Modeling and Control
of an Industrial Distillation Plant
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Modeling and Control of an Industrial Distillation Plant

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presented by
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2001
Modeling and control of distillation columns is a research area that evokes considerable interest. On the one hand, substantial savings are possible with good controllers, on the other hand, distillation columns are often used as test cases for new methods of model based controller design. Strongly nonlinear behavior and high order are the characteristics that present challenges when designing controllers for this multivariable system.

Many case studies deal with well-known binary systems that may even show ideal behavior for their vapor-liquid equilibrium. The industrial reality, however, also uses distillation columns for separating highly non-ideal multicomponent mixtures, using complicated column sequences, as it is the case for the system investigated in this thesis. The work presented here concentrates on problems which arise when an existing industrial distillation plant has to be modeled and controlled, and it points out possible solutions.

A rigorous dynamic model using the description of physical processes is developed for two columns in series that are coupled by a recycle stream. It is shown that steady-state balances and physical reasoning can be used to check the available plant data. For making simulated column profiles match the measured profiles, a new solution is used: Temperature dependent vaporization efficiencies model the non-ideal behavior of the second column. This leads to a flexible description that is able to match simulation results with plant measurements in different operating points.

The model is linearized numerically. Because of the size of the system (1586 state variables, 260 algebraic variables), the columns are linearized individually, leading to models that show good agreement
Abstract

with the nonlinear model. The models are scaled using a fast numerical method. Model reduction using balanced truncation leads to models of order 100 (column 1) and 70 (column 2), which are suitable for controller design.

Subsequently a first set of $H_\infty$-optimal controllers is designed with the S/KS/T weighting scheme, leading to a closed-loop bandwidth of up to 0.1 rad/min. The controllers show good performance in the nonlinear simulations. Reduction of the controller using balanced residualization leads to a smaller system, but the control quality is maintained.
Zusammenfassung


Viele Fallstudien befassen sich mit gut bekannten binären Gemischen, deren Dampf-Flüssigkeits-Gleichgewicht sogar ideales Verhalten zeigt. In der Industrie werden jedoch Destillationskolonnen auch zum Trennen von stark nichtidealigen Mehrstoffgemischen in komplizierten Kolonnenschaltungen verwendet, wie es in dem System, das in dieser Dissertation untersucht wird, der Fall ist. Die hier präsentierte Arbeit konzentriert sich auf die Probleme, die auftreten, wenn eine reale Destillationsanlage modelliert und geregelt werden muss, und sie zeigt mögliche Lösungen dafür.

Zusammenfassung

Das Modell wird numerisch linearisiert. Aufgrund der Größe des Systems (1586 Zustandsgrößen, 260 algebraische Variablen) werden die Kolonnen einzeln linearisiert, was zu einem Modell führt, das gute Übereinstimmung mit dem nichtlinearen Modell aufweist. Die Modelle werden mit einer schnellen numerischen Methode skaliert. Bei der Modellreduktion wird die Methode der „balanced truncation“ verwendet, was zu Modellen der Ordnung 100 (Kolonne 1) und 70 (Kolonne 2) führt, die für den Reglerentwurf geeignet sind.

Anschließend wird das S/KS/T-Gewichtungsschema zum Entwurf erster $H_{\infty}$-optimaler Regler verwendet, deren Bandbreite im geregelten Kreis bis zu 0.1 rad/min beträgt. Die Regler zeigen eine gute Regelqualität in nichtlinearen Simulationen. Balancierte Residualisierung führt zu einer Reduktion der Reglerordnung; die Regelqualität wird jedoch aufrechterhalten.
Acknowledgements

When you start working for a thesis, you usually don’t have any idea of what is expecting you (and people exist who think it is better this way). When you finally write the last sentences, you realize that you have been supported by many people during the last years.

First of all I would like to thank my supervisor Prof. Max Steiner for his support throughout the whole project, for encouraging me when my efforts failed, as well as for being happy with me when I succeeded. His commitment especially during the final weeks of writing this thesis went beyond of what could be expected. I have always enjoyed our discussions about many subjects, no matter if related to control, teaching, or life in general. My thanks go as well to Prof. Dr. Hans-Peter Geering, who agreed to be my co-examiner on short notice. He gave valuable input and showed enthusiasm for the results of the project.

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My parents made it possible for me to study Chemical Engineering at ETH, which was the first of several steps that finally led to this thesis, and I want to thank them for giving me this opportunity.
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My final thanks go to Clemens Hammerschmied. Without him and his support, I am not sure if I were today where I am now. He cheered me up when I was desperate, he celebrated with me when everything was just great, he supported me in times of hard work, he gave me input—he was always there for me.

Zürich, May 2001

Esther Baumann
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Nomenclature

Symbols

$\alpha$ constant for modified Francis’s weir equation
$\beta$ constant for modified Francis’s weir equation
$\gamma_i$ liquid activity coefficient of component $i$, ($-$)
$\eta_H$ Hausen tray efficiency, ($-$)
$\eta_M$ Murphree tray efficiency, ($-$)
$\eta_{v,k,i}$ vaporization efficiency of component $i$ on tray $k$, ($-$)
$\kappa$ condition number
$\kappa^*$ minimum condition number
$\lambda$ eigenvalue
$\Lambda_{i,j}$ Wilson binary interaction parameter for components $i$ and $j$
$\nu_d$ differential index
$\xi$ orifice coefficient, ($-$)
$\xi_{\text{cond}}$ orifice coefficient for condenser, ($1/m^4$)
$\pi_1$ constant for calculating liquid volume fraction
$\pi_2$ constant for calculating liquid volume fraction
$\rho$ mass density of liquid ($kg/m^3$)
Nomenclature

\( \rho' \) mass density of vapor, \( (kg/m^3) \)

\( \sigma \) singular value

\( \sigma \) surface tension, \( (N/m) \)

\( \bar{\sigma} \) maximum singular value

\( \sigma \) minimum singular value

\( \Phi \) liquid volume fraction, \( (-) \)

\( \phi_i \) component volume fraction, \( (-) \)

\( \varphi_i \) fugacity coefficient for component \( i \), \( (-) \)

\( A \) state space matrix

\( A_{active} \) active tray area (cross-section minus downcomer), \( (m^2) \)

\( A_h \) total hole area per tray, \( (m^2) \)

\( a_i \) cubic equation-of-state constant for component \( i \), \( (J^3m^3/mol^2) \)

\( a_{ij} \) constant for Wilson interaction parameter, \( (-) \)

\( a_m \) cubic equation-of-state constant for mixture, \( (J^3m^3/mol^2) \)

\( \Delta_{ig}a_m \) Helmholtz energy departure for mixture, \( (J/mol) \)

\( A_t \) area of tray without downcomer, \( (m^2) \)

\( a_{Tm} \) cubic equation-of-state constant for mixture (not temperature dependent)

\( B \) state space matrix

\( b_i \) cubic equation-of-state constant for component \( i \), \( (m^3/mol) \)

\( b_{ij} \) constant for Wilson interaction parameter, \( (K) \)

\( b_m \) cubic equation-of-state constant for mixture, \( (m^3/mol) \)
Nomenclature

\( C \) state space matrix

\( C_d \) friction factor in Francis's weir formula, (−)

\( C_i \) constants used in different equations

\( c_{p,i}^{ig} \) ideal gas heat capacity for component \( i \), \((J/K \cdot mol)\)

\( D \) state space matrix

\( d \) disturbance at the plant output

\( d_{\text{hole}} \) hole diameter, (m)

\( D_I \) input scaling matrix

\( d_i \) disturbance at the plant input

\( D_O \) output scaling matrix

\( e \) error

\( f_i \) fugacity of component \( i \) in the liquid phase, (Pa)

\( f_i' \) fugacity of component \( i \) in the vapor phase, (Pa)

\( f_i^o \) liquid activity coefficient of pure component \( i \) at mixture temperature, (Pa)

\( g \) acceleration due to gravity, \(9.81 \text{ m/s}^2\)

\( G(s) \) transfer function of a plant

\( G^E \) excess Gibbs energy, (J)

\( g^E \) specific Gibbs energy, \((J/mol)\)

\( H \) enthalpy of liquid holdup, (J)

\( h \) linearization step width

\( h \) specific liquid enthalpy, \((J/mol)\)
Nomenclature

$h'$ specific vapor enthalpy, (J/mol)

$h_{\text{aer},k}$ height of aerated liquid on tray, (m)

$h_{\text{cl}}$ height of clear liquid, (m)

$\Delta_f h_i^{\text{ig}}$ standard enthalpy of formation for ideal gas at 298.15 K and 1 atm for component $i$, (J/mol)

$\Delta_{\text{ig}} h_i^o$ specific enthalpy departure for pure component $i$, (J/mol)

$\Delta_{\text{vap}} h_i^o$ specific enthalpy of vaporization for component $i$, (J/mol)

$h_i^{\text{ig}}$ specific ideal gas enthalpy for a pure component, (J/mol)

$h_m$ specific liquid enthalpy of a mixture, (J/mol)

$h_{\text{ig} m}$ specific enthalpy of a mixture of ideal gases, (J/mol)

$\Delta_{\text{ig}} h_m$ specific enthalpy departure for a liquid mixture, (J/mol)

$h_w$ weir height, (m)

$J$ Jacobian matrix

$K(s)$ transfer function of a controller

$k(z)$ valve pressure drop coefficient

$k_{i,j}$ binary interaction parameter, (−)

$K_{\text{VLE}}^{\text{VLE}}$ vapor-liquid equilibrium constant of component $i$ on tray $k$, (−)

$K_{s,k}$ velocity factor on tray $k$, (m/s)

$L$ liquid flow from tray, (mol/s)

$M$ matrix

$M^*$ mass flow, (kg/s)

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Nomenclature

\[ m_{i,k} \] liquid mass holdup of component \( i \) on tray \( k \), (kg)

\[ MW \] molar mass, (kg/mol)

\( n \) measurement noise

\( n \) number of components, (–)

\( N_i \) moles of component \( i \), (mol)

\( N_k \) liquid holdup on tray, (mol)

\( N_{k,i} \) liquid holdup of component \( i \) on tray \( k \), (mol)

\( nc \) number of components

\( nt \) number of trays, including condenser and reboiler

\( nx \) number of state variables for one column

\( P \) controllability Gramian

\( p \) pump power, (W)

\( p \) pressure, (Pa)

\( \Delta p \) total pressure drop over the tray, (Pa)

\( p_{ci} \) critical pressure for component \( i \), (Pa)

\( \Delta p_{\text{cond}} \) pressure drop in piping to condenser, (Pa)

\( \Delta p_{\text{dry}} \) dry pressure drop, (Pa)

\( p^\circ_i \) pure component vapor pressure, (Pa)

\( \Delta p_{\text{liq}} \) static pressure drop, (Pa)

\( \Delta p_p \) pressure drop in a pump, (Pa)

\( \Delta p_{\text{res}} \) residual pressure drop (Pa)

\( \Delta p_v \) pressure drop over a valve, (Pa)
Nomenclature

\(Q\) observability Gramian
\(r\) reference signal
\(R\) universal gas constant, \(8.31451 \text{ J/K mol}\)
\(\Re\) real part of a complex number
\(\Delta_{ig} s_m\) entropy departure for mixture, \(\text{(J/mol)}\)
\(T\) absolute temperature, \(\text{(K)}\)
\(t\) time, \(\text{(s)}\)
\(T_{ci}\) critical temperature for component \(i\), \(\text{(K)}\)
\(T_{cij}\) averaged critical temperature for components \(i\) and \(j\), \(\text{(K)}\)
\(T_{cm}\) critical mixture temperature, \(\text{(K)}\)
\(T_{\text{ref}}\) reference temperature: \(298.15 \text{ K}\)
\(T_{ri}\) relative temperature of component \(i\), \(T_{ri} = T/T_{ci}, \text{ (–)}\)
\(T_u\) scaling matrix for input variables
\(T_x\) scaling matrix for state variables
\(T_y\) scaling matrix for output variables
\(U\) internal energy of holdup on tray \(k\), \(\text{(J)}\)
\(u\) control signal as calculated by the controller
\(u\) input variable
\(u_P\) control signal applied to the plant
\(V\) vapor flow from tray, \(\text{ (mol/s)}\)
\(v\) molar volume of liquid, \(\text{ (m}^3/\text{mol)}\)
\(v'\) molar volume of vapor, \(\text{ (m}^3/\text{mol)}\)
Nomenclature

\( \nu'_m \)  vapor mixture molar volume, \((m^3/mol)\)

\( V^* \)  volume flow, \((m^3/s)\)

\( V^*_{aer} \)  volume flow of froth, \((m^3/s)\)

\( \nu_{c_i} \)  critical molar volume of component \( i \), \((m^3/mol)\)

\( V^*_{cl} \)  volume flow of clear liquid, \((m^3/s)\)

\( \nu_i \)  molar volume of component \( i \), \((m^3/mol)\)

\( \nu_m \)  liquid mixture molar volume \((m^3/mol)\)

\( V_t \)  total volume of liquid, \((m^3)\)

\( V'_t \)  total volume of vapor, \((m^3)\)

\( W \)  weir length, \((m)\)

\( \omega_h \)  vapor velocity through the holes of tray, \((m/s)\)

\( x \)  state variable

\( x_i \)  liquid mole fraction of component \( i \)

\( x_{k,i} \)  liquid mole fraction of component \( i \) on tray \( k \), \((-)\)

\( y \)  output variable

\( y \)  plant outputs (controlled variables and possibly additional measured variables)

\( y_i \)  vapor mole fraction of component \( i \), \((-)\)

\( y_{k,i} \)  vapor mole fraction of component \( i \) on tray \( k \), \((-)\)

\( y_{eq} \)  equilibrium vapor mole fraction of component \( i \) on tray \( k \), \((-)\)

\( y_m \)  measurements
Nomenclature

Z  liquid compressibility, \( Z = \frac{pV}{RT} \), (−)

z  algebraic variable

z  valve position, (m)

Z'  vapor compressibility, \( Z' = \frac{pV'}{RT} \), (−)

z'  molar vapor compressibility, \( z' = \frac{pv'}{RT} \), (−/mol)

Z_{RA_i}  pure component Rackett compressibility factor, (−)

Z_{RA_m}  mixture Rackett compressibility factor, (−)

Superscripts/Subscripts

'  vapor property

eq  equilibrium

i  component i

ig  ideal gas

j  component j

k  tray k (numbered from top, starting with condenser)

l  component l

m  mixture

°  pure component property

ref  reference

t  total

vap  vaporization

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Nomenclature

Equivalent Component Names

Component 7: Intermediate Component
Component 8: Main Component
Component 9: Heavy Component 1
Component 10: Heavy Component 2
Introduction

Much progress has been made in the world of process control in the last decades. Starting from simple PID controllers which were tuned empirically, more and more sophisticated methods for controller design have been developed which make use of specialized mathematical algorithms.

During the same time, computers have gained an unforeseen importance and power, leading way to simulations using complicated models, to optimizations and much more.

Combining these two aspects, algorithms and computing power, lays the ground for an important discipline of control engineering: Model Based Controller Design. With this approach, detailed models of the system to be controlled are used to design, test and improve controllers.

One area that has always attracted the interest of control engineers is the control of distillation columns, as distillation is the most important separation technique in the chemical process industries. Improving the performance of a distillation column can lead to substantial savings. In addition to the economic aspect, distillation columns are interesting for testing controller design methods, as they are highly nonlinear and constitute a MIMO system of high order.

Closer inspection of the projects published, however, reveals that the columns investigated are often simple systems, separating e.g. bi-
1 Introduction

Binary mixtures with nearly ideal behavior. The physical properties are well characterized and the components involved are known. The industrial reality, however, is different: In many cases, multicomponent mixtures with non-ideal behavior are separated. Instead of one column, several columns are used, which interact with each other. The plant data available is often incomplete and uncertain, and the components involved are only partially known. But still these plants need to be controlled, however disadvantageous the circumstances are.

The aim of this thesis is to show how such industrial distillation plants can be modeled and controlled, which steps are necessary, which problems occur, and how they can be solved. The following tasks are involved:

- Collect plant measurements data.
- Find suitable models of physical properties.
- Reproduce stationary measurements results.
- Create (nonlinear) dynamic model.
- Create linear dynamic model suitable for controller design.
- Design and test controllers.

1.1 The Plant

The plant that is investigated in this thesis consists of three distillation columns in series. They separate a highly non-ideal multicomponent mixture, which contains at least twelve important components. The total number of components, however, is unknown, as it is often the case in the chemical industries. A schematic flowsheet, showing how feeds and products connect the columns, is shown in figure 1.1. The bottom product of the first column is split into two parts and then fed into the second column (on tray 48 and in the reboiler). The distillate flow of the second column is recycled to the first column. The main product is taken from the second column as a side stream. While the
1.1 The Plant

Figure 1.1: Flowsheet of the plant

Explanation:
- --- not modeled
- ➔ feed/product
first two columns are tray columns, the third one is a packed column. Its feed consists of the bottom product of the second column, and its distillate flows back to the second column, forming the second recycle of the system.

Inspection of the mixture which is separated reveals, however, that the third column may not be necessary, if a good controller exists which ensures that the specifications for the main product are met. This thesis will therefore will concentrate on the first two columns, leaving the third column unmodeled. The recycle from column 3 to column 2, however, is included in the model as an external feed, to enable a comparison of measurements and simulations.

The current operation of the plant makes an improvement of the control system desirable: When the feed flow to the first column is changed, the specifications for the main product are no longer met. It typically takes two days to get the plant back on track. Currently, the bottom level of each column is controlled by the corresponding bottom product stream; the pressure drop of the column is controlled by the heat input to the column. The temperature of a tray is used as an indicator for the composition profile; if its setpoint is not reached, the product flows are adjusted manually. Both columns are operated under vacuum. A summary of plant data as obtained from measurements in two operating points is shown in table 1.1.

### 1.1.1 The Control Problem

The following variables can be used as control variables for column 1:

- Reboiler heat input
- Distillate flow rate or reflux flow rate
- Bottom product flow rate

This column is not equipped with a reflux drum, and the condenser holdup is negligible. Therefore the distillate flow and the reflux flow cannot be changed independently, as the sum of both flows must always equal the vapor flow entering the condenser.
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</tr>
<tr>
<td>main component</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>measurement 1:</td>
<td>– 0.854</td>
<td></td>
<td>0.888</td>
<td>0.969</td>
</tr>
<tr>
<td>measurement 2:</td>
<td>– 0.827</td>
<td></td>
<td>0.989</td>
<td>0.975</td>
</tr>
</tbody>
</table>
1 Introduction

Column 1 has to fulfill the following specifications:

- Main component in distillate: less than 1 mass-% (full recovery in bottom product)
- Bottom level controlled
- Pressure drop controlled

Three control variables are available, so three variables can be controlled independently.

Column 2 has to fulfill the following specifications:

- Main component in distillate: more than 90 mass-%
- Main component in side stream: more than 96 mass-%
- Bottom level controlled
- Pressure drop controlled

The manipulated variables for column 2 consist of

- Reboiler heat input
- Distillate flow or reflux flow
- Bottom product flow
- Side stream flow

For this column therefore four variables can be controlled.

