MODELLING AND ADVANCED MULTIVARIABLE
CONTROL STRATEGIES FOR A
PILOT SCALE EXTRACTIVE DISTILLATION
COLUMN

by

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To My Parents...
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Abstract:

A pilot scale distillation column was built jointly with other students to study the separation of an azeotropic mixture of acetone and methanol. An extractive distillation process is used to break the azeotrope using water as a solvent. This is a nonideal, nonlinear, multicomponent system. A VAX 11/750 computer with DPM-23 industrial front-end system was used in a distributed control configuration for control and data archiving of the column. An on-line Varian-6000 gas chromatograph (G.C.) is used for the top and bottoms product analysis.

A complete tray to tray steady state and dynamic mass and energy balance models were developed. The validity of these models has been explored using experimental data over a wide operating region. The simulated behaviour from the dynamic model was compared with the experimental column behaviour for various open loop steps in the reflux flow rate, feed flow rate, feed composition and reboiler duty. The nonlinear behaviour of the system was simulated by the models. A simple model for vapour liquid equilibrium (VLE) calculations was developed and its validity was proven.

The grouping of several trays together as a compartment has a thermodynamic basis and reduces the total number of model equations to be solved. Models with 3, 4 and
5 compartments showed good agreement with the experimental data and with a tray to tray model. A saving of 70% in the computation time was achieved over the tray to tray model. The 5 compartment model was used to develop a reduced order bilinear model of the system using the reflux flow rate and the reboiler duty as manipulated variables. The dynamics of the column were investigated for steps in steam pressure, reflux flow rate and feed flow rate. The system behaviour using the bilinear model and a complete tray to tray model were similar to the actual plant data.

PI control strategies were simulated for single and dual composition control for four different kinds of disturbances. From the simulation studies it was found that for the control strategy with two single loop the conventional pairing of the reflux flow rate and reboiler duty is suitable for only certain kinds of disturbances. Selection of the water flow rate and reboiler duty (steam pressure) as a manipulated variable pairing showed better performance. This was also shown experimentally.

A bilinear optimal controller design was developed which would result in an asymptotically stable system. The optimal controller for a bilinear system is nonlinear in nature, but the control law depends upon the objective function selected. The proof of optimality is given. It was also shown that an optimal controller based on a bilinear equation has a larger region of application than a
controller designed from a linearized model. The optimal controller, along with a reduced order bilinear model, was applied to a simulation and on the pilot plant for dual composition control. Reflux flow rate and reboiler duty were used as the manipulated variable pair. The weighting matrices from the objective function and the constant system matrices from the model were used to solve a Liapunov equation to obtained the matrix used in the control law. The tray temperatures were used to predict compositions for the experimental control studies. A recursive least squares (RLS) method was used to update the predictor parameters when the G.C. analyses were available. An optimal controller with the composition predictor was implemented successfully on the pilot scale extractive distillation column for the servo control problem. A bilinear controller was also applied to the regulatory problem of a feed flow disturbance. It was found that even a multivariable controller based on the reflux flow rate and reboiler duty did not perform well. Subsequently, a bilinear model for the extractive distillation was changed to use water flow rate and reboiler duty as manipulated variables. The controller resulting from this model was implemented successfully on the simulation for 20% feed flow disturbance. It should be noted that the system performance depends upon the performance index used in the design of the bilinear controller.
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Chapter - 1

INTRODUCTION

During the past two decades, improvements in computer hardware have played an important role in the control of chemical processes with replacing analog computers by digital computers. The increased speed of computation has helped to reduce energy consumption and operating costs by allowing the implementation of complex control algorithms. Digital computer control algorithms are easier to implement and provide more flexibility than their analog predecessors. Computer technology has also played a role in modelling various chemical processes, such as reactors, distillation, extraction, heat exchangers and others, by allowing the use of complete mechanistic models involving nonlinear heat and mass transfer equations. Mathematical models play a fundamental role in the understanding of the dynamic behavior and control of any process.

Distillation is one of the most important separation processes in the chemical industries. McAvoy (1981) has reported that 3% of the total U.S. energy consumption in 1977 went into distillation operation. Ogunnaike et al. (1983) suggest that the U.S.A. would save approximately $500 million/year if the energy efficiency of distillation
systems is increased by 10%. Reducing the energy requirement of distillation has been an area of particular interest to many researchers. In conjunction with high energy consumption, distillation columns exhibit nonlinear behavior. The nonlinear behavior of any system is best understood with the help of a mathematical model. In Section 1.1 the literature on the modelling of a distillation column is reviewed, followed by a control review in Section 1.2. Problems associated with Extractive distillation column are discussed in Section 1.3. In Section 1.4 a brief outline of the thesis is presented. In this chapter general reviews on modelling and control are given and a detailed reviews are presented in the appropriate chapters.

1.1 LITERATURE REVIEW- MODELLING:

In this section the literature on modelling of a distillation column will be reviewed. Only selected works are been cited here, but a detailed list of articles is given in the bibliography.

The literature on distillation dynamics is extensive. The first simulation studies were reported for binary systems by Huckaba and coworkers (1963,1965). Christiansen et al. (1979) used a modified Naphtali-Sandoholm column calculation procedure, coupled with the Soave Redlich Kwong equations for generating K-values. This modified
calculation procedure is only valid when the individual stage efficiencies are unity and the K-values are not strongly dependent upon the vapour phase composition.

Ballard et al. (1978) reported a stable algorithm to integrate the stiff MESH (material balance, equilibrium summation of mole fraction and heat balance) ODE(ordinary differential equations), which required calculation of a Jacobian matrix at the beginning of each time step. This was used to implement a second order semi-implicit Runge Kutta algorithm for solving dynamic equations. Prokopakis and Seider (1980) presented results on distillation column dynamics. The method is closely related to that of Ballard et al. (1978). The difference is that they used an adaptive semi-implicit Runge Kutta (SIRK) algorithm to integrate the equations and the coefficients were calculated at each integration step to match the variation in estimates of the local eigenvalues.

Gallund and Höland (1980) developed another algorithm using Gear's multistep integration method. They used a complete distillation model. Kumar et al. (1983) presented another algorithm using Gear's multistep algorithm, but using an enthalpy balance as an approximation for the energy balance. They presented experimental data which was matched with simulation results. The main advantage of Gear's method over SIRK is that it can be applied directly to the systems of nonlinear differential
equations with variable coefficients. Holland and Liapis (1983) have shown that Gear's method is faster than the SIRK method.

In the modelling of distillation columns it is often assumed that the vapour leaving the tray is in equilibrium with the liquid leaving the tray. In actual operation trays rarely operate at equilibrium. Efficiency factors which can be combined easily with equilibrium relations are used to deal with non-equilibrium conditions. These efficiency factors are dependent on the tray location and component characteristics since different components exhibit different mass transfer behaviour. Krishnamurty et al. (1985) published a non-equilibrium tray model in which tray efficiencies are not used. In this method mass and energy balance equations are written for each phase separately. The equations for each phase are connected by the mass and energy balance around the interface, which is assumed to be in thermal equilibrium. The model is developed for steady state conditions only and requires a knowledge of the mass transfer coefficients for each component. For multicomponent systems these calculations become more difficult.

Distillation modelling can be divided into two categories. One uses a tray to tray concept yielding a complete order model, and the other uses a reduced order model. The tray to tray model gives a complete understanding of the physical system over wide operating conditions.
However, such a detailed model has a major disadvantage if it is to be used for on-line control. A typical column may require a large set of differential equations for accurate solution, particularly when nonlinear equilibria or wide ranging operating conditions are important factors. On the other hand, for the case where optimization of a large network is sought, a complete model may be inappropriate from the computational point of view. A reduced order model is often necessary for on-line control. Complex problems like network optimization, quick calculation of the process gain or dynamics, and selection of appropriate control schemes, can be implemented much more efficiently with a reduced order model. Reduced order modelling is a very useful approach for the study of distillation, or any general multistage process. It can be used efficiently in the design and control of such processes. Reduced order models are common in industry, and are typically based on step or impulse tests. Wahl and Harriott (1970) give correlation curves to determine zeros and poles. Waller (1979) presented correlations in the frequency domain, Wood and Berry (1973) presented transfer functions for a binary system and Kumar et al. (1984) published transfer function models for an extractive distillation column. Alternatively, a low order model may be obtained by linearizing the complete tray to tray model and then using model reduction techniques (Davison (1966)). Osborne et al. (1965) obtained a
low order model by writing tray equations in a form similar to packed column equations.

Transfer function models from step or impulse tests can only be applied in a limited operating range. The same problem pertains to models obtained by linearizing the complete model and applying model reduction techniques. In distillation, these methods are simple and effective for an ideal mixture. Wong and Luss (1980) presented a method based on orthogonal collocation in which the composition is estimated as a continuous function of the distance along the column. Polynomials are selected based on the degree of the accuracy required. Cho and Joseph (1983) also used this method. Roots of the collocation polynomials have to be obtained and these roots are taken as states for the control system design. The major disadvantage is that these roots need not coincide with an actual tray number. Therefore, interpolation may be required to get the composition leaving a tray. Orthogonal collocation can be used either directly on the linearized systems or on their partial differential equation formulation. Benallou (1982) has shown that in addition to the mathematical complications introduced by this method, which involve finding the roots of the collocation polynomials and curve fitting of initial conditions, the collocation method can result in fictitious state variables. This is a serious disadvantage of this method. This difficulty has been addressed in part by
Stewart et al. (1985) who developed a grid selection process using a stagewise least square criterion. The grid points, which can be considered as states, are computed as the zeros of the Hahn polynomials. When the degree of collocation is equal to the number of trays, the collocation points coincide with the actual tray number. The other method of obtaining a low order model, the Compartmental method, requires grouping trays as a section. The Compartmental method was proposed by Espana and Landau (1978) and Benallou et al. (1982). In this method, various trays are grouped and the most sensitive tray of the section represents the whole group. This method reduces the number of calculations significantly, although the criteria for the selection of the number of groups is not very clear. For ideal systems, where the variation of the relative volatilities does not vary from plate to plate, the number of compartments can be easily determined. However, for non-ideal systems the choice is not simple. Kumar et al. (1985) presented a compartmental technique to obtain a reduced order model for an extractive distillation column. They concluded that the number of compartments should be selected on the basis of the dynamics of the system as compared to steady state results. The steady state behavior of a 13 tray experimental column was modeled using 5, 4 and 3 compartments. For 15 different operating points the three different reduced order models show good agreement with the experimental data. The dynamics
of the column were investigated for steps in the reboiler duty and reflux flow rate. A reduced order bilinear model was developed mechanistically using the compartmental technique. Although the steady state data were well represented with the three reduced order models, the 3 and 4 order compartmental models did not produce an accurate representation of the dynamics. The 5 compartment model produced satisfactory dynamic results.

A part of the work presented in this thesis is geared towards modelling of an extractive distillation column to get a complete and reduced order models. Since extractive distillation column is a nonlinear process, models will help in understanding the process. Existing compartmental techniques have been modified to produce a reduced order model. This will contribute towards the development and application of compartmental techniques to nonlinear processes. All the simulation work have been tested against experimental work. This also provides experimental data in the open literature, which has been largely hidden in the patent literature.

1.2 LITERATURE REVIEW—DISTILLATION CONTROL:

Control of distillation columns has been a very popular research area. There are several review papers available in the literature (Schwanke et al. (1977),

Most of the published work on distillation control is based on simulation studies of binary systems. In a simple distillation system where pressure is constant, the control objective is to maintain the following variables at their set points:

- Top product composition
- Bottom product composition
- Condenser liquid level
- Reboiler liquid level

using the following manipulated variables:

- Reflux flow rate
- Reboiler duty (boilup rate)
- Distillate flow rate
- Bottoms product flow rate

There are numerous ways by which these manipulated variables can be used. The conventional method is to use reflux flow rate and reboiler duty to control top and bottom product compositions, distillate flow rate and bottom product flow rate to control condenser level and reboiler level respectively. The other type of configuration, in which reflux flow rate is used to control the condenser level and distillate product rate to control the top product composition, has been used successfully on columns which are difficult to control with reflux flow rate and reboiler
duty. This configuration is called direct material balance (Shinskey (1984), Bojnowski et al. (1976)). The material balance configuration is recommended for high reflux ratio columns and the conventional control scheme for the lower reflux ratio columns (Shinskey (1984)). The major disadvantage of the material balance scheme is the sluggish response of the bottom composition loop. Control configurations which include ratio controls are suggested by Shinskey (1984) and Rijndsdorp (1965).

The simultaneous control of overhead and bottom composition in a binary distillation column, using reflux and steam flow as manipulated variables, often proves to be difficult due to coupling effects; the control action by one loop propagates through the column and effects the performance of the other loop and vice versa. McAvoy (1979) investigated these interactions using Bristol's (1966) concept of the relative gain array. McAvoy and Weischedel (1981) compared material balance and conventional control schemes and concluded that the performance is system dependent. McAvoy (1981) suggested that as the purity of the column increases, the interactions between the two composition control loops becomes stronger. Davison (1970) used a simplified distillation model to outlined the conditions which give rise to interaction between the two composition control loops. One of the assumptions that he made is that there is no hydraulic delay in the liquid flow.
In the presence of hydraulic delays, the increased interaction would give different results. The other assumption is that of a binary mixture. In the case of a multicomponent system, the control of top and bottom composition, or top and bottom temperature in the presence of pressure control, may not be simple due to strong interactions. Luyben (1970) used a simulation to study two different approaches to non-interacting control. The first approach employs ideal decoupling, where the closed loop response of each loop is the same as it would be if the closed loop was under manual control, and a second method which uses simplified decoupling. His conclusion was in favor of simplified decoupling. He synthesized decouplers in the frequency domain from a linear model of the column, and then tested their effectiveness on a nonlinear system.

The factors which make the control problem difficult are:

1. The response of a distillation column to a control action is usually slow.
2. There are large numbers of variables and possible control loop configurations.
3. Interactions exist between various control loops.
4. There are nonlinear relationships between the variables.
5. Frequent disturbances from upstream units upset normal column operation.
The purpose of ratio control is to select an appropriate ratio to minimize the coupling effects. Rijnsdorp (1965) suggested the ratio of reflux and top vapour flow as the manipulated variable for the top loop. Stainthorpe and Jackson (1974) used a reflux ratio (reflux to distillate flow rate) as the manipulated variable for the top loop. Rademaker et al. (1975) gave a survey of various ratio control schemes suggested in the literature.

Wood and Berry (1973) used the ratio control system proposed by Rijnsdorp (1967) in which the controller is used to control the ratio of the overhead vapour rate to reflux rate. The setpoint of the ratio controller is adjusted by the signal from the overhead composition controller. In this way, the overhead composition becomes insensitive to variations in the steam flow rate. Their conclusion was that the ratio controller is better than a conventional two point controller. Their results are based on a binary system with a first order plus delay transfer function. Tung and Edgar (1979) presented experimental data along with a simulation model written in multivariable state space format for a binary system. Shimizu and Mah (1983) used an SRV scheme (secondary reflux and vapourization) for binary distillation in state space format. Using simulations they studied decoupling control and show that the existence of a constant feed matrix and a precompensator matrix would completely decouple the system. McAvo and Togas (1981) reported that
material balance control is superior to decoupling for the dual composition control in high purity towers, whereas the reverse is true for low purity columns. Takamatsu et al. (1978) show the influence on the control system, when the decoupling controller is designed using incomplete state variable feedback.

Tyreus (1979) applied the inverse Nyquist Array method to a 30 tray industrial column. It is reported that the multivariable design gives considerable dynamic improvement as compared to multiloop single input single output (SISO) method. On the contrary, Bilec et al. (1979) reports only a minor improvement by using a Direct Nyquist Array Method over SISO method.

Recently, Self Tuning Regulators (STR) have become very attractive. Sastry et al. (1977) used the STR of Astrom and Wittenmark (1973) for adaptive control of the top product composition. They found that this controller was definitely superior to conventional PI control of their column for feed flow rate disturbances. Clough (1981) used a multivariable STR for distillation control by assuming only one process dead-time. Dahlqvist (1981), Morris et al. (1981) applied multivariable STR and Self Tuning Controllers (STC) to distillation columns. Chien, Mellichamp and Seborg (1986) evaluated the performance of a multivariable STC. In their approach the parameters are estimated using the extended least squares rather than the conventional least squares
method, and the approach was extended to handle multiple time delays. The controller was applied successfully on simulation studies. Additional references can be found in the review paper on the application of modern control theory to distillation column by Edgar and Schwanke (1976).

Ogunnaike et al. (1983) reported an experimental study of the multivariable control of a pilot plant distillation column having a side stream drawoff. Although they used a multivariable controller with multiple delays the time delay compensator resulted in only slightly improved performance.

Coppus et al. (1983) used Davison's (1976) robust multivariable feedback feedforward controller for a binary distillation column. Davison's approach is a black box approach which uses input/output data based on the notion of compensator identification as opposed to plant identification for the STR. Through experimentation, they show that the robust controller gives improved control performance compared to that achieved using conventional multiloop PID control. The major limitation of Davison's approach is that it is applicable to plants which can be described by linear time invariant models and which are open loop asymptotically stable.

Takamatsu et al. (1979) used the geometric approach to controller design. In this approach, it is recognized that the properties of a linear system depend on the
structure of the linear subspace generated by the given system. The total system, including the control system, will generate a linear subspace having desirable structure in the state space. By using the design specification of the feedback controller to describe the structure of the subspace generated by the controlled system, the design is treated intuitively. They applied the geometric approach to the disturbance rejection control problem. Guerchet et al. (1983) used this method for decentralised disturbance decoupling control for binary distillation.

One major problem in composition control is the long time delay associated with the composition measurements using analysers. Tray temperatures can be used either in place of the analyser or in addition to the process analysers. Patke and Deshpande (1982) presented a comparative assessment of inferential and parallel cascade schemes for controlling the top product composition of a simulated multicomponent distillation column. In their inferential control scheme a process model is used to infer the composition from the tray temperatures and reflux and steam flows. They concluded that inferential control is useful. The settling time with inferential control was shorter than when a conventional feedback system was used. However only the top product composition was controlled. The application and results of an inferential control scheme to two composition control were not discussed. Fuentes and
Luyben (1983) used a cascading of the composition controller to an intermediate tray temperature. The performance of this configuration depends upon the tuning parameters and type of disturbance. The use of a single tray temperature to infer composition in a multicomponent system is not feasible. For the case of a non-ideal system, where the non-key component composition profile has intermediate maxima and minima, a single temperature inferential control scheme would result in an incorrect composition. Yu and Luyben (1984) adjusted a single tray temperature set point, but it was based on a linear combination of two differential temperature measurements. Johnson (1984) used multiple tray temperatures to infer composition.

Most of the open literature is concerned with binary systems. Literature on the control of multicomponent systems is very scarce. Waller and Gustafsson (1972) reported that in multicomponent systems, the non-key components can show irregular behavior, such as inverse response. Also, the non-key components can have a significant effect on the behavior of the key component. Waller (1981) presented a review of dual composition control of distillation columns. The contents will not be repeated here.

Controllers used in the above studies were based on linearized models of distillation columns. Another class of controllers, based on bilinear models, is gaining importance.
due to its wide range of applicability. Espana and Landau (1978) indicated that distillation columns can be described more accurately by a bilinear model. Benallou (1982) applied a linear feedback controller based on a bilinear model. He has compared his optimal controller with that based on the technique of Derese and Noldus (1980). Benallou used a nearly ideal system for his study. Moreover, no simulation study results were presented to corroborate with experimental data. This is the only literature the author could find in which bilinear controls have been applied to a distillation process.

In this thesis a bilinear model-based optimal controller will be applied to an extractive–distillation column which is a nonlinear process. To understand the control behaviour basic controllers like proportional integral (PI) and PI+decoupler will be applied on the simulation. In this multicomponent system compositions will be inferred from tray temperatures. The study will provide a complete work on the application of bilinear controller to an extractive distillation column. Experimental results on the control studies will be presented. The author could not find an experimental application of nonlinear controller to the extractive distillation column in the open literature. However, it seems that the patent literature contains few linear control studies, but none on nonlinear or bilinear controller.
1.3 EXTRACTIVE DISTILLATION:

Extractive and azeotropic distillation are important unit operations for the separation of either close boiling or azeotropic mixtures of liquids in the petrochemical industry. Common examples include recovery of Butadiene from Butane, butene, and 1-2 Butadiene and the separation of propylene from propane by extractive distillation. In extractive distillation the introduction of a third component which has a higher boiling point than the feed material is used to increase relative volatilities and thereby increase the separation.

Extractive distillation is a two-fold problem. It is a multicomponent distillation and a nonideal system with multiple feeds. The solvent plays an important role in the separation. On each tray of an extractive distillation column there typically needs to be twice the amount of extractive agent as the close boiling point components on each tray of a rectifying column. The solvent should be heated to about the same temperature as the plate onto which it is introduced. Thus, extractive distillation imposes an additional heat requirement.

Additional problems in the case of an extractive distillation, other than those mentioned earlier for simple distillation column are:
1. The amount of the solvent on the trays should be small in order to lower tray loading, but it must be sufficient to break the azeotrope.

2. Extractive distillation requires two columns for complete separation. For economic reasons the solvent recovered in a second column is recycled in the solvent feed to the first column. Thus fluctuations in either composition or flow rate in one stream potentially may cause upsets in both columns.

3. Since the system is multicomponent, the composition of the solution will not be a monotonic function of the flowrates due to the interactions between components.

4. Consequently, a model of an extractive distillation column must be nonlinear with respect to changes in the operating conditions. Thus, the empirical model changes with the operating point.

A limited amount of published work is available on extractive distillation. A few US and British patents exist. Seider and Prokopakis (1983) have recently published work on the dynamics of Azeotropic distillation. The only published work on the control of an extractive distillation available to the author is by Gilles et al. (1980); which is based on a simulation study. Experimental data on extractive
distillation are not available in the open literature, especially when dynamic behavior of the column is to be considered. This has motivated the present work.

1.4 OUTLINE OF THE THESIS:

The following is the layout of each chapter in this thesis.

In Chapter 2 the description of the process and details of the experimental setup are given. The thermodynamics of the system and the differences between extractive and azeotropic distillation are explained. The problems associated with extractive distillation are addressed and the method of solvent selection is explained. The column configuration, the various control loops for smooth operation of the column, the gas chromatograph and the communication between the real-time programs which were developed for data acquisition and control are discussed. The steady state and dynamic models for the extractive distillation column are developed in Chapter 3. These models are based on complete mass and energy balance equations. A brief literature survey on modelling of distillation columns is also presented. Simulation results are compared to the experimental data to study the steady state behavior. Step tests in the reflux flow rate, reboiler duty, feed composition and feed flow rate on the pilot scale
distillation column are compared with results from the
dynamic simulator of the extractive distillation column. The
nonlinearity of the system is exposed and simple transfer
functions are evaluated for controller analysis and design.
A simple method of evaluating the vapour liquid equilibrium
for the system under study is presented and compared with
the more rigorous method developed earlier.

In Chapter 4, the concept of compartments to obtain a
reduced order model is discussed. Various methods of
obtaining a reduced order model are also discussed.
Compartmental models for an extractive distillation column
using 3, 4, and 5 compartments are developed. The heat loss
model used in the modelling of the column is given. The
simulation results for the steady state column operation are
compared with experimental results for 15 different
operating conditions. The amount of computer time saved by
using the compartment models over the complete model
developed in Chapter 3 is also discussed.

The concept of a bilinear system is presented in
Chapter 5. A literature review on the application of
bilinear models for physical systems is given. A bilinear
state space model for the extractive distillation column is
developed using 5 compartments. This model is developed for
the reflux flow rate and reboiler duty as the manipulated
variables. The dynamic response of the bilinear model is
compared with the experimental response.
To understand the control behaviour, the performance of PI (Proportional plus Integral) controllers for single and dual composition control is evaluated in Chapter 6 for various types of disturbances. The controller is applied on the complete tray to tray dynamic simulator described in Chapter 3. Different control schemes, (i.e., decoupling, feed forward control) are also presented. This would also serve as a base case for comparison with various advanced controllers in future work. A simple method is given to calculate the control action required to bring the system back to its original setpoint when different disturbances enter the column.

A bilinear optimal controller which will asymptotically stabilize the system is developed in Chapter 7. Using a numerical example, the advantage of the bilinear controller over a linear controller for a nonlinear process is shown. The bilinear controller is applied to the extractive distillation column on simulation studies in Chapter 8. The objective of the control study in Chapter 8 is to take the system from one operating point to another while minimizing the performance index of Chapter 7. Both single composition and dual composition control problems are considered. A method was been developed to infer the top and bottom product compositions from the tray temperatures. The limitations of the bilinear controller are also discussed.

In Chapter 9, the bilinear optimal controller is
applied to a pilot scale extractive distillation column. A procedure for implementing the controller is given. Both the servo and regulatory problems are considered and the experimental results presented. A PI controller with a steady state decoupler is applied to the experimental column for a feed flow disturbance. When a bilinear optimal controller was applied for the regulatory problem with the conventional manipulated variables, it was found that controller saturates. This raised a few questions about the applicability of the controller for the regulatory problem. Therefore, a reduced order bilinear model was redeveloped for a different set of manipulated variables and the controller was restructured. The simulation results for the new controller are shown in Chapter 9.

The sequence of work presented in the thesis is the same as it occurred during the research work. This seems to be more natural way of presentation than rearranging the work. The description of the redesign of the bilinear optimal controller for water and steam is presented in the chapter 9. This part of the work was done after it was found that the bilinear optimal controller based on steam and reflux flow did not perform well.

Conclusions and recommendations are given in Chapter 10.
Chapter 2

PROCESS DESCRIPTION AND EXPERIMENTAL SETUP

2.1 PROCESS DESCRIPTION INTRODUCTION:

Distillation is a physical process for separating a liquid mixture into its constituents. The separation is possible because when a mixture is vapourised the vapour produced has a different composition than the remaining liquid. This separation technology is several centuries old. Early distillations were of the batch type. An important development in distillation technology was a method of operating the distillation column continuously using several trays. Present day distillation technology is of a multistage, continuous type utilizing a vertical tower. Each tower has several internal contacting devices called stages or trays. The liquid mixture to be separated can enter anywhere, but normally it enters near the center of the column. The section below the feed point is called the stripping zone and the section above is called the rectifying zone. A fraction of the liquid is vapourised in the reboiler at the bottom of the column and vapours leaving the top of column are condensed. The stream collected at the bottom of the column is called the bottoms product. A part of the condensed stream is recycled and the rest is
collected as the top product output. The recycled stream is called reflux and the ratio of the amount of reflux and top product is called the reflux ratio. The top product stream is richer in the lighter components (i.e., components with lower boiling point) of the mixture and the bottoms product has most of the heavier components of the mixture. If the mixture has only two components the process is called binary distillation, and for more than two components it is known as multicomponent distillation.

The number of trays required depends upon the nature of the vapour liquid equilibrium (VLE) curve of the mixture. If the feed components have a large difference in their boiling points, then fewer trays are normally required than for those with close boiling points. For the class of mixtures which form an azeotrope there is a maximum amount of separation, governed by the azeotropic composition, that can be obtained. Increasing the number of trays does not change the product purity. These mixtures are industrially very important, and they are separated with a modified distillation technique. The characteristics of an azeotropic system are discussed in the next section.

2.2 CHARACTERISTICS OF AN AZEOTROPE:

Azeotrope, a Greek, word means "to boil without changing"; i.e., vapours leaving from the liquid have the
same composition as the remaining liquid. Azeotropes occur in binary as well as multicomponent systems. The formation of an azeotrope is a function of the difference in boiling temperatures of the components and the deviation from Raoult's law. Raoult's law states that the vapour pressure of the mixture is a linear function of the molar composition. The single most important cause of such a deviation is the hydrogen bond. All azeotropic mixtures reflect a non-ideal relationship of the components. Azeotropes are classed as minimum boiling and maximum boiling azeotropes. The minimum (maximum) boiling azeotrope is formed when the vapour pressure of some mixture exceeds (is less than) the vapour pressure of any of the pure components (Smith and Van Ness (1981)).

From the above discussion it is clear that once the azeotropic mixture is formed during the distillation process, no further improvement in separation is possible by heating. Mathematically the formation of an azeotrope can be explained as given below.

The necessary condition for a state of equilibrium between vapour and liquid to exist, is that the fugacity \( \bar{f}_v^i \) of each component \( i \) in the vapour phase must be equal to fugacity \( \bar{f}_l^i \) in the liquid stream.

\[
\bar{f}_v^i = \bar{f}_l^i \quad \quad (2.1)
\]
Mixture fugacities may be restated in terms of the fugacities of the pure components:

\[ \bar{f}_i^V = \tau_i^V f_i^V y_i \]  
(2.2)
\[ \bar{f}_i^L = \tau_i^L f_i^L x_i \]  
(2.3)

where

- \( f_i^V \) = fugacity of pure component \( i \) in the vapour phase at the mixture temperature \( T \) and pressure \( P \)
- \( f_i^L \) = fugacity of pure component \( i \) in the liquid phase at the mixture temperature \( T \) and pressure \( P \)
- \( \tau_i^V \) = activity coefficient of component \( i \) in the vapour phase at \( P,T,y_i \)
- \( \tau_i^L \) = activity coefficient of component \( i \) in the liquid phase at \( P,T,x_i \)
- \( x_i \) = molar liquid composition of component \( i \)
- \( y_i \) = molar vapour composition of component \( i \)

The equilibrium relationship for component \( i \) is:

\[ y_i = \tau_i^L K_i x_i / \tau_i^V \]  
(2.4)
\[ K_i = f_i^L / f_i^V \]  
(2.5)

For the ideal vapour phase \( \tau_i^V = 1.0 \) and for the ideal liquid phase \( \tau_i^L = 1.0 \). At low pressures the assumption that the vapour phase is ideal is reasonable.

Under this assumption:
\[ y_i = r_i^1 K_i x_i \]  \hspace{1cm} (2.6)

and the ratio \( (Y_i/X_i)/(Y_j/X_j) \) is defined as the relative volatility:

\[ \alpha_{ij} = \frac{(Y_i/X_i)}{(Y_j/X_j)} = \frac{r_i^1 K_i}{r_j^1 K_j} \]  \hspace{1cm} (2.7)

For the separation to take place \( \alpha_{ij} \approx 1.0 \)

When an azeotrope is formed, \( \alpha_{ij} = 1.0 \); hence any modification of simple distillation to achieve a separation of an azeotropic mixture should be directed at altering \( \alpha_{ij} \). This can be achieved either by changing \( K \) or \( r \). \( K \) is a function of temperature whereas \( r \) is the function of liquid composition.

