text{Cl}_2 \rightarrow \text{C}_2\text{H}_2\text{Cl}_2 + \text{H}_2 \)
- c) \( \text{C}_2\text{H}_4\text{Cl}_2 + \text{HCl} \rightarrow \frac{1}{2} \text{C}_4\text{Cl}_6 + 2\frac{1}{2} \text{H}_2 \)

Conversion: 52.3% \( \text{C}_2\text{H}_4\text{Cl}_2 \)

Selectivity to \( \text{C}_2\text{H}_4\text{Cl}_2 \): 1) 0.993110  
a) 0.002360  
b) 0.001050  
c) 0.003480

**Oxychlorination Reactor (R3)**

Temperature: 240 °C  
Pressure: 1 bar

Main Reaction:
1) \( \text{C}_2\text{H}_4 + 2 \text{HCl} + \frac{1}{2} \text{O}_2 \rightarrow \text{C}_2\text{H}_4\text{Cl}_2 + \text{H}_2\text{O} \)

Side Reactions:
- a) \( \text{C}_2\text{H}_4 + 3 \text{HCl} + 1\frac{1}{2} \text{O}_2 \rightarrow \text{C}_2\text{HCl}_3 + 3 \text{H}_2\text{O} \)
- b) \( \text{C}_2\text{H}_4 + 8 \text{HCl} + 3 \text{O}_2 \rightarrow 2 \text{CCl}_4 + 6 \text{H}_2\text{O} \)
- c) \( \text{C}_2\text{H}_4 + 2 \text{HCl} + \text{O}_2 \rightarrow \text{C}_2\text{H}_2\text{Cl}_2 + 2 \text{H}_2\text{O} \)
- d) \( \text{C}_2\text{H}_4 + 3 \text{HCl} + 1\frac{3}{4} \text{O}_2 \rightarrow \frac{1}{2} \text{C}_4\text{Cl}_6 + 3\frac{3}{4} \text{H}_2\text{O} \)

Conversion 100% HCl

Selectivity to HCl: 1) 0.983350  
a) 0.000787  
b) 0.003141  
c) 0.002424  
d) 0.010298
**Extra Chlorination Reactor (R4)**

<table>
<thead>
<tr>
<th>Temperature: 80 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure: 1.4 bar</td>
</tr>
<tr>
<td>Volume: 5 m³</td>
</tr>
</tbody>
</table>

1) \[ \text{C}_4\text{H}_5\text{Cl} + 5 \text{Cl}_2 \rightarrow \text{C}_4\text{Cl}_6 + 5 \text{HCl} \]

Conversion: 86% C₄H₅Cl

Kinetic constant: 196 H⁻¹

2) \[ \text{C}_2\text{H}_2\text{Cl}_2 + 1\frac{1}{2} \text{Cl}_2 \rightarrow \frac{1}{2}\text{C}_4\text{Cl}_6 + 2 \text{HCl} \]

Conversion: 66% C₂H₂Cl₂

Kinetic constant: 58 H⁻¹

3) \[ \text{C}_2\text{HCl}_3 + \frac{1}{2} \text{Cl}_2 \rightarrow \frac{1}{2}\text{C}_4\text{Cl}_6 + \text{HCl} \]

Conversion: 57% C₂HCl₃

Kinetic constant: 39 H⁻¹

**Separation units**

**Component splitters**

<table>
<thead>
<tr>
<th>S0</th>
<th>S6</th>
<th>S7</th>
<th>S8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top</td>
<td>T [°C]</td>
<td>70</td>
<td>90</td>
</tr>
<tr>
<td>P [bar]</td>
<td>1.5</td>
<td>3.6</td>
<td>3.6</td>
</tr>
<tr>
<td>Bottom</td>
<td>T [°C]</td>
<td>90</td>
<td>100</td>
</tr>
<tr>
<td>P [bar]</td>
<td>2</td>
<td>3.6</td>
<td>3.6</td>
</tr>
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Mole fraction of feed to Top