In this thesis, the assumption is made for both columns that the bottom levels are controlled using the bottom product flows, and that the distillate flow is manipulated.

Altogether this leads to the controller inputs and outputs shown in table 1.2. Note that this table does not imply any special pairing of variables shown.
1.2 Organization of this Thesis

A detailed description of the dynamic model developed, including equations and implementation details, is given in Chapter 2. The problems that occur when trying to model the behavior of an existing plant are illustrated in Chapter 3, followed by an explanation of possible solutions. Linear models suitable for controller design are obtained by linearization, model reduction, and scaling in Chapter 4. Controllers for both columns are designed and tested in Chapter 5. A summary and conclusions are given in Chapter 6.

Table 1.2: Controlled and Manipulated Variables

<table>
<thead>
<tr>
<th>column 1</th>
<th>column 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>manipulated</td>
<td>manipulated</td>
</tr>
<tr>
<td>distillate flow</td>
<td>distillate flow</td>
</tr>
<tr>
<td>main component in distillate</td>
<td>main component in distillate</td>
</tr>
<tr>
<td>reboiler heat</td>
<td>reboiler heat</td>
</tr>
<tr>
<td>pressure drop</td>
<td>pressure drop</td>
</tr>
<tr>
<td>side stream flow</td>
<td>side stream flow</td>
</tr>
</tbody>
</table>
Rigorous Model

Models with various amounts of detail have been used for distillation design and control for a long time. An often-quoted expression in the distillation area, however, is: “There are no two distillation columns that are alike” [1]. For this reason, each time a new model for a distillation column is needed, the decision has to be made all over again which details in the model are necessary for a good description of the column behavior. One of the fundamental questions which have to be answered is which concept is to be used to describe the mass transfer in a distillation column. The two possible approaches are:

- Equilibrium-based approach
- Rate-based approach

The equilibrium-based approach assumes that vapor and liquid leaving a distillation tray are in thermodynamic equilibrium. The foundations for this model were laid by Sorel in 1893, but only in the 1920s, when graphical methods were developed by Ponchon and Savarit first, and by McCabe and Thiele later, its application started to spread. The equilibrium-based model still is the most popular approach. This can be explained (among other reasons) by its long history of application and the fact that its concepts can easily be understood.
2 Rigorous Model

The rate-based approach uses the laws of multicomponent mass transfer to describe the processes in a distillation column. Instead of formulating material and energy balances for each tray, the balances are written for each phase of the tray, leading to two balances where only one balance has been used in the conventional approach. The pair of phase balances is then coupled by interface transport rates [2]. Although using this approach is recommended to obtain a more realistic model for the distillation process [3], it is not widely used yet. One problem is the fact that the number of physical properties needed for the model is much larger than for the equilibrium case. The parameters that are necessary for calculating vapor-liquid equilibria are already difficult to obtain. To describe mass transfer and flow patterns, however, additional parameters and properties are necessary, e.g. diffusivities, surface tensions, thermal conductivities, and heat and mass transfer coefficients. In an industrial environment this information is seldom available, so the rate-based approach is seldom used. Consequently an equilibrium-based model has been chosen for this project.

In the following sections, a rigorous model of a distillation column is developed. After the necessary equations have been introduced, in section 2.8 the calculation sequence will be explained as well as some other mathematical details of the implementation.

For the following equations trays are assumed to be numbered from top to bottom, starting with the condenser as tray 1. For components, the indices \(i, j,\) and \(l\) are used, while index \(k\) is used for trays, denoting either a property that refers to the tray or a property of a stream leaving the tray.

2.1 Summary of the Assumptions for the Dynamic Model

The most important assumptions made during the modeling process are summarized as follows:

- The holdup in the downcomer is negligible due to a special tray construction.
The core of a rigorous model for a distillation column is formed by balances of energy and material for each tray, for the condenser, and for the reboiler. They are represented by nonlinear first order differential equations.

2.2.1 Material Balance

When considering a system with \( n \) components, for each tray \( n \) material balances are necessary to characterize the dynamic behavior. The balances can be written as component balances, which leads to one equation per component. Another possibility is to use \( (n - 1) \) component balances and one total material balance. For this project the first method was chosen. For the distillation tray depicted in figure 2.1, the component balance for component \( i \) is defined as follows:

\[
\frac{dN_{k,i}}{dt} = L_{k-1}x_{k-1,i} - L_kx_{k,i} + V_{k+1}y_{k+1,i} - V_ky_{k,i} \tag{2.1}
\]
2 Rigorous Model

\[ \frac{dU_k}{dt} = L_{k-1}h_{k-1} - L_k h_k + V_{k+1}h'_{k+1} - V_k h_k' \] (2.3)

where \( k \) denotes the tray, \( i \) the component, \( N \) the liquid holdup, \( L \) the liquid flow, and \( V \) the vapor flow.

The following assumptions are made:

- Only liquid holdup is taken into account, because vapor holdup can be neglected for low-pressure columns [1, 4].
- The holdup is perfectly mixed.

The liquid mole fractions \( x_{k,i} \) can then be calculated from the component holdups \( N_{k,i} \):

\[
x_{k,i} = \frac{N_{k,i}}{\sum_{i=1}^{n} N_{k,i}} \] (2.2)

The use of component holdups as state variables instead of mole fractions is less likely to cause problems when the equations are integrated, as for mole fractions the algorithm used has to ensure that they always stay between 0 and 1, whereas for holdups only the lower bound is critical.

2.2.2 Energy Balance

The change of energy on a distillation tray can be described by the following energy balance:
where \( U \) denotes the internal energy of the holdup, and \( h \) and \( h' \) denote the specific enthalpies of the liquid and gas phase, respectively.

As the vapor holdup is neglected, the internal energy term only refers to the liquid holdup. In liquid systems, the internal energy can be approximated by the enthalpy \( H \):

\[
\frac{dH_k}{dt} = L_{k-1}h_{k-1} - L_kh_k + V_{k+1}h'_{k+1} - V_kh'_k
\]  
(2.4)

Under the assumption of perfect mixing, \( H_k \) and \( h_k \) are related as follows:

\[
h_k = \frac{H_k}{N_k}
\]  
(2.5)

### 2.3 Pressure Drop

The vapor crossing tray \( k \) from below will suffer a pressure drop \( \Delta p_k \):

\[
\Delta p_k = p_{k+1} - p_k
\]  
(2.6)

This pressure drop is usually assumed to consist of the static pressure drop \( \Delta p_{\text{liq},k} \) caused by the liquid on the tray, the dry pressure drop \( \Delta p_{\text{dry},k} \) caused by the vapor that flows through the openings (holes, slots, valves) in the tray, and the residual pressure drop \( \Delta p_{\text{res},k} \):

\[
\Delta p_k = \Delta p_{\text{liq},k} + \Delta p_{\text{dry},k} + \Delta p_{\text{res},k}
\]  
(2.7)

The static pressure drop is calculated using the height of the clear liquid on the tray (see section 2.4 for additional information):

\[
\Delta p_{\text{liq},k} = \rho_k g h_{\text{cl},k}
\]  
(2.8)

where \( \rho \) denotes the mass density of the liquid.

The dry pressure drop is usually represented by an orifice-type equation [5]:

\[
\Delta p_{\text{dry},k} = \xi \rho_{k+1} \omega_{h,k}^2
\]  
(2.9)
2 Rigorous Model

The factor $\xi$ can be calculated from various correlations (a selection of them can be found e.g. in [6] and [7]), or be fitted using steady-state data, as done in this project.

The vapor velocity through the holes, $w_{h,k}$, is related to the incoming vapor flow rates:

$$w_{h,k} = \frac{V_{k+1}v'_{k+1}}{A_h}$$

(2.10)

The residual pressure drop is usually interpreted as the excess pressure required to overcome the surface tension when bubbles are formed at the orifice. It depends on the surface tension $\sigma$ and the hole diameter $d_{hole}$ [8]:

$$\Delta p_{res} = \frac{4\sigma}{d_{hole}}$$

(2.11)

In most cases the residual pressure drop is small compared to the other two contributions, so it can be neglected.

The pressure drop that occurs in the piping to the condenser is modeled as a dry pressure drop:

$$\Delta p_{cond} = \xi_{cond}\rho'_2(V_2 \cdot v'_2)^2$$

(2.12)

where $\xi_{cond}$ has been estimated from steady-state simulations.

2.4 Holdup and Flow from Tray

Assuming negligible vapor holdup, the liquid holdup on a tray is usually divided into two parts, the liquid on the tray itself and the liquid in the downcomer. In our case, due to a special tray construction, liquid only stays on the tray, and the downcomer part can be neglected. The liquid holdup is aerated by the incoming vapor. The resulting froth occupies a larger volume than would be required by the pure
2.4 Holdup and Flow from Tray

liquid alone. To take this into account, the liquid volume fraction \( \Phi_k \) is introduced:

\[
\Phi_k = \frac{h_{cl,k}}{h_{aer,k}}
\]  
(2.13)

where \( h_{cl} \) is the theoretical height of the holdup volume if no aeration were present, and \( h_{aer} \) is the height of the aerated liquid on the tray.

Assuming that only liquid holdup is present, the holdup \( N \) and the clear liquid height are then related by

\[
h_{cl,k} = \frac{N_k v_k}{A_t}
\]  
(2.14)

where \( A_t \) denotes the area of the tray without the downcomer.

The volume flow \( V_{aer}^* \) of froth flowing across a weir of length \( W \) can be calculated using Francis’s weir formula [8]

\[
V_{aer}^* = W \left( \frac{C_d^{0.67} g^{0.33}}{1.04} \right)^{1.5} (h_{aer,k} - h_w)^{1.5}
\]  
(2.15)

where \( h_w \) denotes the weir height and \( C_d \) is a friction coefficient.

Equation (2.15) can be generalized to the form

\[
V_{aer}^* = \alpha (h_{aer,k} - h_w)^\beta
\]  
(2.16)

The parameters \( \alpha \) and \( \beta \) depend on the details of the tray geometry. A detailed description of different variants of this modified Francis’s weir equation can be found in [9].

The mole flow of clear liquid from a tray is then obtained from equation (2.16) with the help of the liquid volume fraction \( \Phi \) and the molar volume \( v_m \):

\[
L_k = \frac{1}{v_{m,k}} \Phi_k V_{aer}^* = \frac{1}{v_{m,k}} \Phi_k \alpha (h_{aer,k} - h_w)^\beta
\]

\[
= \frac{1}{v_{m,k}} \Phi_k \alpha \left( \frac{h_{cl,k}}{\Phi_k} - h_w \right)^\beta
\]  
(2.17)
2 Rigorous Model

Several empirical as well as theoretical correlations for predicting $\Phi$ exist. An overview can be found in [8]. The equation by Stichlmair [10] is widely used, but it requires the calculation of surface tensions, for which parameters were not available in this project. Therefore the relatively simple correlation by Bennett [11] has been chosen:

$$\Phi_k = \exp(\pi_1 \cdot K_{s,k})$$

(2.18)

The constants $\pi_1$ and $\pi_2$ have been fitted by Bennett.

The velocity factor $K_{s,k}$ depends on the vapor velocity through the active area and the densities:

$$K_{s,k} = \frac{V_{k+1}V'_{k+1}}{A_{\text{active}}} \sqrt{\frac{\rho'_{k+1}}{\rho_k - \rho'_{k+1}}}$$

(2.19)

2.5 Tray Efficiencies

2.5.1 Theoretical Stage

The theoretical or ideal stage is an important concept in modeling distillation columns. It consists of a device (a tray or a column section) that has a liquid product and a vapor product. All the liquid and vapor entering the stage are intimately contacted and perfectly mixed, and the vapor leaving the stage is in equilibrium with the liquid leaving the stage (see figure 2.1):

$$y_{k,i} \equiv y_{k,i}^\text{eq} = K_{k,i}^{\text{VLE}} x_{k,i}$$

(2.20)

Real behavior can then be described by combining ideal stages with efficiencies which take into account the non-idealities. Efficiencies, however, are difficult to predict, especially for multicomponent mixtures. See [8] for an overview of recommended methods.
2.5 Tray Efficiencies

2.5.2 Section Efficiency

Efficiencies have been defined in several different ways, but the more theoretically sound the definition, the more difficult it is to use practically [8]. The simplest type of efficiencies is the section efficiency $E_0$ which relates the number of actual trays $N_a$ in a section to the number of theoretical trays $N_t$:

$$N_a = \frac{N_t}{E_0} \tag{2.21}$$

The section efficiency is most useful for design studies of binary mixtures, where all calculations are made with ideal trays in a first step and then the necessary number of trays is obtained using the section efficiency in a second step. This approach is unsuitable, however, if information is required about the composition on a certain tray. For multicomponent mixtures, overall section efficiencies have no meaning: The section efficiencies are not identical for different components. This in turn would imply a different number of actual trays for each component, which is not possible.

2.5.3 Murphree Tray Efficiency

The Murphree tray efficiency $\eta_M$ [12] is widely used. It relates the incoming vapor composition $y_{k+1,i}$ to the composition of the liquid and vapor leaving the tray $k$

$$\eta_M = \frac{y_{k,i} - y_{k+1,i}}{y_{k,i}^e - y_{k+1,i}} \tag{2.22}$$

or

$$y_{k,i} = y_{k+1,i} + \left(y_{k,i}^e - y_{k+1,i}\right) \eta_M \tag{2.23}$$

where $y_{k,i}$ is the real mole fraction of the vapor leaving tray $k$, and $y_{k,i}^e$ denotes the mole fraction of the vapor which is in equilibrium with the liquid leaving the tray:

$$y_{k,i}^e = K_{k,i} x_{k,i} \tag{2.24}$$
2 Rigorous Model

Although $\eta_M$ takes on different values for different components and also varies along the column [13], for simulations it is often assumed to be constant. For binary mixtures, $\eta_M$ varies between 0 and 1; for multicomponent mixtures, however, its values lie between $-\infty$ and $+\infty$ [14]. The Murphree tray efficiency is used for column 1. A constant value is used for the efficiencies on all trays for all components.

2.5.4 Hausen Tray Efficiency

The definition by Hausen [15] is not very well known. His objection to the Murphree tray efficiency consists of the fact that, while the compositions of the liquid stream entering the stage are identical for the ideal stage and the actual stage, the vapor compositions differ. His definition retains the form of the Murphree efficiency, but specifies that $y_{eq}$ is the mole fraction of $i$ that would result from an equilibrium flash calculation based on the combined vapor and liquid streams entering the tray:

$$
\eta_H = \frac{y_{k,i} - y_{k+1,i}}{y_{eq,i} - y_{k+1,i}} = \frac{x_{k,i} - x_{k-1,i}}{x_{eq,i} - x_{k-1,i}}
$$

(2.25)

where

$$
y_{eq,i} = K_{eq,i}x_{k,i}
$$

(2.26)

This approach has the disadvantage that efficiencies have to be used not only for calculating the actual vapor composition, but also for calculating the actual liquid composition.

2.5.5 Vaporization Efficiency

A different approach is the use of vaporization efficiencies, which have been investigated by Holland [14]:

$$
y_{k,i} = \eta_{v,i} y_{eq,i} = \eta_{v,i} K_{eq,i} x_{k,i}
$$

(2.27)
2.6 Physical Properties

Choosing suitable methods for calculating physical properties has a fundamental impact on the simulation results. Especially the choice of a model for calculating the vapor-liquid equilibrium (VLE) is critical.

2.6.1 Equation of State

The relationship between the pressure \( p \), the temperature \( T \), and the volume \( V \) for pure components and mixtures is described by an equation of state. Usually this equation is explicit in pressure. Any thermodynamic property, such as fugacity coefficients and enthalpies, can be calculated from the equation of state with the help of fundamental thermodynamic relationships. When using an equation-of-state method, thermodynamic properties are calculated relative to the ideal gas properties of the same mixture at the same conditions.

The Redlich-Kwong equation-of-state is applicable for systems at low or moderate pressures for which the vapor phase exhibits nearly
2 Rigorous Model

ideal behavior [18], which makes it suitable for the system considered in this project.

2.6.1.1 Pure Components

For a pure component, the Redlich-Kwong equation-of-state has the following form [19]:

\[
p = \frac{RT}{v_i - b_i} - \frac{a_i}{v_i^2 + b_i v_i}
\]  (2.28)

The parameters \(a_i\) and \(b_i\) depend on the critical pressure \(p_c\), the critical temperature \(T_c\), and the system temperature \(T\):

\[
a_i = \frac{0.42748023 R^2 T_{c_i}^{2.5}}{p_c T_{c_i}^{0.5}}
\]  (2.29)

\[
b_i = \frac{0.08664035 RT_{c_i}}{p_{c_i}}
\]  (2.30)

2.6.1.2 Multicomponent Mixtures

For multicomponent mixtures, the pure component constants \(a_i\) and \(b_i\) as well as the molar volumes \(v_i\) are replaced by the corresponding properties of the mixture, as shown in the following equation [19]:

\[
p = \frac{RT}{v_m - b_m} - \frac{a_m}{v_m^2 + b_m v_m}
\]  (2.31)

The mixture constants \(a_m\) and \(b_m\) are calculated from the pure component constants \(a_i\) and \(b_i\) by applying mixing rules. General mixing rules for Redlich-Kwong-type equations-of-state are [19]:

\[
a_m = \sum_i \sum_j y_i y_j (a_i a_j)^{0.5} (1 - k_{ij})
\]  (2.32)
2.6 Physical Properties

\[ b_m = \sum_i y_i b_i \]  \hspace{1cm} (2.33)

where \( y_i \) denotes the vapor mole fraction.

For pairs of hydrocarbons, \( k_{ij} \) is usually assumed to be zero, in which case equation (2.32) can be reduced to the following equation:

\[ a_m = \left( \sum_i y_i (a_i)^{0.5} \right)^2 \]  \hspace{1cm} (2.34)

2.6.2 Vapor-Liquid Equilibrium

There are two fundamentally different methods for describing VLE properties [18]:

1. Equation-of-state method

2. Activity coefficient method

Regardless of the method chosen, a mixture is in thermodynamic equilibrium if the requirement is met that the fugacity \( f_i' \) of each component in the vapor mixture is equal to the fugacity \( f_i \) in the liquid mixture:

\[ f_i = f_i' \]  \hspace{1cm} (2.35)

The fugacity of a component in a mixture depends on the following properties:

- Temperature
- Pressure
- Composition of the mixture
2 Rigorous Model

2.6.2.1 Vapor Phase Fugacity

For the vapor phase, the fugacity is always calculated using an equation-of-state:

\[ f_i' = \varphi_i' y_i p \]  
\[ \ln \varphi_i' = - \frac{1}{RT} \int_{\infty}^{V_i'} \left[ \left( \frac{\partial p}{\partial N_i} \right)_{T,V_i,N_{j\neq i}} - \frac{RT}{V_i'} \right] dV_i' - \ln Z' \]

where \( V_i' \) denotes the total volume of vapor and \( Z' = \frac{PV_i'}{RT} \) is the vapor compressibility. For an ideal gas, the fugacity coefficient \( \varphi_i' \) is equal to one, so the following relationship holds:

\[ f_i' = y_i p \]

As the columns are operated at very low pressure, the vapor phase fugacities are close to one. Therefore ideal behavior was assumed.