2.3 AZEOTROPIC AND EXTRACTIVE DISTILLATION:

The ability to alter equation (2.7) is achieved in two types of distillation processes: (1) Azeotropic distillation and (2) Extractive distillation. These processes are used when the feed mixture cannot be separated by simple distillation due to low relative volatility or the presence of an azeotrope. To improve the relative volatility, the activity coefficient is changed by adding another component, called an agent, in the distillation process. In an azeotropic process the agent has approximately the same vapour pressure as that of the feed mixture and forms an
azeotrope with the lighter component, it comes out as an overhead product. In extractive distillation the agent is referred to as a solvent, it has a lower vapour pressure and a higher boiling point than that of the feed mixture. The solvent is added near the top of the column and is removed with the bottoms product. The solvent is recovered in a second column and recycled to the first column. Azeotropic distillation is useful when the overhead azeotropic mixture has a small quantity of the agent. In this case the amount of the agent needed is small and results in a low agent recovery cost. When the feed mixture is a close boiling pair and the agent is required to improve the relative volatility over the entire column height, then extractive distillation is more useful.

2.4 SYSTEM UNDER CONSIDERATION AND SOLVENT SELECTION:

The system chosen for this work is a binary mixture of acetone and methanol. Acetone and methanol form a minimum azeotrope at 54.6°C and 80% mole of acetone (see Hala et al. (1968)). 80% mole of acetone is equivalent to 0.8 mole fraction of acetone in acetone-methanol mixture. The extractive distillation technique is used to break the azeotrope. The choice of a solvent plays an important role in the performance of an extractive distillation. Tassios (1969) has given the following guidelines for the selection
of a solvent: (1) if the difference in the molar volumes of the close boiling hydrocarbons is more than 5%, then a solvent of high polar cohesive energy should be used; (2) if the molar volumes are very close, then choose a solvent having the higher electron affinity. Gerster (1969) suggests that:

(1) if the two components in the mixture differ by at least one double bond, then the presence of a polar solvent increases the volatility of the component having the least number of double bonds;

(2) when the feed components are of a different chemical type, then water should always be considered first as a possible solvent, except in the case where miscibility with water is limited or the vapour pressure of the water is not very low compared to the feed mixture. In general, the solvent should be noncorrosive, nontoxic, cheap and should be easily available.

The selectivity of a solvent expresses its capacity to interact more strongly with one component than with the other. The attraction may be physical or chemical in nature. The selectivity of the solvent is defined as

$$S_{ij} = r_i^1 / r_j^1$$  \hspace{1cm} (2.8)

where \( r \)'s are activity coefficients for the liquid phase.

Tassios (1969) suggests that dispersion forces and forces between dipoles and induced-dipoles are the main
cause for the physical interaction. If the molar volume difference is large and the solvent has a high cohesive energy, then the selectivity is high. The chemical effect is due to the formation of a complex of loosely bound aggregates, which is the result of a Lewis acid/base interaction. Usually the physical interactions are much greater than those due to chemical effects. Since hydrocarbons are usually electron donors, good selectivity from chemical effects is obtained when: (1) the difference between the hydrocarbon ionization potential is large; and, (2) solvent electron affinity is high.

Possible solvent candidates for acetone, and methanol system as given by Schiebel (1948) are given below:

<table>
<thead>
<tr>
<th>Solvent</th>
<th>B.P.</th>
<th>Solvent</th>
<th>B.P.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methyl-ethyl ketone</td>
<td>79.6</td>
<td>Ethanol</td>
<td>78.3</td>
</tr>
<tr>
<td>Methyl-propyl ketone</td>
<td>102.0</td>
<td>Propanol</td>
<td>97.2</td>
</tr>
<tr>
<td>Methyl-iso-butyl ketone</td>
<td>115.9</td>
<td>Butanol</td>
<td>117.8</td>
</tr>
<tr>
<td>Methyl-n-amyl ketone</td>
<td>150.9</td>
<td>Water</td>
<td>100.0</td>
</tr>
<tr>
<td>Ethylene glycol</td>
<td>197.2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

where B.P. means boiling point in degree centigrade

Solvents belonging to the homologous group of
ketones are ideal with acetone and the homologous group of alcohol are ideal with methanol. All solvents can be used to separate the azetrope. Due to the difference in the chemical nature of acetone and methanol, water was selected as the solvent. Other reasons for selecting water are cost, absence of toxicity and availability. Water improves the volatility of the less polar acetone much more than it affects the volatility of methanol. This is due to the fact that water has more affinity for methanol than for acetone. Methanol (CH₃-O-H) can form hydrogen bonds with water in two ways, from the oxygen of the water to the hydrogen of the methanol and from the oxygen of the methanol to the hydrogen of the water. In comparison, acetone (CH₃-C-CH₃) can only form hydrogen bonds with water in one way, from the oxygen of the acetone to the hydrogen of the water. Due to this, the selectivity of water is high enough to improve the separation.

Figure 2.1 shows the complete extractive distillation circuit for this system. A feed mixture of acetone and methanol is separated in the first column using water as the solvent. The overhead product is richer in acetone while the bottoms product consists mainly of methanol and water. The output of the first column enters as the feed to the second column, the solvent stripping column. The top product of the second column is richer in methanol and its bottoms product is mainly water. The bottoms product
Figure 2.1: The Extractive Distillation Unit

of the solvent stripping column is recycled with fresh makeup solvent as the solvent feed to the first column.

Figure 2.2 shows how water changes the activity of acetone and methanol (Grisworld et al. (1949)). Figure 2.3 represents the VLE diagram for an acetone-methanol mixture at different water concentrations. Curve 1 shows the formation of an azeotrope at 80% mole of acetone in absence of water. As the water concentration is increased, the
Figure 2.2: Effect of Water on the Activity Coefficient of Methanol and Acetone

Figure 2.3: VLE Curves for Acetone-Methanol System on Water Free Basis
azeotrope disappears and the separation becomes easier. From this figure it is also clear that a minimum amount of a solvent is required to completely break the azeotrope.

2.5 PROBLEMS WITH EXTRACTIVE DISTILLATION:

The solvent not only modifies the process to increase the separation, but also causes it to become a multicomponent distillation with multifeed. It is also a highly nonideal system. The solvent should be heated to about the same temperature as the tray onto which it is introduced.

Thus, extractive distillation imposes an additional heat requirement. In Chapter 1, control problems associated with simple distillation were discussed. In the case of an extractive distillation, further difficulties encountered are:

(1) the amount of solvent on the trays should be kept to a minimum in order to keep the loading on the trays low, but it should be sufficient to break the azeotrope for separation;

(2) as shown in Figure 2.1, it requires two columns for complete separation. Solvent recovered in the second column is recycled as the solvent feed to the first column (thus, any fluctuation in one column will cause a deviation in the other column);
(3) since this is a multicomponent, non-ideal system the composition trend are generally not monotonic because of interactions between the components.

(4) An accurate model of the distillation system will have to account for changes in the system's behaviour.

From the operational point of view, since liquid loading is increased without much increase in the vapour loading, the tray and downcomer design should be modified accordingly. For the hydrocarbon-solvent system, foaming may arise and this can increase the liquid handling problems.

2.6 MOTIVATION FOR THIS WORK:

A limited amount of published work is available on extractive distillation. A few United States and British patents exist. Seider and Prokopakis (1983) have published work on the dynamics of an azeotropic distillation system. The only published work on the control of an extractive distillation available is by Gilles et al. (1980), which is based on a simulation study. Experimental data on extractive distillation is not available in the open literature. This has motivated the present work.

2.7 EXPERIMENTAL SETUP:

For this study, and other research work, a
distillation column was built in collaboration with Langille (1983) and later modified with help of Yasuchenko (1988) and Mayer (1985). At the present time, the distillation system is comprised of a 15 cm diameter column fabricated from Quick Fit glass segments. There are 13 trays each with a single Teflon bubble cap. The tray spacing is 15 cm. A schematic diagram along with various control loops are shown in Figure 2.4. The maximum pressure rating of the column is 206.7 kPa but all experiments were carried out at atmospheric pressure. Temperatures are measured for both vapour and liquid on each tray. The feed mixture enters the column on the 10th tray from the top and the solvent enters on the 5th tray. A thermosyphon reboiler was used. The overhead product is completely condensed, split, and reheated to provide the liquid reflux stream to the column. Other details about the hardware are given in Langille (1983). The system uses Direct Digital Control which allows for the implementation of advanced control algorithms.

A VAX 11/750 is used as a host computer to control the column through a DPM-23 distributed front-end micro computer system. Four different processes are connected to the main computer and can be run simultaneously. For the distillation control system the configuration and data acquisition circuit is given in Figure 2.5.

The interface communication program to collect data from the real-time process via the front-end to the VAX was
Figure 2.4 Schematic Diagram of the Extractive Distillation Column
developed at McMaster University. A description of this interface is available in Segall et al. (1984) and details are given in Wong (1983), and Yasuchenko (1988). In brief, the DPM-23 front-end system consists of an LS1-11/23 minicomputer with 192 kbytes of memory. The RSX/11S operating system runs in the front-end. The DPM-23 is connected to the VAX via DYS 56 kbaud data network. The VAX and the DPM-23 each have two communication programs for passing data, one for downline loading the complete database at the time of startup and one for regular periodic updating.
of the database. The database permits data sharing between the programs in a manner similar to a common blocks shared by various subroutines. The database has all the information that is passed back and forth between the various program modules.

2.8 LOW LEVEL CONTROL:

The process variables which are logged and used for low level control computations are given in Table 2.1.

All orifice meters are designed for a maximum of 101.0 kPa pressure drop. The feed and solvent flow rates are maintained by control valves CV2 and CV1, respectively. Two separate feed tanks are connected through solenoid valves S1 and S2 which give the ability to introduce changes in feed composition under computer control. The reflux flow rate and the top product flow rate have individual control valves. Various combinations of control schemes for reflux ratio, condenser level control and product stream flow rate can be configured through the on-line computer system. To maintain the various flow rates and levels at the operating set points, low level control loops are used. The performance of these low level controllers play an important role in the smooth operation of the column. The velocity form of a discrete PI (proportional plus integral) algorithm along with high and low saturation limits are used throughout for
TABLE 2.1: Process variables for low level control

<table>
<thead>
<tr>
<th>Variable</th>
<th>Sensor</th>
<th>Label</th>
<th>Figure 2.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed flow</td>
<td>Orifice meter</td>
<td>OM2</td>
<td></td>
</tr>
<tr>
<td>Solvent flow</td>
<td></td>
<td>OM1</td>
<td></td>
</tr>
<tr>
<td>Reflux flow</td>
<td></td>
<td>OM3</td>
<td></td>
</tr>
<tr>
<td>Distillate flow</td>
<td></td>
<td>OM4</td>
<td></td>
</tr>
<tr>
<td>Steam pressure</td>
<td>Differential</td>
<td>PT1</td>
<td></td>
</tr>
<tr>
<td>Reboiler level</td>
<td>pressure</td>
<td>LT1</td>
<td></td>
</tr>
<tr>
<td>Condenser level</td>
<td></td>
<td>LT2</td>
<td></td>
</tr>
<tr>
<td>Feed temperature</td>
<td>Thermocouple</td>
<td>TT1</td>
<td></td>
</tr>
<tr>
<td>Solvent temperature</td>
<td></td>
<td>TT2</td>
<td></td>
</tr>
<tr>
<td>Reflux temperature</td>
<td></td>
<td>TT3</td>
<td></td>
</tr>
</tbody>
</table>

these low level loops. These controllers are executed at the front-end and are not affected if the main computer is non-operational. The low level computer control loops used in this system are shown in Figure 2.4 and are presented in Table 2.2.

Table 2.2: Computer Control Loops

<table>
<thead>
<tr>
<th>Loop#</th>
<th>control variable</th>
<th>manipulated variable</th>
<th>Type</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Feed flow rate</td>
<td>Feed Valve CV2</td>
<td>PI</td>
<td>ml/min</td>
</tr>
<tr>
<td>2</td>
<td>Solvent flow rate</td>
<td>Solvent Valve CV1</td>
<td>PI</td>
<td>ml/min</td>
</tr>
<tr>
<td>3</td>
<td>Reflux flow rate</td>
<td>Reflux Valve CV3</td>
<td>PI</td>
<td>ml/min</td>
</tr>
<tr>
<td>4</td>
<td>Steam pressure</td>
<td>Steam Valve CV7</td>
<td>PI</td>
<td>kPa</td>
</tr>
<tr>
<td>5</td>
<td>Reboiler level</td>
<td>Bottom flow CV4</td>
<td>PI</td>
<td>volts</td>
</tr>
<tr>
<td>6</td>
<td>Condenser drum</td>
<td>Top flow CV5</td>
<td>PI</td>
<td>mm</td>
</tr>
</tbody>
</table>
Table 2.3 gives the controller gains and reset time for the PI controller shown in Table 2.2.

**Table 2.3: Controller parameters for low level controllers**

<table>
<thead>
<tr>
<th>Control loop</th>
<th>Controller gain</th>
<th>Reset action 1.0/sec</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.09 ma/(ml/min)</td>
<td>0.086</td>
</tr>
<tr>
<td>2</td>
<td>0.06 ma/(ml/min)</td>
<td>0.065</td>
</tr>
<tr>
<td>3</td>
<td>0.05 volt/(ml/min)</td>
<td>0.001</td>
</tr>
<tr>
<td>4</td>
<td>0.15 volt/(ml/min)</td>
<td>0.005</td>
</tr>
<tr>
<td>5</td>
<td>-15.0 volt/(ml/min)</td>
<td>0.00001</td>
</tr>
<tr>
<td>6</td>
<td>-3.0 ma/(ml/min)</td>
<td>0.001</td>
</tr>
</tbody>
</table>

For the flow controllers, set-point responses settle within 2-3 minutes with the maximum deviation of 2 ml/min. Only the reboiler level control loop, which is controlled by the bottoms product flowrate, has large fluctuations. This is a common tradeoff between smooth flowrates and level fluctuations.

The pressure signals from the orifice plates are converted to electrical signal through Rosemount pressure transmitters. Table 2.4 gives the type of electrical signals for the various control loops.

Apart from these low level controllers, temperatures for the feed and solvent lines are controlled by Barber Coleman SCR time-proportioning controllers. The setpoints for these temperature controllers are supplied by the
Table 2.4: Circuit type and signal range for low level controls

<table>
<thead>
<tr>
<th>#</th>
<th>Variable</th>
<th>Type</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Feed Valve</td>
<td>Current</td>
<td>4-20 ma</td>
</tr>
<tr>
<td>2</td>
<td>Solvent Valve</td>
<td>Current</td>
<td>4-20 ma</td>
</tr>
<tr>
<td>3</td>
<td>Condenser</td>
<td>Current</td>
<td>4-20 ma</td>
</tr>
<tr>
<td>4</td>
<td>flow Valve</td>
<td>Voltage</td>
<td>0-10 volts</td>
</tr>
<tr>
<td>5</td>
<td>Bottoms flow Valve</td>
<td>Voltage</td>
<td>0-10 volts</td>
</tr>
<tr>
<td>6</td>
<td>Reflux flow Valve</td>
<td>Voltage</td>
<td>0-10 volts</td>
</tr>
<tr>
<td>7</td>
<td>Steam flow Valve</td>
<td>Voltage</td>
<td>0-10 volts</td>
</tr>
<tr>
<td>8</td>
<td>Top flow Valve</td>
<td>Voltage</td>
<td>0-10 volts</td>
</tr>
</tbody>
</table>

program "SUPER", which runs in the detached mode on the VAX host computer. Details of this program are given in Yasuchenko (1988). SUPER collects information about the solvent plate temperature and supplies it as the setpoint to the solvent heater controller H1. For the feed temperature controller, SUPER sends the setpoint as 20°C less than the feed plate temperature. The reason for introducing the feed at a lower temperature is to produce a sharp temperature profile within the column. For the reflux heater, the objective is to maintain the reflux stream at the top tray temperature. SUPER sends the top tray temperature as the setpoint for the feedback controller on the reflux line. Manual heaters are used to base-load these temperature loops. Initially, 4-5 minutes may be required, depending on
the flow rate being used, for these controllers to come up to the setpoint. Thereafter the temperature is maintained within 1.5°C. Each section of SUPER is provided with the maximum and minimum allowable setpoints. This is necessary to check the malfunctioning of the thermocouple readings. These maximum and minimum values are given below:

<table>
<thead>
<tr>
<th>Point</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed temperature</td>
<td>38</td>
<td>47 °C</td>
</tr>
<tr>
<td>Solvent temperature</td>
<td>55</td>
<td>65 °C</td>
</tr>
<tr>
<td>Reflux temperature</td>
<td>52</td>
<td>58 °C</td>
</tr>
</tbody>
</table>

Another provision to safeguard the column operation is an operator override on the temperature setpoint supplied by SUPER. This is used when there is some malfunction in the temperature readings.

Initially, temperature scanning was carried out by INTEL 8085 microcomputer system designed by Langille (1983). However, with the availability of a multiplexer in the front-end computer these temperatures are now scanned directly by the front-end. Temperature results shown in Chapter 3 were taken from the 8085 system and results in other chapters are from the front-end multiplexer.

9 THE GAS CHROMATOGRAPH SYSTEM FOR HIGH LEVEL CONTROL:
As described above, all the low level controllers operated in the front-end, whereas, the higher order controllers for dual composition control operated in the VAX. A gas chromatograph provides the composition data to the VAX via an asynchronous serial communication line linked to a Varian Vista 401 chromatographic data system. A Varian 6000 gas chromatograph together with the Vista 401 are used to analyse the top and bottoms products. The chromatograph is equipped with an automatic sampler and stream selector valve. The bottoms product and top product streams are selected automatically one after another. A Chromosorb 102 chromatographic column is used to analyse the water, methanol, and acetone mixture. Ultra high purity grade helium was used as the carrier gas with a flowrate of 30 ml/min. When the distillation column is not operating, a minimum of 8-10 ml/min of helium flows through the gas chromatograph to secure the detector filament from oxidation. Details about the programming the Vista 401 and other operating conditions (i.e., method building procedures and calibration methods) are given in the Vista 401 manual.

The accuracy of the gas chromatograph (G.C.) data depends on the calibration. The G.C. system has shown good reproducibility. Methanol and Water are polar components and their peaks overlap each other. This affects the analysis specially for the bottoms samples where the water concentration is high. A typical chromatogram for the
Bottoms product is shown in Figure 2.6.

Initially, the G.C. was equipped with a VALCO injection/sampling valve. This has a hot chamber at the entrance to the column and so the sample flashes as it enters the column. For the bottoms product which has very

| CHART SPEED | 1.0 CM/MIN |
| ATTEN: 256 | ZERO: 10% |
| 1 MIN/ TICK |
| 0.307 |
| WATER |
| MOLY |
| 1.282 |
| 0.940 |
| AT: 64 |
| ACET |
| 3.461 |

PECALC
TITLE: BOTTOM PRODUCT ANALYSIS  12:34  17 JUN 85

CHANNEL NO: 1  SAMPLE: BOTTOM  METHOD: BOTTOM

<table>
<thead>
<tr>
<th>PEAK NO</th>
<th>NAME</th>
<th>RESULT</th>
<th>TIME</th>
<th>AREA</th>
<th>SEP</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>WATER</td>
<td>1.2887</td>
<td>0.940</td>
<td>1395390</td>
<td>EV</td>
</tr>
<tr>
<td>2</td>
<td>METH</td>
<td>0.1929</td>
<td>1.282</td>
<td>403122</td>
<td>VV</td>
</tr>
<tr>
<td>3</td>
<td>ACET</td>
<td>0.0136</td>
<td>3.461</td>
<td>42973.6</td>
<td>T</td>
</tr>
</tbody>
</table>

TOTALS: 1.4954  1841490

DIVISOR: 1.00000  MULTIPLIER: 1.00000
NOTES: OCT. 17, 1984

Figure 2.6: Chromatogram of Bottoms Product Analysis
small amounts of acetone it gave incorrect results. It was also observed that the sample volume taken by the VALCO valve depended on the pressure of the stream being sampled. Calibrations were done with manual injections but the samples taken while the process is running are obtained via pumps. The variability and inaccuracy was unacceptable and, the VALCO valve was changed to a true liquid sampling valve. The new valve has an initial cold chamber for the liquid sampling, a thermal barrier with carrier gas purge, and a separate heated flash chamber so that it flashes instantaneously. However, the new valve has extra column length which increases the retention time. The helium flowrate was increased from 30 ml/min to 45 ml/min to reduce the retention time. The new valve is independent of the inlet pressure and gives better analysis than the old VALCO valve. Experimental results presented in Chapter 3 and partly in Chapter 4 are with the old VALCO valve and other results are with new valve.

The VISTAREAD computer program developed by Segall (1983) is used to send data from the Vista 401 to the VAX through an asynchronous line. There are three different channels in the Vista 401 and three different G.C.'s can send data simultaneously. Channel #1 is used for sending the distillation G.C. data. As soon as the data is transferred to the VAX, it is written to a mailbox. The program COMP, which uses Asynchronous System Traps (ASTS), picks up the
data from the mailbox, strips the data to get compositions, and stores them in the file MOPER2.DAT. They are simultaneously sent to the controller program to execute the higher level controllers. The complete analysis and control route is given in Figure 2.7.

The startup and shutdown procedures are given in Langille (1983) and Yasuchenko (1988). Yasuchenko (1988)

Figure 2.7: Analysis and Control Route of the GC Data for the Higher Level Control
also describes the various real-time programs needed for smooth column operation and data acquisition. In brief these programs are:

(1) STILL menu driven program to run the column, plotting run time data, CRT display of the column;

(2) SUPER provides setpoints for feed, solvent and reflux heater controllers;

(3) VISATREAD transfers G.C. data from the VISTA 401 to VAX memory;

(4) COMP gets G.C. data from VAX memory, strips it, stores the data in the file and transfers information for higher level control;

(5) TROLL higher level controller program (user supplied);

(6) RLOG logs the historical data (i.e., temperature, levels, flowrates of the running column);

(7) VAXHOS communication program between front-end and main VAX, also creates the global section.

(8) KILL To shutdown the distillation column operation

The programs VAXHOS, DEP1, and VISATREAD are always
Figure 2.8: CRT Display of the Extractive Distillation Column

running because they are used by all processes connected to the VAX. The operator must check the status of these programs before startup. A menu driven program, STILL, is the main program and displays the various conditions of the column while under operation. Figure 2.8 shows this display at one operating condition.

2.10 CONCLUSIONS:

An extractive distillation process is utilized to
break the minimum boiling azeotrope of methanol and acetone using water as a solvent. Due to the azeotrope formation the system is non-ideal and with a solvent it becomes a multicomponent distillation.

The process, hardware and software systems needed to investigate advanced multivariable control on an extractive distillation is presented. A VAX 11/750 is used as a host computer to control the column through a DPM-23 distributed front-end microcomputer. For the smooth operation of the column, various low level PI controllers are implemented on the front-end. For temperature control Barbar coleman SCR time-proportioning controllers are used. A higher level controller for the dual composition is implemented at the VAX. This is a hierarchial control system which simplifies the investigation and keeps the main computer available for other purposes. A communication program between the front-end and VAX developed at McMaster is flexible enough to implement a variety of control strategies.

It was also observed that the performance of the first VALCO sampling valve was dependent on the inlet pressure and at low acetone concentrations it did not represent the correct composition. A new automatic liquid sampling valve is independent of inlet pressure and gives better results.
Nomenclature

\( f^l_i \) = Fugacity of pure component \( i \) in the liquid phase

\( f^l_i \) = Fugacity of pure component \( i \) in the liquid mixture

\( f^v_i \) = Fugacity of pure component \( i \) in the vapour mixture

\( f^v_i \) = Fugacity of pure component \( i \) in the vapour phase

\( K_i = \frac{f^l_i}{f^v_i} \) K-value for component \( i \)

\( S_{ij} \) = Selectivity of the Solvent defined by equation (2.8)

\( X_i \) = Molar liquid composition of component \( i \)

\( Y_i \) = Molar vapour compositions of component \( i \)

Greek Symbols:

\( \alpha_{ij} \) = Relative volatility given by equation (2.7)

\( \gamma^l_i \) = Activity coefficient of component \( i \) in liquid phase

\( \gamma^v_i \) = Activity coefficient of component \( i \) in vapour phase
Chapter - 3
TRAY TO TRAY MODELS

3.1 INTRODUCTION:

Extractive and azeotropic distillation are important unit operations in petrochemical industries for separating either close boiling or azeotropic mixtures. As explained in the previous chapter, a solvent is introduced to break the azeotrope in the extractive distillation process. These complex thermodynamics make the process itself complex. A digital simulation is useful for the qualitative and quantitative analysis of the column operating performance. It can also be used for the initial design and/or revamping.

The long range objectives of this work are to develop and implement advanced, model based controllers. It is therefore necessary to develop good steady state and dynamic models to represent the process. The first step is to develop such models and compare both the steady state and the dynamic models with experimental data from an extractive distillation column.

Section 3.2 details the steady state simulation developed for an extractive distillation. A comparison of the simulation and experimental results is presented in Section 3.3. The development of the dynamic simulation and
its experimental verification for step changes in reflux flow rate, feed flow rate, reboiler duty and feed composition are given in Section 3.4 and 3.5 respectively. The effect of solvent flow and solvent/feed ratio are given in Section 3.6. The nonlinearity of the system is demonstrated in Section 3.7. In Section 3.8, a simple model for vapour liquid equilibrium calculation for acetone, methanol and water system is given. Section 3.9 contains the conclusions of the chapter.

3.2 STEADY STATE SIMULATION:

Steady state simulation is widely used in design and process studies. On the design side, simulation can provide information about the temperature, flow rates and compositions which can subsequently be used for the optimal design of the distillation column diameter and tray spacing. It may also be used for various energy conservation schemes. On the process side, the relative gain array analysis may be used to select the manipulated variables. A steady state simulation can be used to design a steady state controller. This is useful in the initial investigation of the operability and controllability. Fisher et al. (1985) present a similar justification for simulation. Thus, steady state analysis has advantages in designing, as well as understanding, process control.
In order to obtain the column conditions at different operating points, it is necessary to solve a set of equations describing the mass balance, the enthalpy balance and the equilibrium relationship at the steady state. One method of solving this set of equations is by tearing and partitioning of the system so that temperatures are paired with combined constitutive and phase equilibrium equations, and interstage phase rates are paired with enthalpy balances and mass balances, i.e., the Wang and Henske method (1966). This method is not suitable, however, for the systems having components over a wide boiling point range. Tomich (1970) improved this method by adjusting the temperature and the phase rates simultaneously. The Jacobian of the system with respect to temperature and phase rate is initially calculated by a finite difference approximation and its inverse is updated using the Quasi-Newton method of Broyden (1965). The major disadvantage of this approach is the excessive computation time. In contrast, the Napthali et al. (1971) method uses a Newton-Raphson multivariable scheme, in which all the equations are solved simultaneously. This approach depends on a good initial guess. To compensate the deficiencies of these methods Kumar et al. (1984) suggested an iterative technique, which is described below.

In a continuous distillation column, it is necessary to write the mass and energy balance equations for the system. It is convenient to write these equations for each
tray in the column, for the overhead condenser and for the reboiler. A typical tray in the system can be represented as shown in Figure 3.1.

![Typical Tray Configuration and Nomenclature](image)

**Figure 3.1: Typical Tray Configuration and Nomenclature**

The trays are numbered from the top of the column, with condenser as tray number 1. The following assumptions are made:

- the liquid phase is perfectly mixed
- there is no mixing of vapour as it passes through the liquid pool on the tray, but upon leaving it is perfectly mixed
- the liquid and vapour phases are in thermal equilibrium at the liquid temperature on the tray
- the system is at constant pressure
- no shaft work
- heat losses from the system are negligible
Using these assumptions, Kumar et al. (1984) have derived the following steady state equations.

The component material balance for the jth tray is given by:

\[ V_{j+1}Y_{ij+1}^+ - V_jY_{ij}^- - L_jX_{ij} = 0 \]

The total material balance for the jth tray is given by:

\[ V_{j+1} - L_{j-1} - V_j - L_j + F - W = 0 \]

The enthalpy balance for the jth tray is given by:

\[ V_{j+1}H_{j+1} + L_{j-1}h_{j-1} - V_jH_j - L_jh_j + Fh_f - Wh_w = 0 \]

The component material balance for the condenser is given by:

\[ V_2Y_{2l} = L_1X_{1l} + D X_{1d} \]

and for the reboiler it is given by:

\[ V_bV_{ib} = L_{b-1}X_{ib} + B X_{ib} \]

where b indicates the reboiler.

The enthalpy balance for the condenser is given by:

\[ V_2H_2 = L_1h_1 + D H_d + Q_c \]

and for the reboiler is given by:

\[ V_bH_b = L_{b-1}h_{b-1} + B h_b + Q_b \]
The overall component material balance for the distillation column is:

\[
\sum_{j=1}^{NP} \alpha_j F_j x_{ij} = D x_{id} + B x_{ib} + \sum_{j=1}^{NP} \Gamma_j w_j x_{iw}
\]  

where \( \alpha_j = 1 \) if \( j \)th tray is a feed tray otherwise = 0

\( \Gamma_j = 1 \) if \( j \)th tray is a drawoff tray otherwise = 0

NP = Total number of trays in the distillation column

Liquid and vapour specific enthalpies for the \( j \)th tray are defined by:

\[
H_j = \sum_{i=1}^{N} H_{ij}^* y_{ij}
\]

\[
h_j = \sum_{i=1}^{N} h_{ij}^* x_{ij} - h_{mix}
\]

The performance of each tray is defined by the Murphree efficiency for each component:

\[
E_{ij} = \frac{y_{ij} - y_{ij+1}}{Y_{ij}^* - y_{ij+1}}
\]

The equilibrium at the \( j \)th tray for the \( i \)th component is defined as:
\[
Y_{ij}^* = r_{ij}^1 k_{ij} X_{ij} = K_{ij} X_{ij}
\]
(3.11)

\[
K_{ij} = r_{ij}^1 k_{ij} ; \quad k_{ij} = \frac{P_{ij}^*}{P}
\]
(3.11b)

where the activity coefficient \( r_{ij} \), \( k \)-values and \( K_{ij} \) are functions of composition and temperature, respectively. Equations (3.10) and (3.11) may be combined to give

\[
Y_{ij} = E_{ij} k_{ij} x_{ij} + Y_{ij+1} (1.0 - E_{ij})
\]
(3.12)

or

\[
X_{ij} = \left( -Y_{ij+1} (1.0 - E_{ij}) + Y_{ij} \right) / \left( E_{ij} k_{ij} \right)
\]
(3.13)

Then, multiplying by \( L_j \) on both sides of equation (3.13) and rearranging yields:

\[
L_j X_{ij} = - \left[ \frac{L_j}{V_j E_{ij} k_{ij}} \right] \left[ \frac{V_j}{V_{j+1}} \right] (1.0 - E_{ij}) V_{j+1} Y_{ij+1}
\]

\[
+ \left[ \frac{L_j}{V_j E_{ij} k_{ij}} \right] V_j Y_{ij}
\]
(3.14)

or

\[
I_{ij} = - A_{ij} S_{ij} Y_{ij+1} + A_{ij} Y_{ij}
\]
(3.15)

where

\[
A_{ij} = \frac{L_j}{V_j E_{ij} k_{ij}} ; \quad S_{ij} = \frac{V_j}{V_{j+1}} (1.0 - E_{ij})
\]
(3.16)

\[
I_{ij} = L_j X_{ij} ; \quad V_{ij} = V_j Y_{ij}
\]

Using equation (3.15), the component material balance
equation (3.1) can be rewritten as:

\[ A_{ij-1} v_{ij-1} - v_{ij} (1.0 + A_{ij} + A_{ij-1} S_{ij-1}) + (1.0 + A_{ij} S_{ij}) v_{ij+1} = -(f_i - w_i) \]  

(3.17)

where \( f_i = F X_{iF} \) and \( w_i = W X_{iW} \).