<table>
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<tr>
<th>Compound</th>
<th>S0</th>
<th>S6</th>
<th>S7</th>
<th>S8</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₂H₄</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Cl₂</td>
<td>1</td>
<td>0.5</td>
<td>1</td>
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</tr>
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<td>VCM</td>
<td>1</td>
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<tr>
<td>HCl</td>
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<td>1</td>
</tr>
<tr>
<td>DCE</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Lt</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Clp</td>
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<td>0</td>
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<td>1</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>O₂</td>
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<td>1</td>
</tr>
<tr>
<td>H₂O</td>
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<td>1</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>
## Distillation columns

### Base case

<table>
<thead>
<tr>
<th></th>
<th>$S1$</th>
<th>$S2$</th>
<th>$S3$</th>
<th>$S4$</th>
<th>$S5$</th>
</tr>
</thead>
<tbody>
<tr>
<td># of stages</td>
<td>6</td>
<td>47</td>
<td>6</td>
<td>10</td>
<td>13</td>
</tr>
<tr>
<td>Feeds (on stage)</td>
<td>BS0(2)</td>
<td>BS7(22)</td>
<td>BS2(3)</td>
<td>TS1(3)</td>
<td>BS3(6)</td>
</tr>
<tr>
<td></td>
<td>BS1(37)</td>
<td>BS5(5)</td>
<td>BS2(5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure [bar]</td>
<td>1.4</td>
<td>1.4</td>
<td>3.0</td>
<td>1.11</td>
<td>0.20</td>
</tr>
<tr>
<td>Top</td>
<td>1.415</td>
<td>1.415</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Δ</td>
<td>0.20</td>
<td>0.20</td>
<td>0.20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bottom</td>
<td></td>
<td></td>
<td></td>
<td>1.36</td>
<td>0.25</td>
</tr>
<tr>
<td>Qreb [GJ/hr]</td>
<td>1.4</td>
<td>34</td>
<td>100</td>
<td>1</td>
<td>3.7</td>
</tr>
<tr>
<td>Distillate [kmol/hr]</td>
<td>4.5 (V)</td>
<td>14.5 (L)</td>
<td>5.59 (L)</td>
<td>60 (L)</td>
<td></td>
</tr>
<tr>
<td>Bottom [kmol/hr]</td>
<td></td>
<td></td>
<td>65 (L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Side Draw [kmol/hr]</td>
<td></td>
<td></td>
<td>35 (L st.5)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

|                   | $2.35e-3$ | 0.20 | $2.35e-3$ | 4.94 | 0.46 |
| Condenser area [m$^2$] | 0.41 | 5.05 | 0.40 | 1.02 | 1.85 |
| Drum area [m$^2$]    | 0.57 | 23.9 | 0.54 | 2.14 | 5.89 |
| Holdup [Kmol]       | Reflux | Reflux | Distillate | Reflux | Reflux |
| Free/manipulated    |      |      |      |      |      |
| Reboiler area [m$^2$] | 3.60 | 2.27 | 3.65 | 0.42 | 0.76 |
| Holdup [Kmol]       | 90.7 | 23.9 | 2.15 | 3.45 | 4.39 |
| Free/manipulated    | Bottom | Bottom | Bottom | Bottom | Bottom |
| Trays              | 2-5 | 2-36/37-46 | 2-5 | 2-9 | 2-12 |
| Active area [m$^2$] | 0.55 | 6.00/6.00 | 11.1 | 0.23 | 4.00 |
| Free area [m$^2$]   | 0.07 | 0.72/0.72 | 1.34 | 0.28 | 0.48 |
| Weir height [m]     | 0.05 | 0.05/0.05 | 0.05 | 0.50 | 0.05 |
| Weir length [m]     | 1.50 | 1.60/3.20 | 3.60 | 0.20 | 2.16 |

The base case design of the distillation columns is kept in the alternative flowsheet structures. The different operating values are specified in the following tables.