2.6.2.2 Liquid Phase Fugacity

The liquid phase fugacities can also be calculated from the equation of state [19]:

\[ f_i = \varphi_i x_i p \]

with

\[ \ln \varphi_i = - \frac{1}{RT} \int_{\infty}^{V_i} \left[ \left( \frac{\partial p}{\partial N_i} \right)_{T,V_i,N_{j\neq i}} - \frac{RT}{V_i} \right] dV_i - \ln Z \]

where \( Z = \frac{PV_i}{RT} \) denotes the liquid compressibility.

For describing highly non-ideal behavior, as in the system investigated, a method using activity coefficients is better suited. In this case the following relationship is used:

\[ f_i = x_i y_i f_i^\circ \]
2.6 Physical Properties

where $\gamma_i$ is the liquid activity coefficient of component $i$ in the mixture, and $f_i^\circ$ denotes the liquid activity coefficient of pure component $i$ at the temperature of the mixture.

For an ideal liquid, the activity coefficients are identical to one and the liquid activity coefficients $f_i^\circ$ of the pure components are identical to their vapor pressures $p_i^\circ$, so equation (2.41) reduces to

$$f_i = x_i p_i^\circ$$ (2.42)

**Vapor Pressure** The pure component vapor pressure $p_i^\circ$ is calculated using the extended Antoine equation [18]

$$\ln p_i^\circ = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i} T + C_{5i} \ln T + C_{6i} T^{C_{7i}}$$ (2.43)

Outside of given temperature bounds, $\ln p_i^\circ$ is linearly extrapolated versus $1/T$.

**Wilson Activity Coefficients** Starting point for calculating the activity coefficients $\gamma_i$ is a model for the excess Gibbs energy $G^E$. By using the Gibbs-Duhem equation for multicomponent systems, the activity coefficients can be calculated as follows [19]:

$$RT \ln \gamma_i = \left( \frac{\partial G^E}{\partial N_i} \right)_{T,p,N_j \neq i}$$ (2.44)

The Wilson model proposes the following relationship for the Gibbs energy:

$$\frac{g^E}{RT} = - \sum_i x_i \ln \left( \sum_j x_j \Lambda_{ij} \right)$$ (2.45)

where $g^E$ denotes the specific Gibbs energy:

$$g^E = \frac{G^E}{N}$$ (2.46)
2 Rigorous Model

The interaction parameters $\Lambda_{ij}$ are empirical constants which are usually temperature dependent. A model that is often used is

$$\ln \Lambda_{ij} = a_{ij} + \frac{b_{ij}}{T} \quad (2.47)$$

In many cases $a_{ij}$ is calculated from the molar volumes of the two components (at room temperature):

$$a_{ij} = \ln \frac{v_j}{v_i} \quad (2.48)$$

In this case the following equation holds

$$a_{ij} = -a_{ji} \quad (2.49)$$

Using equation (2.44), the corresponding activity coefficients are

$$\ln \gamma_i = 1 - \ln \left( \sum_j x_j \Lambda_{ij} \right) - \sum_j \frac{\Lambda_{ji} x_j}{\sum_l \Lambda_{jl} x_l} \quad (2.50)$$

The Wilson model was chosen to describe the behavior of the liquid phase in this project as it is especially suited for strongly non-ideal liquids, as long as the mixture does not exhibit a miscibility gap. Mixtures of polar and nonpolar components can be handled [19].

2.6.2.3 Vapor-Liquid Equilibrium Constants

Inserting equations (2.41) and (2.36) into equation (2.35) and solving for $y_i$ leads to the following relationship for the VLE:

$$y_i = \frac{\gamma_i f_i^c}{\varphi_i^c p} x_i = K_{eq}^i x_i \quad (2.51)$$

For ideal substances, we arrive at

$$y_i = \frac{p_i^c}{P} x_i = K_{eq, id}^i x_i \quad (2.52)$$
2.6 Physical Properties

When performing VLE calculations in distillation simulations, the following situation is commonly encountered: The liquid mole fractions \( x \) and the system pressure \( p \) are known, and the system temperature \( T \) and the vapor mole fractions \( y \) have to be calculated. In this case the following procedure is applied: Using a starting value for the boiling point temperature \( T \), the liquid mixture activity coefficients \( \gamma_i \), and the liquid pure component activity coefficients \( f_i^0 \) are determined. The vapor mole fractions \( y_i \) can be calculated subsequently. They have to fulfill the bubble point equation

\[
1 - \sum_i y_i(p, T, x) = 0 \quad (2.53)
\]

therefore the temperature is adjusted until the bubble point equation is fulfilled.

2.6.3 Molar Volume

2.6.3.1 Liquid Phase

The mixture volume \( v_m \) for the liquid phase is calculated by the Rackett equation [19], using critical temperatures \( T_c \) and pressures \( p_c \) of the individual components, the critical temperature of the mixture \( T_{cm} \), and the Rackett compressibility factor \( Z_{RA_m} \) of the mixture:

\[
v_m = R \left( \sum_i x_i \frac{T_{ci}}{p_{ci}} \right) Z_{RA_m} \left[ 1 + \left(1 - \frac{T}{T_{cm}}\right)^{2/7} \right] \quad (2.54)
\]

where \( Z_{RA_m} \) is calculated from the individual component compressibility factors \( Z_{RA_i} \):

\[
Z_{RA_m} = \sum_i x_i Z_{RA_i} \quad (2.55)
\]

The critical temperature of the mixture \( T_{cm} \) is calculated as follows:

\[
T_{cm} = \sum_i \sum_j \phi_i \phi_j T_{ci,j} \quad (2.56)
\]
2 Rigorous Model

with

\[ 1 - k_{ij} = \frac{8 \left( v_{ci} v_{cj} \right)^{0.5}}{\left( v_{ci}^{1/3} + v_{cj}^{1/3} \right)^3} \]  
\[(2.57)\]

\[ T_{cij} = (1 - k_{ij}) \left( T_{ci} T_{cj} \right)^{0.5} \]  
\[(2.58)\]

\[ \phi_i = \frac{x_i v_{ci}}{\sum_i x_i v_{ci}} \]  
\[(2.59)\]

where \( v_c \) denotes the critical volume and \( \phi \) is the component volume fraction.

2.6.3.2 Vapor Phase

The molar volume for the vapor phase, \( v'_m \), is calculated by solving the mixture Redlich-Kwong equation-of-state (2.31) for \( v'_m \), using the method of auxiliary variables [20].

2.6.4 Calculation of Mixture Enthalpy

2.6.4.1 Ideal Gas Properties

Ideal Gas Enthalpy The ideal gas enthalpy of a pure component is calculated using the ideal gas heat capacity [18]:

\[ h_{ig} = \Delta_f h_{ig} + \int_{T_{ref}}^T c_{p,i}^{ig}(T) dT \]  
\[(2.60)\]

where \( \Delta_f h_{ig} \) denotes the standard enthalpy of formation of an ideal gas at 298.15 K and 1 atm, and \( c_{p,i}^{ig} \) is the ideal gas heat capacity.

The application of mixing rules leads to the corresponding property of a mixture:

\[ h_m^{ig} = \sum_i y_i h_{ig} \]  
\[(2.61)\]
### 2.6 Physical Properties

**Ideal Gas Heat Capacity** The ideal gas heat capacity for a component can be calculated with two different approaches. The first possibility is using the DIPPR (Design Institute for Physical Properties) equation [18]:

\[ c_{ig}^p,i = C_1i + C_2i \left( \frac{C_3i/T}{\sinh (C_3i/T)} \right)^2 + C_4i \left( \frac{C_5i/T}{\cosh (C_5i/T)} \right)^2 \] (2.62)

The integral in equation (2.60) then evaluates to

\[ \int_{T_{ref}}^{T} c_{ig}^p,i(T)\,dT = C_1i (T - T_{ref}) + C_2iC_3i \coth \frac{C_3i}{T} - C_2iC_3i \coth \frac{C_3i}{T_{ref}} \\
- C_4iC_5i \tanh \frac{C_5i}{T} + C_4iC_5i \tanh \frac{C_5i}{T_{ref}} \] (2.63)

The second possibility is using a polynomial equation [18], which is applicable for those components for which the DIPPR constants are not available:

\[ c_{ig}^p,i = \begin{cases} 
A_i(T) & \text{for } C_7i \leq T \leq C_8i \\
B_i(T) & \text{for } T < C_7i \\
C_i(T) & \text{for } T > C_8i 
\end{cases} \] (2.64)

with

\[ A_i(T) = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 + C_{6i}T^5 \] (2.65)

\[ B_i(T) = C_{9i} + C_{10i}T^{C_{1i}} \] (2.66)

\[ C_i(T) = \text{linear extrapolation of } A(T) \text{ using slope at } C_{8i} \] (2.67)

#### 2.6.4.2 Liquid Phase

The liquid mixture enthalpy \( h_m \) is calculated from two terms, the enthalpy of an ideal gas mixture and the enthalpy departure function.
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$\Delta_{ig}h_m$, which expresses the difference between the enthalpy of a real liquid mixture and the enthalpy of an ideal gas mixture [18]:

$$h_m = h_m^{ig} + \left( h_m - h_m^{ig} \right)$$

$$= h_m^{ig} + \Delta_{ig}h_m \tag{2.68}$$

Liquid Mixture Enthalpy Departure Function  The enthalpy departure function for a mixture can be calculated from the individual pure component enthalpy departure functions:

$$\Delta_{ig}h_m = \sum_i x_i \Delta_{ig}h_i^\circ \tag{2.69}$$

For vacuum systems, the influence of pressure on liquid enthalpy can be neglected. The pure component liquid enthalpy departure can then be calculated, using the vapor enthalpy departure $\Delta_{ig}h_i^\circ$ and the enthalpy of vaporization $\Delta_{vap}h_i^\circ(T)$:

$$\Delta_{ig}h_i^\circ = \Delta_{ig}h_i^\circ(p_i^\circ, T) - \Delta_{vap}h_i^\circ(T) \tag{2.70}$$

The enthalpy departure for the individual components is calculated at system temperature $T$ and pure component vapor pressure $p_i^\circ$, using an equation-of-state method, as described in equation (2.79).

2.6.4.3 Vapor Phase

The dependence of pressure $p$ on the vapor molar volume $v_m'$ and temperature $T$ can be expressed using the Redlich-Kwong equation-of-state for mixtures, as described in section 2.6.1:

$$p = \frac{RT}{v_m' - b_m} - \frac{a_m}{v_m'^2 + b_m v_m'} \tag{2.71}$$

For the following calculations, the temperature dependency of the constant $a_m$ is shown more clearly by using the following formulation:

$$a_m = \frac{a_{Tm}}{T^{0.5}} \tag{2.72}$$
2.6 Physical Properties

Equation (2.71) is then rewritten as

\[ p = \frac{RT}{v_m' - b_m} - \frac{a_{Tm}/T^{0.5}}{v_m'^2 + b_m v_m'} \]  

(2.73)

The enthalpy departure \( \Delta_{ig}h_m \) can be calculated using fundamental thermodynamic properties [19].

\[ \Delta_{ig}a_m = -\int_{\infty}^{v_m'} \left( p - \frac{RT}{v_m'} \right) dv_m' - RT \ln \frac{v_m'}{v_{im}'} \]  

(2.74)

\[ \Delta_{ig}s_m = -\frac{\partial}{\partial T} \Delta_{ig}a_m \]  

(2.75)

\[ \Delta_{ig}h_m = \Delta_{ig}a_m + T \Delta_{ig}s_m + RT (z' - 1) \]  

(2.76)

with the molar compressibility \( z' = \rho v'/RT \). Using equation (2.73), we get:

\[ \Delta_{ig}a_m = -\int_{\infty}^{v_m'} \left( p - \frac{RT}{v_m'} \right) dv_m' - RT \ln \frac{v_m'}{v_{ig}'m} \]  

\[ = \frac{a_{Tm}}{b_m \sqrt{T}} \ln \frac{v_m'}{v_m' + b_m} + RT \ln \frac{v_m'}{v_m' - b_m} - RT \ln \frac{v_m'}{v_{ig}'} \]  

(2.77)

\[ \Delta_{ig}s_m = -\frac{\partial}{\partial T} \Delta_{ig}a_m \]  

\[ = 0.5 \frac{a_{Tm}}{b_m T^{1.5}} \ln \frac{v_m'}{v_m' + b_m} - R \ln \frac{v_m'}{v_m' - b_m} + R \ln \frac{v_m'}{v_{ig}'} \]  

(2.78)

\[ ^1 \text{In the following equations, it is important not to confuse the specific Helmholtz energy departure } \Delta_{ig}a_m \text{ with the Redlich-Kwong parameter } a_m. \]
2 Rigorous Model

\[ \Delta_{ig} h_m = \Delta_{ig} a_m + T \Delta_{ig} s_m + RT (z' - 1) \]

\[ = \frac{a_{Tm}}{b_m \sqrt{T}} \ln \frac{v_m'}{v_m' + b_m} + RT \ln \frac{v_m'}{v_m' - b_m} - RT \ln \frac{v_m'}{v_m'} \]

\[ + 0.5 T \frac{a_{Tm}}{b_m T^{1.5}} \ln \frac{v_m'}{v_m' + b_m} - RT \ln \frac{v_m'}{v_m' - b_m} \]

\[ - RT \ln \frac{v_m'}{\frac{v_m'}{v_m'}} + RT (z' - 1) \]

\[ = 1.5 \frac{a_{Tm}}{b_m \sqrt{T}} \ln \frac{v_m'}{v_m' + b_m} + RT (z' - 1) \]

\[ = 1.5 \frac{a_m}{b_m} \ln \frac{v_m'}{v_m' + b_m} + RT (z' - 1) \quad (2.79) \]

For pure components, all mixture properties in equation (2.79) \((a_m, b_m, v_m')\) have to be replaced by the corresponding pure component properties.

2.6.4.4 Heat of Vaporization

One way of calculating the pure component heat of vaporization is using the Watson equation [18], which relates the heat of vaporization to be calculated to the known heat of vaporization at a temperature \(T_1\):

\[ \Delta_{vap} h_i^\circ(T) = \Delta_{vap} h_i^\circ(T_1) \left( \frac{1 - \frac{T}{T_{ci}}}{1 - \frac{T_1}{T_{ci}}} \right)^{a_i + b_i \left(1 - \frac{T}{T_{ci}}\right)} \quad (2.80) \]

If Watson parameters are not available, the DIPPR model is used [18]:

\[ \Delta_{vap} h_i^\circ(T) = C_{1i} \left(1 - T_{hi}\right)^{\left(C_{2i} + C_{3i} T_{n} + C_{4i} T_{n}^2 + C_{5i} T_{n}^3\right)} \quad (2.81) \]

where \(T_{hi} = T/T_{ci}\) is the relative temperature for component \(i\). Outside of given temperature bounds, extrapolation of \(\Delta_{vap} h_i^\circ\) versus \(T\) occurs.
2.7 Mass Flows versus Mole Flows

Traditionally, distillation column simulations are performed by specifying flows (reflux, feeds, products) on a molar basis. This choice is natural, considering the fact that the separation is determined by the size of mole flows, and therefore material balances are expressed on a molar basis as well. For the real plant, however, flows are fixed on a mass or volume basis. The transformation from mass or volume flows to mole flows is nonlinear and may become singular [21]. As a consequence, the situation can occur where specifying one set of inputs (flows) and solving the steady-state equations leads to several different sets of outputs (product compositions). This phenomenon is called output multiplicity. Conditions for the occurrence of multiplicities and their consequences are a wide research area of their own and will not be discussed here. The focus is laid on the practical implications for realistic simulation results.

When liquid flows are adjusted, two different situations can be distinguished [22]:

- Liquid flows without measurements
- Liquid flows with measurements

**Liquid Flows without Measurements** Liquid flows can be influenced by changing a valve position. The pressure drop $\Delta p_v$ over the valve can be described as

$$\Delta p_v = k(z)\rho V^* z^2 = k(z)(\rho V^*) V^* = k(z) M^* V^*$$

(2.82)

where $k(z)$ is a function of the valve position $z$. The variable $M^*$ denotes the mass flow, and $V^*$ is the volume flow. The pressure drop across the valve is assumed constant, which is reasonable for a liquid system with slow changes at the pipe inputs and outputs, as it is usually the case for chemical process plants. Changing the valve position then leads to a change of the product $M^* V^*$. 

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For a pump the power $P$ which is needed to overcome a pressure drop $\Delta p$ is defined by:

$$P = \Delta p V^*$$  \hspace{1cm} (2.83)

Assuming constant pressure drop, changing the power is therefore equivalent to changing the volume flow $V^*$.

Liquid Flows with Measurements  In many cases valves are part of a cascaded control loop. The flow is measured and the valve position or the pump power are adjusted to keep the flow close to the desired setpoint. If venturi meters or orifice meters are used, which determine the flow as a function of the pressure drop over a restriction in a pipe, the product $M^*V^*$ is measured. Other devices provide direct measurement results of mass or volume flow, but not of mole flow.

No matter whether the liquid flows are measured or not, the value that is influenced is the mass or volume flow or the product of mass and volume flows. As both flow types are related by the liquid density, which usually is only a weak function of composition, both kinds of flows are equally suitable as simulation inputs. For this reason, all simulations were performed using mass flows as inputs to ensure that the simulation conditions are as close as possible to reality. In addition, component mass holdups were used as state variables and mass fractions were used as controlled variables.

The simulation model converts all input flows from mass flows to mole flows, so the internal calculations are performed using mole flows.

2.8 Implementation of the Dynamic Model

The dynamic model was implemented as a combination of MATLAB and C. MATLAB provides a comfortable interface for controller design, so performing the nonlinear simulations in this environment is desirable. In order to obtain a reasonable simulation speed, however,
2.8 Implementation of the Dynamic Model

the main part of the model was programmed in C and then integrated into MATLAB.

2.8.1 Solution Methods

The complete model is represented by a system of differential and algebraic equations (DAE system):

\[
\begin{align*}
\dot{x} &= F(x, z, u) \\
0 &= G(x, z, u)
\end{align*}
\]  

(2.84)  

(2.85)

Equations (2.84) are the differential equations that result from the material and energy balances, and equations (2.85) are the algebraic equations that are necessary for describing the system, where \(x\) are the state variables, \(z\) the algebraic variables, and \(u\) the input variables. DAE systems are needed for modeling many dynamic systems in chemical, mechanical, and electrical engineering. They may exhibit characteristics fundamentally different from systems of ordinary differential equations [23]. Inconsistent initial conditions or discontinuous inputs may lead to impulsive solutions, a common reason for the failure of standard ODE simulation techniques when applied to DAE systems. The differential index \(\nu_d\) is used as a measure for the differences between ODE and DAE systems:

**Definition** Consider the following system

\[
\begin{align*}
\dot{x} &= F(x, u, z) \\
0 &= G(x, u, z)
\end{align*}
\]  

(2.86)

where \(x \in \mathbb{R}^n\) is the vector of state variables for which we have the explicit differential equations, \(u \in \mathbb{R}^m\) is the vector of input variables, and \(z \in \mathbb{R}^p\) is the vector of algebraic variables that vary according to the algebraic equations.