Similar expressions for all the trays are combined to get the following matrix equation:

\[ A_i v_i = -f_i \]  

(3.17b)

where \( A_i \) is a tridiagonalized matrix. This matrix equation (3.17b) is solved for \( v_i \) by the Thomas algorithm (see Carnahan et al. (1964)). Then, the 'Theta' method of convergence, as described by Holland (1981) is used. In this method, a parameter 'theta' is calculated using the Newton-Raphson method to obtain the corrected distillate flow rate which, in turn, can be compared with the specified distillate flow. New liquid compositions are then calculated using the following equations:

\[ p_i = (d_i)_{CO} / (d_i)_{CA} \]

\[ x_{ij} = \frac{(1_{ij})_{CA} p_i}{\Sigma_{m=1}^{N} (1_{mj})_{CA} p_m} \]

\[ p_m = (d_m)_{CO} / (d_m)_{CA} \]

co stands for corrected flows using a parameter "Theta".
The temperature of the tray is calculated using the Bubble point method corresponding to the corrected composition.

The key parameter in calculating the vapour and liquid equilibria for non-ideal mixtures is the activity coefficient $T_{ij}$. Some data are given in Hala et al. (1968). In order to calculate these phase equilibria, several methods including the Wilson method, the Van Larr equations, the UNIFAC and others may be used. Jackson (1974) used the Wilson method. However, through simulations and comparisons with the literature data, it was found that this method did not give accurate predictions over the range of the data available. The 3rd order Margules method was found to give a more accurate representation of the data. The form of this equation used is:

$$
\text{Log}(T_i) = X_i^2(a_{ij} + 2X_i(a_{ij} - a_{ij})) + 2X_m(a_{mj} - a_{jm})
$$

$$
+ X_m^2(a_{im} + 2X_i(a_{im} - a_{im})) + X_jX_m(a_{ji} + a_{im} - a_{mj})
$$

$$
- c (1 - 2X_i) \quad (3.18)
$$

where the $i$, $j$, $m$ indicate the components. The sequence of calculation is $i=1$, $j=2$, $m=3$, then $i=2$, $j=3$, $m=1$, and finally, $i=3$, $j=1$, $m=2$ and $c = 0.113$.

The constants used for calculating the vapour pressure by the Antoine equation and the activity coefficients are given in Table 3.1. Another method of
calculating the vapour liquid equilibrium (VLE) data for acetone-methanol-water, is based on simple local relations near the operating point and is described later in the chapter.

Table 3.1: Physical Property Correlation

<table>
<thead>
<tr>
<th>Vapour Pressure by Antoine Equation</th>
<th>Log(P) = A - B/(T+C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P = mm of Hg</td>
</tr>
<tr>
<td></td>
<td>T = deg C</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Antoine Coefficients</th>
<th>Margule Coefficients</th>
<th>Liquid Enthalphy (kcal/mole)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>B</td>
<td>C</td>
</tr>
<tr>
<td>Acetone</td>
<td>7.240</td>
<td>1279.87</td>
</tr>
<tr>
<td>Methanol</td>
<td>8.072</td>
<td>1574.99</td>
</tr>
<tr>
<td>Water</td>
<td>7.967</td>
<td>1668.21</td>
</tr>
</tbody>
</table>

Heat of mixing: \[ h_m = a + bx + cx^2 + dx^3 + ex^4 \]

<table>
<thead>
<tr>
<th>Heat of Mixing</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone/methanol</td>
<td>1.017e-03</td>
<td>-0.7534</td>
<td>0.9441</td>
<td>-0.1924</td>
<td>0</td>
</tr>
<tr>
<td>Water/methanol</td>
<td>6.058e-03</td>
<td>0.1719</td>
<td>0.6461</td>
<td>-0.8130</td>
<td>0</td>
</tr>
<tr>
<td>Water/acetone</td>
<td>-6.005e-03</td>
<td>0.3685</td>
<td>-2.1499</td>
<td>5.3065</td>
<td>-3.507</td>
</tr>
</tbody>
</table>

** Int. Critical Tables, 5,155-159

Once a new temperature and composition profile is obtained, the new flow profile is calculated by satisfying the enthalpy balance. The enthalpy balance is performed on the loop enclosing the jth tray and the condenser. Consider this loop as shown in Figure 3.2.
Figure 3.2: Envelope for Enthalpy Balance

The total enthalpy balance is given by:

\[ V_{j+1}H_{j+1} + \sum_{r=1}^{j} \alpha_{r} F_{r} H_{rf} = L_{j} h_{j} + D H_{d} + Q_{c} + \sum_{r=1}^{j} \sum_{r} W_{r} h_{rw} \]  

(3.19)

where \( \alpha_{r} = 1 \) if feed is introduced, otherwise = 0.

\( D_{s} = 1 \) if product is drawn, otherwise = 0.

The component material balance is:
\[ v_{ij+1} \sum_{r=1}^{j} \alpha_r f_{ir} = l_{ij} + D_i + \sum_{r=1}^{j} \Gamma_r w_{ir} \] (3.20)

Multiplying equation (3.9) by \( V_j \) the following equation is obtained for the \( j^{th} \) tray:

\[ V_j H_j = \sum_{i=1}^{N} H_{ij} v_{ij} \] (3.21)

for the \( j+1^{th} \) tray the above equation is:

\[ V_{j+1} H_{j+1} = \sum_{i=1}^{N} H_{ij+1} v_{ij+1} \]

Substituting for \( v_{ij+1} \) from equation (3.20) yields:

\[ V_{j+1} H_{j+1} = \sum_{i=1}^{N} H_{ij+1}^* (l_{ij} + D_i + \sum_{r=1}^{j} \Gamma_r w_{ir} - \sum_{r=1}^{j} \alpha_r f_{ir}) \] (3.22)

\[ = L_j \sum_{i=1}^{N} H_{ij+1}^* x_{ij} + D \sum_{i=1}^{N} H_{ij}^* x_{id} + \]

\[ \sum_{r=1}^{j} \Gamma_r w_{ir} \sum_{i=1}^{N} H_{ij+1}^* x_{iw} - \sum_{r=1}^{j} \alpha_r f_{ir} \sum_{i=1}^{N} H_{ij+1}^* x_{if} \] (3.23)

Substituting equation (3.23) into equation (3.19) produces
\[ L_j = \frac{D (H_d - \sum_{i=1}^{N} H_{ij+1}X_{id}) + Q_c + \sum_{r=1}^{j} \alpha_r F_r (\sum_{i=1}^{N} H_{ij+1}X_{ir} - H_{rf})}{\sum_{r=1}^{N} \Gamma_r W_r (H_{rw} - \sum_{i=1}^{N} H_{ij+1}X_{iw})} \]  

(3.24)

The vapour flow rates are obtained using the total material balance around the loop. Once the new flow profiles are known, calculations are repeated till the temperature changes are less than 0.00005 °C. The flow chart of the above calculation procedure is given Figure 3.3.

3.3 EXPERIMENTAL AND SIMULATION RESULTS (STEADY STATE):

To investigate the steady state behaviour of the column, a number of experiments were carried out at different operating conditions. The initial transients from the cold start required 4-5 hours to settle out. The operating conditions along with the overhead and bottoms compositions from the Gas Chromatograph for various runs are given in Table 3.2. The simulation results and the comparison with the experimental data are given in Table 3.3. The Murphree efficiencies for each tray were adjusted to give the best fit of the data, and these are given in Table 3.4. The distillate flow rates from the experiments
Figure 3.3: Steady State Simulation Flowsheet

Start

Read Column Conditions
Physical Properties
Feed Conditions

Assume a Linear Temperature Profile

is flashing required?

Flash Calculations

No

Assume Flow Profile

Solve Material Balance Equations

From the next page

Continued on the next page
Figure 3.3 Steady State Simulation Flowsheet (continued)

- Find Out $\theta$ and Modified Tray Composition
- Calculate Activity Coefficients
- Calculate Improved Temperature Profile Using Bubble Point
- Is New Temp Profile = Old Temp Profile?
  - Print Result
  - Stop
- Solve Energy Balance Equations To Get Improved Flow Profiles
Table 3.2: Steady State Operating Conditions (Experimental)

<table>
<thead>
<tr>
<th>RUN NUMBER</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FEED</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow ml/min</td>
<td>109.0</td>
<td>111.0</td>
<td>108.0</td>
<td>130.0</td>
<td>108.6</td>
</tr>
<tr>
<td>Temp. °C</td>
<td>40.5</td>
<td>40.0</td>
<td>40.7</td>
<td>40.0</td>
<td>40.0</td>
</tr>
<tr>
<td>Composition Acetone</td>
<td>0.6370</td>
<td>0.5578</td>
<td>0.6370</td>
<td>0.5578</td>
<td>0.6290</td>
</tr>
<tr>
<td>(Mole Frac.) Methanol</td>
<td>0.3630</td>
<td>0.4422</td>
<td>0.3630</td>
<td>0.4422</td>
<td>0.3710</td>
</tr>
<tr>
<td><strong>SOLVENT</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow ml/min</td>
<td>53.5</td>
<td>53.5</td>
<td>53.5</td>
<td>53.5</td>
<td>53.0</td>
</tr>
<tr>
<td>Temp. °C</td>
<td>60.4</td>
<td>64.0</td>
<td>60.4</td>
<td>64.0</td>
<td>60.0</td>
</tr>
<tr>
<td><strong>REFLUX</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow ml/min</td>
<td>142.0</td>
<td>142.0</td>
<td>168.0</td>
<td>146.0</td>
<td>217.9</td>
</tr>
<tr>
<td><strong>TOP PRODUCT</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow ml/min</td>
<td>88.6</td>
<td>81.5</td>
<td>83.3</td>
<td>97.1</td>
<td>80.7</td>
</tr>
<tr>
<td>Composition Acetone</td>
<td>0.8188</td>
<td>0.8002</td>
<td>0.8713</td>
<td>0.7729</td>
<td>0.9053</td>
</tr>
<tr>
<td>(Mole Frac.) Methanol</td>
<td>0.1520</td>
<td>0.1712</td>
<td>0.0996</td>
<td>0.1836</td>
<td>0.0572</td>
</tr>
<tr>
<td>Water</td>
<td>0.0291</td>
<td>0.0286</td>
<td>0.0290</td>
<td>0.0435</td>
<td>0.0375</td>
</tr>
<tr>
<td><strong>BOTTOMS PRODUCT</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow ml/min</td>
<td>73.0</td>
<td>81.0</td>
<td>75.6</td>
<td>95.0</td>
<td>82.2</td>
</tr>
<tr>
<td>Composition Acetone</td>
<td>0.0012</td>
<td>0.0033</td>
<td>0.0019</td>
<td>0.0058</td>
<td>0.0025</td>
</tr>
<tr>
<td>(Mole Frac.) Methanol</td>
<td>0.1255</td>
<td>0.1653</td>
<td>0.1290</td>
<td>0.1857</td>
<td>0.1666</td>
</tr>
<tr>
<td>Water</td>
<td>0.8732</td>
<td>0.8323</td>
<td>0.8691</td>
<td>0.8095</td>
<td>0.8299</td>
</tr>
</tbody>
</table>

were used directly in the simulation.

As stated in Chapter 2, the distillation column has a number of local PI controllers. One of these controllers is used to maintain the level of liquid in the reboiler at a fixed position by manipulating the bottoms product flow rate. Large control actions were required by the reboiler
Table 3.3: Simulated Steady State Operating conditions and Comparison to Experimental Data

<table>
<thead>
<tr>
<th>Run #</th>
<th>Component</th>
<th>Top Product</th>
<th>Bottoms Product</th>
<th>$\Delta C_1$</th>
<th>$\Delta C_2$</th>
<th>Bottoms Flow Rate</th>
<th>$\Delta C_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Acetone</td>
<td>0.8188</td>
<td>0.0137</td>
<td>0.0</td>
<td>-0.0045</td>
<td>-0.0125</td>
<td>-0.3</td>
</tr>
<tr>
<td></td>
<td>Methanol</td>
<td>0.1565</td>
<td>0.1239</td>
<td></td>
<td>0.0016</td>
<td>73.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0.0247</td>
<td>0.8624</td>
<td></td>
<td>0.0109</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Acetone</td>
<td>0.8048</td>
<td>0.0184</td>
<td>-0.0046</td>
<td>-0.0152</td>
<td>81.25</td>
<td>-0.25</td>
</tr>
<tr>
<td></td>
<td>Methanol</td>
<td>0.1736</td>
<td>0.1667</td>
<td>-0.0024</td>
<td>-0.0014</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0.0216</td>
<td>0.8149</td>
<td></td>
<td>0.0174</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Acetone</td>
<td>0.8675</td>
<td>0.0193</td>
<td>0.0038</td>
<td>-0.0174</td>
<td>75.6</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>Methanol</td>
<td>0.1093</td>
<td>0.1397</td>
<td>-0.0097</td>
<td>-0.0107</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0.0232</td>
<td>0.8410</td>
<td></td>
<td>0.0281</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Acetone</td>
<td>0.7781</td>
<td>0.0219</td>
<td>-0.0052</td>
<td>-0.0161</td>
<td>84.8</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Methanol</td>
<td>0.1985</td>
<td>0.1801</td>
<td>-0.0149</td>
<td>0.0056</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0.0234</td>
<td>0.7980</td>
<td></td>
<td>0.0115</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Acetone</td>
<td>0.8909</td>
<td>0.0288</td>
<td>0.0144</td>
<td>-0.0253</td>
<td>80.3</td>
<td>1.9</td>
</tr>
<tr>
<td></td>
<td>Methanol</td>
<td>0.0892</td>
<td>0.1537</td>
<td>-0.0320</td>
<td>0.0129</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>0.0199</td>
<td>0.8175</td>
<td></td>
<td>0.0124</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\Delta C = \text{Difference between Experimental and Simulated}$

$\Delta C_1 = \Delta C \text{ for Top Product Composition (Mole Fraction)}$

$\Delta C_2 = \Delta C \text{ for Bottoms Product Composition (Mole fraction)}$

$\Delta C_3 = \Delta C \text{ for Bottoms Flow Rate (ml/min)}$

level controller. This resulted in large variations in the bottoms product flow rate. However, either the overhead or the bottoms flow rate must be specified in the calculation of the required heat duty, consequently, the overhead
product rate, which had smaller fluctuations as compared to
the bottoms product flow rate, was used in the simulation.
The specified overhead product rate was used with the mass
balance equation to calculate the bottoms product rate. The

<table>
<thead>
<tr>
<th>Tray</th>
<th>Acetone</th>
<th>Methanol</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>4</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>6</td>
<td>0.85</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>7</td>
<td>0.85</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>8</td>
<td>0.85</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>9</td>
<td>0.85</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>10</td>
<td>0.85</td>
<td>0.9</td>
<td>1.0</td>
</tr>
<tr>
<td>11</td>
<td>0.95</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>12</td>
<td>0.95</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>13</td>
<td>0.95</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Reb.</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

results showed good agreement with the experimental
observations.

An examination of the data in Table 3.3 shows that
the largest errors in the simulation were for the acetone
composition in the bottoms product stream. This was due, in
part, to the difficulty in analyzing the bottoms
composition. The reason for this was the resolution of the
chromatograph column for the methanol water system, poor
sampling valve performance and normalization of the G.C. data. Methanol and water are both polar solvents. Therefore, the large water peak dominated the methanol peak, and both were very large compared to the acetone peak. Small errors in these two large, overlapping peaks had a large effect on acetone composition upon normalization. The problem was partly resolved with the sampling valve described in Chapter 2.

The vapour and liquid temperature data corresponding to Run 1 are shown in Table 3.5, along with the simulation results for the same case. The comparison of data shows that the assumption of a equilibrium condition is reasonably satisfied. The experimental and simulated

<table>
<thead>
<tr>
<th>Tray</th>
<th>Liquid</th>
<th>Vapour</th>
<th>Simulated</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>54.89</td>
<td>-</td>
<td>55.90</td>
</tr>
<tr>
<td>2</td>
<td>55.67</td>
<td>55.38</td>
<td>56.35</td>
</tr>
<tr>
<td>3</td>
<td>56.85</td>
<td>56.50</td>
<td>57.24</td>
</tr>
<tr>
<td>4</td>
<td>56.97</td>
<td>57.18</td>
<td>58.38</td>
</tr>
<tr>
<td>5</td>
<td>63.94</td>
<td>63.57</td>
<td>62.02</td>
</tr>
<tr>
<td>6</td>
<td>71.03</td>
<td>70.43</td>
<td>72.74</td>
</tr>
<tr>
<td>7</td>
<td>69.24</td>
<td>68.89</td>
<td>70.79</td>
</tr>
<tr>
<td>8</td>
<td>68.08</td>
<td>67.59</td>
<td>69.98</td>
</tr>
<tr>
<td>9</td>
<td>67.51</td>
<td>67.02</td>
<td>68.84</td>
</tr>
<tr>
<td>10</td>
<td>66.82</td>
<td>66.33</td>
<td>67.04</td>
</tr>
<tr>
<td>11</td>
<td>63.59</td>
<td>64.11</td>
<td>64.34</td>
</tr>
<tr>
<td>12</td>
<td>67.15</td>
<td>67.42</td>
<td>66.78</td>
</tr>
<tr>
<td>13</td>
<td>70.69</td>
<td>71.15</td>
<td>71.59</td>
</tr>
<tr>
<td>Reb.</td>
<td>81.30</td>
<td>-</td>
<td>82.08</td>
</tr>
</tbody>
</table>
temperature data have been plotted in Figure 3.4. The sharp increase in the temperature profile corresponds to the solvent entry point.

Simulated composition profiles, matching the temperature profile, are plotted in Figure 3.5. The methanol composition in the liquid phase shows a maximum just below the feed tray. At the same point temperature profile shows a
local minima. The decrease in the temperature profile is due to the lower feed temperature. The acetone composition in the vapour phase increases rapidly in this region and also in the region around the solvent feed tray. The methanol composition increases above this tray because there is very little water above this tray, and because the equilibrium coefficient for methanol is relatively high in comparison to acetone. Due to the comparatively small increase in relative volatility in the middle section of the column, the acetone
composition shows little increase here. The presence of water on the trays also prevents the increase in vapour composition below the solvent feed tray. The relative volatility data for the temperature profile shown in Figure 3.4 are summarized in Table 3.6. These data reflect the temperature effect through partial pressures and the composition effect through the activity coefficients.

<table>
<thead>
<tr>
<th>Tray</th>
<th>Acetone</th>
<th>Methanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.021</td>
<td>1.050</td>
</tr>
<tr>
<td>2</td>
<td>1.050</td>
<td>1.030</td>
</tr>
<tr>
<td>3</td>
<td>1.106</td>
<td>1.000</td>
</tr>
<tr>
<td>4</td>
<td>1.253</td>
<td>0.968</td>
</tr>
<tr>
<td>5</td>
<td>2.022</td>
<td>1.087</td>
</tr>
<tr>
<td>6</td>
<td>5.878</td>
<td>2.385</td>
</tr>
<tr>
<td>7</td>
<td>5.878</td>
<td>2.770</td>
</tr>
<tr>
<td>8</td>
<td>4.671</td>
<td>1.929</td>
</tr>
<tr>
<td>9</td>
<td>4.179</td>
<td>1.748</td>
</tr>
<tr>
<td>10</td>
<td>3.477</td>
<td>1.497</td>
</tr>
<tr>
<td>11</td>
<td>2.529</td>
<td>1.176</td>
</tr>
<tr>
<td>12</td>
<td>3.075</td>
<td>1.317</td>
</tr>
<tr>
<td>13</td>
<td>4.414</td>
<td>1.749</td>
</tr>
<tr>
<td>Reb.</td>
<td>8.897</td>
<td>3.467</td>
</tr>
</tbody>
</table>

3.4 DYNAMIC MODEL OF AN EXTRACTIVE DISTILLATION COLUMN:

The dynamic model for the column was formulated by
adding the dynamic terms for the tray holdups and the liquid holdups in the reboiler and the overhead condenser. Additional assumptions were that there was constant volumetric liquid holdup and that the fluid dynamic response time was negligible compared with that for mass transfer. Based on these assumptions, Kumar et al. (1984) have developed the following transient equations.

The dynamic component material balance:

\[
\frac{d(M_j X_{ij})}{dt} = V_{j+1} Y_{ij+1} + L_{j-1} X_{ij-1} - V_j Y_{ij} - L_j X_{ij} + F X_{if} - W X_{iw} \quad (3.25)
\]

The total material balance:

\[
\frac{dM_j}{dt} = V_{j+1} + L_{j-1} - V_j - L_j + F - W \quad (3.26)
\]

where \( M \) is the molar tray holdup of the \( j \)th tray. After some manipulation, the following equation can be obtained:

\[
\frac{d( X_{ij})}{dt} = (V_{j+1} Y_{ij+1} + L_{j-1} X_{ij-1} - V_j Y_{ij} - F X_{if} - W X_{iw} - X_{ij}(V_{j+1} + L_{j-1} - V_j - F - W))/M_j \quad (3.27)
\]

The component material balance for the condenser is:

\[
\frac{d(M_{c, X_{i1}})}{dt} = V_2 Y_{i2} - L_1 X_{i1} - D X_{id} \quad (3.28)
\]
and for the reboiler is:

\[
\frac{d(M_b X_{ib})}{dt} = - V_b Y_{ib} + L_{b-1} X_{ib-1} - B X_{ib} \tag{3.29}
\]

The Murphree tray efficiencies, \( E_{ij} \), calculated from the steady state simulation were used in the dynamic simulation in order to calculate the true compositions of the vapour leaving each tray. The relationship for the \( j \)th tray was:

\[
Y_{ij} = Y_{ij+1} + E_{ij}(Y^*_{ij} - Y_{ij+1}) \tag{3.30}
\]

Since no vapour enters the reboiler, the Murphree efficiency was defined differently using the liquid composition in place of the vapour in equation (3.30):

\[
Y_{ib} = X_{ib} + E_{ib}(Y^*_{ib} - X_{ib}) \tag{3.31}
\]

The differential equations were solved at each tray for the liquid and vapour flow rates as a function of time. The enthalpy balance at each tray was defined as:

\[
\frac{d(H_j)}{dt} = V_{j+1} H_{j+1} + L_{j-1} h_{j-1} - V_j H_j - L_j h_j + F h_f - W h_w \tag{3.32}
\]
The change in enthalpy at each time step was assumed to vapourize more or less liquid on the tray; thus, producing a change in the vapour flow rates. The new vapour flow rates were calculated from:

\[ V_j(t+1) = V_j(t) + \frac{(dH_j}{dt}) t \]

\[ (H_j - h_j) t \]

(3.33)

where the subscript \( t \) means the \( t \text{th} \) sampling interval. The vapour flow rates were adjusted by beginning the calculation at the reboiler. The revised liquid flow rates were adjusted from the top of the column.

This set of dynamic equations was solved using the DYNSYS Simulation Package (1975) with the stiff option in Gear's Method for the integrations. This option was required because the difference between the reboiler dynamics and the tray dynamics is 6:1. To reduce the number of equations in the simulation, the integrations were done on the acetone and methanol compositions with the water composition being calculated by difference. At each step, vapour compositions for the entire column are recalculated using the bubble point method to give the new equilibrium temperature profile.

The stiff option in the Gear's method requires that the Jacobian Matrix for the system be calculated. This was done by taking partial derivatives for equation (3.27) with
respect to $x_{ij}$, $x_{ij-1}$ and other terms as required. The Jacobian Matrix for the system is given below:

$$
J_i = \begin{bmatrix}
\frac{\partial}{\partial x_{i1}} \frac{\partial x_{i1}}{\partial t} & \cdots & \frac{\partial}{\partial x_{ib}} \frac{\partial x_{i1}}{\partial t} \\
\vdots & \ddots & \vdots \\
\frac{\partial}{\partial x_{i1}} \frac{\partial x_{ib}}{\partial t} & \cdots & \frac{\partial}{\partial x_{ib}} \frac{\partial x_{ib}}{\partial t}
\end{bmatrix} (3.34)
$$

Some problems were encountered with the automatic step size adjustment in the Gear's Method as the system approached steady state. This resulted in time step sizes which were too large to allow critical dynamics in the nonlinear system to be calculated. The automatic step size adjustment was restricted by specifying a short time interval (i.e., 0.1 hr) for each solution, and using the results of the previous solution as the initial conditions for the next solution.

### 3.5 Experimental and Simulation Results (Dynamic):

The open loop dynamics were investigated by applying step changes in feed rate, reflux rate, feed composition and reboiler duty, but with the liquid levels in the reboiler and the overhead condenser under proportional integral control during these tests. Details of the response of these
control loops may be found in Langille (1983).

In order to estimate the process time constants, and to show the dynamic behaviour of the column, a number of step tests were performed. Step changes in feed composition, feed flow rates, reboiler duty and reflux rates were implemented; both on the experimental equipment, and in the simulation. The initial conditions (i.e., column profiles), for the dynamic simulation were provided by the steady state program. For each case, the experimental data, the simulation results and a fitted set of transfer function models are shown. The key responses are the acetone in the overhead and methanol in the bottoms product composition.

Figure 3.6 shows the response to a step change in feed composition from 0.637 mole percent acetone to 0.5578 mole percent. The acetone composition is well modelled by

The empirical transfer function and the simulation. There is a significant transport lag in this response. The methanol composition in the bottoms follows the direction of the experimental response but it is shifted in time. This is attributed to an error in the initial conditions. It is emphasized here that no parameters were adjusted in the dynamic simulation; except for the tray holdups, which were estimated to be 450 ml, and the reboiler, which was 6 litres. These were fixed for the simulations.

The responses to a step increase in reboiler duty (steam pressure) are shown in Figure 3.7: The bottoms
Figure 3.6: Feed Composition Step Responses

Composition responds very quickly, as expected, and the overhead acetone composition shows a rather long lag caused by mass transport in the column. The general shape of the response from the simulation is different for the experimental overhead composition, although the time to reach equilibrium agrees well with the data.

Figure 3.8 shows the response of the column to a step change in reflux flow rate from 149 ml/min to 180 ml/min. The bottoms composition shows slight non-minimum
phase behaviour. The gains for the reflux step are small. The reason is that a high reflux rate tends to reduce the solvent concentration by increasing the non-solvent components in the liquid phase. Therefore, the advantage of the higher reflux is reduced due to a decrease in the relative volatilities. The non-minimum phase behaviour is shown both in the experimental response and in the simulation. One reason for the difference between the two is the poor resolution of the process chromatograph. It is also assumed there is no heat loss. However, the column was not
insulated and heat losses varied as the environmental
temperature changed.

Figure 3.8: Reflux Flow Rate Step Responses

The response to a step change in feed flow rate from
143.2 to 109.9 mole/hr is shown in Figure 3.9. A slight
non-minimum phase response is shown for the overhead
composition in both the simulation and the experiment. The
acetone composition rises due to the lower column
temperature (for the same reboiler duty). The simulation
does not fit the bottoms composition well. The column
responds less quickly than predicted by the model.
Finally, Figure 3.10 shows the same column response to a step change in feed flow rate. This run was nominally the same as for Figure 3.9 but the response was puzzling since it went in a direction opposite to that of the previous result. This was not initially predicted by the simulation and prompted an investigation of the process itself. The difference stemmed from a malfunctioning in the reflux temperature controller, with the result that the reflux stream was entering the column at a higher temperature than that on the top tray. This is similar in
Figure 3.10: Troubleshooting Feed Flow Rate Step Responses

effect to an increase in the reboiler heat load, and when this was implemented in the simulation the results matched the experimental responses shown in Figure 3.10. The interesting observation one can make here is that a simulation can be very useful for process troubleshooting. It is also noted here that for these multicomponent systems it is much more difficult to predict the effects of changes in the manipulated or load variables than for the equivalent binary systems. The difficulties arise from: system non-linearities, poor or inadequate measurements (compositions are no longer predicted correctly by tray temperatures) and
by operating ranges where desired outputs are uncontrollable by the column manipulated variables.

Table 3.7 shows the fitted transfer function models for all of the step response tests. The models were obtained by nonlinear least squares estimates for models of either first or second order with dead-time form. The criterion for model selection was the minimization of the sum of squares of residuals. Except for the step response of the overhead product to feed composition, which had a large dead-time, all the overhead composition responses are well represented by second order transfer function models. The bottoms compositions tended to be first order dead-time models with larger time constants than the above. This probably reflects the large holdup in the reboiler relative to tray holdups.

3.6 EFFECT OF SOLVENT FLOW:

Figure 3.11 shows the dynamic effect of the solvent flow rate. A severe negative step change from 176.0 mole/hr to 24.5 moles/hr was introduced. From Figure 3.11 it is clear that the top product composition has gone below 80% clearly indicating that the feed composition (0.60, 0.40) and the operating conditions of the column do not allow greater separations.