### Case with R4

<table>
<thead>
<tr>
<th></th>
<th>$S1$</th>
<th>$S2$</th>
<th>$S3$</th>
<th>$S4$</th>
<th>$S5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feeds (on stage)</td>
<td>BS0(2)</td>
<td>BS7(22)</td>
<td>BS2(3)</td>
<td>TS1(3)</td>
<td>BS3(6)</td>
</tr>
<tr>
<td></td>
<td>BS1(37)</td>
<td>BS5(5)</td>
<td>BS2(5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Qreb [GJ/hr]</td>
<td>1.4</td>
<td>34</td>
<td>100</td>
<td>0.9</td>
<td>3.6</td>
</tr>
<tr>
<td>Distillate [kmol/hr]</td>
<td>4.5 (V)</td>
<td>14.5 (L)</td>
<td>3.53 (L)</td>
<td>60 (L)</td>
<td></td>
</tr>
<tr>
<td>Bottom [kmol/hr]</td>
<td></td>
<td></td>
<td>70 (L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Side Draw [kmol/hr]</td>
<td></td>
<td></td>
<td>35 (L st.5)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Alternative A

<table>
<thead>
<tr>
<th></th>
<th>$S1$</th>
<th>$S2$</th>
<th>$S3$</th>
<th>$S4$</th>
<th>$S5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feeds (on stage)</td>
<td>BS0(2)</td>
<td>BS7(22)</td>
<td>BS2(3)</td>
<td>TS1(3)</td>
<td>BS4(4)</td>
</tr>
<tr>
<td></td>
<td>BS1(37)</td>
<td>TS5(38)</td>
<td>BS2(5)</td>
<td>BS8(5)</td>
<td>BS3(6)</td>
</tr>
<tr>
<td>Qreb [GJ/hr]</td>
<td>1.4</td>
<td>37.5</td>
<td>100</td>
<td>0.85</td>
<td>4.0</td>
</tr>
<tr>
<td>Distillate [kmol/hr]</td>
<td>4.5 (V)</td>
<td>14.5 (L)</td>
<td>3.48 (L)</td>
<td>70 (L)</td>
<td></td>
</tr>
<tr>
<td>Bottom [kmol/hr]</td>
<td></td>
<td></td>
<td>70 (L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Side Draw [kmol/hr]</td>
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<td></td>
<td>39 (L st.5)</td>
<td></td>
<td></td>
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</table>
### Alternative B

<table>
<thead>
<tr>
<th>Feeds (on stage)</th>
<th>S1</th>
<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qreb [GJ/hr]</td>
<td>1.4</td>
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<td>100</td>
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<tr>
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<td>4.5 (V)</td>
<td>14.5 (L)</td>
<td>3.10 (L)</td>
<td>60 (L)</td>
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</tr>
<tr>
<td>Bottom [kmol/hr]</td>
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<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Side Draw [kmol/hr]</td>
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### Alternative C

<table>
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<th>S2</th>
<th>S3</th>
<th>S4</th>
<th>S5</th>
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<tr>
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<td>1</td>
<td>3.7</td>
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<td>60.0 (L)</td>
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</tr>
<tr>
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<td>66.35(L)</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Side Draw [kmol/hr]</td>
<td>60 (L st.5)</td>
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### Feed streams

<table>
<thead>
<tr>
<th>C₂H₄</th>
<th>Cl₂</th>
<th>C₂H₄</th>
<th>O₂</th>
<th>DCE</th>
<th>Cl₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>To</td>
<td>R1</td>
<td>R1</td>
<td>R3</td>
<td>R3</td>
<td>S0</td>
</tr>
<tr>
<td>T [°C]</td>
<td>80</td>
<td>80</td>
<td>240</td>
<td>240</td>
<td>80</td>
</tr>
<tr>
<td>P [bar]</td>
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<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Flow [Kmol/hr]</td>
<td>335.6</td>
<td>345</td>
<td>550</td>
<td>275</td>
<td>175</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mole fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₂H₄</td>
</tr>
<tr>
<td>Cl₂</td>
</tr>
<tr>
<td>VCM</td>
</tr>
<tr>
<td>HCl</td>
</tr>
<tr>
<td>DCE</td>
</tr>
<tr>
<td>Lt</td>
</tr>
<tr>
<td>Clp</td>
</tr>
<tr>
<td>RCl</td>
</tr>
<tr>
<td>Tri</td>
</tr>
<tr>
<td>Hv</td>
</tr>
<tr>
<td>H₂</td>
</tr>
<tr>
<td>O₂</td>
</tr>
<tr>
<td>H₂O</td>
</tr>
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</table>