Let us assume that the (smooth) inputs \(u\) of this system are specified. The differential index \(\nu_d\) then is the minimum number of times the algebraic equations or their subset have to be differentiated to yield a set of differential equations for \(z\) [24].
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With this definition, ODE systems can be regarded as a special class of DAE systems with index $\nu_d = 0$. Systems with $\nu_d = 1$ can be solved by specialized algorithms, whereas for $\nu_d > 1$ no suitable software is available (although the solution is possible theoretically).

For the model described in the previous sections, the state variables for each tray and for the reboiler are

- the component mass holdups $m_{i,k}$
- the enthalpy of the liquid holdup $h_k$

No reflux accumulator is present, so there are no state variables in the condenser which is modeled as a total condenser.

The algebraic variables for each tray and the reboiler are

- the temperature $T_k$
- the pressure $p_k$

The condenser pressure is controlled by a vacuum pump, so the only algebraic variable in the condenser is the temperature.

If $G(x, z, u)$ is calculated for an arbitrary set of state variables $x$, algebraic variables $z$, and input variables $u$, the result is not necessarily equal to zero. The integration routine therefore has to make sure that equations (2.85) always hold, either by solving $G$ for $z$ and inserting this solution into equations (2.84) or by a more advanced scheme that uses both groups of equations at once. Independently of the method chosen, a function has to be programmed that calculates $F$ and $G$ for any set of values $x$, $z$, and $u$.

Numerical methods for integrating differential equations fall into two classes: The methods that use one starting value at each integration step (one-step methods) and the methods where the solution is based on several values of the solutions (multi-step methods) [25]. The integrator provided by MATLAB for solving DAE systems belongs to the second class. Two variants can be used, either backward differentiation formulas (BDFs, also known as Gear’s method) or numerical differentiation formulas (NDFs), which are faster, as they allow larger integration step sizes while still retaining stability [26]. This method has been chosen for the dynamic simulations performed.
2.8 Implementation of the Dynamic Model

A prerequisite for the successful integration of a DAE system is the availability of consistent initial values, which means that equations (2.85) have to be fulfilled for \( t = 0 \). A nonlinear least-square solver was used for solving the algebraic equations before starting the integration.

2.8.2 Calculation Sequence

When the derivatives \( F \) and the errors \( G \) are calculated, the right sequence has to be used, because several values are interdependent, as an example may illustrate: Calculating the liquid flow from a tray requires the knowledge of the height of froth above the weir. For calculating this property, the liquid fraction has to be known, which in turn depends on the incoming vapor stream.

The following steps explain in which order \( F \) and \( G \) have to be evaluated when simulating one column, starting from the state variables determined by integration in the last timestep and assumed starting values (provided by the integrator) of the algebraic variables. The additional steps necessary for connecting both columns are explained afterwards.

Holdup properties From the mole holdups, the liquid mole fractions can be calculated. The total holdup is determined. The specific liquid enthalpy is calculated from the total mole holdup and the enthalpy of the liquid holdup.

⇒ Loop from bottom to top (reboiler and all trays)

Vapor-liquid equilibrium The tray temperature and pressure are used to determine the necessary properties for calculating the vapor-liquid equilibrium. The pure component vapor pressure is calculated. When calculating column 1, Wilson activity coefficients are determined, and the vapor mole fractions are calculated using activity coefficients, pure component vapor pressure, tray pressure, composition of liquid holdup, and Murphree efficiency. For column 2, in which an ideal relationship is used for the VLE,
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the vapor mole fractions are calculated using the pure component vapor pressure, the composition of liquid holdup, and the vaporization efficiencies.

**Tray physical properties** The liquid and the vapor mole fractions, the pressure, and the temperature are used for calculating the molar volumes, mass densities, and specific enthalpies.

**Pressure drop (trays only)** Using the tray pressures of the tray below and of the current tray, the total pressure drop for the current tray is calculated.

- **Clear liquid height** The clear liquid height on the tray can be determined using the liquid holdup, the tray area, and the molar volume.
- **Static pressure drop** The static pressure drop can be calculated from the clear liquid height.
- **Dry pressure drop** The dry pressure drop is the difference between total pressure drop and static pressure drop.

**Vapor flow (trays only)** The velocity and the flow rate of the vapor entering the tray are calculated from the dry pressure drop across the tray.

**Liquid flow (trays only)** The liquid fraction of the holdup is determined using the incoming vapor flow rate and physical properties. The height of froth above the weir height is calculated from the clear liquid height, the liquid fraction, and the weir height. The liquid flow leaving the tray can then be determined.

⇐ *Back to the beginning of the loop (calculate next tray)*

**Condenser:**

**Vapor-liquid equilibrium** The composition in the condenser is identical to the composition of the vapor leaving the top tray. The condenser temperature is an algebraic variable which has to be determined with the help of the bubble
2.8 Implementation of the Dynamic Model

point equation: Using pure component vapor pressure coefficients, the condenser pressure, and the temperature estimate provided by the integration routine, the theoretical vapor composition in equilibrium with the liquid is calculated.

Physical properties The liquid mole fractions, the pressure, and the temperature are used for calculating the molar volume, the mass density, and the specific enthalpy.

Pressure drop The pressure drop in the pipe to the condenser is calculated as the difference between the pressure of the vapor leaving the top tray and the column top pressure (condenser pressure). Using the condenser pressure drop equation, the vapor flow rate from the top tray can be calculated.

Reflux flow rate The reflux flow rate is calculated as the difference between the vapor flow rate to the condenser and the distillate flow rate.

Derivatives (from top tray to reboiler):

Material balances The material balances are calculated using the flow rates and compositions of vapor and liquid streams entering and leaving the tray. If feeds or products are present at the tray, the necessary additional terms are included in the balance.

Enthalpy balance The enthalpy balance is calculated using the flow rates and specific enthalpies of the vapor and liquid streams entering and leaving the tray, including possible feed and product streams. For the reboiler, the heat input is added.

Errors (condenser, trays, and reboiler):

Error in boiling point The error in the boiling point equation is calculated.
2 Rigorous Model

**Error in enthalpy (trays and reboiler)** The specific liquid enthalpy is calculated from the holdup enthalpy and from the temperature, pressure, and the liquid composition, and the difference between these two values is determined.

When both columns are simulated including the recycle stream, the component mass flows, the temperature, and the pressure of the distillate of column 2 form additional algebraic variables: For calculating the derivatives and errors of column 1, not only the state variables and algebraic variables of column 1 are used but also the assumed distillate properties of column 2.

Component mass flows, temperature, and pressure of the bottom product of column 1 are then used, together with state variables and assumed algebraic variables of column 2, to calculate the errors and derivatives of column 2.

The additional error equations consist of the difference between the assumed values for the distillate properties and their values, as calculated when treating column 2. See section 4.3.3.2 for additional information about the size of the resulting model.

2.8.3 Pattern of the Jacobian Matrix

The Jacobian matrix $J$ for the DAE system which is shown in equations (2.84) and (2.85) is defined as follows:

$$J = \begin{bmatrix} \frac{\partial F}{\partial x} & \frac{\partial F}{\partial z} \\ \frac{\partial G}{\partial x} & \frac{\partial G}{\partial z} \end{bmatrix} \quad (2.87)$$

The inputs $u$ are assumed to be externally specified, therefore they do not show up in this definition.

The integration routine has to evaluate the Jacobian matrix function repeatedly during the simulation. If a system consists of $N_{\text{DAE}}$ differential and algebraic equations, the size of the Jacobian matrix is $N_{\text{DAE}} \times N_{\text{DAE}}$. For staged separation processes, large parts of the Jacobian matrix are identical to zero. The sparsity pattern of the Jacobian matrix shows which entries may be non-zero, or in other words,
2.8 Implementation of the Dynamic Model

on which algebraic variables and state variables the balance equations and algebraic equations depend. If the sparsity pattern is provided, only the non-zero values have to be evaluated, which greatly speeds up the simulations.

2.8.3.1 Modeling a Distillation Column Using Ideal Stages

If a distillation column is modeled using the concept of an ideal stage, the vapor and the liquid leaving the tray are assumed to be in equilibrium. To determine the composition of the vapor leaving the tray, only the temperature, the pressure, and the component holdups of the tray investigated are necessary. As a consequence the derivatives of the component holdups and the tray enthalpy as well as the errors in the algebraic equations can only depend on the properties of the tray investigated, of the tray below (due to the influence of the incoming vapor), and of the tray above (due to the influence of the incoming liquid). The Jacobian pattern then takes on a block diagonal form, as shown in figure 2.2.

2.8.3.2 Modeling a Distillation Column Using Murphree Efficiencies

If a distillation column is modeled using Murphree efficiencies, the vapor leaving a tray is no longer in equilibrium with the liquid on the tray. The vapor composition then depends not only on the tray temperature, the tray pressure, and the tray component holdups, but also on the composition of the vapor leaving the tray below (which in turn depends on the temperature, the pressure, and the composition of that tray as well as the vapor leaving the tray below that tray and so on). As a consequence, the properties of any tray are influenced by the properties of all trays below that tray, leading to an upper triangular matrix for the Jacobian pattern, as depicted in figure 2.3. The calculation effort therefore is substantially higher than for a model using ideal stages.
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Figure 2.2: Pattern of the Jacobian matrix for a column model using ideal stages or vaporization efficiencies

Figure 2.3: Pattern of the Jacobian matrix for a column using Murphree efficiencies
2.8 Implementation of the Dynamic Model

2.8.3.3 Modeling a Distillation Column Using Vaporization Efficiencies

Vaporization efficiencies do not change the structure of the DAE system in comparison to the model that uses ideal stages. The advantageous block diagonal form of the Jacobian pattern shown in figure 2.2 is retained, leading to much shorter calculation times than when using Murphree efficiencies.

2.8.4 Scaling of the Nonlinear System

For simulation purposes the values for the state and algebraic variables should be of comparable size. Using the units that are most comfortable from an engineer’s point of view may not lead to the mathematically best scaling. For this reason the following units were chosen:

- Enthalpy in GJ
- Temperature in K
- Pressure in mbar
- Holdup in kg

2.8.5 Ensuring Physically Meaningful Values

The simulations showed that an important issue is to insure that only physically meaningful values can occur. The integration routine is not prepared to do boundary checking for algebraic or state variables, so the user has to take care of this task. The component holdups for components that only exist in traces are especially sensitive. If they take on (even small) negative values, the physical properties routines may deliver unexpected results. Just setting the component holdups to zero if a negative value occurs is not sufficient, however. If their derivatives become negative as well, the simulation routines abort as they fail to meet the simulation tolerances. Setting the corresponding derivatives to zero in this case enables the simulation to finish, unfortunately with substantially longer simulation times. Speed can be
2 Rigorous Model

Improved when the simulation tolerances are relaxed. In this case, however, the maximum step size has to be chosen very small, otherwise the simulation tends to get stuck at points where derivatives change sign: The step size is reduced repeatedly until the minimum allowed step size is reached, where the simulation aborts.

2.9 Summary

In this chapter, the equations describing the dynamic behavior and the physical properties of a distillation column have been introduced. Murphree and vaporization efficiencies are used to relate the real behavior of a distillation column tray to the behavior of an ideal stage. The complete dynamic model forms a DAE system which is solved using a multistep solver. To remain close to reality, mass flows are used as inputs instead of mole flows.
Real World Model

This chapter gives an overview of the special considerations which are necessary when a model is developed for a distillation plant that is already in use and not only in the planning stage. Several of the problems that can occur in this situation are shown, and possible solutions and methods for model improvements are explained.

3.1 Modeling Existing Distillation Plants

When modeling an existing distillation plant, the first step is the decision as to which kind of model to use. Generally, two main classes of models can be distinguished.

The first possibility is to obtain an experimental model by system identification techniques. Using purely mathematical methods, the input-output behavior of the system is analyzed and a model is created. An overview of methods suitable for distillation columns can be found in [27]. A case study on applying nonlinear identification techniques to a high-purity distillation column is described in [28].

In general, the following four main steps have to be performed:

1. Planning and performing of experiments
3 Real World Model

2. Selection of a suitable model structure (e.g. ARMAX, ARX, Hammerstein [29])

3. Estimation of parameters

4. Validation of the model

Repeated application of these steps theoretically leads to a suitable model. In practice, however, repetition of dynamic tests may not be possible for a production plant, because the normal operation process would be disturbed, so the experiment should be designed to obtain all the necessary data in a short time; only steps two to four can be iterated in this case.

The behavior of linear systems can be described well by these models, and in many cases even the use of a linear model for a nonlinear system leads to good results.

If a nonlinear model is desired or necessary, however, the selection of the model structure becomes a difficult task. Knowledge of the processes taking place in the system has to be used to find a suitable structure, and the number of iterations necessary for obtaining a usable model rapidly increases.

A model with an unsuitable structure can never represent the reality well, no matter which parameters are used. For this reason the use of neural networks has become popular: They do not require a-priori assumptions on the structure. Unfortunately this method has the drawback that a large data set has to be available for training the networks, a condition that may be hard to fulfill for a production plant.

The main disadvantage of these purely experimental models is the fact that they represent the system by a black box. No insight on the processes taking place in the system is available, and the parameters used no longer have any physical meaning. No prediction is possible of what happens outside of a small neighborhood of the region in which the model was obtained, or how the change of certain operating parameters influences the model.

The second main type of model is the theoretical model: The physical and chemical processes which are relevant for the system behavior are identified and described using balances, thermodynamic relation-
3.1 Modeling Existing Distillation Plants

The models obtained this way are called *white box* models, if all the necessary parameters are known. This approach results in models like the rigorous model described in chapter 2.

The modeling of distillation columns as staged processes has a long tradition. In the early years, only steady-state behavior was investigated. These simulations were used for column design and optimization. Later the availability of computers made it possible to cover the dynamic behavior as well [4]. This kind of rigorous models is easily interpretable, but it also exhibits fundamental disadvantages. In addition to the considerable modeling effort, it also heavily depends on the availability of parameters for calculating physical properties and tray hydraulics. For simple systems or laboratory situations, this may not be a matter of concern, but for a real production plant it may lead to the following problems:

- Physical properties data is incomplete, inaccurate, or not available at all.
- Only some of the components that are involved in the process are known.
- Although parameters used for column design may be available (pressure drop coefficients, hydraulic parameters, …), they do not necessarily match the values of the actual plant.

To overcome these problems, often a *gray box* model is used for describing existing distillation plants. It combines the structure of the rigorous model with fitted parameters, thereby exploiting the advantages of both types of models.

Prerequisite for any model is the availability of reliable plant data. In the chemical process industries, however, the following situation is commonly encountered:

- Composition analysis data is available only for a subset of components.
- Measurement data is not available with the accuracy desired for modeling purposes.
Methods for composition analysis are not properly verified.

Performing experiments is time consuming and not always possible, as the constraints for product quality must *always* be met.

For large columns and systems with many components the size of the model is prohibitive for simple data fitting.

Only if each of these problems is solved, a usable model will result. When a distillation plant is modeled using a rigorous model, the first challenge consists of selecting the set of equations which is suited best for the system investigated. This requires making the proper simplifying assumptions to include only those details that are absolutely necessary for the purpose of the model. After successfully mastering this step, a set of parameters has to be found which makes the model represent reality. This constitutes the second challenge in the modeling process. For these reasons obtaining an adequate dynamic model is responsible for about 80–90% of the total work when using model based control [30].

At the beginning of the modeling process, however, the results are often far from being usable. An example of the results from the initial phase of modeling the distillation plant examined in this project is depicted in figure 3.1. It shows measured values for the mole fraction of the main component, as obtained from analyzing liquid samples taken from trays of the second column. The simulated values were obtained by performing a stationary simulation of the complete plant using ASPENPLUS, with the ten most important components included that had been named by the project partner. Both columns were simulated using Murphree tray efficiencies. Wilson activity coefficients were selected for describing the non-ideal behavior of the liquid phase.

When trying to come up with a usable model which matches plant data, checking the following items is recommended:

- Streams
- Components
- Profiles
3.2 Checking Streams

Modeling of a chemical production plant often starts from steady-state data, which is readily available in many cases today. However these data sets cannot be used for simulation without pre-processing. The values of flow measurements contradict each other in most cases, violating the basic requirement that steady-state data has to fulfill the steady-state balances. The following questions have to be asked:

- Is the plant in a stationary point during the measurement?
- Does the measurement data contain (large) errors?

In all of these steps steady-state data is used, because dynamic data is difficult to obtain, and the dynamic model has to match the results of stationary measurements as well. All simulations in this stage of the project were performed using the RADFRAC model of ASPENPLUS, while the dynamic model was implemented afterwards using a combination of MATLAB [31] and C, as discussed in chapter 2.
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For process units that are part of a large plant, the properties of the feed are influenced by upstream process units and cannot be controlled tightly. Even if the dynamics are slow, their influence may be increased by the fact that taking samples simultaneously is not always possible, as obtaining samples takes some time, and the sampling locations are not always close to each other.

Even if true steady-state is reached, measurement errors and noise cause differences between the real values and the measurement results. As an example the errors in the mass balances for column 1 and column 2 when using the data obtained from measurement 1 are shown in table 3.1.

When data reconciliation techniques are used, an attempt can be made to remove the errors from the measurement data and to estimate the true values of the measured variables by applying statistical methods (maximum likelihood estimations) and least-square optimizations [32]. For a complex plant with many components, large columns, and additional couplings by recycles, this purely mathematical method soon comes up against its limiting factors. Even though modern flowsheeting programs provide routines for data reconciliation, they are not able to arrive at an improved data set in this case. The underlying algorithms and routines cannot be inspected, so investigating the reason for a failure is not possible. Specifically influencing the outcome of the reconciliation runs therefore turns into a time consuming and inefficient process of trial and error.

<table>
<thead>
<tr>
<th>Table 3.1: Error in mass balance (measurement 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>column 1</td>
</tr>
<tr>
<td>total mass flow to column (kg/hr)</td>
</tr>
<tr>
<td>total mass flow from column (kg/hr)</td>
</tr>
<tr>
<td>difference (kg/hr)</td>
</tr>
</tbody>
</table>
Substantial progress can be made, however, by applying physical reasoning and checking component streams, as the following example shows: The distillate stream can never contain more low boiling components than the complete amount of low boiling components entering the system. If the measurements do not agree with this fact, either the composition or the flow of the streams involved are wrong. Careful inspection and adjustment of the values may lead to more improvements than using highly sophisticated mathematical methods, although several iterations may be necessary.

3.3 Checking Components

When investigating a distillation process, the components involved play a key role, as their physical properties determine the behavior of the separation. Even though this may seem like a trivial fact, in reality the set of components used for simulations often needs thorough checking: For the company running a distillation plant, only a few components may be of importance, as only these components have to meet product specifications, for selling purposes, for environmental reasons, or for making other subsequent processing steps possible. In many cases, only these components are known and it is only for them that methods for composition analysis exist. A common problem is the fact that using gas chromatography does not reveal mass fractions directly: Care has to be taken that the necessary weighting factors for converting area percent into mass percent have been determined with the necessary accuracy. Even though additional components may be important for the simulation of the system, they may be unknown or not characterized with the necessary precision.