The effect of the solvent to feed ratio can be seen from Run 2 and Run 4 (given in Table 3.2). In Run 4 the feed
Table 3.7  Transfer Functions

<table>
<thead>
<tr>
<th>Manipulated Variable</th>
<th>Top Product (Acetone)</th>
<th>Bottoms Product (Methanol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed composition (0.637 to 0.5578) Acetone</td>
<td>$0.53 e^{-7.0s}$ $(30.3s + 1)$</td>
<td>$-0.366 e^{-8.0s}$ $(45.0s + 1)$</td>
</tr>
<tr>
<td>Steam Pressure 152.7 to 172.4 kPa(gauge)</td>
<td>$-0.0045 e^{-5.0s}$ $400s^2 + 26.88s + 1$</td>
<td>$-0.0015 e^{-2.0s}$ $(37.0s + 1)$</td>
</tr>
<tr>
<td>Reflux Flow Rate 149.0 to 180.0 ml/min</td>
<td>$0.00132 e^{-6.0s}$ $883s^2 + 25.43s + 1$</td>
<td>$0.00065 e^{-17.0s}$ $(52.8s + 1)$</td>
</tr>
<tr>
<td>Feed Flow Rate (142.8 to 109.0 ml/min</td>
<td>$-0.00151$ $900s^2 + 48.0s + 1$</td>
<td>$-0.00177$ $(90.0s + 1)$</td>
</tr>
</tbody>
</table>

ratio is lower, giving rise to a lower relative change in the volatility of acetone to methanol. The consequence is that the separation is poor compared with that in Run 2. This indicates that the solvent flow rate to feed flow rate ratio has a critical role on controlling the top product composition. To illustrate this point, the solvent liquid composition profile for the column for Run 2, 4 and 5 are shown in Figure 3.12. From these it is clear that the nature of the profile is the same for all cases in that there is a
sudden increase in the solvent composition at the solvent and feed trays, as expected. However, the factor that governs the separation is the region between the two feed points. The profile steepness declines from Run 4 to Run 2 to Run 5 in the reverse order of the acetone separation. From this it is concluded that for better separation in extractive distillation, the solvent concentration profile between the feed points should be as flat as possible. The profile will depend upon the solvent flow rate, the feed flow rate, the feed composition and the reflux flow rate.
3.7 NONLINEAR BEHAVIOUR OF THE COLUMN:

To illustrate the nonlinear behaviour of the column, steady state gains for 10% disturbances in feed composition, feed flow rate, reflux flow rate, and reboiler duty were calculated for two different operating conditions for the column. These are summarized in Table 3.8. The nonlinear effects are particularly significant for the feed flow rate changes and for the feed composition changes. This is an
Table 3.8: Steady State Gain (absolute) for 10% Disturbance

<table>
<thead>
<tr>
<th></th>
<th>Gain (Top)</th>
<th>Gain (Bottom)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>FEED COMPOSITION</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ist Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(0.5578, 0.4422)</td>
<td>0.0259</td>
<td>-0.0186</td>
</tr>
<tr>
<td>IIInd Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(0.65, 0.35)</td>
<td>0.310</td>
<td>-0.0204</td>
</tr>
<tr>
<td><strong>FEED FLOW RATE</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ist Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>109.87 Moles/hr</td>
<td>0.0136</td>
<td>0.0183</td>
</tr>
<tr>
<td>IIInd Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>100.00 Moles/hr</td>
<td>0.0265</td>
<td>0.0238</td>
</tr>
<tr>
<td><strong>REFLUX FLOW RATE</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ist Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>142 ml/min</td>
<td>0.0414</td>
<td>0.0124</td>
</tr>
<tr>
<td>Feed Comp (0.5578, 0.4422)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IIInd Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>142 ml/min</td>
<td>0.415</td>
<td>0.0146</td>
</tr>
<tr>
<td>Feed Comp (0.673, 0.327)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>REBOILER DUTY</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ist Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1628.12 Kcal/hr</td>
<td>0.0937</td>
<td>-0.0485</td>
</tr>
<tr>
<td>IIInd Condition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1709.0 Kcal/hr</td>
<td>0.0846</td>
<td>-0.0500</td>
</tr>
</tbody>
</table>

Gain (Top) = Acetone Composition
Gain (Bottoms) = Methanol Composition
important result because it illustrates the importance of the complete simulation. Fitted transfer functions could only be used to derive control schemes in a region for which the implied linearization was valid. By contrast, the detailed nonlinear models show valid responses throughout the operating range of this column. Even transfer functions derived from these models could be used for control system design purposes only in the close vicinity of the operating point.

3.8 SIMPLE MODEL FOR VLE CALCULATIONS FOR ACETONE-METHANOL AND WATER SYSTEM:

The models in Sections 3.1 and 3.3 use the 3rd order Margules's equation to calculate activity coefficients and the Antoine equation to calculate vapour pressure. One of the most time consuming procedures in the simulation of a distillation process is the calculations of the vapour-liquid equilibrium (VLE) data. As the number of components increase the equations become more and more rigorous, and solving them requires more CPU time. In this section, a simple local model for calculating the K-values for acetone, methanol and water system is presented.

The VLE for a N-component system is defined in terms of the equilibrium ratio $K_i$ as:
\[ K_i = \frac{Y_i}{X_i} = \frac{r_i P_i^*}{\phi_i P} \]  \hspace{1cm} (3.35)

for \( i = 1, 2 \ldots N \)

The activity coefficient, \( r_i \), is calculated either by the Wilson equation or by other equations. When the 3rd order Margule's equation is used for calculating the activity coefficient, approximately 45 mathematical operations (- + / *) are required for each component at each step. For the process where the assumption of an ideal vapour phase is valid, \( \phi_i \) can be set to be 1 and equation 3.35 becomes:

\[ K_i = \frac{r_i P_i^*}{P} \]

\[ \ln(K_i) = \ln(r_i) + \ln(P_i^*) - \ln(P) \]  \hspace{1cm} (3.36)

In terms of relative volatilities this is:

\[ \frac{K_i}{K_{re}} = \frac{r_i P_i^*}{r_{re}^* P_{re}} \]

\[ \ln(K_i / K_{re}) = \ln(r_i) - \ln(r_{re}) + \ln(P_i^*) - \ln(P_{re}^*) \]  \hspace{1cm} (3.37)

where \( re \) stands for the reference component.

The vapour pressure, \( P_i^* \), is calculated using the two
parameter Antoine equation given as:

$$\ln \left( P_i^* \right) = (VP1)_i - (VP2)_i / T$$

and

$$\ln \left( P_i \right) - \ln \left( P^* \right) = G_i - \left( Z_i / T \right) - G_{re} \left( Z_{re} / T \right)$$

(3.38)

The RHS can be approximated so that:

$$\ln \left( P_i^* \right) - \ln \left( P^* \right) \approx g_i + \left( z_i / T \right)$$

(3.39)

It is assumed that the ternary mixture behaves as a pseudo-binary mixture. This is a reasonable assumption in the three component distillation, since normally all three components do not vary from 0-100% within the column. In the ternary system under study, methanol varies between 10-30% within the column; therefore, it is assumed that the ternary mixture resembles a pseudo binary mixture. The Margule equation for the binary mixture is given as:

$$\ln( r_i ) = x_2^2 ( \beta_2 + \beta_1 x_1 )$$

(3.40)

This equation is used to approximate the activity coefficient in equation (3.36) and (3.37). Equation (3.36) can be approximated as:

$$\ln \left( K_i \right) = (1 - x_i)^2 ( FC1_i + FC2_i x_i ) + FC3_i \ln \left( P_i^* \right) - \ln \left( P \right) + FC4_i$$

(3.41)
Similarly for equation (3.37), the following approximate model is chosen:

\[
\ln \frac{K_i}{K_{re}} = \frac{FC1_i}{T} + FC2_i(1 - X_{re})^2 + FC3_i(1-X_i)2 + FC4_i
\]

(3.42)

Parameters of equations (3.41) and (3.42) are calculated through nonlinear regression. Since only a range of \(Y\) and \(X\) are selected, models given by equations (3.41) and (3.42) are called local models. Through the complete tray to tray simulation described in Section 3.1, \(56\) \(K\)-data were generated. Since water is the heaviest component and its activity does not change very much, it is selected as the reference component.

The following parameters are obtained using a nonlinear least squares estimate routine.

For water the parameters in equation (3.41) are:

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Confidence Interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>FC1 = 1.38850</td>
<td>( 1.436 1.341 )</td>
</tr>
<tr>
<td>FC2 = 0.04102</td>
<td>( 0.2807 -0.1986)</td>
</tr>
<tr>
<td>FC3 = 1.1371</td>
<td>( 1.197 1.077 )</td>
</tr>
<tr>
<td>FC4 = -2.3413</td>
<td>( -1.894 -2.789 )</td>
</tr>
</tbody>
</table>

Using water as the reference component, the methanol parameters in equation (3.42) are:
Parameters  	Confidence Interval
FC1 = -94.0339  
( -86.49  -101.69 )
FC2 = -0.9686  
( -0.9146  -1.1023 )
FC3 = 0.5766  
( 0.6352  0.5183 )
FC4 = 2.6673  
( 2.781  2.5545 )

Using methanol as the reference component, the parameters for the acetone are:

Parameters  	Confidence Interval
FC1 = 175.8103  
( 198.9  152.7 )
FC2 = 0.21986  
( 0.3002  0.1395 )
FC3 = 1.985  
( 2.119  1.857 )
FC4 = -3.3209  
( -2.845  -3.796 )

From the parameters result, it seems FC2 for water is not statistically significant. To show the validity of the proposed model, 8 sets of data were generated using the simulation program at different operating points. The liquid composition and the temperature data from simulation results were used as the input data for the model. The composition error variance and the maximum absolute value of the residual for the three components for all 8 conditions are given below:
<table>
<thead>
<tr>
<th></th>
<th>error variance</th>
<th>Max. absolute error</th>
</tr>
</thead>
<tbody>
<tr>
<td>acetone</td>
<td>6.26 E-05</td>
<td>1.94 E-02</td>
</tr>
<tr>
<td>methanol</td>
<td>3.58 E-05</td>
<td>1.46 E-02</td>
</tr>
<tr>
<td>water</td>
<td>1.48 E-05</td>
<td>1.19 E-02</td>
</tr>
</tbody>
</table>

In the above analysis, the reference component for acetone was changed from water to methanol. The composition error variance for the acetone with water as the reference component was 1.55E-04. The reason for a larger variance is attributed to a larger K-value difference between acetone-water than for acetone-methanol. Therefore, the reference component was changed from water to methanol. Figure 3.13 shows the comparison of the composition profiles for the three components from the model presented in Section 3.1 and from the simple local VLE model. Figure 3.13 shows good agreement between the two models.

The above results show the validity of this method. Its main attributes are:

1. It requires only 11 mathematical operations to give the K-values. Thus, reducing the calculation time significantly.

2. The ability of the model to produce good VLE data in the operating region and its simple form suggest it can be used easily for the steady state and the dynamic simulation.
Figure 3.13: Comparison of Vapour Phase Steady State Composition Profile

- - - 3rd order Margule's Method
--- --- Simple Local VLE Model
3.9 REMARKS:

1. The vapourization efficiency defined as:

\[ Y_{ij} = F_{ij}^* i_j k_{ij} X_{ij} \]  

(3.43)

can also be used instead of Murphree efficiencies defined by equation (3.10). Calculations were carried out using the vapourization efficiencies given in Table 3.9. The final results for the different cases were close to the results presented in Table 3.4.

2. The simulation can be used easily for systems other than acetone, methanol, and water. One would need to supply the appropriate data in Table 3.1 to calculate the activity coefficients and vapour pressures. Both vapour pressure and activity coefficients are calculated in separate routines and can be changed easily if methods other than 3rd Margule's and Antoine equations are used. The user also has to supply the efficiency factors, which depend upon the system under study and upon the experimental equipment from which data is obtained. The assumptions of a total condenser and constant column pressure are also limitations of the simulation. However, for the partial condenser case, only equation (3.4) has to be changed. For systems where the
Table 3.9: Vapourization Efficiencies for the Column

<table>
<thead>
<tr>
<th>Tray</th>
<th>Acetone</th>
<th>Methanol</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>1.0</td>
<td>1.0</td>
<td>1.1</td>
</tr>
<tr>
<td>3</td>
<td>1.0</td>
<td>1.0</td>
<td>1.05</td>
</tr>
<tr>
<td>4</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>1.08</td>
<td>1.05</td>
<td>1.0</td>
</tr>
<tr>
<td>6</td>
<td>1.05</td>
<td>1.06</td>
<td>1.0</td>
</tr>
<tr>
<td>7</td>
<td>1.03</td>
<td>1.04</td>
<td>1.0</td>
</tr>
<tr>
<td>8</td>
<td>1.0</td>
<td>1.03</td>
<td>1.0</td>
</tr>
<tr>
<td>9</td>
<td>0.97</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>10</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>11</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>12</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>13</td>
<td>0.98</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Reb.</td>
<td>0.95</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

pressure drop is appreciable, equation (3.11 b) has to be modified to:

\[ K_{ij} = r_{ij} k_{ij} \]

\[ k_{ij} = \frac{p^*_i}{p_j} \]  \hspace{1cm} (3.11c)

where \( p_j \) is the pressure at the jth tray.

The user can easily incorporate a variable pressure because the \( k_{ij} \) are calculated in a separate routine.

3. Since the primary objective of this project was to
understand the system behaviour, the simulation does not include a heat-loss model. The experimental distillate flow rate was used to calculate the required heat duty. However, for control studies based on the reboiler heat duty as a manipulative variable, one needs to use the supplied steam pressure to calculate the corresponding distillate flow rate. This calculation procedure requires a heat loss model. This is presented in the next chapter.

3.10 CONCLUSIONS:

Steady state and dynamic mass and energy balance models have been developed for an extractive distillation system separating acetone and methanol using water as a solvent. The importance of a good simulation for nonlinear multicomponent systems is highlighted. The simulations have been fitted to process operating data by adjusting the Murphree and vapourization efficiencies. Literature data were used in the equilibrium calculations for the three component mixture. A simple model for VLE calculations was developed for the system, and its validity was demonstrated. The dynamic models used the results from the steady state simulations and adjusted only the tray holdups. Transfer function models were fitted to the step response test to allow simple controller testing. Generally, the simulations gave good agreement with experimental results over a broad
range of nonlinear operating conditions. The nonlinear
behaviour of the column was adequately simulated by the
models. Finally, the importance of the solvent in increasing
the separation was shown.
NOMENCLATURE

a = Coefficients for 3rd order Margule equation (3.18)
A_{ij} = Absorption factor of component i at tray j
A_i = Tridiagonalised matrix for equation (3.17b)
B = Bottoms product flow rate moles/hr
ΔC = Difference between Experimental and Simulated
ΔC_1 = ΔC for Top Product Composition (Mole Fraction)
ΔC_2 = ΔC for Bottoms Product Composition (Mole fraction)
ΔC_3 = ΔC for Bottoms Flow Rate (ml/min)
(d_i)_C0 = Corrected distillate flow rate using Theta
(d_i)_C_a = Calculated distillate flow rate in simulation
D = Distillate flow rate moles/hr
D_i = Component distillate flow rate for component i
E_{ij} = Murphree efficiency of component i at tray j
E_{i,j} = Vapourization efficiency of component i at tray j
f_i = Feed flow rate of component i moles/hr
\tilde{f}_i = Component feed flow vector used in equation (3.17b)
F = Total feed flow rate moles/hr
F_r = Feed flow rate at r^{th} tray
f_{ir} = Component feed flow rate at r^{th} tray
FC1 = Constant for equations (3.41) and (3.42)
FC2 = Constant for equations (3.41) and (3.42)
FC3 = Constant for equations (3.41) and (3.42)
FC4 = Constant for equations (3.41) and (3.42)
$g_i = \text{coefficient for equation (3.38)}$

$h_j = \text{liquid enthalpy of the stream leaving} \ j\text{th tray (kcal/(mole.hr))}$

$h_{ij}^* = \text{Liquid enthalpy of component i at tray j (kcal/(mole.hr))}$

$h_f = \text{Feed enthalpy (kcal/(mole.hr))}$

$H_{rf} = \text{Enthalpy of the feed entering at r\text{th tray}}$

$H_b = \text{Enthalpy of the vapour stream leaving reboiler}$

$h_m = \text{Heat of mixing (kcal/(mole.hr))}$

$h_{rw} = \text{Enthalpy of the liquid drawoff at r\text{th tray}}$

$h_w = \text{Enthalpy of the liquid drawoff (kcal/(mole.hr))}$

$h_d = \text{Enthalpy of the distillate (kcal/(mole.hr))}$

$H_j = \text{Vapour enthalpy of the stream leaving j\text{th tray (kcal/(mole.hr))}}$

$H_{ij}^* = \text{Vapour enthalpy of the component i at tray j}$

$k_{ij} = \frac{P_i}{P} \text{k-value of component i at tray j}$

$K_{ij} = k_{ij} r_{ij}$

$l_{ij} = \text{liquid flow rate of component i at tray j}$

$L_j = \text{Liquid flow rate leaving j\text{th tray (moles/hr)}}$

$L_{b-1} = \text{Liquid flow from tray above the reboiler}$

$M_b = \text{Reboiler molar holdup}$

$M_c = \text{Condenser molar holdup}$

$M_j = \text{Molar holdup of j\text{th tray}}$

$N = \text{Number of components in the system}$

NP = Total number of trays
\( P_i^* \) = Vapour pressure of component \( i \) (mm of Hg)
\( P_i = (d_i)_{CO}/(d_i)_{CA} \)
\( P \) = Total pressure of the system (mm of Hg)
\( Q_C \) = Condenser heat duty (kcal/hr)
\( Q_B \) = Reboiler heat duty (kcal/hr)
\( s \) = Laplace variable
\( S_{ij} \) = Defined by equation (3.16)
\( T \) = Temperature in °C
\( t \) = \( t^{th} \) sampling time

\( v_{ij} \) = Vapour flow rate for \( i^{th} \) component leaving \( j^{th} \) tray
\( v_j \) = Vapour flow rate leaving tray \( j \) (moles/hr)
\( VP1 \) = coefficient 1 for 2 parameters Antoine equation
\( VP2 \) = coefficient 2 for 2 parameters Antoine equation
\( v_i \) = Component vapour flow rate for component \( i \) vector used in equation (3.17b)
\( w_i \) = Liquid drawoff of component \( i \) (moles/hr)
\( w_{ir} \) = Liquid drawoff of component \( i \) at \( r^{th} \) tray
\( W_j \) = Liquid drawoff from tray \( j \) (moles/hr)
\( X_i \) = Liquid composition for component \( i \) used in section 3.7
\( X_{ib} \) = bottoms product composition for component \( i \)
\( X_{id} \) = distillate composition for component \( i \)
\( X_{if} \) = feed composition of component \( i \)
\( X_{ij} \) = Liquid composition of component \( i \) at tray \( j \)
\( X_{iw} \) = liquid composition of drawoff
\( Y_{ij} \) = vapour composition of component \( i \) at tray \( j \)
$Y_{ij}^* =$ Equilibrium vapour composition of component $i$ at tray $j$

$Y_{ib} =$ Vapour composition of component $i$ leaving reboiler

$Z_i =$ coefficient for equation (3.38)

$z_i =$ coefficient for equation (3.39)

GREEK SYMBOLS:

$\tau_{ij} =$ Activity coefficient of component $i$ at tray $j$

$\alpha =$ 1 for feed plate, otherwise = 0

$\Gamma =$ 1 for drawoff plate, otherwise = 0

$\phi_i =$ fugacity coefficient of component $i$

$\beta_1, \beta_2 =$ Coefficients for 2nd order margules method for binary mixture

= Partial derivatives

Subscripts:

$b =$ reboiler

c = condenser

$ca =$ calculated quantity

$co =$ corrected quantity

d = distillate

$f =$ feed

$i =$ component

$j =$ tray number
\[ j+1 = \text{tray just below the } j\text{th tray} \]
\[ j-1 = \text{tray just above the } j\text{th tray} \]
\[ m = \text{component number for equation (3.18)} \]
\[ \text{mix} = \text{mixing} \]
\[ \text{re} = \text{reference component} \]
\[ t = t \text{ sampling time} \]
Chapter - 4

COMPARTMENTAL MODEL OF AN EXTRACTIVE DISTILLATION COLUMN

4.1 INTRODUCTION:

In the previous chapter a tray-to-tray model of an extractive distillation column was presented. The tray to tray model gives a complete understanding of the physical system over a wide range of operating conditions. However, a distillation column normally has a large number of trays; there are several industrial columns consisting of more than a hundred trays. Therefore, a simulation based on tray to tray equations requires a large computation effort, particularly for a nonlinear and multicomponent systems. The application of this type of simulation in control studies has the major disadvantage of producing a large number of state variables. This not only effects the computation time, but it also requires a large memory space. For the case where optimisation of a large network is sought, a complete model may be inappropriate from a computational viewpoint. A reduced order model is often necessary for online control since complex problems like network optimisation, quick calculation of process gains and dynamics, and selection of
appropriate control schemes can be implemented much more efficiently with a reduced order model than with a complete model. Since the objective of this work was to implement a model-based advanced controller, a reduced order model for a pilot scale distillation column was sought.

A brief review of the literature on the methods used in the production of reduced order models has been discussed in Chapter 1. In this chapter a compartmental method with a thermodynamic basis is developed and used to obtained a reduced order model of an extractive distillation column. The mass and energy balance equations for the compartments are developed in Section 4.2. A heat loss model for the experimental equipment is presented in Section 4.3. Section 4.4 summarises all the steps needed to solve for the steady state profiles. The model predictions over a wide operating space are compared with experimental data in Section 4.5. The conclusions are given in Section 4.6.

4.2 STEADY STATE COMPARTMENTAL MODEL:

The model introduced here is a steady state compartmental model in which trays are grouped to reduce the total number of mass and energy balance equations. The reasoning for combining trays into a compartment is that, although there may be a sharp temperature profile within the column, there are certain sections in which the profile can
be approximated by a linear function. All trays in this section are grouped together and called a compartment. The selection of a compartment can also be made on the basis of relative volatility. The size of the compartment depends upon various $K$-values and the degree of accuracy required. Each of these compartments is considered as one stage, thus reducing the total number of effective stages. For an ideal system this analysis can considerably reduce the number of effective stages and thus save computation time.

Figure 4.1 shows a typical compartment with $N$ trays for the case where no feed stream enters. The total material balance for the $j^{th}$ compartment:

$$L'_{j-1} - V'_j - L'_j + V'_{j+1} = 0 \quad (4.1)$$

Figure 4.1: Typical Compartmental Configuration
where the prime indicates that the flow rates are the compartmental values.

The compartmental component material balance for the \( j \)th compartment and the \( i \)th component is:

\[
L'_{j-1}X_{ij-1} - V_j'Y_{ij} - L'_jX_{ij} + V'_{j+1}Y_{ij+1} = 0
\]  \( (4.2) \)

The enthalpy balance equation is:

\[
L'_{j-1}h_{j-1} - V_j'\hat{h}_j - L'_j\hat{h}_j + V'_{j+1}\hat{h}_{j+1} = 0
\]  \( (4.3) \)

By defining an effective \( K \)-value for the compartment the following equation can be written:

\[
Y_{ij} = K'_{ij}X_{ij}
\]  \( (4.4) \)

It should be noted that \( T_j \neq T_j^* \) (where \( T_j^* \) refers to the liquid temperature) in Figure 4.1 because the vapour and liquid streams leaving the compartment are not at true equilibrium.

In general, equations (4.1) to (4.4) are similar to those described for tray to tray calculations. The only difference in the two representations lies in the method by which the thermodynamic properties (mainly \( K \)-value) are calculated. A true equilibrium is assumed for the tray to tray model. In the present model this relationship is obtained in the following manner.

In Figure 4.1 the compartmental flow rates are
defined as:

\[ v_{ij}' = v_j v_{ij} \quad , \quad l_{ij}' = L_j x_{ij} \]  \tag{4.5}

\[ A_{ij}' = L_j \left( \frac{K_{ij} v_j'}{v_j} \right) \quad , \quad l_{ij}' = A_{ij}' v_{ij}' \]  \tag{4.6}

\( A_{ij}' \) is defined as the effective compartmental absorption factor for compartment \( j \) and component \( i \).

Substituting equation (4.5) into equation (4.2) yields:

\[ l_{ij-1}' - v_{ij}' - l_{ij}' + v_{ij+1}' = 0 \]  \tag{4.7}

Substitute for \( l_{ij}' \) from equation (4.6) to get:

\[ l_{ij-1}' - (A_{ij}' + 1) v_{ij}' + v_{ij+1}' = 0 \]  \tag{4.8}

In Appendix A, it is shown how equation (4.8) can be changed so that the equation has only vapour flow rate variables. In general it can be written as:

\[ A_{ij-1}' v_{ij-1}' - (A_{ij}' + 1) v_{ij}' + v_{ij+1}' = 0 \]  \tag{4.9}

\( A_{ij-1}' \) is a modified compartmental absorption factor which depends upon the number of trays in the compartment, the flow profile, the temperature profile, and the compartmental absorption factor of the previous compartment.
Note that the subscript "i" for the component is dropped from here onwards, but the equations are valid for all components.

Using the method of induction the expressions for $A_j$ for a compartment with 1, 2, 3 and 4 trays are derived in Appendix A, and results are shown in Table 4.1. From Table 4.1, the following general equations for $A_{j-1}$ and $A_j$ can be obtained for a compartment with $N$ trays.

$$A_{j-1} = \left[ \sum_{k=2}^{N} \left( \frac{k}{p=N} A_p \right) + 1 \right] A_{j-1} \quad (4.11)$$

$$A_j = \left[ \sum_{k=1}^{N} \left( \frac{k}{p=N} A_p \right) \right] \quad (4.12)$$

for $N = 1$

$$\left[ \sum_{k=2}^{N} \left( \frac{k}{p=N} A_p \right) + 1 \right] = 1.0$$

where the $A_p$ are the absorption factors for each tray within the compartment and are defined as:

$$A_{ip} = \frac{I^*}{E_{ip} V_p K_{ip}} \quad (4.12)$$

$$K_{ip} = \tau_{ip} P_{ip} / P \quad (4.13)$$
where

- \( E_{ip} \) is defined as the efficiency factor at tray \( p \) for component \( i \)
- \( \gamma_{ip} \) is defined as the activity coefficient at tray \( p \) for component \( i \)
- \( P_{ip}^* \) is vapour pressure for component \( i \) at the \( p \)th tray
- \( P \) is the total pressure.

### Table 4.1: Compartmental Component Material Balance

<table>
<thead>
<tr>
<th>Case</th>
<th># Trays</th>
<th>Relationship Tray and Compartment</th>
<th>( \lambda_{j-1}^* \lambda_{j-1}^* )</th>
<th>( \lambda_{j+1}^* )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>( v_{j-1}' = v_0 ) ( v_j' = v_1 ) ( v_{j+1}' = v_2 )</td>
<td>1</td>
<td>( A_1 + 1 )</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>( v_{j-1}' = v_0 ) ( v_j' = v_1 ) ( v_{j+1}' = v_3 )</td>
<td>( A_2 + 1 )</td>
<td>( A_2 A_1 + A_2 + 1 )</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>( v_{j-1}' = v_0 ) ( v_j' = v_1 ) ( v_{j+1}' = v_4 )</td>
<td>( A_3 A_2 + A_3 + 1 )</td>
<td>( A_3 A_2 A_1 + A_3 A_2 + A_3 + 1 )</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>( v_{j-1}' = v_0 ) ( v_j' = v_1 ) ( v_{j+1}' = v_5 )</td>
<td>( A_4 A_3 A_2 + A_4 A_3 + A_4 + 1 )</td>
<td>( A_4 A_3 A_2 A_1 + A_4 A_3 A_2 + A_4 A_3 + A_4 + 1 )</td>
</tr>
</tbody>
</table>
Using the definition in equations (4.10) and (4.11), equation (4.9) becomes:

\[
\left[ \frac{N}{k} \sum_{p=N}^{k} A_p + 1 \right] A_{j-1} \left[ V_{j-1} - \left[ \frac{N}{k} \sum_{p=N}^{k} A_p + 1 \right] V_j + V_{j+1} \right] = 0 \quad (4.14)
\]

There are important points to note about equation (4.14). \( A_p \) can be calculated easily since the \( K \)-value for the individual trays and components can be obtained from the thermodynamics, given the temperatures, pressures, and liquid compositions. The first term in equation (4.14) is a product of two terms. The effective \( A' \) value from the previous compartment is modified by a factor of

\[
\left[ \frac{N}{k} \sum_{p=N}^{k} A_p + 1 \right]
\]

If a compartment has only one tray, i.e., if \( N=1 \), equation (4.14) reduces to:

\[ A'_{j-1} V_{j-1} - (A_1 + 1) V_j + V_{j+1} = 0 \]

which is exactly the same as if a tray to tray model is used. This shows agreement between the tray to tray and
compartmental model.

$E_{ip}$ used in equation (4.12) is the total efficiency factor which includes all model mismatch. These can be used as the adjustable parameters in the final fitting of the model to plant data.

The above analysis can be extended for a compartment with multiple feeds and drawoffs as shown in Figure 4.2.

Figure 4.2: Compartment with Multiple Feeds and Drawoffs
The general equation for the compartment is given as:

\[
\sum_{k=2}^{N} \left( \frac{\pi}{p=N} \frac{k}{\lambda_p} \right) + 1 \right] A_{j-1} v_{j-1} - \left[ \sum_{k=1}^{N} \left( \frac{\pi}{p=N} \frac{k}{\lambda_p} + 1 \right) \right] v_j^j + v_{j+1}^j
\]

\[
= NF - \sum_{m=1}^{N} \left( \sum_{k=fm+1}^{k} \frac{\pi}{p=N} \frac{k}{\lambda_p} + 1 \right) l_{fm}
\]

\[+ \sum_{m=1}^{NW} \left( \sum_{k=wm+1}^{k} \frac{\pi}{p=N} \frac{k}{\lambda_p} + 1 \right) l_{wm}
\]

(4.15)

where \(fm\) is the feed tray number in the compartment and \(wm\) is the drawoff tray number in the compartment. However, care should be taken about the validity of the assumptions while applying equation (4.15).

Equation (4.15) and equation (4.3) will now be used to model a distillation column under the following assumptions.

1. The vapour phase is assumed to follow the ideal gas law.
2. No shaft work.
3. Linear temperature, flow and composition profiles within the compartment.

Although it is assumed that the profiles can be approximated by a linear function, in the case of the feed
entry into a compartment mixing rule is used to get the compositions and temperature of the feed tray. This will be explained later in the chapter as the algorithm is developed.

For the pilot plant distillation column discussed in Chapter 2, one of the ways for the compartment layout is illustrated in Figure 4.3 for the five compartment model.

![Diagram](image)

**Figure 4.3:** 5 Compartmental Structure of the Extractive Distillation Column
The following equations are valid for all components.