The same feed streams are used for the alternative flowsheet structures.
### Linear systems

#### Nominal values

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<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>86</td>
<td>82</td>
<td>70</td>
<td>87</td>
<td>85</td>
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<tr>
<td>l₂</td>
<td>565</td>
<td>548</td>
<td>567</td>
<td>567</td>
<td>571</td>
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</tbody>
</table>

#### Scale factors

| l₁ | 100 – nominal value |
| l₂ | 600 – nominal value |
| l₃ | 500                 |

D₂, SS₂, Q₂, D₄, Q₄ 25% of nominal value

**FDEC** 75 kmol/hr

**X₁₃** 0.012 kmol/kmol

#### Static gain matrices

##### Base case

<table>
<thead>
<tr>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
<th>D₄</th>
<th>Q₄</th>
<th>F_{DCE}</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>l₁</td>
<td>-0.0753</td>
<td>-0.2609</td>
<td>-5.7420</td>
<td>-0.3755</td>
<td>-0.0791</td>
<td>0.2949</td>
</tr>
<tr>
<td>l₂</td>
<td>-0.2119</td>
<td>-0.5267</td>
<td>-3.5737</td>
<td>-0.4371</td>
<td>-0.0706</td>
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<tr>
<td>l₃</td>
<td>0.4106</td>
<td>0.0296</td>
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<td>-2.8289</td>
<td>-0.6161</td>
<td>0.1737</td>
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##### With R4

<table>
<thead>
<tr>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
<th>D₄</th>
<th>Q₄</th>
<th>F_{DCE}</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>l₁</td>
<td>-0.0764</td>
<td>-0.1835</td>
<td>-4.3254</td>
<td>-0.1541</td>
<td>-0.0409</td>
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<tr>
<td>l₂</td>
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<td>-0.3020</td>
<td>-2.2979</td>
<td>-0.2153</td>
<td>-0.0613</td>
<td>0.1374</td>
</tr>
<tr>
<td>l₃</td>
<td>0.7368</td>
<td>0.1555</td>
<td>-0.9083</td>
<td>-2.1351</td>
<td>-0.7268</td>
<td>0.1491</td>
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</tbody>
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##### alt. A

<table>
<thead>
<tr>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
<th>D₄</th>
<th>Q₄</th>
<th>F_{DCE}</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>l₁</td>
<td>0.2256</td>
<td>-0.1068</td>
<td>-1.9066</td>
<td>-0.3415</td>
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<tr>
<td>l₂</td>
<td>0.6712</td>
<td>-0.8716</td>
<td>-3.9383</td>
<td>-0.3514</td>
<td>-0.0527</td>
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<tr>
<td>l₃</td>
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<td>-0.9299</td>
<td>-2.4417</td>
<td>-0.8547</td>
<td>0.1645</td>
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</table>

##### alt. B

<table>
<thead>
<tr>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
<th>D₄</th>
<th>Q₄</th>
<th>F_{DCE}</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>l₁</td>
<td>0.0052</td>
<td>-0.3392</td>
<td>-6.3101</td>
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<td>l₂</td>
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<tr>
<td>l₃</td>
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<td>0.3396</td>
<td>-0.9385</td>
<td>-3.4397</td>
<td>-0.7294</td>
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##### alt. C

<table>
<thead>
<tr>
<th>D₂</th>
<th>SS₂</th>
<th>Q₂</th>
<th>D₄</th>
<th>Q₄</th>
<th>F_{DCE}</th>
<th>X₁₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>l₁</td>
<td>0.3774</td>
<td>-0.3966</td>
<td>-4.4765</td>
<td>-0.4973</td>
<td>-0.2244</td>
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<tr>
<td>l₂</td>
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<td>-1.1474</td>
<td>-3.8844</td>
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<td>-0.0752</td>
<td>0.2280</td>
</tr>
<tr>
<td>l₃</td>
<td>0.3683</td>
<td>0.2229</td>
<td>-0.8173</td>
<td>-1.4331</td>
<td>-0.5364</td>
<td>0.1150</td>
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Summary