The main components for the system investigated were named by the project partner. Initial simulations soon showed, however, that this set of components was unsuitable for reproducing the steady-state measurement data available. The compositions in the product streams of column 1 showed negligible deviations from the measurements; for column 2, where the main product is removed as a side stream, the
product compositions contained large errors, and the profiles did not match the measurements.

These differences were explained as follows: According to the simulations, all the components with a boiling point lower than the main component are removed in the first column. The main component is the component with the lowest boiling point for the mixture separated in the second column. As a result the distillate and the side stream consist of pure main component in the simulation. In reality, as shown by gas chromatography analyses, a group of components is present with a boiling point that lies slightly below the boiling point of the main component; these components leave the second column in the distillate and in the side stream, leading to a main product that contains a certain amount of impurities. When the selected set of components is not chosen properly, matching the real plant behavior is impossible, regardless of the parameter values used. Finding a representative component and adding it to the simulations therefore greatly improved the matching.

3.4 Checking Profiles

Even using corrected measurement data and an improved set of components does not guarantee that the simulation results match the profile measurement data. For the first column, the simulated product compositions show good agreement with the measured data. As the main product is taken from the second column, the first column was not investigated any further. For the second column, however, the product compositions in the simulations showed a much higher purity than the measurement, indicating an easier separation—a column with only a few trays would be sufficient according to the simulations.

The standard solution that is usually suggested if this kind of mismatch occurs is to use the Murphree efficiency $\eta_M$ and adjust its value until the simulated column profile matches the measurements. Simulations with various values for $\eta_M$ were performed, but in our case this approach did not prove successful. The behavior of the real plant could not be reproduced using Murphree efficiencies. Obviously this
type of efficiency was not able to represent the deviation of the real system from ideal behavior in this case.

Another possible reason for profile mismatch are unsuitable VLE models or parameters. In our case, the simulated system showed a more ideal behavior than the real system. As the main part of the non-ideal behavior is described by the activity coefficients, VLE measurements can be used to improve the parameters characterizing these coefficients [33].

The model used for the activity coefficients was the Wilson model (see section 2.6.2.2), which had been chosen due to theoretical considerations. The core of the Wilson model consists of the binary interaction parameters $\Lambda_{ij}$, which are defined as follows:

$$\ln \Lambda_{ij} = a_{ij} + \frac{b_{ij}}{T}$$ (2.47)

The standard approach for identifying the interaction constants $a_{ij}$ and $b_{ij}$ is performing a series of experiments with binary mixtures. As $a_{ij} \neq a_{ji}$ and $b_{ij} \neq b_{ji}$, this rapidly leads to a large number of experiments for an increasing number of components. Assuming $N$ components, the number $N_P$ of parameters required can be calculated as

$$N_P = 2N(N - 1)$$ (3.1)

A more attractive way seems to be fitting multiple interaction constants simultaneously using multicomponent VLE measurements. This approach was applied successfully to pseudo-measurements: A simulation of the plant was performed and using the results, vapor and liquid equilibrium compositions were obtained from the column profile of the second column. Together with the simulated temperatures and pressures, this data set was used for fitting all necessary interaction parameters at once. When investigating the real plant, several mixtures using samples taken from the second column were prepared and VLE measurements were performed. The data obtained this way was then used for fitting binary interaction parameters, but no real improvement could be achieved: Independently of the routine and the simulation parameters chosen, the optimization aborts after a few steps because the step width approaches zero.
3 Real World Model

Therefore a different method for describing the VLE was chosen. In chapter 2 the following relationship for the VLE has been introduced:

\[
y_i = \frac{\gamma_i f_i^0}{\varphi_i^p} x_i = K_i^{\text{VLE}} x_i
\]

(2.51)

The equilibrium constant \(K_i^{\text{VLE}}\) is a function of temperature, pressure, and composition. Vaporization efficiencies have been defined as follows:

\[
y_{k,i} = \eta_{\text{vle}} y_{k,i}^{eq} = \eta_{\text{vle}} K_{k,i}^{\text{VLE}} x_{k,i}
\]

(2.27)

Examination of the elements forming the equilibrium constant shows that the main part of the non-ideality stems from the activity coefficients \(\gamma\), whereas the vapor phase fugacities are close to one, indicating nearly ideal behavior. For this reason, the decision was made to combine all the non-ideality in the vaporization efficiency and use an ideal VLE constant:

\[
y_{k,i} = \eta_{\text{vle}}(x, T) \frac{p_i^0}{p} x_i = \eta_{\text{vle}}(x, T) K_{i}^{\text{VLE, id}} x_i
\]

(3.2)

Using these considerations the vaporization efficiency in principle depends on composition and temperature. An interesting approach for finding a relationship between compositions and vaporization efficiencies is the use of neural networks: Their advantage consists of the fact that no knowledge of the structure of the dependency is required; their disadvantage, however, is the fact that a large amount of data is necessary for being able to train the networks. After fitting vaporization efficiencies as described in the next section, a neural net was trained which related the efficiency values to the liquid compositions on the trays. Although the training data could be reproduced satisfactorily, prediction performance was poor: Changing the composition values by small amounts led to large changes in the vaporization efficiencies predicted, which made this model unsuitable for simulation purposes.

For the following steps therefore the simplifying assumption is made that the vaporization efficiencies are only temperature depen-
dent. This has the advantage that fewer parameters have to be estimated from the limited set of data available. The simulation results presented in section 3.4.1.3 show that this assumption is justified, as the simulation profiles match the measured profiles in different operating points.

### 3.4.1 Estimating Temperature Dependent Vaporization Efficiencies

To find the relationship between \( \eta_{vi} \) and temperature, profile measurements of the second column are used. Theoretically, a function, e.g. a polynomial, could be fitted for each component, trying to match the measurement data using optimization and data fitting techniques available in the simulation package used. However, these one-step methods fail if a large number of components, trays, and parameters is present. Therefore a different, multi-step approach was chosen.

#### 3.4.1.1 Preparation of Measurements

As the results for the first column showed good agreement with the measurements, emphasis was laid on the second column. Profile data for compositions and temperatures was available, but only for a few trays. Efficiencies had to be calculated for all trays, so an interpolation using splines was performed to obtain an estimation of the missing data. For this purpose it was assumed that the profiles do not exhibit any discontinuities between the points of measurement. As an example, the measurement data and the interpolated values for the main component are shown in figure 3.2.

#### 3.4.1.2 Fitting Vaporization Efficiencies

The profiles generated by interpolation are combined with the real measurement data for subsequent data reconciliation runs (using a least square algorithm), in which the complete plant is simulated. Initially, vaporization efficiencies for all components present in the sec-
ond column were fitted for all trays. Simulations showed that the column profiles are hardly influenced by the vaporization efficiencies of those components that are only present in traces. In addition, the efficiencies of the two components with the highest boiling points did not show any significant influence on the profiles either. For this reason, the efficiencies for all of these components were set to one.

The values of the vaporization efficiencies fitted for the remaining components present in the column, however, vary strongly from tray to tray. Even though discontinuities for Murphree efficiencies have been reported (see [13] for an overview), no such information was found for vaporization efficiencies. In addition, a closed mathematical form for describing the vaporization efficiencies is aimed at, which is more difficult to achieve if smoothness is lacking. For this reason, the fitted value for tray $k$ is replaced by the average vaporization efficiency of trays $(k - 1)$ to $(k + 1)$. Some outliers are manually adjusted. These new values are then used as starting values for the next data reconciliation run, which after some iterations leads to a usable, smooth set of efficiencies.
3.4.1.3 Formulating the Relationships

Vaporization efficiencies have now been fitted for each tray. A numerical set of efficiencies for all trays is good enough for many applications. Dynamic simulations used for controller design, however, also involve changes of operating points and flow schemes, which could render these values unusable. Therefore a closed mathematical form is desired, providing enough flexibility. In principle, any kind of equation could be used to relate the efficiencies to temperatures, but the relationship chosen has to meet several requirements:

- Smoothness
- No unrealistic values for temperatures outside the fitting range
- Easy fitting is possible
- Programming of the function in C and FORTRAN is possible

Third-order splines were selected because of the smoothness of their derivatives, which avoids discontinuities that could result in problems with dynamic simulations. For temperatures below the value at the column top, the efficiencies calculated at the top temperature are used. The same procedure is used at the column bottom, using the bottom temperatures and efficiencies, respectively. This ensures that no unrealistic values can occur. As splines are essentially polynomials, programming is straightforward. For fitting, the MATLAB Spline Toolbox [34] was used which provides an easy-to-use interface to the algorithms needed. The efficiencies obtained in the stationary runs and the splines fitted to represent them are shown in figures 3.3–3.6. The peaks coincide with the feed and product locations, respectively. Note that the efficiency values are kept constant at high temperatures for the intermediate component and at low temperatures for the heavy component 2: The exact values are not important in this range, as the amount of component present is zero.

No prediction can be made as to how the values of the vaporization efficiencies influence the VLE as the example in table 3.2 shows. The pressure and the vaporization efficiencies were kept constant in these
3 Real World Model

Figure 3.3: Efficiencies of the intermediate component

Figure 3.4: Efficiencies of the main component
3.4 Checking Profiles

Figure 3.5: Efficiencies of the heavy component 1

Figure 3.6: Efficiencies of the heavy component 2
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calculations, and the liquid mole fractions were varied. A value of \( \eta_v > 1 \) enlarges the ratio \( y'_i/x_i \). But the new vapor compositions also have to fulfill the bubble point equation:

\[
\sum_{i=1}^{n} y'_i(p, T) = 1
\] (3.3)

The change of the equilibrium constant will therefore cause a change of the bubble point temperature, which in turn can increase or decrease the vapor mole fraction of the corresponding component, depending on the combination of values chosen. The vapor compositions are calculated using the following relationship:

\[
y'_i = \eta_v \frac{p^c_i(T'_\text{bub})}{p} x_i
\] (3.4)

and

\[
y_i = \frac{p^c_i(T\text{bub})}{p} x_i
\] (3.5)

The boiling points \( T_{\text{bub}} \) and \( T'_{\text{bub}} \) are calculated by solving the boiling point equation for the respective temperature.

Using external FORTRAN functions, the splines describing the vaporization efficiencies were included in the ASPENPLUS simulations. A comparison of the measurement and steady-state simulation results obtained this way can be found in figures 3.7–3.10. Especially in the top section, where the main product leaves the column as a side stream, the new model shows very good matching performance. The large improvement for the main component is clearly visible when the original simulation shown in figure 3.1 and the new simulation in figure 3.8 are compared.

In order to test if the formulation of vaporization efficiencies has the necessary flexibility, simulations using a second set of measurement data were performed. The operating point used for verification (denoted measurement 2) is characterized by a smaller total flow of the main feed to column 1 (approximately 85% of its value in measurement 1). These simulation results are shown in figures 3.11–3.14.
3.4 Checking Profiles

**Figure 3.7:** Mole fraction of the intermediate component (measurement 1)

**Figure 3.8:** Mole fraction of the main component (measurement 1)
3 Real World Model

![Graph of Heavy Component 1](image1)

- Figure 3.9: Mole fraction of the heavy component 1 (measurement 1)

![Graph of Heavy Component 2](image2)

- Figure 3.10: Mole fraction of the heavy component 2 (measurement 1)
3.4 Checking Profiles

Figure 3.11: Mole fraction of the intermediate component (measurement 2)

Figure 3.12: Mole fraction of the main component (measurement 2)
3 Real World Model

Figure 3.13: Mole fraction of the heavy component 1 (measurement 2)

Figure 3.14: Mole fraction of the heavy component 2 (measurement 2)
Table 3.2: Influence of vaporization efficiency values on vapor compositions, calculated using $\eta_v = 1$ for the intermediate component, $\eta_v = 10$ for the main component and $\eta_v = 2$ for the heavy component.

<table>
<thead>
<tr>
<th>component</th>
<th>$T_{\text{bub}}$</th>
<th>$T'_{\text{bub}}$</th>
<th>$x$</th>
<th>$y$</th>
<th>$y'$</th>
<th>result</th>
</tr>
</thead>
<tbody>
<tr>
<td>intermediate</td>
<td>360.2</td>
<td>333.2</td>
<td>0.152</td>
<td>0.372</td>
<td>0.136</td>
<td></td>
</tr>
<tr>
<td>main</td>
<td>360.2</td>
<td>333.2</td>
<td>0.277</td>
<td>0.297</td>
<td>0.699</td>
<td>increase</td>
</tr>
<tr>
<td>heavy 1</td>
<td>360.2</td>
<td>333.2</td>
<td>0.571</td>
<td>0.331</td>
<td>0.165</td>
<td></td>
</tr>
<tr>
<td>intermediate</td>
<td>345.9</td>
<td>333.7</td>
<td>0.571</td>
<td>0.841</td>
<td>0.521</td>
<td></td>
</tr>
<tr>
<td>main</td>
<td>345.9</td>
<td>333.7</td>
<td>0.152</td>
<td>0.080</td>
<td>0.397</td>
<td>increase</td>
</tr>
<tr>
<td>heavy 1</td>
<td>345.9</td>
<td>333.7</td>
<td>0.277</td>
<td>0.079</td>
<td>0.082</td>
<td>increase</td>
</tr>
<tr>
<td>intermediate</td>
<td>352.4</td>
<td>324.3</td>
<td>0.277</td>
<td>0.518</td>
<td>0.168</td>
<td></td>
</tr>
<tr>
<td>main</td>
<td>352.4</td>
<td>324.3</td>
<td>0.571</td>
<td>0.421</td>
<td>0.806</td>
<td>increase</td>
</tr>
<tr>
<td>heavy 1</td>
<td>352.4</td>
<td>324.3</td>
<td>0.152</td>
<td>0.061</td>
<td>0.026</td>
<td></td>
</tr>
</tbody>
</table>

This second operating point leads to a different shape of the composition profiles especially in the top section of the column. Nevertheless, the matching between simulated and measured profiles is good in this section, where the main product is removed. In the middle, the differences between simulation and measurement increase, but the situation improves again in the bottom column section.

The profile of the main component shows a noticeable increase of the liquid mole fraction in the middle part of the column (instead of the expected decrease), followed by a sudden decrease at the feed location on tray 48. Simulations using ideal properties with Murphree efficiencies and Wilson activity coefficients with Murphree efficiencies revealed, however, that these models exhibit a similar behavior, as can be seen in figure 3.15. Obviously, the shape of the profile is not caused by the use of vaporization efficiencies.

After testing the steady-state model in two operating points, the formulation for vaporization efficiencies was implemented in the dynamic model, leading to a flexible nonlinear model of the plant.
3 Real World Model

![Figure 3.15: Comparison of different simulation methods for measurement 2](image)

3.5 Summary

This chapter has given an overview of model types suitable for distillation models. Gray box models that combine the structure of a model based on physical relationships with experimentally determined parameters are favored for existing distillation plants. Checking the stream measurements, the set of components used, and the profiles are essential steps in obtaining realistic results. As a new approach, spline functions relating vaporization efficiencies to temperature are used to capture the non-ideal behavior of the plant, which leads to a model that is able to match the steady-state behavior of the distillation plant in two different operating points, providing the necessary flexibility for subsequent dynamic simulations.
This chapter will explain the different steps needed to create a linear dynamic model that is suitable for controller design, starting from the model developed in chapters 2 and 3. Methods for scaling and order reduction are introduced and compared.

4.1 Introduction

Rigorous models used for testing control configurations as well as plant strategies are used as a replacement for the real plant in many cases. These detailed models, which contain many differential, algebraic and sometimes also partial differential equations, are usually unsuitable for the controller design process itself, which has different requirements:

Linearity Many methods that are widely used today need a linear process model. Recently, however, several examples of controllers based directly on nonlinear models have been published as well. See [35] for an overview of different methods.
4 Simplified Models for Controller Design

**Low order** Model based methods of controller design, as e.g., $H_\infty$ and LQG, provide controllers with an order at least as high as the order of the plant. The capabilities of process control systems, however, seldom allow for the implementation of such complicated systems. One way to circumvent this is to reduce the order of the calculated controller by numerical techniques. High-order plant models, however, also cause prolonged calculation times and are prone to numerical difficulties in the design process.

**Ordinary differential equations** For controller design, partial differential equations have to be approximated by ordinary differential equations.

In the following we will concentrate on the first two properties, as partial differential equations are not part of the column models used in this project.

Two main methods can be distinguished for arriving at a linear, low-order process model:

1. Using simplifying modeling assumptions (*Physical Simplification*)
2. Using purely mathematical methods (*Mathematical Simplification*)

In many cases both methods are combined: First the order of the model is reduced by simplifying assumptions, then the model is linearized numerically.

## 4.2 Simplification Methods

### 4.2.1 Physical Simplification

Using process knowledge, simplifying assumptions can reduce the order and complexity of the process model. They may also lead to linear models at the same time.
4.2 Simplification Methods

4.2.1.1 Neglecting Dynamic Processes

Assumptions can help to eliminate some of the state variables. Examples are:

1. Negligible vapor holdup
2. Fast vapor energy dynamics
3. Fast flow dynamics
4. Fast liquid energy dynamics

Assumptions 1 and 2 are more or less standard in distillation publications, because the interest is focused on composition dynamics and control. Assumption 3 is only reasonable if composition dynamics are much slower than flow dynamics. Assumption 4 changes the energy balance on each tray from a differential equation to an algebraic equation. See [4] for a detailed overview.

4.2.1.2 Reducing the Number of Components

Even if several simplifying assumptions are applied, the model can still be of very high order if a large number of components is present. Two different approaches exist to reduce the number of components in this case:

In the first one, some components are lumped together, resulting in so-called pseudo-components. In this case, balances are written only in terms of these pseudo-components. The main problems are the selection of the components and the calculation of the physical properties.

The second approach tries to apply continuous thermodynamics to the modeling of the distillation process. This method replaces the discrete values of mole fractions by continuous distribution functions, which are then used for calculating the physical properties [36]. The successful application to steady-state multicomponent distillation has been reported [37], and an extension to distillation dynamics is expected.

In general, the methods of continuous thermodynamics are suited well for mixtures with a large number of components (e.g. petroleum
fractions) but not for mixtures with less than ten components. For the latter, pseudo-components should be used.

4.2.1.3 Reducing the Number of Stages

For reducing the number of stages, usually the dynamics of a number of stages is approximated by the dynamics of a smaller number of pseudo-stages.

In this case a distillation column is considered as a compartmental system [38], in which several stages are lumped together to form an equivalent stage. The resulting low-order model is nonlinear. It preserves material balances and steady-state gains. The model parameters are not just arbitrary numbers but they are related to the process. The main problem lies in finding rules on how to divide a given column into compartments. Besides that, the simplified model can show fundamentally different dynamics (inverse responses that have not been observed in the full model).

A modification of this approach is suggested in [39]. For a system with \( n \) components, the component material balances are written for each tray, resulting in \((n - 1)\) equations per tray, but only one differential equation is used for the total holdup in the compartment. The following assumptions are made:

- The total holdup is of the same size on all trays in a compartment.
- Vapor and liquid flows within one compartment are uniform.
- The temperature profiles between adjoining reference trays are linear.
- The pressure drop over each tray in a compartment is equal to the pressure drop over the sensitive tray of that compartment.