For the condenser (compartment number 1):

\[ v_1' - l_1' + v_2' = 0 \]  \hspace{1cm} (4.16)

For the general compartment the equation is:

\[ \left[ \sum_{k=2}^{N} \left( \pi \frac{A_p}{p} \right) + 1 \right] l_{j-1}' \leq \left[ \sum_{k=1}^{N} \left( \pi \frac{A_p}{p} \right) + 1 \right] v_j' + v_{j+1}' = \delta A_f l_f \]  \hspace{1cm} (4.17)

In equation (4.17) \( \delta \) is equal to 1.0 if the feed is introduced and is zero otherwise. In writing the above equations, the component subscript has been dropped. Therefore, \( l_{j-1}' \) and \( v_j' \) refer to the component flow rates.

To solve these equations it is convenient to enclose the condenser with a succession of compartments moving down the column. Consider an envelope consisting of top (j-1) compartments and a condenser, where j is greater than 1. The component material balance for this envelope is given by:

\[ l_{j-1}' = v_j' - v_1' + \sum_{m=1}^{NF} l_{fm} \]  \hspace{1cm} (4.18)
where NF is the total number of feeds in the current envelope. Equation (4.18) is valid for all components. Substituting equation (4.18) in equation (4.17) and simplifying for only one feed and no drawoff in the compartment yields:

\[- \left[ \sum_{k=2}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right] v'_{1} - \left[ \sum_{p=N}^{1} \pi_{p} A_{p} \right] v'_{j} + v'_{j+1} = 0 \]

\[- \delta \left( \sum_{k=f_{1}+1}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right) l_{f_{1}} \]

\[+ \left( \sum_{k=2}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right) \sum_{m=1}^{NF} l_{f_{m}} \]  \hspace{1cm} (4.19)

The equation for the compartment containing the reboiler is similar and is:

\[- \left[ \sum_{k=2}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right] v'_{1} - \left[ \sum_{p=N}^{1} \pi_{p} A_{p} \right] v'_{j} = 0 \]

\[- \delta \left( \sum_{k=f_{1}+1}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right) l_{f_{1}} \]

\[+ \left( \sum_{k=2}^{N} \left( \sum_{p=N}^{k} \pi_{p} A_{p} \right) + 1 \right) \sum_{m=1}^{NF} l_{f_{m}} \]  \hspace{1cm} (4.20)

Equations (4.18) to (4.20) constitute a set of algebraic equations which can be solved to get component flow.
rates. A standard IMSL subroutine LEQT2F was used. The "Theta" method of convergence described by Holland (1975) was applied to get the required distillate flow rate and liquid and vapour compositions leaving each compartment. Based on the linear composition profile within the compartment, bubble point calculations are performed to get the top and bottom temperatures of each compartment. If a feed is introduced within the compartment, or between two compartments, then a mixing rule is used to calculate the profiles. In these cases sudden changes in the profiles due to feed entry can be captured easily. The mixing rule is as follows. For the compartment as shown in Figure 4.4.

Figure 4.4: Compartment with One Feed and No Drawoff
Suppose a profile for the property "Z" is required; Z may be temperature or composition.

Calculate the increment for the property \( Z \):

\[
Z_a = \frac{Z_2 - Z_1}{N}
\]  
(4.21)

where \( Z_2 \) and \( Z_1 \) are the properties at the outlet and inlet respectively of the compartment stream and \( N \) is the number of trays in the compartment. Then the value of that property on a tray within the compartment above the feed tray is:

\[
Z_p = Z_1 + (Z_a)p \quad \text{for } p = 1, \text{ to } f-1
\]  
(4.22)

At the tray \( f \) where the feed is introduced a mixing rule is used to calculate the property:

\[
Z_f = \frac{L_F Z_{f-1} + L_F Z_F}{(L_F + L_{f-1})}
\]  
(4.23)

A modified increment is used to calculate the property \( Z \) for the trays after the feed tray:

\[
Z_b = \frac{Z_2 - Z_f}{(N-f+1)}
\]  
(4.24)

Then the value of \( Z \) on these remaining trays is calculated:

\[
Z_p = Z_f + Z_b(p-f) \quad \text{for } Z = f, N
\]  
(4.25)
When Z is the temperature, it is assumed that the heat capacity of the mixing streams before and after mixing is nearly equal. If the feed is introduced between the compartments, then the mixing rule is used only to obtained the composition of the mixed stream. The top temperature of the compartment is calculated from the the bubble point method based on the new composition.

Since these equations are coupled the solution must be iterative. Given a composition and temperature profile, the next step in solving the compartmental model is to get the flow profile using the energy balance equation. This is a similar procedure to that used in the tray to tray model Chapter 3 and is not repeated here. Heat loss from the column is calculated based on the temperature profile using the model is given in Section 4.3.

Since the objective was to use the steam pressure for the control studies, it is supplied as the input to the simulation and the program then calculates the distillate flow rate and new flow profile. Once the new flow profile is known than an iterative scheme given in Section 4.4 is followed.

4.3 HEAT LOSS MODEL:

The following heat loss model was used:
\[ H_{ls} = c \left( \frac{\Delta T}{X_L} \right)^{0.25} (\Delta T) S_a \]  

The equation is similar to the heat loss due to natural convection given in Perry's handbook (1985). To compensate for the model mismatch due to other forms of heat losses, the parameter "c" in equation (4.22) was estimated to best fit the experimental results.

\[ \Delta T = \frac{(T_L + T_b)}{2} - T_{env} \]

- \( T_L \) = Top tray temperature in °C
- \( T_b \) = Reboiler temperature in °C
- \( T_{env} \) = Environmental temperature in °C
- \( X_L \) = Column length = 3.6 meters
- \( c \) = 21.37
- \( S_a \) = Surface area

**4.4 FLOWSHEET:**

The constants used for calculating the physical properties (i.e., vapour pressure, liquid and vapour enthalpies and activity coefficients) are given in Table 3.1. The simulation calculations are iterative in nature. A summary of steps of the calculation procedure is given below and in Figure 4.5.

1. Select the number of compartments and the number of
trays within each compartment.

2. Assume a set of temperatures for each compartment; two temperatures are assumed, one for the top of the compartment and one for the bottom.

3. Assume a set of vapour flow rates $V_j$.
   The corresponding liquid flow rates are calculated using the mass balance equation:

   $$ V_{j+1} + \sum_{m=1}^{NF} F_m = L_j + D $$

   (4.27)

4. Assume activity coefficients $\gamma_{ip}$ for components in all trays.

5. Calculate a linear temperature and flow profile within each compartment. Only one flow needs to be calculated linearly while the other should be calculated using equation (4.27).

6. Calculate the coefficients of equations (4.19) and (4.20).

7. Solve the set of algebraic equations (4.19) and (4.20) to get the compartmental component flow rates.

8. Use the Theta method to calculate the liquid and vapour composition profiles.

9. If feed is introduced, apply the mixing rule and then calculate the linear liquid composition profile.
within each compartment.

10. Calculate the activity coefficients for all components at all trays within each compartment.

11. Calculate the top and bottom compartment temperatures using bubble point calculations.

12. If the column is not insulated, calculate the net heat losses from the column using the heat loss model; i.e., equation (4.26).

13. If the new temperature profile is same as the old temperature profile (i.e., profile changes are less than 0.0005 °C), stop the simulation; otherwise go to step 14.

14. Using the new temperature and composition profiles, a new flow profile is obtained by energy balance. This step is performed in the same fashion as for the tray to tray calculations. The only difference is that the results are the liquid and vapour flow rates leaving each compartment rather than those leaving each tray. Once the new flow profile is known then go to step 5.

4.5 RESULTS AND DISCUSSION:

In order to test the model the three different configurations shown in Table 4.2 were used. Model #1 refers to a complete tray to tray model. Fifteen different
Figure 4.5: Flowsheet of the Algorithm

START

SELECT # OF COMPARTMENT AND CONFIGURATION

READ SYSTEM VARIABLES

ASSUME TEMPERATURE AND FLOW PROFILE

ASSUME ACTIVITY COEFFICIENTS

ASSUME LINEAR TEMPERATURE AND FLOW PROFILE WITHIN COMPARTMENTS

GET A SET OF COMPARTMENT COMPONENT BALANCE EQUATIONS

CONTINUED ON THE NEXT PAGE
Use LEQT2F to solve to get compartment component flow rates.

Use Theta method.

Linear composition profile within compartment using mixing rule.

Calculate top and bottom temperatures using bubble point method.

Is old temp. = new temp. profile?

Yes: Stop

No:

Calculate activity coefficients at each tray.

Perform heat loss calculations and energy balance to get new flows.
Table 4.2: Different Model Configuration

<table>
<thead>
<tr>
<th>Number of Compartment</th>
<th>Configuration</th>
<th>Solvent Compartment &amp; Tray</th>
<th>Feed Compartment &amp; Tray</th>
</tr>
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<td>Model# 2 5</td>
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<td>4 (1)</td>
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<tr>
<td>Model# 3 4</td>
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<td>4 (1)</td>
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<td>Model# 4 3</td>
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<td>3 (1)</td>
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</table>

operating conditions were chosen for the investigation. These conditions are given in Table 4.3. The results for the four models and corresponding experimental data are given in Table 4.4. The efficiency factors in equation (4.12) represent not only the vapourization efficiencies, but are also used as parameters to take care of model mismatch arising from the linearity assumption. Therefore, these factors are different for the different models, but are the same for all operating conditions for any one model. A different approach based on the nonequilibrium tray model presented by Krishnamurty et al. (1985) can also be used. In this method efficiency factors are not required, but one needs to know mass transfer coefficients which makes the calculation procedure more complex. Since the objective is to develop a model useful for control studies, optimization
Table 4.3: Steady State Operating Data (Experimental)

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Table 4.4: Simulated Steady State Conditions and Comparison to Experimental Data

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Table 4.4 (continued): Simulated Steady State Conditions and Comparison to Experimental Data

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</tr>
<tr>
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Avg. CPU Time (sec) 27.44 8.28 7.99 7.36
% Time Saving 69.8 70.6 73.0
and quick gain calculations simplicity of the equations is retained by using the efficiency factor approach rather than mass transfer coefficient approach. It is common practice in distillation column models to use either Murphree or the vapourisation efficiencies to match the simulations to the experimental data. In this study the $E_{ij}$ are used in place of these efficiency factors. The total number of parameters is the same as for the tray to tray model. These factors are given in Table 4.5.

Predicted compositions from four different models and the measured compositions for the acetone in the top product and methanol in the bottoms product are compared in Figures 4.6 and 4.7 respectively. All four models predict the composition equally well. It is observed that Model 2 (5 compartmental model) gave composition prediction closest to the complete tray to tray model.

To illustrate the comparison to experimental data, Figures 4.8 to 4.10 show the composition profiles obtained from the tray to tray model and the three different compartmental models for run 1. Figure 4.10 also shows the different sections for the 5 compartmental model. The sharp increase in the water composition at the solvent tray is obtained from the mixing rule. Similarly the mixing rule gives the drop in the composition at the feed tray. Since both the solvent and the feed enters at the first tray of compartments 3 and 4 respectively (see Table 4.2), the
<table>
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<td>1.17</td>
<td>0.82</td>
<td>0.99</td>
<td>1.16</td>
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</tbody>
</table>
Figure 4.6: Comparison of Top Product Acetone Composition

Figure 4.7: Comparison of Bottoms Product Methanol Composition
mixing rule was applied on the composition only. A linear composition profile within the compartment was obtained between the outlet composition and the composition resulting from the mixing rule. The results are in good agreement with each other. Figure 4.11 shows the experimental temperature profile along with the simulation results. The results of mixing calculations can be seen at the solvent and the feed tray. All models show a drop in the temperature profile in agreement with the experimental data. The nonlinear nature of the composition profiles is also captured by the mixing rule. Model 3 and Model 4, which lump the reboiler in the last compartment, require that two more parameters be assumed. These include the temperature difference between the reboiler and the tray above it. This was assumed to be 10°C (based on previous experience). Secondly the vapour flow leaving the reboiler was assumed to be 12 moles/hr less than the vapour flow leaving the last compartment.

In general, the compartmental models give results which are in good agreement with the tray to tray and experimental results. The largest error in the simulation are in acetone composition in the bottoms product stream for runs 1 to 7. In the real column, the chromatographic analysis of the bottoms product is difficult due to the large quantity of water in the bottoms product. This gives rise to a large peak in the chromatogram which overlaps with the methanol peak. Both peaks are very large compared to the
Figure 4.8: Comparison of Different Models Steady State Acetone Composition (Simulation)

Figure 4.9: Comparison of Different Models Steady State Methanol Composition (Simulation)
Figure 4.10: Comparison of Different Models Steady State Water Composition (Simulation)

Figure 4.11: Comparison of Different Models Steady State Temperature Profile (Experimental and Simulation)
acetone peak. Small errors in these two large peaks have a large effect on the measurement of the acetone composition when a normalisation calculation is performed. The unexpected large error for run 3 is due to a malfunctioning in the process gas chromatograph. As was explained in Chapter 2, the sampling valve was changed at this point and runs 8 to 15 were conducted with a new sampling valve. Considerable improvement in the agreement on acetone composition in the bottoms product can be seen in these experiments with the new sampling valve. Table 4.4 also shows the average computation time for the different models; savings of up to 73% can be achieved. This illustrates the usefulness of the compartmental model for quick calculation and optimization purposes.

In choosing the compartmental size, care should be taken for those components for which the K-value is less than 1.0. If a large number of trays are grouped together the coefficients of equations (4.17) to (4.19) are very different. As a result, accuracy may be lost. In the present system, water has a K-value ranging from 0.29 to 0.49. Therefore the following should be considered when selecting the compartments. First of all, select the section of the column which has an approximately linear temperature profile. Then check whether any of the components has a K-value less than 1.0. If so, run the compartmental simulation and check for the accuracy. If it passes the
accuracy test the model is adequate, otherwise reduce the compartment size. Most IMSL routines have such accuracy tests.

In the model, if the reboiler duty is specified, the program calculates the distillate flow rate from the energy balance equation. At every iteration, a new distillate flow is obtained. The actual distillate flow rate to be used can be calculated from

$$D_{it} = \sigma D_{it-1} + (1.0 - \sigma) D_{\text{new}}$$  \hspace{1cm} (4.29)

"it" is the present iteration number
"it-1" previous iteration number
$D_{\text{new}}$ is the unfiltered distillate flow in the it iteration
$\sigma$ filter constant

It was observed that filtered distillate flow rates with $\sigma=0.4$ converge faster than unfiltered flows ($\sigma=0.0$). In the particular case corresponding to run 1, Figure 4.12 shows the advantage of using the filtered data. With the unfiltered distillate flow, the algorithm does not converge in 50 iterations but with the filtered data it converges rapidly. All simulation results presented in Table 4.5 use $\sigma=0.4$. The value of $\sigma$ depends on the system under study.

One criticism which can be made about the algorithm is the number of parameters needed for the efficiency
Figure 4.12: Variation of the Distillate Flow Rate with Filter Constant

facators. The total number of parameters in the reduced-order and the tray to tray models are the same, whereas, the nature of a reduced order model suggests that it should need fewer parameters. In fact, the number of parameters required depends upon the nature of the system under study and the desired degree of accuracy. Calculations for the five compartmental model were repeated with the efficiency factors given in Table 4.6. In this case a single efficiency factor is used for each compartment and for each component. In this way, the total number of parameters was reduced from 45 to 15. Results for the 5-compartmental model with 15
Table 4.6: Efficiency Factors for 5 Compartmenal Model, One Factor for one Compartment

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Acetone</th>
<th>Methanol</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>2</td>
<td>0.95</td>
<td>1.0</td>
<td>1.02</td>
</tr>
<tr>
<td>3</td>
<td>1.01</td>
<td>1.04</td>
<td>0.93</td>
</tr>
<tr>
<td>4</td>
<td>0.90</td>
<td>0.89</td>
<td>1.24</td>
</tr>
<tr>
<td>5</td>
<td>1.03</td>
<td>0.95</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Parameters are compared to those for the 5-compartment model with 45 parameters for all 15 cases considered previously. These are presented in Figures 4.13 and 4.14. Even for this non-ideal azeotropic system, the comparison shows the favourable results for the 15 parameter model. Deviation from the experimental data is larger for the 15 parameter model than for the 45 parameter model. This is due to the nonlinear behaviour of the column. For an ideal linear system, one efficiency factor for one compartment would show much better results.
Figure 4.13: Comparison of Top Product Acetone Composition for 45 Efficiency Factors Model with 15 Factors Model

Figure 4.14: Comparison of Bottoms Product Methanol Composition for 45 Efficiency Factors Model with 15 Factors Model
4.6 CONCLUSIONS:

A compartmental model is developed and used to obtain a steady state model for an extractive distillation column. The number of equations to be solved in multicomponent distillation can be considerably reduced by using compartmental models. For the extractive distillation system, results show good agreement with experimental data and with the more rigorous tray to tray models. Savings of 73% in computation time were achieved. The nonlinear nature of the composition profiles is captured by using the mixing rule. It was observed that when the reboiler heat duty is known, a filtered distillate flow rate gives faster convergence.

The simulation was also performed with 15 efficiency factors in which a single efficiency factor is used for each compartment and for each component. In this way the total number of parameters was reduced from 45 to 15. For this azeotropic system the comparison with a 45 parameter model shows favourable results for a 15 parameter model.

The model can be used for any distillation system by providing the appropriate physical property data and compartment configuration.

The 5 compartmental model gives results which are closest to the tray to tray results. Therefore, this configuration will be used to formulate the system to get a
state space model for the control studies.
**NOMENCLATURE:**

\[
A_{ip} = \frac{L_p}{(E_{ip} K_{ip} V_p)} \quad \text{Absorption factor at the } p\text{th tray for the } i\text{th component}
\]

\[
A_{ij} = \frac{L_j}{K_j V_j} \quad \text{Absorption factor for the Compartment } j \text{ for the } i\text{th component}
\]

\[
A_{ij}^" = \text{Modified compartmental absorption factor given by equation (4.10)}
\]

\[
c = \text{Parameter for the equation (4.26)}
\]

\[
D = \text{Distillate flow rate moles/hr}
\]

\[
D_{new} = \text{Unfiltered distillate flow rate}
\]

\[
E_{ip} = \text{Efficiency factors at the } p\text{th tray for the } i\text{th component}
\]

\[
f_{m} = \text{feed tray number within compartment for } m\text{th feed}
\]

\[
f = \text{Feed tray number within the compartment}
\]

\[
F = \text{Feed flow rate moles/hr}
\]

\[
F_{m} = \text{Feed flow rate of } m\text{th feed}
\]

\[
h_j = \text{Molar liquid heat enthalpy of the stream leaving } j\text{th compartment kcal/hr}
\]

\[
H_j = \text{Molar vapour heat enthalpy of the stream leaving } j\text{th compartment kcal/hr}
\]

\[
H_{ls} = \text{Heat loss from the column kcal/hr}
\]

\[
K_{ij} = \frac{Y_{ij}}{X_{ij}} \quad \text{compartmental } K\text{-value for } j\text{th compartment and for } i\text{th component}
\]

\[
K_{ip} = r_{ip} P_{ip} / P \quad \text{plate } K\text{-value}
\]

\[
L_p = \text{Molar liquid flow rate leaving } p_{th} \text{ tray moles/hr}
\]

\[
L_j' = \text{Molar liquid flow rate leaving compartment } j \text{ moles/hr}
\]
\[ l_{ij} \] = Molar component liquid flow rate leaving the compartment \( j \) for the \( i \)th component moles/hr

\[ L_f \] = Molar liquid flow rate leaving feed tray in the compartment

\[ L_F \] = Molar feed flow rate

\[ l_{fm} \] = Molar component liquid flow rate for the \( m \)th feed moles/hr

\[ l_{wm} \] = Molar component liquid flow rate for the \( m \)th drawoff moles/hr

\[ N \] = Number of trays in the compartment

\[ NC \] = Number of components

\[ NF \] = Total number of feeds in the envelope

\[ NW \] = Total number of drawoffs

\[ N_{fd} \] = Total number of feeds entering in the compartment

\[ N_{dw} \] = Total number of drawoff streams from the compartment

\[ P_{ip}^* \] = Vapour pressure for component \( i \) on tray \( p \)

\[ P \] = Total system pressure

\[ S_a \] = Surface area of the column for heat loss in equation (4.26)

\[ T_b \] = Reboiler temperature in °C

\[ T_{env} \] = Environmental temperature in °C

\[ T_j \] = Vapour temperature leaving the compartment \( j \)

\[ T_j^* \] = Liquid temperature leaving the compartment \( j \)

\[ T_t \] = Top tray temperature in °C

\[ \Delta T \] = Temperature difference defined by equation (4.27)

\[ X_{ij} \] = Liquid composition leaving the compartment \( j \) for the \( i \)th component
\( X_L \) = Length of the column meters
\( V_p \) = Molar vapour flow leaving the tray \( p \) moles/hr
\( V_j' \) = Molar vapour flow leaving the compartment \( j \) moles/hr
\( V_{ij}' \) = Molar component vapour flow rate leaving the compartment \( j \) for the \( i \)th component
\( W_{m} \) = drawoff tray number in the compartment for the \( m \)th draw
\( Y_{ij} \) = Vapour composition leaving the compartment \( j \) for the \( i \)th component
\( Z \) = temperature or composition property for the mixing rule
\( Z_1 \) = \( Z \) at inlet of compartment
\( Z_2 \) = \( Z \) at outlet of compartment
\( Z_a \) = increment per tray for the \( Z \) property for the \( i \)trays above the feed tray
\( Z_F \) = Feed properties
\( Z_f \) = property at the feed plate
\( Z_p \) = \( Z \) at the \( p \)th tray
\( Z_b \) = Increment per tray for the \( Z \) property for trays below the feed tray

Subscripts:
\( j \) = \( j \)th compartment
\( j+1 \) = compartment below the \( j \)th compartment
\( j-1 \) = Compartment above the \( j \)th compartment
\( i \) = component
\( p \) = \( p \)th tray
\( m \) = feed or drawoff stream number
\( \lambda \) = iteration number
Greek Symbols:

\( \gamma_{ip} \) = Activity coefficient for \( i \)th component at \( p \)th tray

\( \delta = \begin{cases} 
1 & \text{if feed is introduced} \\
0 & \text{otherwise} 
\end{cases} \)

\( \sigma = \text{Filter constant for distillate flow rate} \)
Chapter 5

REDUCED ORDER BILINEAR MODEL OF AN EXTRACTIVE DISTILLATION COLUMN

5.1 INTRODUCTION:

In the previous chapter, reduced order steady state models of an extractive distillation column based on the compartmental technique were developed. The objective of this chapter is to develop a reduced order dynamic simulation which can be used for designing a model based controller using the reflux flow rate and the reboiler duty (steam pressure) as manipulated variables. In Chapter 3 it was shown that the system under study exhibits nonlinear behaviour. A complete nonlinear model would result in a complex controller structure, but a linear representation restricts the region of application. Therefore, a reduced order bilinear form is sought because it is a compromise between a linear and a nonlinear representation.

A brief description of a bilinear system, its advantages over a linear case, and its application in different fields, are discussed in Section 5.2. A bilinear model of a distillation column is developed in Section 5.3. The various steps involved in setting up and running the
simulation are given in Section 5.4. The simulated responses for step changes in reflux flow rate, feed flow rate, and reboiler duty are compared with the experimental data and a tray to tray model in Section 5.5. Section 5.6 covers the conclusion.

5.2 BILINEAR SYSTEMS:

A theoretical representation of any system, whether chemical, biological, socio-economic, ecological etc., uses some kind of a mathematical model. The type of the model used depends on the system understudy. In general a dynamic representation can be described as:

\[ \dot{X} = f(X, U, t) \]  

(5.1)

\( X(0) \) is specified

where

\( \dot{X} = \) Vector of variables of interest

\( U = \) Vector of input variables

\( t = \) time

\( \dot{\text{(dot)}} = \) time derivative of the variable

If equation (5.1) is a nonlinear differential equation, it is usually linearized around some operating condition. Linearizing the system leads to a straight
forward solution of a relatively low dimensional model as compared with the original nonlinear case. However, linearization causes a loss in accuracy and restricts the region of application. On the otherhand, nonlinear equations are difficult to solve and frequently require large dimensionality. Therefore, a compromise has to be sought which has the simplicity of a linear system and acceptable accuracy. A bilinear system carries some of these properties and has attracted much attention in recent years.

For systems like biological growth, nuclear fission, chemical processes involving flow and concentration, the dynamics are represented by product terms which are strictly bilinear in nature. A bilinear representaion of the system is an advancement over the linear representation of a nonlinear system.

A system is considered to be a bilinear if it has a mathematical model which is linear in the state and control variable, but their products appear in the system equation. A simple equation for a bilinear system is:

\[ \dot{X} = AX + \sum_{i=1}^{m} B_i U_i X + CU \]  \hspace{1cm} (5.2)

\[ X = DX, \quad X(0) = \text{specified} \]  \hspace{1cm} (5.3)

where

\[ X \]  \hspace{1cm} \text{is the state vector of dimension n x 1}
\( U \) is the control vector of dimension \( m \times 1 \)  
\( A \) is \( n \times n \) system matrix  
\( B_i \) is \( n \times n \) matrix for \( i = 1, 2, \ldots, m \)  
\( C \) is \( n \times m \) control matrix  
\( Y \) is \( 1 \times 1 \) output vector  
\( D \) is \( 1 \times n \) matrix  

whereas, a linear representation of the same system is:

\[
\begin{align*}
\dot{X} &= AX + CU \quad (5.4) \\
Y &= DX, \quad \dot{X}(0) = \text{specified} \quad (5.5)
\end{align*}
\]

The bilinear term \( \sum B_i U_i X \) in equation (5.2) allows a bilinear model to more accurately represent a specific system than the linear representation of equations (5.4) and (5.5). If the system is strictly linear in nature then the set of \( B_i \) matrices are null. Mohler (1972, 1973, 1974), Brockett (1972) and D'Alessandro et al. (1974) have presented the necessary theory concerning the realization and structure of bilinear dynamical systems.

Bilinear systems have been used to represent many processes in engineering and other areas. Some of these processes are strictly bilinear in nature, whereas other processes can be approximated by manipulating the dynamic equation. Costanza et al. (1983) have presented an algorithm to help constructing a bilinear model by using the generalized Hankel matrices. Mohler and Kolodziej (1980) have
given an overview of bilinear system theory and its application. A few of these applications are discussed below.

Mohler and Frick (1979) analysed a deterministic and stochastic bilinear approximation of the population model applied to human demography. This model is applicable to chemical, biological and inventory problems.

Aoki (1975) and Koening (1975) have given several examples in micro and macro economics for the use of bilinear models including parametric control via investment and tax rates, and a simple monetary model.

Pattern (1972) presented a grassland bilinear system model in the field of agriculture. The additive control includes sunlight, temperature, and moisture with a parametric control modelling of harvest rate and grazing.

Carotenuto et al. (1985) use a bilinear distributed parameter system of the hyperbolic type coupled with lumped parameters for the modelling of a solar power plant.

Biological bilinear systems includes CO₂ concentration in the blood, blood flow, regulation of temperature, and water balance. Such physiological processes have been discussed by Mohler (1973).

Rastrick (1978) developed a time series analysis of a discrete bilinear system. This has been applied to the problem of approximate sunspot and earthquake activity by output to a white noise driven bilinear system.
Slemrod (1978) studied the problem of controlling a force to a flexible body as a bilinear system.

Sudarshan et al. (1985) discussed an optimization of a bilinear system to design optimal strategies for cancer chemotherapy by control of the proliferation kinetic of cell population. A multicompartmental model for cell proliferation was combined with a pharmacokinetic model to obtain a bilinear model. Using the optimization technique, the optimal dose and optimal period is determined for minimizing the total quantity of the drug used given a specified rate of cure constraint.

Cebuhar et al. (1984) used a bilinear model to control chemical stirred tank reactors (CSTRs). A bilinear model was developed by manipulating the dynamic equation and a comparison with a linear representation was presented. Through the simulation study, the superiority of a bilinear model over a linear model was shown.

Espana and Landau (1978) and Benalib (1982) modelled the dynamics of a distillation column as a bilinear system.

The identification of a bilinear system has also attracted many investigators. Karan and al. (1978) used an approach based on Walsh function expansion. In this method, the system variables are first expanded in Walsh functions. Then, the differential input-output model is combined to get an integral form, which is finally converted to a set of linear algebraic equations by using the integral matrix.
Cheng and Hsu (1982), and Jan and Wong (1981) used block pulse functions for identification. Chou et al. (1986) used a shifted Chebysev series to identify a time varying bilinear system. Liu et al. (1984) used the operational properties of the integration and a product of Chebysev polynomials. In this method, they used a truncated Chebysev series. Kubrusly et al. (1984) presented a correlation type technique, which requires a stochastic approximation algorithm for estimating the unknown parameters of a discrete time bilinear model. Gabor et al. (1984) presented an identification technique when input-output data is available. In their analysis unobservable outputs and observable inputs are related by a bilinear model. Cases where the output is contaminated with a white noise and autoregressive moving average models are given.

Chyi Hwang et al. (1984) used the Galerkin method (Finlayson and Scriven 1966) with shifted Langendre polynomials as trial function for identifying the system parameters. The method is similar to the Walsh function approach. The system variables are expanded in shifted Langendre series. The original input output model is converted into a linear algebraic equation by setting the weighted integrals of the residuals to zero.

Palanisamy et al. (1985) analysed a bilinear system via a single term Walsh function. The main advantage over the complete Walsh function is in reduced computer time.
Benallou (1982) used a mechanistic approach for the identification of the time invariant model of the distillation column. In this method, data at steady state is combined with various physical parameters, (i.e., activity coefficients, efficiency factors, holdups and others) to get the parameters of a bilinear model.

5.3 BILINEAR MODEL OF A DISTILLATION PROCESS:

The dynamic equations of the distillation process as described in Chapter 3 contain composition and flow terms. The nonlinearity occurs for the following reasons:

1. The nonlinearity of the activity coefficient and vapour pressure relationship used in the calculation of the $K$ value.