The central question in this thesis is "How to design and optimize complex plants with superior dynamic behavior and controllability features". Such complex plants, which are usually highly integrated, involve interactions through recycles of materials and energy. As far as only steady state operation is concerned, the design procedure incorporates already systematic methods. However, a systematic approach of the plant dynamics, at the conceptual design stage, which aims to create better flowsheet alternatives from controllability point of view, is not yet available. The goal of this work is to study both fundamental issues, as the dynamics of recycles and plantwide controllability, as well as to develop computer analysis tools, which can contribute to formulate a systematic approach for the optimal dynamic design of a complex chemical plants.

The first issue described in chapter 2, deals with the development of a 'Systematic Approach of Plantwide Controllability'. The proposed method combines steady state design with dynamic modeling and controllability analysis tools, both static and in the frequency domain. In addition to well-know controllability analysis tools, as Relative Gain Array and Singular Value Decomposition, new tools are introduced to analyze the link between design, recycles and performance of plantwide control structures. These tools are the Performance Relative Gain Array, the Closed Loop Disturbance Gain and the Relative Disturbance Gain. For the first time, they are applied in this thesis for multivariable plantwide control purposes. This is in contrast with previous studies, directed almost exclusively to individual units or academic exercises.

The approach is applied in Chapter 3 to the 'Plantwide Controllability of Impurities in a Plant with Recycles', namely to study the dynamics of impurities in a complex Vinyl Chloride Monomer (VCM) plant. In a first stage we demonstrate that interactions between recycles may be exploited to create viable plantwide control structures, which may imply variables belonging to different units. Such control structures would be infeasible when only the stand-alone behavior of units is considered. Thus, the controllability properties of complex plants
are determined by the competition between positive feedback effects, typically recycles, and negative feedback effects, like exit streams and chemical reactors. As a consequence, an extra reactor for the conversion of impurities is introduced to improve the controllability. Hence, the use of chemical conversion to eliminate components accumulating in recycles may be viewed as a general design rule for recycle systems. Controllability tools, particularly SVD and CLDG, can be used to assess quantitatively both the reactor design and some structural changes of the flowsheet.

Chapter 4 is devoted to ‘Recycle Interaction Effects on Plantwide Controllability’. This thesis presents for the first time a quantitative approach of this crucial industrial issue, particularly with implications on retrofitting. Thus, we demonstrate how connectivity between existing units can be seen as a degree of freedom in designing plants with recycles. The introduction of a chemical converter of impurities generates several flowsheet alternatives with different controllability properties, some being better as the original flowsheet. Again, the interaction between the recycle loops enables a better control of the material balances of components. It is demonstrated that the recycle structure strongly affects the nominal operating point of the plant, which in turn affects the controllability. Therefore, the evaluation of controllability properties of the new recycle structures has as an important consequence the need to redesign the whole plant, this time from a plantwide control perspective.

The above case study demonstrates that through dynamic flowsheeting, with control features incorporated, essential knowledge is obtained both on design and operation. In addition, the large dynamic plant models give access to a whole class of controllability tools that usually are applied on small problems. Consequently, a large dynamic model requires an adequate reduction in size, which is not a trivial problem.

Chapter 5 deals with the ‘Large Scale Model Reduction’. Standard reduction algorithms often fail for large systems. Therefore, a method is introduced to find low rank approximate solutions to large Lyapunov equations by using Oblique Projection Methods on Krylov subspaces of the Controllability and Observability spaces. It is demonstrated that the system is balanced by using approximate solutions, which enables the selection of the most important states to be included in the reduced model. It is also described how the projection methods are used to generate reduced state space realizations directly, without balancing.

We also demonstrate that decomposition of a large system into a number of subsystems improves the large-scale model reduction methods. A dynamic VCM plant model with a state space realization of 668 states cannot be reduced by standard methods. Application of the Krylov model reduction scheme on the full realization also fails. However, when the system
is decomposed into 10 subsystems, each containing a small range of eigenvalues, the realization can be reduced easily into 115 states without affecting the input-output behavior significantly.