With these assumptions, the equations for total holdup, bubble point, flow dynamics and pressure drop only have to be solved once for each compartment. Feed trays and trays with side streams have to be regarded as “one-tray compartments”. With this method, Murphree tray
efficiencies can be used in calculations without producing any erroneous inverse response. Results show good steady-state and dynamic agreement between simulations and measurement data.

Another approach involves the reduction of the models using orthogonal collocation methods, as reported in e.g., [40, 41] (for more information see [27]). The advantages are that the resulting model retains the nonlinearity, it can be used for multicomponent distillation, free choice of thermodynamic subroutines is possible, a full order solution is not necessary, and the computation time is reduced significantly. The main disadvantage is that gains are not retained exactly.

4.2.2 Mathematical Simplification

The type and the order of models can also be changed by purely mathematical methods.

To obtain a linear model and/or a low-order model, a system identification of the rigorous model in the time or frequency domain can be performed. In this case, the rigorous model takes the place of the real plant. System identification is widely covered by specialized literature; see [27] for an overview of methods and models especially suitable for distillation systems.

An alternative is the numerical linearization of the nonlinear rigorous model to arrive at a linear model. The order of this model can then be decreased by numerical model reduction. This is the procedure used in this project. Model reduction is also suitable for further reducing models obtained by system identification.

4.3 Linearization

4.3.1 Systems of Ordinary Differential Equations

The following equations represent a system of ordinary differential equations (ODE)

\[ \dot{x} = F(x, u) \]  
\[ y = H(x, u) \]
where $x$ denotes the state variables, $u$ are the input variables (disturbances, reference values), and $y$ are the measured variables. This system can be linearized in an operating point OP by differentiating all equations with respect to $x$ and $u$:

$$\dot{\tilde{x}} = \left( \frac{\partial F}{\partial x} \right)_{OP} \tilde{x} + \left( \frac{\partial F}{\partial u} \right)_{OP} \tilde{u}$$

$$\tilde{y} = \left( \frac{\partial H}{\partial x} \right)_{OP} \tilde{x} + \left( \frac{\partial H}{\partial u} \right)_{OP} \tilde{u}$$

where deviations from the operating point are denoted by using a tilde on top of the original name. Calculating partial derivatives analytically can be a difficult task for large systems. Therefore they are often approximated numerically, e.g., with 4th order difference formulas [42]:

$$\frac{\partial F(x)}{\partial x} = \frac{-F(x + 2h) + 8F(x + h) - 8F(x - h) + F(x - 2h)}{12h} + O(h^4)$$

where $h$ denotes the step width.

This approach is only useful if steps to both sides of the operating point are allowed. This assumption does not always hold for distillation columns. If component holdups are used as state variables, they may be zero at some tray for some component. In this case, further decrease of $x$ leads to physically impossible values. For this reason a two-point forward difference formula was chosen:

$$\frac{\partial F(x)}{\partial x} = \frac{F(x + h) - F(x)}{h} + O(h)$$

### 4.3.2 Systems of Differential and Algebraic Equations

Assume a system of differential and algebraic equations (DAE system) with index $\nu_d = 1$ (see section 2.8.1):
4.3 Linearization

\[ \dot{x} = F(x, z, u) \quad (4.7) \]
\[ 0 = G(x, z, u) \quad (4.8) \]
\[ y = H(x, z, u) \quad (4.9) \]

Note the similarity to the ODE system of equations (4.1)–(4.2). This system will now be linearized in a stationary operating point OP by differentiating all equations (4.7)–(4.9) with respect to \( x, z \) and \( u \):

\[
\dot{\tilde{x}} = \left( \frac{\partial F}{\partial x} \right)_{\text{OP}} \tilde{x} + \left( \frac{\partial F}{\partial z} \right)_{\text{OP}} \tilde{z} + \left( \frac{\partial F}{\partial u} \right)_{\text{OP}} \tilde{u} \quad (4.10)
\]
\[
0 = \left( \frac{\partial G}{\partial x} \right)_{\text{OP}} \tilde{x} + \left( \frac{\partial G}{\partial z} \right)_{\text{OP}} \tilde{z} + \left( \frac{\partial G}{\partial u} \right)_{\text{OP}} \tilde{u} \quad (4.11)
\]
\[
\tilde{y} = \left( \frac{\partial H}{\partial x} \right)_{\text{OP}} \tilde{x} + \left( \frac{\partial H}{\partial z} \right)_{\text{OP}} \tilde{z} + \left( \frac{\partial H}{\partial u} \right)_{\text{OP}} \tilde{u} \quad (4.12)
\]

For a system with index \( \nu_d = 1 \), \( \left( \frac{\partial G}{\partial z} \right) \) is invertible, so that equation (4.11) can be solved for \( \tilde{z} \):

\[
\tilde{z} = - \left[ \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial x} \right) \right]_{\text{OP}} \tilde{x} - \left[ \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial u} \right) \right]_{\text{OP}} \tilde{u} \quad (4.13)
\]

and can then be substituted for \( \tilde{z} \) in equations (4.10) and (4.12):

\[
\dot{\tilde{x}} = \left[ \left( \frac{\partial F}{\partial x} \right) - \left( \frac{\partial F}{\partial z} \right) \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial x} \right) \right]_{\text{OP}} \tilde{x} + \left[ \left( \frac{\partial F}{\partial u} \right) - \left( \frac{\partial F}{\partial z} \right) \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial u} \right) \right]_{\text{OP}} \tilde{u} \quad (4.14)
\]
\[
\tilde{y} = \left[ \left( \frac{\partial H}{\partial x} \right) - \left( \frac{\partial H}{\partial z} \right) \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial x} \right) \right]_{\text{OP}} \tilde{x} + \left[ \left( \frac{\partial H}{\partial u} \right) - \left( \frac{\partial H}{\partial z} \right) \left( \frac{\partial G}{\partial z} \right)^{-1} \left( \frac{\partial G}{\partial u} \right) \right]_{\text{OP}} \tilde{u} \quad (4.15)
\]
4 Simplified Models for Controller Design

4.3.3 Linearization of the Plant Model

4.3.3.1 Finding an Operating Point

For linearizing the rigorous dynamic model, a stationary operating point is chosen. The model has been programmed in a form that $F(x, z, u)$ (derivatives) and $G(x, z, u)$ (algebraic equation errors) are calculated for any given set of $x$, $z$, and $u$. Finding a stationary point is equivalent to solving the following equation system:

$$0 = F(x, z, u)$$  \hspace{1cm} (4.16)
$$0 = G(x, z, u)$$  \hspace{1cm} (4.17)

where $u$ (inputs like feed properties, reboiler heat input, reflux flows) is specified. In principle a least-square solver could be applied to the function programmed for the dynamic model, solving it numerically for $x$ and $z$. In practice, however, the starting values for the solver have to be very close to the actual solution for the algorithm to succeed, which makes this method unattractive.

For this reason, a different approach is used: The rigorous model is equipped with proportional type level controllers. A stationary run using ASPENPLUS is performed and the results of this calculation are then used as initial values for the dynamic model. Note that, as the ASPENPLUS model equations are not the same equations as those used in the dynamic model, the stationary points of the two models differ, and the dynamic model is not in steady-state with these initial values. After a suitably long dynamic simulation time, a stationary point is reached, and the level controllers are removed.

As an alternative, simulations can be performed by mimicking startup behavior. The composition of the main feed is chosen as initial composition for the tray holdups. A linear pressure profile is assumed. Running the dynamic simulation is then similar to starting up the column. The advantage of this method is that no additional external program is needed for generating initial values. The disadvantage, however, is that, because the initial values are far away from the values reached for steady-state, the simulation times can be very long.
4.3 Linearization

4.3.3.2 Model Order

Assuming that the condenser does not have any holdup, the number of state variables per column can be calculated as follows:

\[
nx = n_{\text{component holdup}} + n_{\text{enthalpy}} = nc \cdot (nt - 1) + (nt - 1) = (nc + 1) \cdot (nt - 1)
\]  

(4.18)

where \( nc \) denotes the number of components and \( nt \) denotes the number of trays including condenser and reboiler. For an individual column with \( nt = 62 \) trays and \( nc = 12 \) components 793 state variables are present. Combining both columns therefore leads to a system with 1586 state variables.

The algebraic variables are the temperatures on the trays, in the condenser and the reboiler, and the pressures on the trays and in the reboiler. The condenser pressure is assumed to be constant (controlled by the vacuum pump). Altogether this leads to

\[
nz = n_{\text{temperature}} + n_{\text{pressure}} = nt + (nt - 1) = 2nt - 1
\]  

(4.19)

Again using \( nt = 62 \), the model of one column contains 123 algebraic variables. When both columns are combined, additional algebraic variables are necessary to describe the properties (compositions, pressure, and temperature) of the recycle loop:

\[
nz_{\text{recycle}} = nc + 2
\]  

(4.20)

The model of the complete plant therefore contains 260 algebraic variables. The information on the system size is summarized in table 4.1.

4.3.3.3 Linear Models

For the model of the complete plant, in a first attempt the rigorous dynamic model with both distillation columns was linearized numerically, using the techniques described above. This leads to a model of order 1586. The subsequent model reduction of this model failed due to excessive memory requirement and computing time.
4 Simplified Models for Controller Design

Table 4.1: System size

<table>
<thead>
<tr>
<th></th>
<th>one column</th>
<th>complete plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of state variables</td>
<td>793</td>
<td>1586</td>
</tr>
<tr>
<td>number of algebraic variables</td>
<td>123</td>
<td>260</td>
</tr>
</tbody>
</table>

Therefore a multistep approach was applied next: Both columns were linearized \textit{individually} in the operating point of the complete plant, leading to two linear models of order 793. For each model, scaling and order reduction were performed. Component mass flows, temperature, and pressure of the product streams were included as additional output variables. The individual scaled and reduced column models showed good agreement with the full linear model; after combining the two parts to the full plant, however, linear and nonlinear simulations did not match. The integrative behavior of the columns was suspected to be responsible for the problems; repeating the same procedure with level controllers included, however, did not improve the situation, so individual models of the columns with level controllers were created, and controllers were designed with these models.

For all models, the forward difference formula (4.6) was applied to evaluate the necessary derivatives numerically. To take into account the fact that the variables involved are of different orders of magnitude and may also become zero, the step width \( h \) is chosen to consist of an absolute and a relative part:

\[
h = \delta_{\text{abs}} \left( 1 + \delta_{\text{rel}} |x_{\text{OP}}| \right)
\]  

(4.21)

For choosing the best values of \( \delta_{\text{abs}} \) and \( \delta_{\text{rel}} \), the model of the first column without level controllers is linearized, using different combinations of \( \delta_{\text{abs}} \) and \( \delta_{\text{rel}} \). Then two simulations are performed with each model of this set of linear models:

1. The total flow of main feed is increased by 10%.
2. The component flow of the main component in the main feed is increased by 5%, while the component flow of the heaviest component is decreased by 5% (total flow remains constant).
Linear and nonlinear simulation results for important output variables (see table 4.2 for a complete listing) are compared, using the integral squared error $ISE$:

$$ISE_i = \int_0^{1\text{hr}} \left( y_{i,\text{lin}}(t) - y_{i,\text{nonlin}}(t) \right)^2 dt$$  \hspace{1cm} (4.22)

where $i$ denotes the output variable. The mass fraction in the distillate for the component with the highest boiling point (component 12) and the mass fraction in the bottom product for the six components with the lowest boiling points (components 1–6) were skipped, as their values are close to zero.

One hour is chosen as the integration limit to emphasize the importance of the initial response for control purposes, as recommended by [43]. To facilitate the comparison of the values, they have been scaled using the following relationship:

$$ISE_{\text{scal},i} = \frac{ISE_i - \min(ISE_i)}{\max(ISE_i) - \min(ISE_i)}$$ \hspace{1cm} (4.23)

The mean value is then calculated as follows:

$$\overline{ISE}_{\text{scal}} = \frac{1}{N} \sum_{i=1}^{N} ISE_{\text{scal},i}$$ \hspace{1cm} (4.24)

where $N$ is the number of outputs considered. Plots of $\overline{ISE}_{\text{scal}}$ values for both simulations individually as well as combined are shown in figures 4.1, 4.2, and 4.3. The numerical results can be found in tables 4.3, 4.4, and 4.5.

To ensure a good set of parameters for all simulations, the combination of $\delta_{\text{rel}}$ and $\delta_{\text{abs}}$ is chosen that shows the smallest $\overline{ISE}_{\text{scal}}$ for both simulations combined:

$$\delta_{\text{rel}} = 10^{-2} \quad \delta_{\text{abs}} = 10^{-4}$$ \hspace{1cm} (4.25)

Examples of simulation results for the linear system that has been linearized with these parameters and for the nonlinear system are shown in figures 4.4 and 4.5. They show good agreement. Column 2 was linearized using the same values for $\delta_{\text{rel}}$ and $\delta_{\text{abs}}$. 

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4 Simplified Models for Controller Design

Table 4.2: Output variables used for determination of linearization parameters

<table>
<thead>
<tr>
<th>place</th>
<th>variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>distillate</td>
<td>mass fraction component 1</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 2</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 3</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 4</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 5</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 6</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 7</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 8</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 9</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 10</td>
</tr>
<tr>
<td>distillate</td>
<td>mass fraction component 11</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 7</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 8</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 9</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 10</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 11</td>
</tr>
<tr>
<td>bottom product</td>
<td>mass fraction component 12</td>
</tr>
<tr>
<td>condenser</td>
<td>temperature</td>
</tr>
<tr>
<td>bottom product</td>
<td>temperature</td>
</tr>
<tr>
<td>reboiler</td>
<td>holdup</td>
</tr>
<tr>
<td>reboiler</td>
<td>pressure</td>
</tr>
</tbody>
</table>
4.3 Linearization

- Figure 4.1: $\bar{ISE}_\text{scal}$ for change of feed flow

- Figure 4.2: $\bar{ISE}_\text{scal}$ for change of feed composition
4 Simplified Models for Controller Design

Figure 4.3: $\overline{\text{ISE}}_{\text{scal}}$ for both simulations

Figure 4.4: Time response for simulation 1: change in mass fraction for heavy component 1 in bottom product
4.3 Linearization

Table 4.3: $\overline{{\text{ISE}}_{\text{scal}}}$ for change of feed flow

<table>
<thead>
<tr>
<th>$\delta_{\text{rel}}$</th>
<th>$10^{-5}$</th>
<th>$10^{-4}$</th>
<th>$10^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-5}$</td>
<td>0.096422</td>
<td>0.123475</td>
<td>0.487417</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.096164</td>
<td>0.122569</td>
<td>0.489402</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>0.096179</td>
<td>0.123821</td>
<td>0.510698</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>0.098556</td>
<td>0.133774</td>
<td>0.896835</td>
</tr>
</tbody>
</table>

Table 4.4: $\overline{{\text{ISE}}_{\text{scal}}}$ for change of feed composition

<table>
<thead>
<tr>
<th>$\delta_{\text{rel}}$</th>
<th>$10^{-5}$</th>
<th>$10^{-4}$</th>
<th>$10^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-5}$</td>
<td>0.581844</td>
<td>0.550760</td>
<td>0.404675</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.581762</td>
<td>0.549933</td>
<td>0.399859</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>0.580902</td>
<td>0.542201</td>
<td>0.357340</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>0.572428</td>
<td>0.463847</td>
<td>0.450987</td>
</tr>
</tbody>
</table>

Table 4.5: $\overline{{\text{ISE}}_{\text{scal}}}$ for both simulations combined

<table>
<thead>
<tr>
<th>$\delta_{\text{rel}}$</th>
<th>$10^{-5}$</th>
<th>$10^{-4}$</th>
<th>$10^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-5}$</td>
<td>0.339133</td>
<td>0.337118</td>
<td>0.446046</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.338963</td>
<td>0.336251</td>
<td>0.444631</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>0.338540</td>
<td>0.333011</td>
<td>0.434019</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>0.335492</td>
<td>0.298811</td>
<td>0.673911</td>
</tr>
</tbody>
</table>
4 Simplified Models for Controller Design

![Graph](image)

Figure 4.5: Time response for simulation 2: change in mass fraction for heavy component 1 in bottom product

4.4 Scaling

To prevent numerical problems, the linear systems have to be scaled appropriately. Starting point is the system obtained by linearizing the rigorous model:

\[
\frac{dx}{dt} = Ax + Bu \quad \text{(4.26)}
\]
\[
y = Cx + Du \quad \text{(4.27)}
\]

All variables can then be scaled by scaling matrices \(T\) that are usually diagonal:

\[
\hat{x} = T_x^{-1}x \quad \text{(4.28)}
\]
\[
\hat{u} = T_u^{-1}u \quad \text{(4.29)}
\]
\[
\hat{y} = T_y^{-1}y \quad \text{(4.30)}
\]
The scaled system is then described by

\[
\frac{d\hat{x}}{dt} = \hat{A}\hat{x} + \hat{B}\hat{u} = T_x^{-1}AT_x\hat{x} + T_x^{-1}BT_u \hat{u} \tag{4.31}
\]

\[
\hat{y} = \hat{C}\hat{x} + \hat{D}\hat{u} = T_y^{-1}CT_x\hat{x} + T_y^{-1}DT_u \hat{u} \tag{4.32}
\]

The scaled variables and the scaled state space matrices are identified by a tilde. A measure for the quality of scaling is the condition number \( \kappa \). For any matrix \( M \) of size \( n \times n \), the condition number is defined as the ratio between its maximum singular value \( \sigma(M) \) and its minimum singular value \( \sigma(M) \):

\[
\kappa(M) = \frac{\sigma(M)}{\sigma(M)} \tag{4.34}
\]

For control purposes a system with a condition number close to one is desirable: In this case, the gain does not depend on the direction of the inputs.

Various methods exist for choosing suitable scaling matrices. One approach is explained in [44]: Each variable is divided by its maximum expected or allowed change. This, however, does not always lead to satisfying results; the system can still be ill-conditioned, and for a large number of variables, the scaling values are not always obvious.

Another approach relies on purely mathematical methods. An optimization procedure is used to find the optimal set of scaling matrices to guarantee a low condition number over all frequencies. For systems with a large number of inputs and outputs, this leads to a large optimization problem. An easier way is to optimize the scaling matrices only for a frequency that is important for the behavior of the system, as e.g., for steady state or for the bandwidth frequency. The optimum scaling matrices are then calculated. The minimum condition number \( \kappa^*(M) \) that can be reached by scaling is defined as [45]

\[
\kappa^*(M) = \inf_{D_O,D_I \in \mathbb{R}^{n \times n}} \kappa(D_O M D_I) \tag{4.35}
\]

with the input scaling matrix \( D_I \) and the output scaling matrix \( D_O \).
4 Simplified Models for Controller Design

The following relationship holds:

$$\kappa^*(M) = \inf_{D, O, D_I \in D_{n \times n}^+} \sigma^2 \left( \begin{bmatrix} D_1^{-1} & 0 \\ 0 & D_0 \end{bmatrix} \begin{bmatrix} M^{-1} & D_1 \\ 0 & D_0^{-1} \end{bmatrix} \right)$$

$$= \inf_{D, O, D_I \in D_{n \times n}^+} \sigma^2 \left( D \begin{bmatrix} 0 & M^{-1} \\ M & 0 \end{bmatrix} D^{-1} \right)$$

$$= \inf_{D, O, D_I \in D_{n \times n}^+} \sigma^2 (DND^{-1}) \quad (4.36)$$

where $D$ and $N$ have been introduced as abbreviations for the respective matrices.