In the first case, simplification is difficult since the nonlinear relations are required for the calculation for the activity coefficients and vapour pressures. Even the simple local models presented in Chapter 3 are nonlinear in nature. In the second case, the product of flow and composition appears as a bilinear term, which leads directly to the use of a bilinear model form. Espana and Landau
(1978) have shown the advantages of a bilinear model over the linear model. They expressed internal flows in terms of the column inputs (reflux flow rate, reboiler duty, and feed flow rate) and used the tray material balance to derive the dynamic equations. Consider a distillation column with NP plates. If the liquid compositions from each tray are considered as state variable then the total number of state variables will be (NP+2) for each component. For two inputs, a total of three ((NP+2) x (NP+2)) matrices and one ((NP+2) x 2) matrix is required. If NP is large (as is the case for many distillation columns), increased dimensionality for the computation is required. It is therefore necessary to use a reduced order model. A reduced order model is also useful for online control studies. Espana and Landau (1978) presented a low order bilinear model for a binary distillation column in which the assumption of equimolal overflow was made. Eight parameters needed for the identification for the model were estimated from the dynamic model. Benallou (1982) presented another model based on the compartmental modelling technique. In this approach the assumption of constant molar flow allowed the outlet vapour and liquid compositions of the compartments to be related to the sensitive tray composition through the compartmental separation factors. These factors were considered to be constant and were calculated from the initial steady state results.
Both of the techniques discussed above assume a constant molar flow and have been applied to an ideal system. (methanol-water by Espana and Landau, and n-butanol, s-butanol, and ter-butanol by Benallou). Furthermore, a linear equation was used by Espana and Landau to calculate the vapour composition from the liquid composition. This approximation is good only for an ideal system. Benallou also used constant separation factors. Even for an ideal system these factors will change if the column is perturbed by 10-20%. For a non-ideal system, these may be very different. These factors need to be updated from one time step to the next. Benallou modelled a distillation column as a set of two compartments. As discussed earlier in Chapter 4, increasing the compartment size may result in a serious inaccuracy for the non-ideal system, in which one or more components has a K-value less than unity. Furthermore, due to the sharp temperature and composition profiles, it may not be possible to consider a distillation column as a set of two compartments and to use only one tray to represent a compartment.

In the following section, an approach to bilinear modelling is presented which combines the methods of Espana and Benallou with the compartmentalization discussed in Chapter 4. Since the objective is to develop a model-based controller, the formulation is based on the reboiler duty and reflux flow rate as manipulated variables. The technique...
is applied to the nonideal system.

The following assumptions are made for the purposes of analysis:

- The liquid phase is completely mixed.
- Vapour holdup is negligible.
- Fluid dynamic response is neglected.
- Constant volumetric holdup is assumed on each tray.
- The total molar holdup of the compartment is equal to the sum of the molar holdups of the trays in the compartment.
- Temperature and flow profiles within the compartment are linear.
- Feed enters as a liquid state.

Consider a compartment with N trays as shown in Figure 4.1 of Chapter 4.

The holdup of compartment \( j \) is:

\[
M_j = \sum_{p=1}^{N} M_{0p} \tag{5.6}
\]

\( M_0 = \) tray hold up

The total material balance equation for the \( j \)th compartment is:
\[ M_j = V'_{j+1} + L'_{j-1} - V'_j - L'_j \quad (5.7) \]

The component material balance for the \( j \)th compartment and \( i \)th component is:

\[ M_j x'_{ij} + M_j x_{ij} = V'_{j+1} y'_{ij+1} + L'_{j-1} x_{ij-1} - L'_{j} x_{ij} - V'_j y_{ij} \quad (5.8) \]

Combining equations (5.7) and (5.8) the following equation is obtained:

\[ M_j x'_{ij} = V'_{j+1} (y'_{ij+1} - x'_{ij}) + L'_{j-1} (x_{ij-1} - x_{ij}) - V'_j (y_{ij} - x_{ij}) \quad (5.9) \]

Let the internal flows \( L'_j \) and \( V'_j \) be a linear combination of input variables, \( U_1 \) and \( U_2 \), where \( U_1 = \text{reflux rate} \) and \( U_2 = \text{reboiler duty supplied - heat loss} \).

\[ L'_j = \sum_{k=1}^{2} \beta_{kj} U_k \quad (5.10) \]

\[ V'_j = \sum_{k=1}^{2} \alpha_{kj} U_k \quad (5.11) \]

Initial \( \alpha_j \) and \( \beta_j \) can be calculated from the steady state.
data. This approach is similar to the one presented by Espana.

$L_j$ and $V_j$ can alternatively be given as the following:

\begin{align*}
L'_j &= U_1 + \beta'_j \quad (5.12) \\
V'_j &= \eta U_2 + \alpha'_j \quad (5.13)
\end{align*}

where $\alpha'_j$ and $\beta'_j$ are calculated from the initial steady state. In the first representation, equations (5.10) and (5.11), flows are represented as a linear combination of input variables. In the second representation equations (5.12) and (5.13), the liquid flow leaving a compartment is given by the summation of reflux rate and a parameter $\beta'_j$, which represents the mass and heat transfer effects by which liquid flows change from one stage to the other. Similarly, vapour flow rate is given as the summation of the net vapour produced at the reboiler and a parameter $\alpha'_j$, which again represents the moles of vapours changed due to mass and heat transfer effects. The amount of vapour produced at the reboiler is given by $\eta U_2$, where $U_2$ is defined earlier. In this chapter, bilinear model equations are developed for the first representation and is referred to as a bilinear model of type I. Corresponding equations for a bilinear model of type II, for equations (5.12) and (5.13), are given in Appendix B.
In equation (5.9), $Y_{ij}$ is not in equilibrium with $X_{ij}$. In fact $Y_{ij}$ and $X_{ij}$ are related by:

$$Y_{ij} = K_{ij} X_{ij}$$

(5.14)

Benallou terms these $K_{ij}$ as separation factors in the $j$th compartment for the $i$th component. Using equations (5.14) (5.10) and (5.11) and after some manipulations, equation (5.9) may be written in the following vector form:

$$M_j X_{ij} = \sum_{k=1}^{2} U_k \begin{bmatrix} \beta_{j-1k} - (\alpha_{j+1k}^+ \beta_{j-1k}^+ \alpha_{jk}(K_{ij}')) \end{bmatrix} \begin{bmatrix} X_{ij-1} \\ X_{ij} \\ X_{ij+1} \end{bmatrix}$$

(5.15)

Three elements in the row vector of equation (5.15) are separated by the commas.

A general dynamic material balance equation for the compartment with feeds, reboiler and condenser is given as:

$$M_j X_{ij} = \delta F_j (X_{iF} - X_{ij}) +$$

$$\sum_{k=1}^{2} U_k \begin{bmatrix} \beta_{j-1k} - (\alpha_{j+1k}^+ \beta_{j-1k}^+ \alpha_{jk}(K_{ij}')) \end{bmatrix} \begin{bmatrix} X_{ij-1} \\ X_{ij} \\ X_{ij+1} \end{bmatrix}$$

(5.16)
Commas are used to separate the elements of a row vector in equation (5.16). And \( X_{IF} \) is the composition of the \( i \)th component in the feed entering in the \( j \)th compartment. The above equation can also be used to represent a compartment with the condenser or the reboiler with the following specifications:

for a compartment with condenser \( \beta_{0k} = 0 \)
for a compartment with reboiler \( \alpha_{NC+1,k} = 0 \)
where \( NC \) is the total number of compartments
\( \delta = 1 \) if feed is introduced otherwise \( = 0 \)

On the basis of equation (5.16), the 13 tray extractive distillation was modelled with the configuration given in Table 4.3.

The following equations are written without component subscripts. However, the equations should be considered for all components. Equations are developed for the 5-compartmental model for which the configuration is given in Table 4.3. Consider the following state vector

\[
X^T = [X_1, X_2, X_3, X_4, X_5]
\]

(5.17)

where

\( X_1 = \) distillate composition
\( X_j = \) liquid composition leaving
\[ j \text{th compartment } j=2,3,4 \]
\[ x_5 = \text{Bottoms product composition} \]

Equation (5.16) can be written for all components and compartments to get the following matrix equation:

\[ \dot{x} = Ax + B_1 u_1 x + B_2 u_2 x + e \]  \hspace{1cm} (5.18)
\[ y = dx \quad ; \quad x(0) = \text{Initial Steady State} \]

where, \( e \) is the disturbance vector and expressions for \( A, B_1, B_2, D \) and \( E \) matrices are given below. The dimension of the equation are defined in equations (5.2) and (5.3) with \( n=5 \) and \( m=2 \).

\[
A = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{-F_1}{M_3} & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{-F_2}{M_4} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]  \hspace{1cm} (5.19)
For $k = 1, 2$ \( B_k = \)

\[
\begin{bmatrix}
\frac{\alpha_{2k}}{M_1} & \frac{\alpha_{2k} K'_2}{M_1} & 0 & 0 & 0 \\
\beta_{1k} & -\frac{(\alpha_{3k} + \beta_{1k} + \alpha_{2k}(K'_2 - 1))}{M_2} & \frac{\alpha_{3k} K'_3}{M_2} & 0 & 0 \\
0 & \frac{\beta_{2k}}{M_3} & -\frac{(\alpha_{4k} + \beta_{2k} + \alpha_{3k}(K'_3 - 1))}{M_3} & \frac{\alpha_{4k} K'_4}{M_3} & 0 \\
0 & 0 & \frac{\beta_{3k}}{M_4} & -\frac{(\alpha_{5k} + \beta_{3k} + \alpha_{4k}(K'_4 - 1))}{M_4} & \frac{\alpha_{5k} K'_5}{M_4} \\
0 & 0 & 0 & \frac{\beta_{4k}}{M_5} & -\frac{(\beta_{4k} + \alpha_{5k}(K'_5 - 1))}{M_5}
\end{bmatrix}
\]
A reduced order bilinear model for a distillation column is completely described by the set of equations (5.18) to (5.22).

5.4 FLOWSHEET AND ALGORITHM:

The various steps involved in setting up and running the simulation are given below:

1. Read the steady state data as the initial conditions.
2. Calculate the compartmental molar holdup using equation (5.6).
3. Set time = 0 and get the disturbance data.
4. Calculate $\beta$ and $\alpha$ from the steady state data
5. Calculate various initial $K'$-values using equation (5.14) and the composition profile.
6. Solve the set of differential equations at time $= t$
7. Assume the linear composition profile within the compartment.
8. Calculate temperature at the top of the compartment and the bottom using bubble point procedures.
9. Calculate the vapour composition leaving the compartment (result of step 8).
10. Calculate the new $K'$-values to be used in the next time interval using the new composition profile and equation (5.14).
11. Calculate the linear temperature profile within the compartment.
12. Calculate the heat loss at time $= t$ using a model presented in Chapter 4.
13. If time $t < t_{\text{max}}$ go to step 6 otherwise stop

In the above analysis, the separation factors $K'$ can be varied from one time step to the next. This can be done in the following manner. Solve the set of simultaneous differential equations at the $(t+1)^{\text{th}}$ time step knowing the
conditions at the tth step. Once the composition profile is obtained at the outlet of each compartment, a linear composition profile is assumed within the compartment as in the steady state case. The bubble point calculations are carried out at the top and the bottom of the compartment to get the temperature profile. This procedure gives the vapour composition leaving the compartment. The new separation factor $K_{ij}$ is defined by:

$$K_{ij}^{(t+1)} = \frac{Y_{ij}^{(t+1)}}{X_{ij}^{(t+1)} \ast E_{ij}^{(t+1)}}$$

where the superscript denotes the time step. The $E_{ij}$ are the average efficiency factors for the jth compartment and the ith component. These factors depend upon the type of disturbance and the liquid composition leaving the compartment. The initial efficiency factor matrix specified at $t=0$ is updated at each time step using the average correction factor matrix. The elements of this correction factor matrix are calculated from the steady state compartmental simulation. The efficiency factor matrix is updated in the following manner:

$$E_{ij}^{(t)} = E_{ij}^{(t=0)} + CF_{ij}(X_{ij}^{(t)} - X_{ij}^{(t=0)}) \quad (5.19)$$

where $(t)$ indicates values at time $= t$. The elements of $CF$ are given in Table 5.1.
Table 5.1: Correction Factor Matrix

<table>
<thead>
<tr>
<th>Acetone</th>
<th>Methanol</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>-0.75</td>
<td>0.48</td>
<td>-0.67</td>
</tr>
<tr>
<td>0.18</td>
<td>9.2</td>
<td>0.38</td>
</tr>
<tr>
<td>0.09</td>
<td>3.40</td>
<td>0.11</td>
</tr>
<tr>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The initial steady state data comes from the output of the compartmental simulation described in Chapter 4. Once the initial conditions and the elements of A, B₁, B₂, and D matrices are known, the set of equations are solved using DYNSYS simulation package (1975) with the stiff option for Gear's method of integration. The integrations were done on acetone and methanol. Water composition response was obtained by the difference.

5.5 Experimental and Simulation Results:

Open loop tests on the real column were performed by introducing step changes in the manipulated variables, i.e., reboiler duty (steam pressure) and reflux rate. Responses for acetone in the overhead product and methanol in the bottoms product compositions are plotted in Figures 5.1 to 5.6 along with dynamic results obtained from both the tray
to tray and the bilinear models of type I and type II.

Figure 5.1 shows the response to a step change in the feed flow rate from 110.0 to 130.0 ml/min. Both the bilinear and tray to tray model predictions show good agreement with the experimental data. The consistent difference between the predicted dynamics and the experimental data is due to an initial offset, which comes from the steady state simulation.

Figure 5.2 shows the response to a step change in the reflux flow rate from 165 to 122 ml/min. The bilinear models predict dynamics similar to those from the tray to tray model. For the acetone in the top product, the gain term predicted by the bilinear models is low, whereas the complete tray to tray model predicts the correct gain. For the methanol in the bottoms product, the bilinear models predict the correct gain. The correct gains corresponds to the one calculated from the experimental data. The low gain for the bilinear models is attributed partly to the constants α_{ij} and β_{ij} in equations (5.10) and (5.11), and α_{j} and β_{j} in equations (5.12) and (5.13). These factors would be different at a new operating point.

Figure 5.3 shows the response to a step change in the reflux flow rate from 155 to 185 ml/min. In this case the acetone in the top product is predicted fairly well by both models, whereas the methanol in the bottoms product is not predicted well. The bilinear model discrepancy is due to
Figure 5.1: Step Change in Feed Flow 110 to 130 ml/min

Figure 5.2: Step Change in Reflux Flow 165 to 122 ml/min
Figure 5.3: Step Change in Reflux Flow 155 to 185 ml/min

Figure 5.4: Step Change in Steam Pressure 151.7 to 127.5 kPa(gauge)
the nonideality of the system. This causes the actual correction factor matrix to change from one operating point to another. However, an average correction factor matrix was used in the bilinear model simulation.

Figure 5.4 shows the response to a step change in the reboiler steam pressure from 151.7 kPa(gauge) (144.6 ml/min) to 127.5 kPa(gauge) (136.0 ml/min). The acetone in the top product is predicted well by the bilinear and the tray to tray model. The constant offset in the tray to tray model is due to an initial offset from the steady state simulation. However, a strange behaviour is obtained for the methanol in the bottoms product for the bilinear model. This again is due to the use of a constant correction factor matrix. The comparison is further complicated by the fact that this particular set of experimental data was obtained when the gas chromatograph sampling valve was not functioning properly.

Figure 5.5 shows the response to a step change in the reboiler steam pressure from 131.0 (138.0 ml/min) to 158.6 kPa(gauge) (147.0 ml/min). In this case both compositions are predicted well and contrary to Figure 5.5 no strange behaviour is seen. This demonstrates the asymmetric behaviour of the distillation column.

These tests of the dynamic predictions were also carried out with the 4 compartmental model. It gave inadequate dynamic predictions and lower gains were obtained
Figure 5.5: Step Change in Steam Pressure 131.0 to 158.6 kPa(gauge)

from the model. The reason for the low gains predicted by the 4 compartment bilinear model for the bottoms product is due to the large variation in the K-value resulting from the compartmentalization. For the tray to tray model, the K value at the reboiler for the acetone is about 17 and for the methanol is about 3.5, whereas for the 4 compartmental model the K value at the last compartment for the acetone is about 35 and for methanol it is 1.2. The large increase in the acetone and decrease in the methanol K-values contributes to the poor dynamics. This shows that combining a large number of trays in a single compartment in order to
obtained a low order model may produce false dynamics for a non-ideal system. Thus, the criterion of selecting the number of compartments should be based on the dynamics of the model rather than on its steady state behaviour. For the actual extractive distillation under study, a 5 compartmental model is adequate and will be used for further control studies.

From Figures 5.1 to 5.5 it is found that responses from type I and type II bilinear models are similar.

The values of $\alpha_kj$ and $\beta_kj$ in equations (5.10) and (5.11) and $\alpha_j$ and $\beta_j$ in equations (5.12) and (5.13) were reevaluated at new operating conditions after the final steady state was reached. It was found that these factors varied depending upon the disturbance and its magnitude. For the step down in reflux flow disturbance the factors vary by as much as 15%, but for the feed flow rate variations the change was only 4%. It was also observed that these factors change by only 9% for the reflux changes. For the reboiler duty up or down dynamics the changes were about 7%.

One of the reasons for the difference in the dynamics produced from the bilinear models and tray to tray models is the assumption of constant factors in equations (5.10) to (5.11) and (5.12) to (5.13). Changing these factors from one time step to another would mean that all elements of matrices $A$, $B_1$, and $B_2$ in equations (5.18) to (5.20) are time variant. As was explained earlier in the chapter, the
objective was to develop a model suitable for designing controllers for on-line operation. The mathematics for controller design from the time variant linear models is quite complex; for the bilinear model it would be even more complex. Therefore, the assumption of constant factors was made.

To compare the performance of the tray to tray model and the bilinear model of type II, six open loop steps were simulated for a period of operation of 27 hours. These steps and their magnitudes are given in Table 5.2. The simulations are shown in Figure 5.6. From the figure it is clear that the two models produce similar results. The small variations in the responses are due to the assumption of linear profiles within the compartment, and the use of a constant correction factor matrix. This result shows that a bilinear model can be used to represent the process dynamics and for development of a model-based controller.

5.6 CONCLUSIONS:

A reduced order bilinear model of an extractive distillation column was developed based on the compartmentalization technique. The internal flows were represented by two different methods to obtain two kinds of bilinear model. The dynamics of the column were investigated for steps in the reboiler duty, reflux flow rate, and feed
Table 5.2: Initial Operating Conditions and Various Steps for Figure 5.6 Study

Initial Conditions

Feed:
- Flow = 110.0 ml/min
- Composition:
  - Acetone = 0.6968
  - Methanol = 0.2819
  - Water = 0.0213

Solvent:
- Flow = 45.0 ml/min

Reflux Flow = 160.0 ml/min

Steam Pressure = 144.7 kPa (gauge)

Room Temperature = 24 °C

Steps:

<table>
<thead>
<tr>
<th>Time (hr)</th>
<th>Type</th>
<th>Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.0</td>
<td>Reflux Flow</td>
<td>160.0 to 180 ml/min</td>
</tr>
<tr>
<td>7.0</td>
<td>Feed Flow</td>
<td>110.0 to 135 ml/min</td>
</tr>
</tbody>
</table>
| 11.0     | Feed composition      | 0.6968 to 0.75 Acetone
                   | 0.2819 to 0.25 Methanol
                   | 0.0213 to 0.0 Water
| 15.0     | Steam Pressure        | 144.7 to 158.6 kPa (gauge)       |
| 19.0     | Reflux Flow           | 180.0 to 165.0 ml/min            |
| 23.0     | Steam Pressure        | 158.6 to 137.9 kPa (gauge)       |
Figure 5.6: Comparison of Responses for Multisteps (simulation)

flow rate. The responses predicted from the two bilinear models and the tray to tray model were very similar to the actual plant data. The difference in the bilinear models is due to the assumption of the constant factors to represent the flows. These factors can vary by up to 15%.

It was also observed that the dynamics for the 4 compartmental model was not acceptable as it resulted in very low gains. This was due to the large variation in the K-value in the last compartment. This also shows that a criterion for the selection of the model should be based on the dynamic results in contrast to the steady state
simulation results. Through simulation, it was shown that bilinear model gives similar dynamics to a tray to tray model for 6 steps.
Nomenclature

A = n x n system matrix
B_i = n x n matrix for i\textsuperscript{th} input in Equation (5.2)
C = n x m Control matrix
CF_ij = Correction factor element for i\textsuperscript{th} component and j\textsuperscript{th} compartment
D = 1 x n matrix in equation (5.3)
E = Disturbance vector of dimension 1 x n
E_ij = Average efficiency factor for the j\textsuperscript{th} compartment and i\textsuperscript{th} component
F_1 = Molar solvent rate (feed #1)
F_2 = Molar feed rate (feed #2)
K_ij = K-value for the j\textsuperscript{th} compartment and i\textsuperscript{th} component
L'_j = Molar liquid flow leaving the j\textsuperscript{th} compartment
M_0 = Tray molar holdup
M_j = Molar holdup for compartment j
N = Number of trays in a compartment
NC = Total number of compartments
t = Time
U = Vector of input variables of dimension m
U_1 = Reflux flow rate
U_2 = Net heat supplied
V'_j = Molar vapour flow leaving the j\textsuperscript{th} compartment
X = State vector of dimension n
X_ij = Liquid composition leaving the compartment j and i\textsuperscript{th} component
X_j = Liquid composition leaving j\textsuperscript{th} compartment used as elements of vector X
\( X_{iF} \) = Composition of the \( i^{th} \) component in the feed
\( \dot{X}(0) \) = State vector at time 0
\( Y_{ij} \) = Vapour composition leaving the compartment \( j \) and \( i^{th} \) component

Greek:
\( \alpha_{ij} \) = Constants for Equation (5.11)
\( \beta_{ij} \) = Constants for Equation (5.10)
\( \alpha_j \) = Constants for Equation (5.13)
\( \beta_j \) = Constant for Equation (5.18)
\( n \) = Constant to convert heat supplied to vapour produced at the reboiler.
\( \delta \) = 1 if feed is introduced otherwise = 0

Subscripts:
\( j \) = Compartment number
\( p \) = Tray number within compartment
\( i \) = Component number
\( k \) = Input variable number

Superscript:
\( (t+1) \) = \((t+1)^{th}\) step
Chapter - 6

APPLICATION OF SIMPLE CONTROLLERS
TO AN EXTRACTIVE DISTILLATION

6.1 INTRODUCTION:

In the previous chapter steady state and dynamic models for an extractive distillation were presented and results were compared with experimental data. In this chapter a simulation of the dynamic model is used to understand the column behaviour under feedback control. Different conventional control strategies (i.e., PI, decoupler, feedforward and combinations of these) are tested for the regulatory problem. The primary controlled variables are acetone composition in the top product and methanol composition in the bottoms product. This selection was dictated by the need for good reproducibility in the Gas Chromatograph analysis of the column output streams when these schemes are applied to the pilot plant. The objective of the regulatory problem is to keep the compositions of the top and/or bottoms products near to their initial steady state levels in spite of disturbances. The results presented in this chapter are based on simulation studies. The maximum and minimum values of the manipulated variables correspond
to the actual physical limitations on the column are given in Section 6.1, along with the description of the PI controller used. A brief theory of decoupling and the design of the steady state decoupler are presented in Section 6.2. Section 6.3 covers the simulation control runs for both single composition and dual composition control. A simple method based on the assumption of a linear system is presented in Section 6.4 to calculate the control action required for disturbance rejection. The conclusions are summarized in Section 6.5.

6.2 PI CONTROL:

Proportional - Integral (PI) controllers were used for single composition and dual composition control. The controllers were tuned by trial and error to give a desired degree of stability for a load disturbance. The performance was considered acceptable if there were no large amplitude oscillations in the controlled and the manipulated variables. For single composition control either the acetone composition in the top product or the methanol composition in the bottoms product was controlled. The composition not under control was free to move. For the dual composition control runs both the acetone in the top and the methanol in the bottoms products were controlled simultaneously. In
either case, it is assumed that the column pressure is constant at 105 kPa. The following manipulated variables were considered:

1. Reflux flow rate to control the acetone in the top product
2. Solvent flow rate to control the acetone in the top product
3. Reboiler duty (steam pressure) to control the methanol composition in the bottoms product.

For dual composition control, two sets of manipulated variables were selected. Set 1 consists of reboiler duty (steam pressure) and reflux flow rate and Set 2 used solvent (water) flow rate and reboiler duty (steam pressure).

Reboiler heat duty is altered by changing the steam pressure in the reboiler. Therefore, steam pressure will be used in place of the reboiler duty. It is assumed that the steam entering the system is saturated. The variation of the steam flow rate with the steam pressure is given in Figure 6.1. The following linear relationship was determined from the experimental column and used in the simulation studies:

\[ F = 66.734 + 0.527 \, P \]  
\( (6.1) \)
where

\[ F = \text{Experimental steam flow rate in ml/min} \]
\[ P = \text{Pressure in kPa(gauge)} \]

![Graph showing steam flow rate vs steam pressure](image)

Figure 6.1: Steam Pressure vs Steam Flow Rate

The minimum and the maximum values of the manipulated variables allowed are given in Table 6.1.

For smooth column operation and proper tray loading, the reflux flow rate should be maintained between 120.0 and 220.0 ml/min. This also incorporates the limitation on the reflux heater to maintain the desired reflux temperature at the higher flow rate. Steam pressures between 117.2 and 172.3 kPa(gauge) (17.0 and 25.0 psig) produce sufficient
Table 6.1: Minimum and Maximum Values of The Manipulated Variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam Pressure</td>
<td>kPa (gauge)</td>
<td>117.2</td>
<td>172.3</td>
</tr>
<tr>
<td>Reflux flow rate</td>
<td>ml/min</td>
<td>120.0</td>
<td>220.0</td>
</tr>
<tr>
<td>Water flow rate</td>
<td>ml/min</td>
<td>35.0</td>
<td>55.0</td>
</tr>
</tbody>
</table>

vapour velocity for the proper mixing on each tray without foaming. The constraint on the water flow rate is mainly to break the azeotrope. It was shown in Chapter 3 that decreasing the water flow rate reduces the acetone purity in the top product. At a higher water flow rate, because of its higher heat capacity, more energy is required. All these values were obtained from experience gained by running the experimental column.

The velocity form of the PI controller is used with a control interval of 7 minutes. The selection of the control interval is governed by the Gas Chromatograph (G.C.) which takes 7 minutes to analyse and communicate composition data to the host computer, a VAX 11/750.

6.3 DECOUPLING:

To reduce the interaction between the SISO (single
input single output) loops used in dual composition control, a compensator was added. The compensation term used to reduce the interaction effect is called a decoupler. Controller performance can be improved significantly by using a decoupler.

For distillation column control, decoupling has been used by Waller (1974), Shinskey (1977), McAvoi (1981) and several others. Sinskey (1977) suggests one-way decoupling, in which only one compensation element exists between the two loops, instead of the usual two-way or full decoupling. It can be either steady state decoupling or dynamic decoupling depending on the system. Since a dynamic decoupler may result in difficult controller structures, a steady state decoupling is used to eliminate the steady state interaction effects. A good review of the application of decouplers to distillation column control is given by Waller (1974). The decoupler used in this study is designed in the following manner:

\[
\begin{align*}
X_1 &= \text{Acetone composition in the top product} \\
X_2 &= \text{Methanol composition in the bottoms product} \\
C_1 &= \text{Manipulated variable \# 1} \\
C_2 &= \text{Manipulated variable \# 2}
\end{align*}
\]
Then the deviation in $x_1$ and $x_2$ can be written as:

$$
\Delta x_1 = \frac{\partial x_1}{\partial c_1} \Delta c_1 + \frac{\partial x_1}{\partial c_2} \Delta c_2 \quad (6.2)
$$

$$
\Delta x_2 = \frac{\partial x_2}{\partial c_1} \Delta c_1 + \frac{\partial x_2}{\partial c_2} \Delta c_2 \quad (6.2)
$$

where

$$
\frac{\partial x_1}{\partial c_1} \bigg|_{c_2}
$$

means partial derivative of $x_1$ with respect to $c_1$ with $c_2$ remaining constant. A block diagram of the decoupler is given in Figure 6.2. The D matrix is made up of the decoupler elements. For simple decoupling with $D_{11} = D_{22} = 1.0$ and using the steady state gains, $D_{12}$ and $D_{21}$ can be written as:

$$
D_{12} = - \begin{bmatrix}
\frac{\partial x_1}{\partial c_2} \\
\frac{\partial x_1}{\partial c_1}
\end{bmatrix}
$$

$$
D_{21} = - \begin{bmatrix}
\frac{\partial x_2}{\partial c_1} \\
\frac{\partial x_2}{\partial c_2}
\end{bmatrix}
$$
The elements $D_{12}$ and $D_{21}$ can be calculated easily using the average steady state gains for up and down dynamics. For this column, the following values are calculated:

- **Reflux/Steam**: $D_{12} = 12.0$, $D_{21} = 0.05$
- **Water/Steam**: $D_{12} = 7.27$, $D_{21} = -0.4$

The performance of the controller was tested for disturbances which would change the system in the four
combinations shown in Figure 6.3. This figure represents only the direction of the deviation from the initial steady state and not the nature of the dynamics; these may be different from those shown in the figure.

Disturbance types I and II were obtained by changing the feed flow rate from 104.0 to 116.0 ml/min for type I and from 104.0 to 92.0 ml/min for type II. Types III and IV resulted from a change in the room temperature from 24.0 to 26.0 °C for type III and from 24.0 to 22.0 °C for type IV. These four different types of disturbance are selected because any process with two variables can only move around its nominal operating conditions in these four ways. It should be noted here that the dynamic simulation used in this chapter includes the heat loss model, described in Chapter 4.