Up to this point the thesis demonstrates that the systems approach, including a linear model reduction step, might be used to evaluate several design and control alternatives in order to compare their performances with respect to some control objective. In this approach each alternative is analyzed separately. However, it could be more interesting to built-up a 'superstructure' with the alternatives suggested by the systematic approach, where the evaluation of controllability would be handled simultaneously. Flowsheet structure and units design might be kept free for optimization. Plantwide controllability criteria, necessary for a controllable plant design, can be added as additional constraints.

Therefore, we consider another approach, described in Chapter 6, devoted to 'Dynamic Optimization of Flowsheet and Control Structures'. We compare two basically different approaches for solving these dynamic optimization problems. In the first approach, a dynamic model is solved by standard integration within the optimization routine, placed in an outer loop. The optimization problem itself contains the object function and additional constraints to ensure a controllable plant design. This two step approach has the advantage that the optimization problem is small, while fast integration routines can be used to solve the dynamic model. However, a disadvantage is that the gradient function of the optimization problem can only be developed numerically. This requires many additional function evaluations, including the integration of the dynamic model. Therefore, in some cases it might be interesting to add the dynamic model directly to the optimization problem as additional constraints. This requires the discretization of the model equations for which the method of orthogonal collocation on finite elements can be used. A disadvantage of this method is that the size of the optimization problem is enlarged considerably. However, since the gradient function can be developed analytically, the number of function evaluations is reduced and therefore the optimal solution might be found in less time.

We have shown that both methods are applicable on small problems and that it depends on the problem characteristics which one is the better choice. The problem of the Trambouze reaction in a batch reactor with discrete charges is solved much faster with the direct approach, while the optimal controller settings of a dynamic vapor-liquid flash drum are found more easily with the two step approach. In conclusion, if the dynamic model can be collocated on a reduced number of finite elements, it is interesting to try the direct method. For systems with a complex dynamic behavior it is better to use the two step method.
Not investigated in this thesis is the influence of a mixed integer problem formulation of flowsheet and control superstructures on the dynamic optimization methods. That will be a subject for further research.
De centrale vraag in dit proefschrift is ‘Hoe ontwerp en optimaliseer je complexe fabrieken met goed dynamisch gedrag en goede regeleigenschappen’. Zulke complexe fabrieken zijn meestal in hoge mate geïntegreerd en ondervinden veel interactie door het terugvoeren van materiaal en energie. Voor zover alleen stabiele toestanden worden beschouwd bevat de ontwerpprocedure al systematische methoden. Echter, een systematische aanpak van de dynamica van het proces, tijdens de conceptontwerfase, teneinde alternatieve processtructuren met betere regeleigenschappen te creëren, is nog niet beschikbaar. Het doel van dit werk is enerzijds het bestuderen van fundamentele aspecten, zoals de dynamica van recyclestromen en de regeleigenschappen van hele fabrieken, en anderzijds het ontwikkelen en implementeren van computer analyse technieken welke kunnen bijdragen tot het formuleren van een *systematische aanpak* voor het *optimaal* dynamisch ontwerpen van een complexe chemische fabriek.

Het eerste aspect, uitgewerkt in hoofdstuk 2, betreft de ontwikkeling van een ‘Systematische Aanpak van de Regeleigenschappen van de Fabriek als Geheel’. De voorgestelde methode combineert het ontwerpen van de stabiele toestanden met dynamisch modeleren en technieken voor de analyse van de regeleigenschappen, zowel statisch als in het frequentiedomein. Naast bekende analysetechnieken, zoals Relative Gain Array en Singular Value Decomposition, worden nieuwe technieken geïntroduceerd voor het analyseren van het verband tussen het ontwerp, de recyclestromen en de prestatie van regelstructuren voor de hele fabriek. Deze technieken zijn de Performance Relative Gain Array, de Closed Loop Disturbance Gain en de Relative Disturbance Gain. Ze worden in dit proefschrift voor het eerst toegepast voor de analyse van de regeleigenschappen van de hele fabriek. Dit is in tegenstelling tot eerdere studies, die bijna allemaal betrekking hebben op individuele apparaten of academische problemen.