For positive diagonal matrices $D$ finding $\kappa^*(M)$ is a convex optimization, which therefore has only one minimum. A possible way to determine this minimum is using the function $\text{mu}$ from the MATLAB “Mu-Analysis and Synthesis Toolbox” (Mu-Tools [46]). This function is designed to calculate an upper bound of the structured singular value, a task which requires the same type of optimization. For nonsquare $M \in \mathbb{R}^{n_{\text{rows}} \times n_{\text{cols}}}$ the real inverse is not defined and the left or right inverse is used instead in this case.

$$M^{-1} \Rightarrow \begin{cases} 
M^T \cdot (MM^T)^{-1} & \text{for } n_{\text{rows}} < n_{\text{cols}} \\
(M^T M)^{-1} M^T & \text{for } n_{\text{rows}} > n_{\text{cols}}
\end{cases} \quad (4.37)$$

An interesting alternative has been presented in [47], where a computationally inexpensive method is shown for finding good scaling matrices without reaching the optimum value. In the first step, all inputs and outputs are divided by their steady-state values. Then scaling matrices are found iteratively: Start with $M_k = M$ which has a condition number of $\kappa_k$. Then repeat the following steps:

1. For each column $c_i$ of $M_k$, calculate the 2-norm $\|c_i\|$. The input scaling matrix $D_{Ik}$ is then defined by

$$D_{Ik} = (\text{diag}\{\|c_1\|, \|c_2\|, \ldots, \|c_{n_{\text{cols}}}\|\})^{-1} \quad (4.38)$$

2. For each row $r_i$ of $M_k$, calculate the 2-norm $\|r_i\|$. The output scaling matrix $D_{Ok}$ is then defined by

$$D_{Ok} = (\text{diag}\{\|r_1\|, \|r_2\|, \ldots, \|r_{n_{\text{rows}}}\|\})^{-1} \quad (4.39)$$
4.4 Scaling

3. Calculate the new system:

\[ M_{k+1} = D_{Ok} M_k D_{Ik} \quad (4.40) \]

4. Calculate the condition number:

\[ \kappa_{k+1} = \frac{\sigma(M_{k+1})}{\sigma(M_k)} \quad (4.41) \]

Continue with step 1 if \( \frac{\kappa_{k+1} - \kappa_k}{\kappa_k} > \epsilon \), else break.

The final scaling matrices are calculated as

\[ D_I = \prod_k D_{Ik} \quad (4.42) \]
\[ D_O = \prod_k D_{Ok} \quad (4.43) \]

The procedure rapidly converges and the difference between the calculated value of the condition number and the minimum condition number is small. The method is easy to use and it does not depend on specialized routines, so it was chosen for this project.

The system that has to be scaled contains the input and output variables as defined in section 1.1.1. The input variables consist of the reboiler heat input and the distillate flow for column 1 and the reboiler heat input, the distillate flow, and the side stream flow for column 2. The output variables for column 1 are the bottom pressure (which is equivalent to the column pressure drop) and the mass fraction of the main component in the distillate stream. For column 2 the output variables consist of the bottom pressure and the mass fraction of the main component in the distillate stream and in the side stream.

The desired closed-loop bandwidth was chosen as 0.01 rad/min. This corresponds to a time constant of 100 min. The scaling matrices for both columns were determined at the chosen closed-loop bandwidth.

Figures 4.6 and figure 4.7 show the singular values of the scaled and the unscaled systems. Figure 4.8 depicts the corresponding condition numbers, which have been decreased substantially.
4 Simplified Models for Controller Design

- Figure 4.6: Singular values for unscaled (left) and scaled system (right): Column 1

- Figure 4.7: Singular values for unscaled (left) and scaled system (right): Column 2
4.5 Model Reduction

4.5.1 Introduction

The goal of model reduction is approximating a dynamic system of high order by a low-order system which makes the maximum error over all frequencies (infinity norm) suitably small. For process control a low-order controller is required, which can be achieved using different methods:

**Controller reduction:** The full plant model is used for controller design and the controller is reduced afterwards [48].

**Plant reduction:** The plant model is reduced and the controller is designed using this simpler model.

Controller reduction is the preferred method, as in this case the full information about the dynamic behavior of the plant can be used for the design. For systems with several hundreds of state variables, however, this may lead to excessive computation times and numerical problems when solving the controller design equations. For this reason, the following three-step approach is chosen:
4 Simplified Models for Controller Design

1. Reduce individual linear column models to medium size
2. Design controller
3. Reduce controller

4.5.2 Mathematical Formulation

Let \((A, B, C, D)\) be a minimal realization of a stable system \(G(s)\). The state vector \(x\) of this system has the dimension \(n\) and can be split into two parts:

\[
x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}
\]  \hspace{1cm} (4.44)

where \(x_1\) are the \((n - k)\) state variables that are kept, and \(x_2\) are the \(k\) state variables that are to be eliminated. With appropriate partitioning of \(A, B, C, \) and \(D\), the state space representation can be written as

\[
\dot{x}_1 = A_{11}x_1 + A_{12}x_2 + B_1u \\
\dot{x}_2 = A_{21}x_1 + A_{22}x_2 + B_2u \\
y = C_1x_1 + C_2x_2 + Du
\]  \hspace{1cm} (4.45)

The reduced system then consists of the following equations:

\[
\dot{x}_1 = A_rx_1 + B_ru \\
y = C_rx_1 + D_ru
\]  \hspace{1cm} (4.46, 4.47)

Depending on the assumptions that are made for calculating \(A_r, B_r, C_r, \) and \(D_r\) the following methods can be distinguished [44]

- Truncation
- Residualization
4.5 Model Reduction

4.5.2.1 Truncation

For truncation those parts of the system matrices referring to the state variables \( x_2 \) are removed, so the reduced system is

\[
A_r = A_{11} \tag{4.48}
\]
\[
B_r = B_1 \tag{4.49}
\]
\[
C_r = C_1 \tag{4.50}
\]
\[
D_r = D \tag{4.51}
\]

The transfer functions of the reduced system and of the original system match at infinite frequency, as the \( D \) matrices are identical:

\[
\lim_{\omega \to \infty} G(j\omega) = \lim_{\omega \to \infty} \left( C(j\omega I - A)^{-1}B + D \right) = D \tag{4.52}
\]
\[
\lim_{\omega \to \infty} G_r(j\omega) = \lim_{\omega \to \infty} \left( C_1(j\omega I - A_{11})^{-1}B_1 + D \right) = D \tag{4.53}
\]
\[
\lim_{\omega \to \infty} G(s) - G_r(s) \leq \sum_{i=k+1}^{n} \frac{\sigma(c_i b_i^T)}{|\Re(\lambda_i)|} \tag{4.55}
\]

where \( k \) is the number of states removed. The variables \( c_i \) are the column vectors forming the \( C \) matrix and \( b_i^T \) are the row vectors forming the \( B \) matrix.
4 Simplified Models for Controller Design

Balanced Truncation State similarity transformations are used for balancing a system, which means that its controllability and observability Gramians $P$ and $Q$ are equal and diagonal:

$$P = Q = \text{diag} (\sigma_1, \sigma_2, \ldots, \sigma_n)$$  \hspace{1cm} (4.56)

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n > 0$ are the ordered Hankel singular values of $G(s)$. Each state variable of a balanced system corresponds to a Hankel singular value. A large Hankel singular value means that the corresponding state variable has a large influence on the input-output behavior of $G(s)$. For balanced truncation the states corresponding to the smallest Hankel singular values are removed.

A bound for the error norm is given by

$$\|G(s) - G_r(s)\|_\infty \leq 2(\sigma_{k+1} + \sigma_{k+2} + \cdots + \sigma_n)$$  \hspace{1cm} (4.57)

4.5.2.2 Residualization

Truncation discards selected states. Residualization sets the derivatives to zero for the states $x_2$ that are eliminated. The resulting equations are solved for $x_2$:

$$\dot{x}_2 = 0 = A_{21} x_1 + A_{22} x_2 + B_2 u$$  \hspace{1cm} (4.58)

$$x_2 = -A_{22}^{-1} (A_{21} x_1 + B_2 u)$$  \hspace{1cm} (4.59)

Substituting eq. (4.59) into the original state space equations (4.45) gives the following representation of the reduced system:

$$A_r = A_{11} - A_{12} A_{22}^{-1} A_{21}$$  \hspace{1cm} (4.60)

$$B_r = B_1 - A_{12} A_{22}^{-1} B_2$$  \hspace{1cm} (4.61)

$$C_r = C_1 - C_2 A_{22}^{-1} A_{21}$$  \hspace{1cm} (4.62)

$$D_r = D - C_2 A_{22}^{-1} B_2$$  \hspace{1cm} (4.63)

The steady-state gain is preserved as stationary behavior has been assumed for $x_2$, but the behavior for $\omega \to \infty$ is different from the original system. An important fact is that, even if the $D$ matrix of the original system is identical to zero, this does not have to be the case for the reduced system, as can easily be seen from equation (4.63).
4.5 Model Reduction

**Modal Residualization**  For modal residualization, the system is first transformed to Jordan form and then the derivatives of the fastest modes are set to zero.

**Balanced Residualization**  In balanced truncation, the least controllable and observable states are discarded. In balanced residualization, their derivatives are set to zero. The error bound for the balanced residualization is the same as for the balanced truncation (see equation (4.57)).

### 4.5.2.3 Optimal Hankel Norm Approximation

In this approach, the Hankel norm of the error between the original system and the reduced system is minimized, so the error is close to being unobservable and uncontrollable.

The Hankel norm of the error between $G(s)$ and the optimal approximation $G_r(s)$ is equal to the $(k+1)^{th}$ Hankel singular value of $G(s)$

$$\|G(s) - G_r(s)\|_H = \sigma_{k+1}(G(s))$$  \hspace{1cm} (4.64)

As the Hankel norm does not depend on the $D$ matrix of the system, the $D$ matrix can be chosen to reduce the infinity norm of the error as well. In this case the following relationship holds for the reduced model $G_r^D(s)$:

$$\sigma_{k+1} \leq \|G(s) - G_r^D(s)\|_\infty \leq \sigma_{k+1} + \sigma_{k+2} + \cdots + \sigma_n$$  \hspace{1cm} (4.65)

To improve the approximation in certain frequency regions, frequency weights $W_1$ and $W_2$ can be applied. In this case, the Hankel norm of $W_1^{-1}(G(s) - G_r(s))W_2^{-1}$ is minimized.

### 4.5.3 Implementation

Starting from the scaled linear model which has been obtained in sections 4.3 and 4.4, model reduction is performed using functions from
4 Simplified Models for Controller Design

Table 4.6: Number of state variables

<table>
<thead>
<tr>
<th></th>
<th>original system</th>
<th>balanced (default $\epsilon$)</th>
<th>balanced, stable</th>
<th>$\epsilon$ for stable system</th>
</tr>
</thead>
<tbody>
<tr>
<td>column 1</td>
<td>793</td>
<td>85</td>
<td>122</td>
<td>$6.48 \cdot 10^{-15}$</td>
</tr>
<tr>
<td>column 2</td>
<td>549</td>
<td>113</td>
<td>147</td>
<td>$7.62 \cdot 10^{-18}$</td>
</tr>
</tbody>
</table>

the MATLAB Mu-Tools [46], which were more reliable than the corresponding routines from the “Robust Control Toolbox” [49]. The following commands are available from the Mu-Tools:

- **sysbal** balancing systems
- **strunc** truncation of systems
- **sresid** residualization of systems
- **hankmr** optimal Hankel norm approximation

First, the system is balanced by **sysbal**, which uses the algorithm by Moore, described in [50]. The command requires the definition of a tolerance $\epsilon$: Any Hankel singular value less than $\epsilon$ is considered zero; the corresponding states are removed from the system by truncation. If the value chosen for this tolerance is too small, an unstable system can result, even though the original system is stable. The default tolerance chosen by MATLAB is

$$
\epsilon = \max(\sigma_1 \cdot 10^{-12}, 10^{-16})
$$

(4.66)

where $\sigma_1$ is the largest Hankel singular value of the system.

The size of the resulting systems when using different tolerances is shown in table 4.6. As stability is required for the different model reduction techniques, the tolerance is chosen to ensure stability while keeping the maximum number of states; its value is shown in the last column of table 4.6. In the case shown here, the default tolerance is sufficiently large. These considerations are important when using...
optimal Hankel norm approximation or residualization, where the reduced system may be unstable if the balanced system is unstable; it is not important for truncation (provided that the final order is smaller than the critical order), as the unstable part is removed in the truncation process.

Afterwards, the model of column 1 is reduced to 100 state variables, which is one eighth of the original size. This reduced model still contains the necessary dynamic information, but does not lead to problems with computation time and memory. Optimal Hankel Norm reduction, balanced truncation, and balanced residualization were performed.

Plots are shown for the $2 \times 2$ system containing the plant inputs and outputs used for control (inputs: reboiler heat, distillate rate; outputs: mass fraction of main component in distillate, bottom pressure). Step responses were calculated using the full linear model (without scaling) and the reduced models obtained with different methods. As an example, figure 4.9 contains the response of the distillate mass fraction of the main component to a step in the reboiler heat input. In addition the error in the response is shown in figure 4.10. It is calculated as

$$\text{error} = \Delta w_{\text{reduced model}} - \Delta w_{\text{full model}}$$

(4.67)

The step responses calculated using the model obtained by truncation and residualization cannot be distinguished from the response of the full model. Only the model obtained by optimal Hankel Norm reduction shows a larger error in the response. The responses of the other input-output combinations are of a comparable quality, so they are not shown here.

The singular values of the linear models obtained by different reduction methods are shown in figure 4.11, again they cannot be distinguished from each other. For controller design the model obtained by truncation was used, because this method leads to good representation of high frequencies, which are important for control.

In column 2, not all components are usually present (they have already been removed in column 1). This knowledge can be used to reduce the linear model before applying numerical reduction techniques: The inputs, outputs, and state variables of these components
4 Simplified Models for Controller Design

- **Figure 4.9**: Response of distillate mass fraction of main component to a one percent step in reboiler heat (column 1)

- **Figure 4.10**: Absolute error: Response of distillate mass fraction of main component to a one percent step in reboiler heat (column 1)
are removed by taking away the corresponding lines and columns of
the state space matrices, leading to a model of order 549.

The $3 \times 3$ system relevant for control contains the reboiler heat input,
the distillate and the side stream mass flow as inputs, and the mass
fraction of the main component in the distillate and in the side stream
and the column bottom pressure as outputs. As for column 1, this
model is reduced to approximately one eighth of the original number
of state variables, using the different reduction techniques discussed
above. The models obtained this way are of order 70. The response
of the mass fraction of the main component in the distillate product to
a one percent step of the reboiler heat input (using unscaled models)
is shown in figure 4.12 and again illustrates the good quality of the
reduced models. The error of the reduced models for the same step
response in shown in figure 4.13.

Again the step responses and the singular values which are shown
in figure 4.14 cannot be distinguished for the different types of models,
and the model obtained by truncation is chosen for controller design.
4 Simplified Models for Controller Design

Figure 4.12: Response of distillate mass fraction of main component to a one percent step in reboiler heat (column 2)

Figure 4.13: Absolute error: Response of distillate mass fraction of main component to a one percent step in reboiler heat (column 2)
4.6 Summary

In this chapter, a linear model suitable for controller design has been developed. After reaching a stationary operating point by using dynamic simulation, the column models have been linearized numerically, using a two-point forward difference formula. The condition numbers have been improved by scaling. Balanced truncation was shown to be a good method of model reduction for these models. These steps lead to a linear model with two inputs, two outputs and 100 state variables for column 1 and a model with three inputs, three outputs and 70 state variables for column 2.

Figure 4.14: Singular values for Column 2
The aim of this chapter is to design controllers using the models that have been developed in chapters 2 to 4. To obtain controllers that work in spite of modeling uncertainties, the $H_\infty$ method has been chosen, since it leads to robust controllers. After presenting the basic ideas of robust control, a set of controllers is designed and tested in simulations.

5.1 Introduction

The availability of fast computers encourages the use of simulation models for controller design and testing. As any model can only describe a part of reality, one of the main tasks of modern controller design is dealing with uncertainty. A good controller should therefore be robust, which means that it should still show good performance (robust performance) and stabilize the system (robust stability) in presence of uncertainty. This uncertainty can have several origins [27]:

- Parameters in the model are only known approximately or not at all.
5 Robust Control

- Measurement devices are not perfect; the controlled inputs are usually operated in a cascade manner, which gives rise to uncertainty in plant inputs.

- At high frequencies the behavior of the plant is often unknown.

- The parameters in the model can change with the operating point.

- The nonlinearity of the plant is not captured by the (often linear) model.

For this reason, several methods have been developed that try to ensure that the controller works well even if the real plant differs from the plant model used for controller design. The most important methods are

- LQG/LTR

- \( \mu \)-optimal control

- \( H_\infty \) control

The LQG/LTR method combines an optimal controller and a state observer to obtain stability and robustness. Static weights are used for the design of the controller, which makes it less flexible than \( H_\infty \) control, where dynamic weights are used. In addition, LQG/LTR may lead to high controller gains [44].

When using \( \mu \)-synthesis, frequency dependent uncertainty functions describe in detail the behavior of the uncertainties at different points of the plant. This leads to a structured uncertainty matrix which has non-zero elements only in the diagonal. Formulating the individual uncertainty functions requires a profound knowledge of the plant dynamics. \( H_\infty \) control on the other hand assumes an unstructured uncertainty matrix. \( \mu \)-synthesis leads to less conservative results than \( H_\infty \) control, but the effort needed is considerable and not always justified: The successful design and implementation of a controller for a binary distillation column is reported in [51], for which \( \mu \)-synthesis has been
5.1 $H_\infty$ controller design

used. The comparison of $\mu$-synthesis and $H_\infty$ control in [52], however, shows that results of the same quality can be obtained by $H_\infty$ with less effort.

Altogether the $H_\infty$ method offers a large amount of flexibility and quality while keeping the effort required at an acceptable level. For these reasons it was used in this project.

5.2 $H_\infty$ controller design

In the following section, the mathematical details will be kept at a minimum; mainly the ideas will be shown that are necessary for understanding the proceedings. For more background information the reader is referred to e.g. [44, 53–55].

Designing a continuous-time $H_\infty$ controller consists of several different steps:

1. Define scalar goals for the plant (maximum errors, settling times, etc.) that ensure good performance and robustness.

2. Translate these goals into the desired closed-loop transfer functions of the plant.

3. Use an approximate inverse of the desired transfer functions as weights.

4. Calculate the controller that keeps the maximum value of the weighted transfer functions below one for all frequencies.

Implementation usually requires discrete-time controllers. They can be obtained from the continuous-time controllers by different transformation methods as shown in [53]. In the following sections, however, only the four points mentioned above will be considered.