6.4 CONTROL RUNS - SIMULATION:

The initial operating condition data is given in Table 6.2. The various simulation control studies are given in Table 6.3, and are summarised below:
Figure 6.3: Different Types of Disturbances

A = Acetone in Top Product
M = Methanol in Bottoms Product
6.4.1 REFLUX/STEAM COMBINATION: CASE 1

The objective is to control only the acetone composition in the top product. The bottoms product is free to move. The manipulated variable is the reflux flow rate. Figure 6.4 shows the simulated response of the column for the Type I disturbance. The following parameters for the PI controller (tuned by trial and error) are used:

Table 6.2: Initial Operating Conditions

<table>
<thead>
<tr>
<th>FEED</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow Rate</td>
<td>110.0 ml/min</td>
</tr>
<tr>
<td>Temperature</td>
<td>43.0 °C</td>
</tr>
<tr>
<td>Composition</td>
<td></td>
</tr>
<tr>
<td>Acetone</td>
<td>0.6429</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.3312</td>
</tr>
<tr>
<td>Water</td>
<td>0.0258</td>
</tr>
<tr>
<td>SOLVENT</td>
<td></td>
</tr>
<tr>
<td>Flow Rate</td>
<td>45.0 ml/min</td>
</tr>
<tr>
<td>REFLUX</td>
<td></td>
</tr>
<tr>
<td>Flow Rate</td>
<td>165.0 ml/min</td>
</tr>
<tr>
<td>STEAM</td>
<td></td>
</tr>
<tr>
<td>Pressure</td>
<td>144.8 kPa (gauge)</td>
</tr>
<tr>
<td>Flow Rate</td>
<td>143.09 ml/min</td>
</tr>
<tr>
<td>Room Temperature</td>
<td>24.0 °C</td>
</tr>
<tr>
<td>ACETONE (Top)</td>
<td>0.8912</td>
</tr>
<tr>
<td>METHANOL (BOTTOMS)</td>
<td>0.1592</td>
</tr>
</tbody>
</table>
\[ K = 900.0 \ (\text{ml/min})/(\text{mole fraction}) \]

\[ T = 2.00 \text{ hr} \]

The reflux flow rate changes from 165.0 to 173.0 ml/min. Due to the dead-time present in the system, it starts to move away from the setpoint before the controller brings the acetone composition back to the desired level. By increasing the controller gain the initial response time can be decreased. Therefore, a split gain controller was tried; i.e., if the absolute error was more than 0.3\%, then use a gain of 1500.0, otherwise use 900.0 (ml/min)/(mole fraction). It was observed that the higher controller gain showed its effect in reducing the response time. However, a higher gain also produced enough inertia to make the system oscillate. Since the bottoms product is not controlled methanol composition deviated from 0.1591 to 0.1725. This is due to increasing the reflux flow rate which increases the methanol composition in the bottoms product.

**CASE 2**

In this experiment the methanol composition in the bottoms product is controlled using the steam pressure for the Type I disturbance. Figure 6.5 shows the response for the following controller parameters:
### Table 6.3: Various Control Studies Performed

<table>
<thead>
<tr>
<th>Case #</th>
<th>Type of Control</th>
<th>Manipulated Variable</th>
<th>Dist. Type</th>
<th>Controller Type</th>
<th>Figure #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sing. Comp. (Top)</td>
<td>Reflux</td>
<td>I</td>
<td>PI</td>
<td>6.4</td>
</tr>
<tr>
<td>2</td>
<td>Sing. Comp. (Bot)</td>
<td>Steam</td>
<td>I</td>
<td>PI</td>
<td>6.5</td>
</tr>
<tr>
<td>3</td>
<td>Sing. Comp. (Top)</td>
<td>Reflux</td>
<td>II</td>
<td>PI</td>
<td>6.6</td>
</tr>
<tr>
<td>4</td>
<td>Sing. Comp. (Bot)</td>
<td>Steam</td>
<td>II</td>
<td>PI</td>
<td>6.7</td>
</tr>
<tr>
<td>5</td>
<td>Dual Comp.</td>
<td>Reflux &amp; Steam</td>
<td>I</td>
<td>PI</td>
<td>6.8</td>
</tr>
<tr>
<td>6</td>
<td>Dual Comp.</td>
<td>Reflux &amp; Steam</td>
<td>III</td>
<td>PI+Decoupler</td>
<td>6.9</td>
</tr>
<tr>
<td>7</td>
<td>Dual Comp.</td>
<td>Reflux &amp; Steam</td>
<td>III</td>
<td>PI+Decoupler</td>
<td>6.10</td>
</tr>
<tr>
<td>8</td>
<td>Dual Comp.</td>
<td>Reflux &amp; Steam</td>
<td>IV</td>
<td>PI+Decoupler</td>
<td>6.11</td>
</tr>
<tr>
<td>9</td>
<td>Sing. Comp. (Top)</td>
<td>Water</td>
<td>I</td>
<td>PI</td>
<td>6.12</td>
</tr>
<tr>
<td>10</td>
<td>Sing. Comp. (Top)</td>
<td>Water</td>
<td>II</td>
<td>PI</td>
<td>6.13</td>
</tr>
<tr>
<td>11</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>I</td>
<td>PI+Decoupler</td>
<td>6.14</td>
</tr>
<tr>
<td>12</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>I</td>
<td>PI+Decoupler</td>
<td>6.15</td>
</tr>
<tr>
<td>13</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>II</td>
<td>PI+Decoupler</td>
<td>6.16</td>
</tr>
<tr>
<td>14</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>III</td>
<td>PI+Decoupler</td>
<td>6.17</td>
</tr>
<tr>
<td>15</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>IV</td>
<td>PI+Decoupler</td>
<td>6.18</td>
</tr>
<tr>
<td>16</td>
<td>Dual Comp.</td>
<td>Water &amp; Steam</td>
<td>I</td>
<td>PI+Decoupler</td>
<td>6.19</td>
</tr>
</tbody>
</table>

Sing. Comp. (Top) = Acetone in the Top Product

Sing. Comp. (Bot) = Methanol in the Bottoms Product

Dual Comp. = Acetone in the Top Product and Methanol in the Bottoms Product

Dist. Type = Disturbance type
\[ K = -689.5 \text{ kPa(gauge)/mole fraction} \]
\[ T = 5.00 \text{ hr} \]

The controller is observed to perform well. The response time in this case is lower than that in Case 1. The shorter response time is attributed to a smaller dead-time. The controller changes the steam pressure from 144.8 to 158.6 kPa(gauge). The acetone in the top product changes from 0.8915 to 0.8623.

**CASES 3 and 4**

In Case 3, the acetone composition is controlled for a type II disturbance. It is interesting to note that for this type of disturbance the controller tuning from Case 1 causes oscillation in the output and in the reflux flow rate, which makes the performance unacceptable. Therefore, the controller parameters are changed to the following:

\[ K = 700.0 \text{ (ml/min)/mole fraction} \]
\[ T = 1.0 \text{ hrs} \]

This shows the necessity of gain scheduling depending on the disturbance. The necessity of gain scheduling for the
nonlinear, asymmetric systems has also been reported by Shinskey (1979) and Tsogas et al. (1985). The controller performance with the new parameters is shown in Figure 6.6. The reflux flow rate changes from 165.0 to 160.0 ml/min. When the type I disturbance used in Case 1 was repeated with these new controller parameters (Case 3), it was found that the rise time and settling time were longer than those with the original Case 1. This is typical of a nonlinear system. As explained in Chapter 3, the process gain varies with the type of disturbance and the operating conditions. Therefore, different controller gains are required. Figure 6.7 shows the results of controlling the bottoms product for the type II disturbance, Case 4. In this case, the controller parameters were not changed but the change in the steam pressure is larger than that in case 2. This is a consequence of the asymmetric nature of the extractive distillation column. The steam pressure changes from 144.8 to 117.2 kPa(gauge) and hits the lower constraint.

Since only a single composition was controlled, controller performance for the type III and IV disturbances was not tested. The nature of these disturbances can be found in either type I or type II disturbances. However, for the dual composition control all four types of disturbance were tested. For single loop, single composition control, it was found that the reflux can be used to control the acetone in the top product and steam pressure can control the
methanol in the bottoms product. The asymmetric nature of the column demands gain scheduling for the top controller depending on the disturbance type.

**CASES 5 and 6**

In these cases, the use of reflux and steam pressure for dual composition control is tested for the type I disturbance. Figure 6.8 shows the system performance for this pair for the following controller parameters:

\[
\begin{align*}
K & = 900.0 & T & = 2.0 & \text{top loop} \\
K & = -689.5 & T & = 5.0 & \text{bottom loop}
\end{align*}
\]

Neither the top composition nor the bottom composition comes back to the desired setpoint. Both the reflux flow rate and steam pressure saturate at their maximum values. As the reflux flow increases the bottoms product starts to move away from its setpoint. The bottoms product controller tries to bring it back by increasing the steam pressure, which decreases the acetone composition and this causes the top controller to call for an even higher reflux flow rate. This situation continues and both controllers run out of
operating space. Once the controllers saturates the system follows the open loop behaviour. Different controller parameters were tried, but none worked satisfactorily. This suggests that at this operating point, this pairing can not be used for dual composition control with PI controllers for the type I disturbance. Similar results were obtained for the type II disturbance. The performance also indicates the strong interaction between two loops. Mayer(1985) has also shown the similar results for PI controllers on the extractive distillation column on an experimental study for feed flow rate disturbances. To reduce the interactions the PI controllers with the decoupler designed earlier was implemented in Case 6 with the following parameters:

<table>
<thead>
<tr>
<th>K</th>
<th>T</th>
<th>Decoupler Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>500.0</td>
<td>1.2</td>
<td>12.0</td>
</tr>
<tr>
<td>-517.1</td>
<td>2.0</td>
<td>0.05</td>
</tr>
</tbody>
</table>

The performance shown in Figure 6.9 for this control strategy was also unacceptable. Both the steam pressure and reflux flow again saturated, but took longer than PI controllers alone. The poor performance can be attributed to the small operating space as well as to interactions.
CASES 7 and 8

The performance of the reflux/steam was tested for the type III disturbance for dual composition control. A PI+decoupler controller was used with the following parameters:

<table>
<thead>
<tr>
<th>K</th>
<th>T</th>
<th>Decoupler Gain</th>
<th>Loop</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000.0</td>
<td>1.2</td>
<td>12.0</td>
<td>top loop</td>
</tr>
<tr>
<td>-413.7</td>
<td>2.0</td>
<td>0.05</td>
<td>bottom loop</td>
</tr>
</tbody>
</table>

The controller performance is shown in Figure 6.10. The controller eventually brings the composition back to the desired setpoints. The response time is very large. Because of the dead-time for the top product composition, the initial reflux flow rate goes up as a result of the decoupler action. After the dead-time is over (i.e., once the top controller action starts to over effect) the reflux flow rate is reduced. Figure 6.11 corresponding to Case 8 shows the controller performance for the type IV disturbance. In this case, the PI+decoupler controller performance is acceptable. The controller parameters are the same as for the type III disturbance. The dead-time in the top product causes the reflux flow to go down initially.

These results show that when a PI+ decoupler
controller is used, the reflux/steam pairing is suitable for dual composition control for only certain types of disturbances. This is due to the strong interactions between the two loops. It may be possible for a multivariable, model-based controller to work under these circumstances. The test of this hypothesis is presented in the Chapter 8 where the reflux/steam bilinear optimal controller designed in the previous chapter is reported.

6.4.2 WATER/STEAM COMBINATION:

The reason for introducing a solvent in extractive distillation is to change the relative volatilities of the components in the system. As discussed in Chapter 2, the change in relative volatility depends on the amount of solvent (water) present. Thus, when the solvent flow changes the problems discussed in Chapter 2 complicate the control problem. However, it provides extra flexibility from the control point of view. Solvent flow rate can be used as a manipulated variable. This tackles the control problem on a more fundamental basis, i.e., controlling the relative volatility. The suitability of water to control the top product composition is investigated in the following simulation studies.
CASES 9 and 10

Figure 6.12 shows the response for the type I disturbance. When only the top product composition was controlled using water flow rate as the manipulated variable. The PI controller parameters are:

\[
K = 400.0 \text{ (ml/min)}/\text{(mole fraction)} \\
T = 1.25 \text{ hrs}
\]

The water flow rate changes from 45.0 to 49.0 ml/min. Comparing Figure 6.4 in Case 1 with Figure 6.12 it is clear that the performance of this controller is much better. The maximum deviation of the top product is 0.005 which is the same as in Case 1. The methanol composition in the bottoms product initially rises but eventually returns almost to its initial level. This very small deviation in the final methanol composition may only be true for this particular operating point. Changing the operating point, or injecting a different disturbance, may produce different results. Figure 6.12 shows an initial increase in methanol composition in response to the feed flow rate disturbance and subsequent dilution of the methanol in the bottoms product as the top controller increases the solvent flow rate. This analysis shows that for the type I disturbance,
water is a better choice than the reflux flow rate as a manipulated variable.

Figure 6.13, corresponding to Case 10 shows the response for type II disturbance for the same controller parameters. The controller performance is acceptable. The top product is controlled as desired and at the same time it reduces the final deviation in the bottoms product from its initial steady state as compared to Case 3.

**CASE 11**

After testing the suitability of water for a single composition control, its pairing with steam pressure for dual composition control is investigated in this case. The controller parameters for two PI controllers were taken from their single loop parameters and are given below:

<table>
<thead>
<tr>
<th></th>
<th>K</th>
<th>T</th>
</tr>
</thead>
<tbody>
<tr>
<td>top loop</td>
<td>400.0</td>
<td>1.25</td>
</tr>
<tr>
<td>bottom loop</td>
<td>-689.5</td>
<td>5.0</td>
</tr>
</tbody>
</table>

However, this set of parameters resulted in an oscillatory behaviour, suggesting a strong interaction between two loops. Therefore, these parameters were retuned, and Figure 6.14 shows the performance for the type I disturbance with
the following parameters:

\[
\begin{align*}
K & \quad T \\
200.0 & \quad 1.0 & \text{top loop} \\
-137.9 & \quad 1.0 & \text{bottom loop}
\end{align*}
\]

The controller brings the top composition back to the setpoints. The response time is larger than in Figure 6.12 due to the interaction effects. Neither controller saturates. The final water flow rate is 51.0 ml/min from 45.0 ml/min and steam pressure moves from 144.8 to 147.6 kPa(gauge). Comparing this response with Figure 6.8, which was for the reflux/steam-pairing, shows that the water/steam handles this type of disturbance better than the reflux/steam pairing.

**CASE 12**

To reduce the interaction effects, PI controllers with a decoupler were implemented in this simulation for the type I disturbance. The decoupler gains were calculated as explained earlier in the chapter. The controller performance for the following parameters is given in Figure 6.15.

\[
\begin{align*}
K & \quad T & \quad \text{Decoupler Gain} \\
175.0 & \quad 1.2 & \quad 7.27 & \text{top loop}
\end{align*}
\]
The controller performance is acceptable. The maximum deviation from the setpoint for the top product acetone composition is only 0.003 mole fraction and for the bottoms product methanol composition is 0.0025 mole fraction. Both compositions come back to the setpoints. Water flow rate changes from 45.0 to 49.7 ml/min whereas steam pressure changes from 144.8 to 148.25 kPa(gauge) around 3.5 hr (which corresponds to the maximum deviation in the bottoms product composition), but finally it settles at 144.8 kPa(gauge). In Case 7, it was observed that for the type I disturbance only water can control both the top and the bottoms product composition. The final water flow rate is nearly the same in both cases. But the response times for both compositions are smaller in this case. A comparison of the maximum deviation in the compositions between Case 12 and Case 9 is given below:

<table>
<thead>
<tr>
<th></th>
<th>Top product (acétone)</th>
<th>Bottoms product (methanol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 12</td>
<td>0.003</td>
<td>0.0025</td>
</tr>
<tr>
<td>Case 9</td>
<td>0.005</td>
<td>0.009</td>
</tr>
</tbody>
</table>
From the above comparison it is clear that the controller for this case is better than for Case 9.

CASE 13

Figure 6.16 shows the controller performance for the type II disturbance. The controller performs well but the response time is larger than in Case 12. The controller parameters are the same as in the Case 12. There is also a slight oscillation in the composition around the setpoint. However, the amplitude of the oscillation is very small. One of the reasons for the difference in the performance is that the different type of disturbance produces interactions of different nature. Moreover, the column is nonlinear and shows asymmetric dynamics. The decoupler gain selected for one type of disturbance may not be optimum for another kind of disturbance. However, the main objective is to show that water/steam can be used for type II disturbance without saturation of the manipulated variables.

CASES 14 and 15

Figure 6.17 presents the controller performance for the type III disturbance for water/steam pairing. The controller type and its parameters are the same as in Case 12. Comparing this performance with reflux/steam of Case 7,
it can be seen that the response time and the maximum deviation are lower for this case. The methanol composition shows oscillation with low amplitude, which is acceptable in most cases. Figure 6.18 for Case 15, shows the controller performance for the type IV disturbance. The controller parameters are unchanged. Again, water/steam works well.

CASE 16

Figure 6.19 shows the effect of adding a feedforward controller for the feed flow disturbance to the PI+decoupler of Case 12. Since feed flow disturbances can be measured instantaneously the use of a feedforward controller should result in better performance. In this case, the feedforward element acts on the solvent flow rate, which is also used in the feedback control loop. The feedforward gain is calculated based on the constant feed/solvent ratio at the initial steady state and it is equal to 0.3636 in this case. The performance, as expected, is improved over the PI or PI+decoupler controller. This control structure results in maximum deviations which are lower than the PI+decoupler case.
6.5 CALCULATION OF THE REQUIRED CONTROL ACTION

BASED ON LINEAR ASSUMPTION:

In the previous section it was shown that reflux/steam was not a suitable pairing for dual composition control for type I or II disturbances. These disturbances are introduced by changing the feed flow rate. Under a linear system assumption, the changes in acetone and methanol composition which result from changing the manipulated variables can be given as:

$$
\begin{bmatrix}
\Delta A \\
\Delta M
\end{bmatrix}
= 
\begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix}
\begin{bmatrix}
\Delta U_1 \\
\Delta U_2
\end{bmatrix}
$$

(6.5)

\( \Delta A \) = change in acetone composition in the top product
\( \Delta M \) = change in methanol composition in the bottoms product
\( \Delta U_1 \) = change in manipulated variable # 1
\( \Delta U_2 \) = change in manipulated variable # 2

The objective of the analysis in this section is to determine the changes in the manipulated variables which are required to bring the system back to the nominal operating point after it is disturbed. Equation (6.6) is used to calculate the required control action to compensate for the deviation:
\[
\begin{bmatrix}
\Delta U_1 \\
\Delta U_2 
\end{bmatrix}
= \begin{bmatrix}
H_{11} & H_{12} \\
H_{21} & H_{22}
\end{bmatrix}^{-1}
\begin{bmatrix}
\Delta \lambda \\
\Delta M
\end{bmatrix}
\tag{6.6}
\]

The new values of \( U_1 \) and \( U_2 \) are given as:

\[
U_i = U_{i0} + \Delta U_i 
\tag{6.7}
\]

for \( i = 1, 2 \)

The pairing of manipulated variables is suitable if \( U_1 \) and \( U_2 \) satisfy the following conditions:

\[
U_{imin} < U_i < U_{imax}
\tag{6.8}
\]

for \( i = 1, 2 \)

The limits of \( U_1 \) and \( U_2 \) are given in Table 6.1. If equation (6.8) is violated, then the pairing is not suitable.

The above analysis was applied to the extractive distillation column for the three possible manipulated variables; i.e., reflux flow rate, steam pressure and water flow rate. The following procedure was used:

1. Calculate the small signal gains at two operating points by giving the following variations in the manipulated variables:
reflux flow rate 1.0 ml/min
steam pressure 0.6895 kPa(gauge)
water flow rate 1.0 ml/min

2. The second operating point is obtained from the first operating point by introducing the desired disturbance.

3. At each operating point, gains for the up and down dynamics were calculated and the average of these are given in columns 1 and 2 of Table 6.4. Gains used in equation (6.6) are the average of columns 1 and 2 of Table 6.4 and are given in column 3 of Table 6.4.

4. The average gains from Table 6.4 are used with equation (6.6) to obtain the results in Table 6.5.

<table>
<thead>
<tr>
<th></th>
<th>Ist point</th>
<th>2nd point</th>
<th>average</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Acetone</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>reflux</td>
<td>0.0009175</td>
<td>0.000962</td>
<td>0.0009397</td>
</tr>
<tr>
<td>steam</td>
<td>-0.01031</td>
<td>-0.01</td>
<td>-0.010155</td>
</tr>
<tr>
<td>water</td>
<td>0.0014915</td>
<td>0.00150</td>
<td>0.001496</td>
</tr>
<tr>
<td><strong>Methanol</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>reflux</td>
<td>0.000249</td>
<td>0.000249</td>
<td>0.000249</td>
</tr>
<tr>
<td>steam</td>
<td>-0.003135</td>
<td>-0.00297</td>
<td>-0.003050</td>
</tr>
<tr>
<td>water</td>
<td>-0.002115</td>
<td>-0.0022</td>
<td>-0.0021577</td>
</tr>
</tbody>
</table>

The first operating point is given in Table 6.2. The
second operating point is obtained by introducing a step in the feed flow rate from 104.0 to 110.0 ml/min.

It is clear from Table 6.5 that,

1. For the feed flow disturbance (Case a), the reflux/steam pair require large control actions and the required manipulated variable settings are out of the operating space. Using this pair may result in saturation. This happened during the type I disturbance when the PI controller was implemented.

2. The water/reflux and water/steam pairings resulted in more satisfactory control action. The pairing shows good results for a large feed flow disturbance (Table 6.5 Case b).

3. For the small disturbance (Case c in Table 6.5) reflux/steam satisfies the constraint equation but the magnitude of the action is very large as compared to the other two pairings. Use of the reflux/steam would consume more energy as compared to the other pairings.

4. The reflux/steam pairing works satisfactorily for the disturbance of Case d in Table 6.4, which corresponds to the type III disturbance. This shows that reflux/steam is suitable only for certain types of disturbances. Water/steam or water/reflux can also be used.

The results obtained from this simple analysis based on the linear system assumption match with the controller
### Table 6.5: Calculation of the Required Control Action

<table>
<thead>
<tr>
<th>Initial States</th>
<th>( \Delta R )</th>
<th>( \Delta B )</th>
<th>( \Delta W )</th>
<th>( \Delta R )</th>
<th>( \Delta W )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0.8912, 0.1592)</td>
<td>Reflux/Steam</td>
<td>Water/Steam</td>
<td>Reflux/water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Case a</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feed Disturbance</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>110 to 116.5 ml/min</td>
<td>184.53</td>
<td>115.5</td>
<td>2.36</td>
<td>0.18</td>
<td>-0.21</td>
</tr>
<tr>
<td>(0.8878, 0.1644)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Case b</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feed Flow Disturbance</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>110 to 126.92 ml/min</td>
<td>510.1</td>
<td>318.9</td>
<td>6.6</td>
<td>2.2</td>
<td>-0.35</td>
</tr>
<tr>
<td>(0.8817, 0.1735)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Case c</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feed Flow Disturbance</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>110.0 to 111.6 ml/min</td>
<td>31.98</td>
<td>19.9</td>
<td>0.41</td>
<td>-0.14</td>
<td>-0.01</td>
</tr>
<tr>
<td><strong>Case d</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Room Temperature</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>24 to 26 °C</td>
<td>-41.7</td>
<td>28.1</td>
<td>-0.55</td>
<td>-15.8</td>
<td>25.30</td>
</tr>
<tr>
<td>(0.8687, 0.1511)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6.6 CONCLUSIONS:

Simple conventional control strategies have been simulated for single and dual composition control. Four kinds of disturbance were considered for the regulatory control problem. From the simulation studies it was found that reflux can be used to control the acetone in the top product and steam pressure can control the methanol in the bottoms product provided that the control strategy is single loop. For this strategy, however, controller parameters need to be changed depending on the type of disturbance or the nature of the dynamics. For dual composition control, the conventional pairing of reflux/steam is suitable only for the type III or IV disturbances when it is used with PI+decoupler. For the type I or II disturbances both manipulated variables saturate for the PI or PI+decoupler control configurations. The selection of water/steam as a pairing shows better performance for all four types of disturbances when used with PI+decouplers for extractive distillation. Due to the strong interaction between two loops, PI+decoupler performs better than the PI controller alone. It is also observed that the feed forward controller along with PI+decoupler further improves the performance for the kind of disturbances which can be measured. Solvent flow
rate is used as a feedforward element.

A simple method based on a linear system assumption was used to calculate the control action required to compensate for the change in the composition produced by the various disturbances. This simple method revealed that the reflux/steam pairing required a large control action and that the final manipulated variables go out of the specified operating space. It also showed that the water/steam pairing this able to regulate the disturbance without saturation. The results obtained by this simple method are in agreement with the controller performance results.

Based on these results, it can be concluded that reflux/steam is not a good choice when two independent SISO controllers are used. However, nothing can be said about the performance of the pairing for the model-based, advanced multivariable controllers which will be tested in the next chapters.
NOMENCLATURE.

\( \Delta A \) = Change in the Acetone Composition
\( A \) = Acetone in the top product
\( \Delta B \) = Change in the steam pressure
\( C_1 \) = Manipulated variable 1
\( C_2 \) = Manipulated Variable 2
\( \Delta C_1 \) = Change in \( C_1 \)
\( \Delta C_2 \) = Change in \( C_2 \)
\( D_{11}, D_{12} \) = Decoupler elements
\( D_{21}, D_{22} \) = Decoupler elements
\( F \) = Experimental Steam Flow Rate in ml/min
\( K \) = Controller Gain
\( H \) = Average System Gain Matrix
\( \Delta M \) = Change in the Methanol Composition
\( M \) = Methanol in bottoms product
\( P \) = Steam pressure kPa(gauge)
\( \Delta R \) = Change in reflux flow rate
\( T \) = Reset Time
\( \Delta U_1 \) = Change in the Manipulated Variable 1
\( \Delta U_2 \) = Change in the Manipulated Variable 2
\( U_i \) = \( i \)th manipulated variable
\( U_{imax} \) = Maximum Value of the \( i \)th Manipulated Variable
\( U_{imin} \) = Minimum Value of the \( i \)th Manipulated Variable
\( U_{is} \) = Steady State Value of the \( i \)th Manipulated Variable
\( \Delta W \) = Change in water flow rate
\[ X_1 = \text{Acetone Composition in the Top Product} \]

\[ X_2 = \text{Methanol Composition in the Bottoms Product} \]
Figure 6.4: Single Loop Top Product Control using Reflux Flow Rate, PI Controller Type I Disturbance
Figure 6.5: Single Loop Bottoms Product Control using Steam Pressure (PI Controller) Type I Disturbance
Figure 6.6: Single Loop Top Product Control using Reflux Flow Rate (PI Controller) Type II Disturbance
Figure 6.7: Single Loop Bottoms Product Control using Steam Pressure (PI Controller) Type II Disturbance
Figure 6.8: Dual Composition Control using Reflux Flow Rate and Steam Pressure (PI Controller) Type I Disturbance
Figure 6.9: Dual Composition Control using Reflux Flow Rate and Steam Pressure (PI + Decoupler Controller), Type I Disturbance
Figure 6.10: Dual Composition Control using Reflux Flow Rate and Steam Pressure (PI + Decoupler Controller, Type IV Disturbance)
Figure 6.11: Dual Composition Control using Reflux Flow Rate and Steam Pressure (PI + Decoupler Controller, Type III Disturbance)
Figure 6.12: Single Composition Control for Top Product using Water (PI Controller) Type I Disturbance
Figure 6.13: Single Composition Control for Top Product using Water (PI Controller) Type II Disturbance
Figure 6.14: Dual Composition Control using Water and Steam Pressure (PI Controller) Type I Disturbance
Figure 6.15: Dual Composition Control using Water and Steam Pressure (PI + Decoupler Controller) Type I Disturbance
Figure 6.16: Dual Composition Control using Water and Steam Pressure (PI + Decoupler Controller) Type II Disturbance
Figure 6.17: Dual Composition Control using Water and Steam Pressure (PI + Decoupler Controller). Type III Disturbance
Figure 6.18: Dual Composition Control using Water and Steam Pressure (PI + Decoupler Controller) Type IV Disturbance.
Figure 6.19: Dual Composition Control using Water and Steam Pressure (PI + Decoupler + Feedforward Controller)
Type I Disturbance
Chapter - 7

DEVELOPMENT OF BILINEAR OPTIMAL CONTROLLER

7.1 INTRODUCTION:

In the previous chapter, simple controllers based on the PI controller structure were applied to an extractive distillation column simulation. A bilinear optimal controller which would guarantee asymptotic stability for the system, is developed in this chapter. Section 7.2, defines the bilinear control problem in general. The present control problem statement is given in Section 7.3. The desired controller structure is developed in Section 7.4. The controller developed in this chapter is based on penalizing the control vector. Controller resulted from this would be robust for impulse disturbances only. This type of analysis is selected because it is conventional method and widely used. A form of the bilinear controller for a single variable case is presented in Section 7.5. In Section 7.6 the importance of a bilinear controller over a linear controller is shown with the help of a numerical example. An optimal controller from a bilinear model is applied to the linear system problem in Section 7.7. Conclusions are given in Section 7.8.
7.2 BILINEAR CONTROL PROBLEM:

The superiority of a bilinear model over its linear counterpart was discussed in Chapter 5. The improvement in the bilinear case is due to the $\sum B_i U_i X$ term in the bilinear representation. Consequently, a controller derived from a bilinear model of a nonlinear process should be more effective than one designed from a linear model. Mohlar and Rink (1969) have shown that a linear system with input constraints which is not controllable can be made controllable by adding a multiplicative control law; controllability can be achieved via a bilinear structure.

Deresse (1980) developed a linear feedback optimal controller for a bilinear process. The final controller structure minimized a quadratic performance index criterion, but did not fully utilize the flexibility of the bilinear structure. Jacobson (1976) developed an optimal controller structure for a nonlinear system. The system is given as:

$$X = f(X) + \sum_{i=1}^{m} D_i(X) U_i$$  \hspace{1cm} (7.1)

$f(X)$ and $D_i(X)$ are functions of $X$, $U_i$ are control variables for $i=1,2,...,m$, and $D_i(X)$ are continuous in the state variable $X$. Jacobson's controller structure is:
where $w_x(x)$ is a radially bounded positive definite function and $w_x(x)f(x)$ is negative semidefinite.

This controller globally stabilizes the system while minimizing the following performance function:

$$J = \int_0^\infty \left( q(x) + \frac{1}{2} \sum_{i=1}^m u_i^2 \right) dt$$

where

$$q(x) = -w_x(x)f(x) + \frac{1}{2} \sum_{i=1}^m \left( w_x(x)d_i(x) \right)^2$$

Longchamp (1980) developed a pure stabilizing controller for a bilinear system. The resulting feedback controller is of the bang-bang type, with a quadratic term in the state switching function.

**7.3 Present Problem Statement:**

The problem considered in this chapter is to design a controller for a bilinear system which is asymptotically stable and minimizes a quadratic performance index. The problem can be stated as follows.

Develop a optimal control policy for a system given as:
\[
\dot{X} = A X + \sum_{i=1}^{m} B_i X U_i + C U
\] (7.3)

where \( X \) is a state vector of order \( 1 \times n \)

\( A \) and \( B_i \) are the \( n \times n \) matrices

\( U \) is the control vector of order \( 1 \times m \)

\( C \) is the matrix of dimension \( n \times m \)

which is asymptotically stable and minimizes the following cost function:

\[
J = \frac{1}{2} \int_0^\infty \left[ X^T Q X + X^T S C_i^* R_i^{-1} C_i^* T S X + U^T R U \right] dt \quad (7.4)
\]

where \( Q \) and \( S \) are positive definite symmetric matrices, \( R \) is a diagonal matrix with \( R_i > 0 \) and

\[
C_i^* = B_i X + C_i
\]

where \( C_i^* \) and \( C_i \) are the \( i \)th column vector of \( C^* \) and \( C \) matrices.