De aanpak wordt in hoofdstuk 3 toegepast op de ‘Regeling van Onzuiverheden in een Fabriek met Recyclestromen’, met name voor het bestuderen van de dynamica van onzuiverheden in
een complexe Vinyl Chloride Monomeer (VCM) fabriek. In eerste instantie tonen we aan dat de interacties tussen recyclstromen gebruikt kunnen worden voor het creëren van uitvoerbare regelstructuren voor de hele fabriek, waarbij de variabelen afkomstig kunnen zijn van verschillende apparaten. Zulke regelstructuren zouden onmogelijk zijn als alleen het gedrag van de individuele apparaten in beschouwing zou worden genomen. Dus, de regeleigenschappen van complexe fabrieken worden bepaald door de competitie tussen meekoppelingseffecten, zoals recyclstromen, en de tegenkoppelingseffecten zoals uitgaande stromen en chemische reactoren. Op basis hiervan wordt er een extra reactor geïntroduceerd voor de conversie van onzuiverheden om de regeleigenschappen te verbeteren. Het gebruik van chemische conversie voor de eliminatie van componenten die accumuleren in recyclstromen kan gezien worden als een algemene ontwerpregel voor recyclesystemen. De technieken voor de analyse van de regeleigenschappen, met name SVD en CLDG, kunnen worden gebruikt voor een kwantitatieve beoordeling van zowel het reactorontwerp als structurele veranderingen van het stroomschema.

Hoofdstuk 4 is gewijd aan de ‘Recycle Interactie Effecten op de Regeleigenschappen van de Hele Fabriek’. Dit proefschrift presenteert voor de eerste keer een kwantitatieve aanpak van dit cruciale industriële probleem, in het bijzonder met betrekking tot het aanpassen van bestaande fabrieken. We tonen aan hoe de verbindingen tussen bestaande apparaten beschouwd kunnen worden als vrijheidsgraden in het ontwerpen van fabrieken met recyclstromen. De introductie van een chemische reactor voor de conversie van onzuiverheden genereert een aantal alternatieve processtructuren met verschillende regeleigenschappen. Sommige zijn beter dan de originele structuur. Ook hier maakt de interactie tussen de recyclstromen een betere regeling van de materiaalbalansen van componenten mogelijk. We laten zien dat de recyclestructuur een grote invloed heeft op het nominale operatiepunt van de fabriek, wat weer effect heeft op de regeleigenschappen. Daarom heeft de evaluatie van de regeleigenschappen van de nieuwe recyclestructuren als belangrijk gevolg de noodzaak van het opnieuw ontwerpen van de hele fabriek, deze keer met vooruitzicht op de regeling van de hele fabriek.

De bovenstaande studie laat zien dat door dynamisch ontwerpen, met daarin opgenomen aspecten van regeling, essentiële kennis wordt verkregen van zowel ontwerp als operatie. Daarnaast bieden de grote dynamische fabrieksmodellen de mogelijkheid voor het toepassen van een hele reeks technieken voor de analyse van regeleigenschappen die normaal alleen worden toegepast op kleine problemen. Als gevolg hiervan vereist een groot dynamisch model een adequate reductie in grootte, wat geen triviaal probleem is.
Hoofdstuk 5 behandelt ‘Grootschalige Modelreductie’. Standaard reductietechnieken falen vaak voor grote systemen. Daarom introduceren we een methode waarbij de oplossingen van grote Lyapunov vergelijkingen worden benaderd door gebruikmaking van Oblique Projectiethoden op Krylov deelruimten van de Controleerbaarheids- en Observeerbaarheidsruimten. We laten zien dat het systeem gebalanceerd kan worden met de benaderde oplossingen, waardoor de meest belangrijke toestanden geselecteerd en in het gereduceerde model opgenomen kunnen worden. We beschrijven ook hoe de projectiethoden gebruikt kunnen worden om gereduceerde toestandsrealisaties direct te genereren, zonder te balanceren.