5.2.1 Mathematical Background

In figure 5.1, a general feedback system with disturbances is shown. The following names are used:
5 Robust Control

Figure 5.1: General feedback system with disturbances

- $K(s)$ transfer function of the controller
- $G(s)$ transfer function of the plant
- $r$ reference signal
- $e$ error
- $u$ control signal as calculated by the controller
- $d_i$ disturbance at the plant input
- $u_p$ control signal applied to the plant
- $d$ disturbance at the plant output
- $y$ plant outputs (controlled variables and possibly additional measured variables)
- $y_m$ measurements
- $n$ measurement noise

Different properties of the feedback system are characterized by closed-loop transfer functions, concentrating either on the plant input or plant output.

5.2.1.1 Input Transfer Functions

The behavior of the plant input is analyzed using the input sensitivity function $S_u$ and the input complementary sensitivity function $T_u$. The function $S_u$ shows how $d_i$ influences the control signal $u_p$ entering the
5.2 $H_\infty$ controller design

plant, whereas $T_u$ describes the influence of $d_i$ on the calculated plant input $u$ [54]. The term complementary reflects the fact that $S_u$ and $T_u$ are related by

$$S_u + T_u = I \quad (5.1)$$

They are defined as follows [55]

$$S_u = (I + KG)^{-1} \quad (5.2)$$

$$T_u = KG \left( I + KG \right)^{-1}$$

$$= K \left( I + G K \right)^{-1} G$$

$$= (I + KG)^{-1} KG \quad (5.3)$$

5.2.1.2 Output Transfer Functions

The plant output is analyzed using the output sensitivity function $S_e$ and the output complementary sensitivity function $T_e$. The function $S_e$ shows the influence of the disturbance $d$ on the plant outputs $y$, whereas $T_e$ shows the influence of the reference signal $r$ on the output $y$ of the plant. They are defined as follows [55]

$$S_e = (I + G K)^{-1} \quad (5.4)$$

$$T_e = G K \left( I + G K \right)^{-1}$$

$$= G \left( I + K G \right)^{-1} K$$

$$= (I + G K)^{-1} G K \quad (5.5)$$

with

$$S_e + T_e = I \quad (5.6)$$

5.2.1.3 Bandwidth

The closed-loop bandwidth is an important property of a controlled system. Bandwidth can be defined as the frequency range over which control is effective [44], or, if good steady state control is required ($\omega = 0$), as the upper bound of this frequency range.
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5.2.2 Goals and Closed-Loop Transfer Functions

The most important design objectives in feedback control can be summarized as follows:

1. Nominal stability: The controller must stabilize the nominal model.

2. Robust stability: The controller must stabilize a plant with deviations from the model used for controller design.

3. Good disturbance rejection (no influence of $d$ and $d_i$)

4. Good tracking performance of $y$ with respect to the reference signal $r$

5. No influence of measurement noise $n$

6. Small values of plant inputs $u_P$

7. Controller must be realizable.

Reaching these goals requires the sensitivity and the complementary sensitivity functions to take on certain shapes in different frequency ranges. The following equations help to illustrate this fact. The plant output $y$ can be expressed as

$$y = d + GK(r - n - y) + Gd_i \tag{5.7}$$

Solving for $y$ leads to

$$y = (I + GK)^{-1}(d + GK(r - n) + Gd_i)$$
$$= S_e d + T_e r - T_e n + S_e Gd_i \tag{5.8}$$

The controller output $u$ is calculated as follows:

$$u = K(r - n - d - Gd_i - Gu) \tag{5.9}$$
Solving for $u$ leads to

$$u = (I + KG)^{-1} K (r - n - d - G d_i) = K S_e (r - n - d - G d_i)$$  \hspace{1cm} (5.10)

Equations (5.8) and (5.10) translate performance and robustness requirements into corresponding requirements for the closed-loop transfer functions. For disturbance rejection, $S_e$ should be close to zero, as is visible from the first term of equation (5.8). This is important for low frequencies, as for high frequencies the sensitivity approaches unity and cannot be influenced. Good tracking performance means that $y$ closely follows $r$, which is only the case for $T_e \approx I$ (equation (5.8), second term). For small control signals, $K S_e$ should be kept small (equation (5.10)). As a result, calculating $H_\infty$ controllers becomes a loop-shaping procedure.

### 5.2.3 S/KS/T Loop Shaping Scheme

The S/KS/T scheme, which has been chosen for this project, is probably the best-known loop-shaping scheme. Its name stems from the fact that $S$, $K S$, and $T$ are shaped in the design process. A graphical representation of the plant and the necessary weights can be found in figure 5.2. When this method is used for controller design, the $H_\infty$ norm of the transfer function $T_{zr}$ is minimized:

$$T_{zr} = \begin{bmatrix} W_e S_e \\ W_u K S_e \\ W_y T_e \end{bmatrix}$$  \hspace{1cm} (5.11)

The second line is only present to fulfill mathematical prerequisites for the existence of a controller. In practice, $W_u$ is chosen small and constant, so it has no large influence on the $H_\infty$ norm.

The remaining weights that have to be chosen are $W_e$ and $W_y$. Both must be asymptotically stable.
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Figure 5.2: Augmentation scheme for shaping at the plant output

5.3 Controller Design for Column 1

5.3.1 Controller Inputs and Outputs

The manipulated and the controlled variables have already been defined in section 1.1.1:

**Manipulated variables:** Reboiler heat and distillate rate

**Controlled variables:** Pressure drop and mass fraction of the main component in the distillate

The column top pressure has been assumed constant, so controlling the pressure drop is equivalent to controlling the bottom pressure. It has been assumed that the bottom level is controlled by the bottom product flow.

5.3.2 Weights

The weights that have been chosen for the controller design are depicted in figure 5.3 together with the achieved singular values for $T_e$ and $S_e$. The mathematical representation of the weights is shown in
5.3 Controller Design for Column 1

Figure 5.3: Weights for controller design

equations (5.12)–(5.14). A closed-loop bandwidth of \( \omega_0 = 0.01 \text{ rad/min} \) has been assumed, with a corresponding time constant of \( \tau = 100 \text{ min} \).

\[
W_e = \begin{bmatrix} W_{e,i} & 0 \\ 0 & W_{e,i} \end{bmatrix} \quad \text{with} \quad W_{e,i} = \frac{0.5s + \omega_0}{s + 0.01\omega_0} \quad (5.12)
\]

\[
W_y = \begin{bmatrix} W_{y,i} & 0 \\ 0 & W_{y,i} \end{bmatrix} \quad \text{with} \quad W_{y,i} = \frac{s + 0.5 \cdot 10\omega_0}{0.001s + 10\omega_0} \quad (5.13)
\]

\[
W_u = \begin{bmatrix} 10^{-4} & 0 \\ 0 & 10^{-4} \end{bmatrix} \quad (5.14)
\]

5.3.3 Simulation Results

For testing the controller, a simulation was performed in which the total mass flow of the main feed was increased by 10\%. Figure 5.4
Figure 5.4: Change of main component distillate mass fraction in column 1 shows the change of the distillate mass fraction for the main product, and figure 5.5 depicts the bottom pressure, as simulated using

- the rigorous nonlinear model for column 1 *without* pressure and composition control (but with level control)
- the linear model *with* pressure and composition control
- the nonlinear model *with* pressure and composition control

The controlled variables settle fast and with only a small steady-state error. The linear and the nonlinear simulations lead to nearly identical results. The corresponding manipulated variables are shown in figures 5.6 and 5.7.
5.3 Controller Design for Column 1

![Figure 5.5: Change of bottom pressure in column 1](image)

Figure 5.5: Change of bottom pressure in column 1

![Figure 5.6: Change of manipulated variable (distillate flow rate) for column 1](image)

Figure 5.6: Change of manipulated variable (distillate flow rate) for column 1
5 Robust Control

Figure 5.7: Change of manipulated variable (reboiler heat input) for column 1

5.4 Controller Design for Column 2

5.4.1 Controller Inputs and Outputs

According to section 1.1.1, the manipulated and the controlled variables are

**Manipulated variables:** Reboiler heat, distillate rate, and rate of side stream

**Controlled variables:** Pressure drop, mass fraction of main component in distillate, and mass fraction of main component in the side stream

As for column 1, pressure drop and bottom pressure are equivalent, and the bottom level is controlled by the bottom product flow.
5.4 Controller Design for Column 2

5.4.2 Weights

The weights chosen for the controller design show dynamics similar to those chosen for column 1. They are displayed in figure 5.8 together with the achieved singular values for \( T_e \) and \( S_e \). The mathematical representation of the weights can be found in equations (5.15)–(5.17). To ensure a fast response, a closed-loop bandwidth of \( \omega_0 = 0.1 \text{ rad/min} \) has been assumed which corresponds to a time constant of \( \tau = 10 \text{ min} \).

\[
W_e = \begin{bmatrix}
W_{e,i} & 0 & 0 \\
0 & W_{e,i} & 0 \\
0 & 0 & W_{e,i}
\end{bmatrix}
\quad \text{with} \quad W_{e,i} = \frac{0.5s + \omega_0}{s + 0.01\omega_0}
\]

(5.15)

\[
W_y = \begin{bmatrix}
W_{y,i} & 0 & 0 \\
0 & W_{y,i} & 0 \\
0 & 0 & W_{y,i}
\end{bmatrix}
\quad \text{with} \quad W_{y,i} = \frac{s + 0.5 \cdot 10\omega_0}{0.001s + 10\omega_0}
\]

(5.16)

\[
W_u = \begin{bmatrix}
10^{-4} & 0 & 0 \\
0 & 10^{-4} & 0 \\
0 & 0 & 10^{-4}
\end{bmatrix}
\]

(5.17)

5.4.3 Controller Reduction

The controller obtained is of order 76. To arrive at a low-order controller for column 2, the controller was reduced using balanced residualization. This method retains the stationary behavior of the controller, which has been shown to be desirable [53]. The controller obtained by this method is of order 30; the singular values for \( T_e \) and \( S_e \) can hardly be distinguished from the values for the full controller.
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5.4.4 Simulation Results

For testing the controller, the total mass flow of the largest feed stream was increased by 10%. Figure 5.9 shows the change of the distillate mass fraction for the main product, figure 5.10 contains the change of the main component mass fraction in the side stream, and figure 5.11 depicts the change of the bottom pressure as simulated using

- the rigorous nonlinear model for column 2 without pressure and composition control (but with level control)
- the linear model with pressure and composition control
- the nonlinear model with pressure and composition control
- the nonlinear model with pressure and composition control, using the reduced controller

The corresponding manipulated variables are shown in figures 5.12–5.14. All controlled variables are brought back to their setpoints within a short time. Note that the reduced controller (denoted by stars) and
5.4 Controller Design for Column 2

Figure 5.9: Change of main component distillate mass fraction in column 2

The full controller (thick line) lead to nearly identical responses. The variations of the manipulated variables are quite large, which is an indication that the bandwidth chosen is not optimal yet.

Figure 5.10: Change of main component side stream mass fraction in column 2
5 Robust Control

Figure 5.11: Change of bottom pressure in column 2

Figure 5.12: Change of manipulated variable (distillate flow rate) for column 2
5.4 Controller Design for Column 2

- Figure 5.13: Change of manipulated variable (reboiler heat input) for column 2

- Figure 5.14: Change of the manipulated variable (side stream flow rate) for column 2
5 Robust Control

5.5 Summary

A multivariable controller has been designed for each column. The $H_\infty$ design method using the S/KS/T augmentation scheme has been chosen for this purpose. Although the model used for controller design is a linear model of much lower order than the full nonlinear model, the controllers show good performance. They are able to keep the controlled variables close to their setpoints. A reduction of the bandwidth of the controller for column 2 might lead to a decrease of the changes in the manipulated variables. For the controller of column 2 an order reduction was performed and the resulting controller was tested with the full nonlinear model, which did not lead to any substantial loss of control quality. It therefore has been shown in this chapter that the models developed in the chapters 2 to 4 can be used successfully for controller design.
6

Conclusions

At the beginning of the chapter the results of this thesis are summarized. Open questions are then addressed in the following outlook. The thesis is concluded by a discussion of lessons learned and of the role that modern simulation tools play when complicated real-world systems are simulated.

6.1 Summary

Within this project the full process of model based controller design has been carried out. First, a detailed dynamic model of two interconnected distillation columns has been developed by describing the physical processes taking place in a distillation column, using balance equations, hydraulic information, and physical properties data. An important aspect was the modeling of the non-ideal behavior of the columns: While for an ideal stage of a distillation column vapor and liquid are in equilibrium, this is not the case for a real column. Murphree efficiencies and vaporization efficiencies were used to capture the difference.

The steady-state behavior of the model was compared to available plant measurements, showing large deviations. Inaccurate physical properties data, missing components, and measurement errors were
6 Conclusions

identified as the causes for mismatch. After eliminating these sources of errors, the plant and the model still did not match. Especially the second column showed large deviations for the profile measurements available. By introducing temperature dependent vaporization efficiencies, which were fitted iteratively and then modeled using splines, good agreement between measurements and simulations could be obtained for two different operating points.

In the next step a linear model was obtained from the nonlinear models. Numerical linearization of the complete plant model was possible in principle, but the subsequent model reduction steps failed due to the size of the system, which had an order of 1586. Linearization, scaling, and reduction of the individual columns showed good results, but the model of the complete plant obtained by re-combining these models showed large deviations from the nonlinear behavior. For this reason, the columns were linearized separately including level controllers. A fast iterative scaling procedure was applied to the resulting linear models which led to condition numbers close to the minimum achievable condition number for the frequency chosen. Model reduction by balanced truncation led to two models of acceptable size (order 100 for column 1, order 70 for column 2), which were still able to represent the input-output behavior of the columns excellently. Using these models a first set of $H_\infty$ controllers using the S/KS/T scheme was designed and tested in nonlinear simulations. The controlled variables rapidly returned to their setpoints when changes of the feed flow were simulated. Even a reduction of the controller order to 30 did not lead to a reduction of performance.

6.2 Outlook

Although the controllers that have been designed lead to a good quality of control, they are not ready for implementation yet, they merely represent the first steps into that direction after the successful completion of the modeling process. To arrive at the final set of controllers several questions should be investigated, e. g.:
6.3 Lessons Learned

- Is the current choice of controlled and manipulated variables, which closely follows the current operating practice, optimal for the desired control objectives?

- Can the weights used in the design process be further improved?

- How large is the advantage of using the GS/T scheme instead of the S/KS/T scheme? This would result in controllers that do not invert the plant, leading to greater robustness especially for ill-conditioned systems like distillation columns [54].

- The current controllers depend on composition measurements, which are not readily available. What happens if only temperatures are available for providing estimates of the controlled variables?

- Can the quality of control be maintained when the continuous-time controllers are converted to discrete-time controllers?

Thorough testing of the final controllers in both operating points for several different disturbances are a necessary condition for the successful implementation.

6.3 Lessons Learned

When this project was started, it looked as if a number of standard tasks would have to be mastered using tools readily available, to arrive at a model suitable for controller design. Reality, however, was different. For a system of this size (order greater than 1500) and complexity (highly non-ideal VLE relationship, recycle streams), not much experience exists and many methods reach their limits. As a consequence, each of the steps described above raises a hoard of questions and problems that can only be solved by a combination of computing power, imagination, and often new methods. Many detail problems have to be tackled successfully before moving on.

As a consequence, the question arises, whether trying to model systems of this size is sensible, using the tools, computers, and methods
available today. Numerical problems can hardly be avoided and simulation times run into hours. Although the dream of an engineer probably still is the exact model, it remains questionable how big an effort is necessary \textit{and} acceptable to develop and implement this model—which, exact or not, will still only show a part of the real behavior. And in the modern chemical process industries no company is willing to pay for these projects, unless very certain estimations on the achievable savings exist at the beginning. Maybe going back to simpler models is still the right solution today, trying to find a better balance between physical modeling and system identification techniques.

### 6.4 Modern Simulation Tools—Pro and Contra

Performing dynamic or steady-state simulations of a distillation column used to be a task for experts with a sound knowledge of the processes taking place in a distillation column as well as of the mathematical methods and algorithms required to perform the necessary calculations. Several books have been published, often by chemical engineers, in which the knowledge of these two fields (e.g. [56]) is combined.

Today the situation seems to have changed completely: Off-the-shelf software is able to perform distillation design calculations, apply shortcut methods, perform data reconciliation, optimizations, dynamic distillation simulations, and much more. Graphical user interfaces help to enter consistent specifications. By pressing a button or setting a flag, different models can be chosen without needing in-depth knowledge of the processes taking place in the column and how to describe them. The mathematical algorithms are provided in an easy-to-use manner. Large databases offer physical properties data, hydraulic parameters, and if some data is missing, estimation routines try to come up with sensible values. Although many different programs exist (the software directory of “Chemical Engineering Progress” lists 474 products for the category “Process De-
sign/Simulation” [57]), many of them are suitable for specialized tasks only. A product package that is widely used in industry and academia is the Aspen Engineering Suite, which offers programs for performing steady-state and dynamic simulations, using library models as well as custom models.

Working with large systems, however, like in this project, soon reveals several problems of such modern simulation tools. They attempt to provide the user with as many defaults as possible, such that a simulation can be performed without the need of much knowledge. In this process default values are often used without proper documentation and explanation of the values that have been chosen. An extreme example may illustrate this: It is possible to perform a rigorous distillation simulation using ASPENPLUS without providing any information about the components present—just providing arbitrary names for them is sufficient, even if these components cannot be found in any of the databases present. No warning appears during the simulations, no information is given about the defaults that are used.

The mathematical algorithms used for optimizations, integration, or steady-state simulations are hidden beneath the surface, so the user does not have to deal with the complicated details. This approach works very well until a situation occurs where the algorithms provided are not able to solve the problem posed. In this case finding specific measures as a cure to the problem or explaining the reason for the failure are often impossible, because the implementation of the algorithms is not transparent.

Modern simulation tools are comfortable environments, as long as more or less standard tasks have to be performed. If, however, a problem setup requires solutions to more complex, non-standard tasks, implementing them may become a challenge.

The tendency to offer all-in-one solutions has the disadvantage that integrating external routines is often not catered for and no open interfaces are provided. A step into the right direction, however, is made within the CAPE-OPEN project, which tries to define and implement standardized interfaces for process design software.

The lack of transparency in the end often requires that the com-
6 Conclusions

Complete simulation program is written from scratch, because this is the only way to have full control over what happens in the simulation. The methods used in this case may not be as sophisticated as those included in the commercial software packages, but they can be influenced efficiently, because all details are known.

And even transparent software, naming MATLAB as an example, where the source code of many functions (including the integration routines) is visible, is not free of problems: In the beginning of a simulation project, hardly any knowledge of the numerics and algorithms hidden behind the functions provided is necessary. Again, problems that are not excessively complex can be solved in a fraction of the time that was needed in earlier years, when everything had to be programmed by the user. Sometimes, however, these functions are no longer able to deliver usable results, e.g. because of numerical problems. In this case, from one moment to the next, the user should be able to understand the complete algorithm and has to become an expert on numerics and algorithms.
Bibliography


Bibliography


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Bibliography


Curriculum Vitae

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