We tonen ook aan dat de decompositie van een groot systeem in een aantal deelsystemen de grootschalige modelreductie verbetert. Een lineair dynamisch model van een VCM fabriek met 668 toestanden kan niet worden gereduceerd met standaard technieken. Toepassing van het Krylov modelreductie schema op de volledige realisatie faalt ook. Echter, als het systeem wordt opgesplitst in 10 deelsystemen, elk een klein interval van eigenwaarden bevattende, kan de realisatie eenvoudig worden gereduceerd tot 115 toestanden zonder het invoer-uitvoer gedrag significant te beïnvloeden.

Tot aan dit punt demonstreert het proefschrift dat de systeamaanpak, inclusief een lineaire modelreductie stap, kan worden gebruikt voor het evalueren van verschillende ontwerp- en regelalternatieven teneinde een vergelijking te kunnen maken van hun prestaties met betrekking tot een zeker regeldoel. In deze aanpak wordt elk alternatief apart bestudeerd. Het kan echter interessanter zijn om een ‘superstructuur’ op te bouwen met de alternatieven die gegenereerd worden door een systematische aanpak van de processsynthese. De evaluatie van de regeleigenschappen kan dan simultaan worden uitgevoerd. De structuur van het processeschema en het ontwerp van de individuele apparaten kunnen vrijgehouden worden voor optimalisatie. Criteria voor de regeleigenschappen van de hele fabriek, nodig voor een regelaar fabrieksontwerp, kunnen worden toegevoegd als extra randvoorwaarden.

Daarom bekijken we een andere aanpak, beschreven in hoofdstuk 6, gewijd aan ‘Dynamische Optimalisatie van Proces- en Regelstructuren’. We maken een vergelijking tussen twee in beginsel verschillende aanpakken voor het oplossen van deze dynamische optimalisatieproblemen. In de eerste aanpak wordt een dynamisch model opgelost met standaard integratietechnieken binnen de optimalisatieroutine, die in een buitenloop geplaatst is. Het optimalisatieprobleem zelf bevat de doelfunctie en aanvullende randvoorwaarden om een regelaar ontwerp van de fabriek te garanderen. Deze twee-staps methode heeft als voordeel dat het optimalisatieprobleem klein is, terwijl snelle integratieroutines gebruikt
kunnen worden om het dynamische probleem op te lossen. Een nadeel is echter dat de gradiëntfunctie van het optimalisatieprobleem alleen numeriek bepaald kan worden. Daarvoor zijn veel extra functieevaluaties nodig, inclusief de integratie van het dynamische model. Daarom kan het in sommige gevallen interessant zijn om het dynamiisch model direct toe te voegen aan het optimalisatieprobleem als aanvullende randvoorwaarden. Dit vereist de discretisatie van de modelvergelijkingen, waarvoor de methode van orthogonale collocatie op eindige elementen kan worden gebruikt. Een nadeel van deze methode is dat de omvang van het optimalisatieprobleem behoorlijk vergroot wordt. Echter, omdat de gradiëntfunctie nu analytisch bepaald kan worden is het aantal functieevaluaties gereduceerd en daarom kan de optimale oplossing sneller gevonden worden.

We hebben aangetoond dat beide methoden toegepast kunnen worden op kleine problemen en dat het afhankelijk is van de karakteristieken van het probleem welke methode een betere keuze is. Het probleem van de Trambouze reactie in een batch reactor met discrete beladingen wordt veel sneller opgelost met de directe aanpak terwijl de optimale regelparameters van een dynamisch vloeistof-damp scheidingsvat gemakkelijker gevonden worden met de twee-staps methode. Concluderend, als het dynamische model kan worden gecolloceerd op een beperkt aantal eindige elementen is het interessant om de directe aanpak te proberen. Voor systemen met een complex dynamisch gedrag is het beter om de twee-staps methode te gebruiken.

Niet bestudeerd in dit proefschrift is de invloed van een Mixed Integer probleem formulering van proces- en regelstructuren op de dynamische optimalisatiemethoden. Dat is een onderwerp voor verder onderzoek.
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