7.4 DEVELOPMENT OF THE CONTROLLER STRUCTURE:

From the Liapunov direct method (see Douglas (1972)), a dynamic system is asymptotically stable iff there exists a Liapunov function. This is some scalar function \( V(X) \) of the state vector which has following properties:
\[ V(\bar{X}) > 0 \quad ; \quad V(\bar{X}) < 0 \text{ for } \bar{X} \neq \bar{X}_e \quad \text{(7.5a)} \]

\[ V(\bar{X}) = \dot{V}(\bar{X}) = 0 \text{ for } \bar{X} = \bar{X}_e \quad \text{(7.5b)} \]

where \( V(\bar{X}) \) = time derivative of \( V(\bar{X}) \)

\( \bar{X}_e \) = Equilibrium state vector

This makes \( V(\bar{X}) \) is a positive definite function.

Equation (7.3) can be rewritten in the following manner:

\[ \dot{\bar{X}} = A\bar{X} + \sum_{i=1}^{m} B_i \bar{X} U_i + \sum_{i=1}^{m} C_i U_i \quad \text{(7.6)} \]

where \( C_i \) are the column vectors of the matrix \( C \), and the variables \( \bar{X} \) and \( U \) are defined in terms of deviation variables. Equation (7.6) can be rewritten as:

\[ \dot{\bar{X}} = A\bar{X} + \sum_{i=1}^{m} (B_i \bar{X} + C_i) U_i \quad \text{(7.7)} \]

Defining a new variable \( C^* \) having dimension of \( n \times m \):

\[ C_i^* = B_i \bar{X} + C_i \]

such that equation (7.7) becomes:
\[ \dot{X} = AX + C^*U \]  \hspace{1cm} (7.8)

Note that \( C^* \) is a function of the state vector \( X \).
Consider the following function as a Liapunov candidate:

\[ V(X) = \frac{1}{2} X^T S X \]  \hspace{1cm} (7.9)

with \( S \) = Positive definite symmetric matrix thus

\[ V(X) > 0 \text{ for } X \neq X_e \]

Differentiate equation (7.9) with respect to (wrt) time to get:

\[ 2 \dot{V}(X) = X^T S \dot{X} + \dot{X}^T S X \]  \hspace{1cm} (7.10)

Substitute from equation (7.8) for \( \dot{X} \) and \( \dot{X}^T \) into equation (7.10) yields:

\[ 2 \dot{V}(X) = X^T AS X + U^T C^*TS X + X^T S A X + X^T S C U \]

\[ = X^T (A^T S + S A) X + U^T C^*TS X + X^T S C^*U \]  \hspace{1cm} (7.11)

Through the dimensional check it can be shown that \( U^T C^*TSX \) is a scalar quantity and \( S \) is a symmetric, this term
can be rearranged:

\[ u^T c^* T s^* x = x^T s^* c^* u \]  \hspace{1cm} (7.12)

Substituting equation (7.12) into equation (7.11) results in:

\[ 2 \dot{V}(x) = x^T ( A^T s + s A ) x + 2 x^T s c^* u \]  \hspace{1cm} (7.13)

The Lyapunov criterion for stability, equation (7.5b)

\[ V(x) < 0 \quad \text{for} \quad x \neq x_0 \quad \text{will be satisfied if the following are true:} \]

a) \[ A^T s + s A = \text{negative definite} \]  \hspace{1cm} (7.14a)

b) \[ x^T s c^* u = \text{non positive} \]  \hspace{1cm} (7.14b)

The conditions which guarantee \[ V(x) < 0 \] are not unique, but the conditions defined in equations (7.14a) and (7.14b) will satisfy the requirement.

Since \( Q \) is a positive definite matrix, condition (7.14a) is satisfied by:

\[ A^T s + s A = -Q \]  \hspace{1cm} (7.15)
Condition (7.14b) involves the control action, \( U \), and will be discussed later. If equation (7.14b) can be satisfied, then the system is asymptotically stable provided that \( A \) and \( S \) satisfy equation (7.15).

In order to obtain the optimal control policy, define the Hamiltonian as:

\[
H = \frac{1}{2} \dot{X}^T Q X + \frac{1}{2} X^T S C^* R^{-1} C^* T S X + \frac{1}{2} U^T R U \\
+ \mu^T (A X + C^* X)
\]  \hspace{1cm} (7.16)

The necessary condition for unconstrained optimal control is:

\[
\frac{\partial H}{\partial U} = 0
\]  \hspace{1cm} (7.17)

and the stopping condition for the free choice of time is:

\[
H = 0 \quad \text{along the optimal trajectory} \quad (7.18)
\]

and selection of \( \mu \) should satisfy the adjoint equation:

\[
\dot{\mu} = -\frac{\partial H}{\partial X}
\]  \hspace{1cm} (7.19)

Differentiating the Hamiltonian, equation (7.16), wrt \( U \) and using the necessary condition, the following results are
obtained:

\[
\frac{\partial H}{\partial \mathbf{u}} = 0 = R \mathbf{u} + \mathbf{c}^T \mathbf{u}
\]  

(7.20)

and the control law is given as:

\[
\mathbf{u}^* = - R^{-1} \mathbf{c}^T \mathbf{u}
\]  

(7.21)

where \( \mathbf{u}^* \) is the control vector.

To show that the optimal control law of equation (7.20) minimizes the performance index, the 2nd derivative of the Hamiltonian wrt to \( \mathbf{u} \) should be a positive definite matrix. Differentiating equation (7.16) one more time wrt \( \mathbf{u} \) yields:

\[
\frac{\partial^2 H}{\partial \mathbf{u}^2} = R^T
\]  

(7.22)

Since \( R \) is a positive definite matrix, equation (7.22) guarantees that the control law of equation (7.21) will minimize the Hamiltonian.

Suppose \( \mathbf{u} \) in equation (7.21) is selected as:

\[
\mathbf{u} = S \mathbf{x}
\]  

(7.23)

and \( S \) is selected as given in equation (7.15). Substituting equation (7.23) into equation (7.21) yields:
\[
U^* = - R^{-1} C^* S X
\]  
(7.24)

where \( C^* S X \) is \( m \times 1 \) and \( R \) is \( m \times m \)

To show that the above control law is optimal and the resultant system is stable, the following conditions should be proved to be true.

a) Equation (7.14b) (i.e., \( X^T S C^* U \) is non positive) must be true.

b) The stopping condition \( (H = 0) \) must be satisfied along the optimal trajectory.

c) The selection of \( u = S X \) must be consistent with equation (7.19).

These conditions are investigated now.

Condition a: \( X^T S C^* U \) = non positive

Substituting the value of \( U \) from equation (7.24) into the LHS of equation (7.14b)

\[
X^T S C^* U = - X^T S C^* R^{-1} C^* S X
\]  
(7.25)
The RHS of equation (7.25) is by definition a negative quadratic expression and it will always be non-positive. The Liapunov criterion for stability is satisfied.

Condition b: $H = 0$ along the optimal trajectory

Substituting equation (7.24) and equation (7.23) in equation (7.16) the following equation is obtained:

$$H = \frac{1}{2} X^T Q X + \frac{1}{2} \left( X^T S C^* R^{-1} C^* T S X \right)$$

$$+ \frac{1}{2} \left( X^T S C^* R^{-1} R^{-1} C^* T S X \right) + X^T S A X$$

(7.26)

$$- X^T S C^* R^{-1} C^* T S X$$

The term $X^T S A X$ is a scalar, therefore:

$$X^T S A X = (X^T S A X)^T = X^T A^T S X$$

therefore, $X S A X^T$ can be written as

$$X^T S A X = \frac{1}{2} \left( X^T S A X + X^T A^T S X \right)$$

Using equation (7.15)

$$X^T S A X = -\frac{1}{2} X^T Q X$$

(7.27)

and substituting equation (7.27) into equation (7.26) yields:
\[ H = \frac{1}{2} \mathbf{X}^T \mathbf{Q} \mathbf{X} + \frac{1}{2} \left( \mathbf{X}^T \mathbf{S} \mathbf{C}^* \mathbf{R}^{-1} \mathbf{C}^* \mathbf{T} \mathbf{S} \mathbf{X} \right) \\
   + \frac{1}{2} \left( \mathbf{X}^T \mathbf{S} \mathbf{C}^* \mathbf{R}^{-1} \mathbf{C}^* \mathbf{T} \mathbf{S} \mathbf{X} \right)^T - \frac{1}{2} \mathbf{X}^T \mathbf{Q} \mathbf{X} \\
   - \mathbf{X}^T \mathbf{S} \mathbf{C}^* \mathbf{R}^{-1} \mathbf{C}^* \mathbf{T} \mathbf{S} \mathbf{X} \\
   = 0 \]

Therefore, the stopping condition is satisfied along the optimal trajectory.

Condition c: Selection of \( \mu = \mathbf{S} \mathbf{X} \) is consistent with equation (7.20)

The proof of this condition is given in Appendix C. The result of Appendix C is that the selection of \( \mu = \mathbf{S} \mathbf{X} \) is consistent.

Therefore, the control policy given by equation (7.24) results in an asymptotically stable system for equation (7.2) and simultaneously minimizes the performance index of equation (7.4)

7.5 FORM OF THE OPTIMAL CONTROLLER:

Consider a bilinear process with one state and one control variable. The process can be written as:

\[ \mathbf{x} = \mathbf{a} \mathbf{x} + \mathbf{b} \mathbf{u} \mathbf{x} + \mathbf{c} \mathbf{u} \quad (7.28) \]
\[ x = ax + c^*u \]  
\[ \text{where } c^* = bx + c \]

The performance index equivalent to equation (7.4):

\[ J = \frac{1}{2} \int_0^\infty \left( xq x + x s c^* \frac{1}{r} c^* s x + u r u \right) dt \]  
\[ \text{(7.30)} \]

and the optimal control law of equation (7.25) is:

\[ u^* = -\frac{1}{r} (bx + c) sx \]
\[ u^* = -(\frac{1}{r} b ss x^2 + \frac{1}{r} c ss x) \]
\[ u^* = -(K_1 x^2 + K_2 x) \]  
\[ \text{(7.31)} \]

where \( K_1 = \frac{1}{r} b s \)
\( K_2 = \frac{1}{r} c s \)

On the other hand, a linear process given as:

\[ \dot{x} = ax + cu \]

would generate an optimal controller which would minimize the performance index of equation (7.30):

\[ u^* = -K_2 x \]  
\[ \text{(7.32)} \]

where \( K_2 \) is same as in equation (7.31)

Comparing the two controllers given in equation
(7.31) and equation (7.32), it is clear that the bilinear model and bilinear design procedure generates a controller structure which is nonlinear, whereas the linear model—procedure generates a linear controller.

The bilinear controller can be applied to the real process in the following manner.

1) Select the matrices $R$ and $Q$. These can be selected arbitrarily depending upon the penalty on the states and control elements.

2) Calculate the $G$ matrix using equation (7.15) to ensure asymptotic stability of the process under feedback control.

3) Measure or observe the state vector elements at each control interval.

4) Use equation (7.24) to calculate the control action to bring the process back to its nominal operating conditions.

Note that both the state vector and control vector are in the deviation form, that is:

$$ x = x_{act} - x_e $$

$$ u = u_{act} - u_e $$

Therefore, the actual value of the manipulated variable should be

$$ u_{act} = u + u_e $$

(7.33)
7.6 COMPARISON OF BILINEAR AND LINEAR SYSTEM PERFORMANCE:

In this section, the controllers developed in the previous sections for a bilinear and a linear process are compared through a numerical example. The problem statement is given below:

Consider the following process:

\[ x = -x + 2x u + 5u \]  
(7.34)

operating around the equilibrium point \((0,0)\). The objective is to design an optimal controller which will minimize the performance index of equation (7.30) with \(q = 2\) and \(r = 1\). The bilinear controller is to be applied for different initial conditions (different impulses) and its performance compared to that obtained from the controller designed from the linearised model of the process. The objective of the application of the controller is to bring the system to its normal operating point (i.e., \((0,0)\)) after impulses of different magnitude.

Bilinear Case:

Using the system equation (7.34) and equation (7.15) with \(q=2\), the value of \(s\) is given as
-s -s = -2
s = 1

The optimal control law is given by equation (7.24) and (7.31) with the weighting factor \( r = 1 \):

\[
u = -2 x^2 - 5x \quad (7.35)\]

**Linearised Case:**

The linearised model equation of the process (7.34) around the (0,0) equilibrium point can be obtained by the Taylor series method as:

\[
x = -x + 5u \quad (7.36)\]

The optimal controller based on equation (7.36) as given by equation (7.32) is:

\[
u = - \frac{1}{r} c s x
\]

where \( r = 1 \), \( c = 5 \) and \( s \) is calculated from equation (7.15) as:

\[-s -s = -2 ; \quad s = 1\]

and the optimal control law is:
\[ u = -5x \]  

(7.37)

Remember that the variables in equations (7.36) and (7.37) are in deviation form.

The controllers (7.36) and (7.37) were tested on the simulation of the process (7.35) for different initial conditions; these corresponded to impulses of different magnitudes. The DVERK routine from the IMSL library was used with a step size of 0.0001 to solve the system equation. Table (7.1) shows the performance index for the two controllers. The performance index (7.4) is:

\[ J = \frac{1}{2} \int_0^\infty \left( 2x^2 + x^2(2x + 5)^2 + u^2 \right) \, dt \]

for the true process.

**Table 7.1: Comparison of Performance for a Bilinear and Linearized Controller**

<table>
<thead>
<tr>
<th>Initial Condition of the State</th>
<th>Linearized Model Controller</th>
<th>Bilinear model Controller</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>0.515</td>
<td>0.501</td>
</tr>
<tr>
<td>5.0</td>
<td>17.420</td>
<td>12.640</td>
</tr>
<tr>
<td>10.0</td>
<td>99.770</td>
<td>51.63</td>
</tr>
<tr>
<td>-1.0</td>
<td>0.528</td>
<td>0.502</td>
</tr>
<tr>
<td>-3.0</td>
<td>diverges</td>
<td>4.49</td>
</tr>
</tbody>
</table>
From Table (7.1) it is clear that the controller based on the bilinear model gives lower performance index than the controller designed from the linearized model of the process around \((0,0)\). For the initial condition of \(x = -3.0\) the controller from a linearized model diverges, whereas, a controller from the bilinear model brings the state back to its original equilibrium point. This shows that a bilinear controller can operate in a larger asymptotically stable space than controller based upon a linearized model. For this example the linear, optimal controller is a suboptimal controller, whereas, the bilinear controller is a globally optimal controller.

The reason why a linear controller diverges for an initial condition of \(x = -3.0\) is clear if the process is linearized around \(x = -3.0\). The equilibrium point of the system for \(x = -3.0\) is \((-3.0, 3.0)\). The linearized process equation around \((-3.0, 3.0)\) is:

\[
\dot{x} = 5x - u
\]  \((7.38)\)

which has a root in right half plane in the Laplace domain.

The above example shows the limitation of a controller designed from a linearized model of the process. For the best results from the linearized model, it is necessary to relinearize when the operating conditions are changed. A controller based on the bilinear model shows \(\)
larger state space region of optimal stable operation.

7.7 APPLICATION OF THE CONTROLLER OF SECTION 7.4 TO A LINEAR PROCESS:

In this section, the bilinear optimal controller method developed in Section (7.2) is applied to a strictly linear process. The method is illustrated using an example taken from Douglas (1972).

The state equation is:

\[ x = a x + c u \]  \hspace{1cm} (7.39)

and the performance index is:

\[ J = \frac{1}{2} \int_0^\infty (x^2 + r_d^2 u^2) \, dt \]  \hspace{1cm} (7.40)

The linear optimal controller is derived as:

\[ u_{\text{opt}} = - \frac{a}{c} \left( 1 + \sqrt{1 + r^*} \right) x \]  \hspace{1cm} (7.41)

where \[ r^* = \frac{c^2}{a^2 r_d^2} \]

in which a solution of a second order differential equation is required. (For details see the Douglas (1972), page 265).
In order to use the method developed earlier to design a bilinear optimal controller for the system (7.39), which minimizes the performance index of equation (7.40) one must rewrite the performance index of equation (7.4) for one state and one control element case:

\[ J = \frac{1}{2} \int_0^\infty \left( x^2 q + \frac{x^2 s^2 b^2}{r} + r u^2 \right) dt \quad (7.42) \]

For this example, \( r = r_d \) to match the penalty on \( u \) in equation (7.40).

The two performance indices of equation (7.40) and (7.42) are equivalent under the following conditions:

\[ q + \frac{s^2 c^2}{r} = 1 \quad (7.43) \]

From equation (7.15), Liapunov stability requires that:

\[ q = -2 a s \quad (7.44) \]

Substitute \( q \) from equation (7.44) into equation (7.43) to get:

\[ -2 a s + \frac{s^2 c^2}{r} - 1 = 0 \quad (7.45) \]

Equation (7.45) has two roots given by:
\[ s = \frac{2a \pm \sqrt{(4a^2 + 4c^2/r)}}{2c^2/r} \]  

(7.46)

and for a positive \( s \) the root is:

\[ s = \frac{ar}{c^2} \left( 1 + \sqrt{1 + c^2/a^2r} \right) \]  

(7.47)

Now from equation (7.24) the optimal control law is:

\[ u_{\text{opt}} = -\frac{1}{r} c s x \]

\[ u_{\text{opt}} = -\frac{a}{c} \left( 1 + \sqrt{1 + c^2/a^2r} \right) x \]  

(7.48)

The control law of equation (7.48) is identical to the linear control law of equation (7.41). Using this bilinear method, the need to find a solution of a second order differential equation was replaced by the need to solve a second order algebraic equation.

7.8 CONCLUSIONS:

An optimal controller design for a bilinear system equation was developed so that the controlled system would be asymptotically stable. The proof of the optimality is given from the first principals. Optimal control law from a bilinear system is nonlinear in nature, contrary to a linear control law from a linearized model. It was also shown
through an example that an optimal controller based on a bilinear equation has a larger region of application than a controller designed from a linearized model. Finally, the developed procedure was applied to a linear process by manipulating the performance index parameters. The final optimal control law obtained was the same as obtained from the classical linear optimal control theory.
**NOMENCLATURE**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A )</td>
<td>System Matrix of ( n \times n ) order</td>
</tr>
<tr>
<td>( A^T )</td>
<td>Transpose of ( A ) matrix</td>
</tr>
<tr>
<td>( B_i )</td>
<td>Matrix for the ( i )th input bilinear term in the system equation</td>
</tr>
<tr>
<td>( C )</td>
<td>Control vector matrix of ( n \times m ) order</td>
</tr>
<tr>
<td>( C_i )</td>
<td>( i )th column vector of matrix ( C )</td>
</tr>
<tr>
<td>( C_i^* )</td>
<td>( B_i X + C )</td>
</tr>
<tr>
<td>( C^* )</td>
<td>( n \times m ) order matrix whose ( i )th column is ( C_i^* )</td>
</tr>
<tr>
<td>( D_i(X) )</td>
<td>Function of ( X ) used in defining equation (7.1)</td>
</tr>
<tr>
<td>( f(X) )</td>
<td>Function of state vector ( X )</td>
</tr>
<tr>
<td>( H )</td>
<td>Hamiltonian defined in equation (7.16)</td>
</tr>
<tr>
<td>( J )</td>
<td>Performance index</td>
</tr>
<tr>
<td>( K_1, K_2 )</td>
<td>Variables defined in equation (7.31)</td>
</tr>
<tr>
<td>( n )</td>
<td>Order of the system</td>
</tr>
<tr>
<td>( m )</td>
<td>Order of the control vector</td>
</tr>
<tr>
<td>( q )</td>
<td>Weighting factor for state in the performance index</td>
</tr>
<tr>
<td>( Q )</td>
<td>Weighting factor matrix associated with state vector</td>
</tr>
<tr>
<td>( R )</td>
<td>Weighting factor matrix associated with control vector</td>
</tr>
</tbody>
</table>
\( R_i \) = Weighting factor for one element of the control vector
\( r_d \) = Penalty on \( U \) in Douglas example
\( r^* \) = Function of \( r_d \), and system variables, defined in equation (7.41)
\( S \) = Matrix defined in equation (7.15)
\( s \) = Scaler defined for one state system by equation (7.15)
\( U_i \) = \( i \)th manipulated variable in deviation form
\( U \) = Vector of length \( m \) of manipulated variables
\( U_e \) = Vector of equilibrium value of \( U \)
\( U_{act} \) = Actual value of the manipulated variable
\( U^* \) = Optimal values of the manipulated variables
\( V(\dot{X}) \) = Liapunov function
\( W(\dot{X}) \) = Function of \( X \)
\( W_x(\dot{X}) \) = Derivative of \( W(\dot{X}) \) wrt \( X \)
\( \dot{X} \) = State vector in deviation form of order \( n \)
\( X_e \) = Vector of equilibrium states of the state vector \( \dot{X} \)
\( X_{act} \) = Actual value of the state vector

GREEK SYMBOL:

\( \mu \) = Lagrange multiplier vector of order \( n \)
SUPERSCRIPTS:

\( T \) = transpose of the matrix

\( \cdot (\text{dot}) \) = Time derivative of the function
Chapter 8

APPLICATION OF BILINEAR OPTIMAL CONTROL
TO AN EXTRACTIVE DISTILLATION COLUMN

8.1 INTRODUCTION:

There is a considerable amount of literature available on the application of linear controllers to chemical processes especially to distillation columns. On the other hand, reports on the experimental application of non-linear controllers to non-ideal distillation systems are rare. Espana and Landu (1978) and Benallou (1982) applied a bilinear optimal controller to a distillation column. As stated earlier in Chapter 4, both studies were done on near ideal systems.

In this chapter the bilinear optimal controller design developed in the previous chapter is applied to an extractive distillation column. For this non-linear and non-ideal system controller based on bilinear model would perform better than the one based on linear model or log transformation of linear model. A complete tray to tray dynamic model developed in Chapter 3 is used to study the system performance. Results presented in this chapter are
based on simulation studies; experimental results will be presented in the next chapter. The objective is to take the system from one operating point to another operating point while minimizing the performance index given in Chapter 7. The development of the chapter is in steps. First, controller performance for single composition control is evaluated, and then the controller is applied to dual composition control for the servo problem. The performance is acceptable if the system has moved from its initial operating condition to the desired operating point and there are no fluctuations or saturations in the manipulated or controlled variables. The controller will also be tested using predictors.

Section 8.2 gives a bilinear state equation of the column in terms of deviation variables and from this model the controller structure is developed. Simulation results of single composition control, where acetone in the top product is controlled for various $Q$ and $R$ matrices (defined in Chapter 7 for the performance index) are presented in Section 8.3. In Section 8.4, the dual composition control problem is considered, where acetone in the top product and methanol in the bottoms product are controlled simultaneously. In order to make this simulation analysis more representative of the actual experimental conditions, temperatures are used to predict compositions. The design of this predictor and results of using it for dual composition
control are given in Section 8.5. A few remarks on the controller design are given in Section 8.6. Conclusions are presented in Section 8.6.

8.2 SYSTEM DESCRIPTION AND CONTROLLER STRUCTURE:

A 5 compartmental bilinear model derived in Chapter 5 is used to design an optimal controller. The system equation is given as:

\[ \dot{X} = A \cdot X + U_1 \cdot B_1 \cdot X + U_2 \cdot B_2 \cdot X + D \quad (8.1) \]

where \( X \) = state vector of \( 1 \times n \)

\( U_1 \) = Reflux flow rate

\( U_2 \) = Steam pressure

\( D \) = Disturbance vector

Matrices \( A, B_1, B_2, \) and \( D \) are given in Chapter 5. If control variables are manipulated so as to correct the deviations of the output variables from their desired values, the procedure can convert an unstable process to a stable process. The variables in equation (8.1) are absolute variables, they can be converted to the deviation form for control purpose in the following manner.

At the steady state equation (8.1) is:
$$0 = \dot{X}_s + U_{1s} B_1 X_s + U_{2s} B_2 X_s + \bar{U} \quad (8.2)$$

where subscript "s" denotes the steady state values.

Subtract equation (8.2) from (8.1) to get:

$$\ddot{X} - \dot{X}_s = A (\dot{X} - \dot{X}_s) + U_1 B_1 \dot{X} - U_{1s} B_1 X_s + U_2 B_2 X - U_{2s} B_2 X_s \quad (8.3)$$

Defining the following deviation variables:

$$\dot{\bar{X}} = \dot{X} - \dot{X}_s \quad (8.4)$$
$$\bar{U}_1 = U_1 - U_{1s} \quad (8.5)$$
$$\bar{U}_2 = U_2 - U_{2s} \quad (8.6)$$

after some manipulations equation (8.3) can be written in deviation variables in the following form:

$$\ddot{\bar{X}} = \bar{A} \bar{X} + \bar{U}_1 B_1 \bar{X} + \bar{U}_2 B_2 \bar{X} + \bar{C} \bar{U} \quad (8.7)$$

where

$$\bar{A} = A + U_{1s} B_1 + U_{2s} B_2 \quad (8.8)$$

$$\bar{C} = [ B_1 X_s \mid B_2 X_s ] \quad (8.9)$$

and $A$, $B_1$, $B_2$ were defined earlier. $C$ is an augmented matrix.

A 5 compartmental bilinear model given in chapter 5 can be converted to the form shown in equation (8.7) by using equations (8.8) and (8.9) and knowing the initial steady state. The final form of the $A$ and $C$ are given below:
\[
C = \begin{bmatrix}
  x_{1is} & K'_{11}x_{2is} - x_{1is} \\
  M_1 & M_1 \\
  x_{2is} - x_{2is} & K'_{31}x_{3is} & K'_{21}x_{2is} \\
  M_2 & M_2 \\
  x_{2is} - x_{3is} & K'_{41}x_{4is} & K'_{31}x_{3is} \\
  M_3 & M_3 \\
  x_{3is} - x_{4is} & K'_{51}x_{5is} & K'_{41}x_{4is} \\
  M_4 & M_4 \\
  x_{4is} - x_{5is} & (K'_{51} - 1)x_{5is} & \frac{1}{M_5} \\
  M_5 & M_5 \\
\end{bmatrix}
\]

Matrices \( B_1 \) and \( B_2 \) remain unchanged and are repeated here for the completeness of equation (8.7).

\[
B_1 = \begin{bmatrix}
  0 & 0 & 0 & 0 & 0 \\
  \frac{1}{M_2} & \frac{-1}{M_2} & 0 & 0 & 0 \\
  0 & \frac{1}{M_3} & \frac{-1}{M_3} & 0 & 0 \\
  0 & 0 & \frac{1}{M_4} & \frac{-1}{M_4} & 0 \\
  0 & 0 & 0 & \frac{1}{M_5} & \frac{-1}{M_5} \\
\end{bmatrix}
\]
\[
B_2 = \begin{bmatrix}
\frac{-n}{M_1} & \frac{nK'_{21}}{M_1} & 0 & 0 & 0 \\
0 & -\frac{nK'_{31}}{M_2} & \frac{nK'_{41}}{M_2} & 0 & 0 \\
0 & 0 & -\frac{nK'_{31}}{M_3} & \frac{nK'_{41}}{M_3} & 0 \\
0 & 0 & 0 & -\frac{nK'_{41}}{M_4} & \frac{nK'_{51}}{M_4} \\
0 & 0 & 0 & 0 & -\frac{(nK'_{51})}{M_5}
\end{bmatrix}
\]

(8.13)

In equation (8.11), \( X_{ki} \) means the kth element of the state vector \( X \) for component \( i \). Thus, matrices \( A \), \( B_2 \), \( C \) will be different for different components. For a complete order bilinear model these equations have to be combined properly. This will be further clarified later in the chapter.

The objective of dual composition control problem is to control the acetone in the top product and methanol in the bottoms product for the system given by equation (8.7) whose coefficients are defined by equations (8.10) to (8.13) and to minimize the following performance index:

\[
J = \frac{1}{2} \int_0^\infty \left[ X^T Q X + \tilde{X}^T S \tilde{C} R^{-1} \tilde{C}^T S \tilde{X} + U^T R U \right] dt
\]

(8.14)

where \( Q \) is \( n \times n \) matrix selected arbitrarily.

\( R \) is \( m \times m \) is a diagonal matrix with \( R_{kk} > 0.0 \)

\( S \) is \( m \times n \) matrix which satisfies equation (..15).
The optimal controller design which minimizes the performance index of equation (8.14) is given by equation (7.24) and is:

\[ \ddot{U}^* = -R^{-1} \dddot{C}^T \dddot{S} \dddot{X} \]  

(8.15)

where the kth column of \( \dddot{C}^* \) is given by:

\[ \dddot{C}_k^* = B_k \dddot{X} + \dddot{C}_k \text{ for } k = 1, m \]

where \( \dddot{C}_k \) means the kth column of \( \dddot{C} \) matrix and \( B_k \) is a matrix of \( n \times n \) corresponding to the kth input in the system equation. Matrix \( \dddot{S} \) satisfies the following Lyapunov equation:

\[ \dddot{A}^T \dddot{S} + \dddot{S} \dddot{A} = -Q \]

(8.16)

Superscript \( T \) in all the above equations corresponds to the transpose of the vector or matrix. The method suggested by Hoskin (1977) is used to solve equation (8.16) to get \( \dddot{S} \) matrix.

\( \dddot{U}^* \) obtained from equation (8.15) is in deviation form; therefore, the correct control signal which should be set is given as:

\[ \dddot{U} = \dddot{U}^* + \dddot{U}_s \]

(8.17)

The selection of \( Q \) and \( R \) depends upon the type of response desired. These matrices will be selected arbitrarily.
system has to move from one point to the other point (i.e., a servo problem) then Kwakernaak and Sivan (1972) suggest using $U_S$ which corresponds to the final state variable. This can be obtained from the compartmental steady state simulation developed in Chapter 4. The steady state compartmental simulation is not perfect, so $U_S$ for the servo move will not be the correct value and final $\Delta U$ will not be zero after servo change.

The control studies are divided into two parts. In the first part a single composition is controlled. The objective here is to control the acetone composition in the top product. In the second part dual composition problem is considered where both acetone in the top product and methanol in the bottoms product are controlled. The summary of the various control studies done in this chapter is given in Table 8.1.

In Table 8.1 $U_f$ means that $U_S$ for equation (8.17) corresponds to $U$ for the final states which was calculated from the steady state program. $U_{in}$ refers to the initial $U$ vector at the initial steady state conditions. $T_c$ is the control interval and 'inf' means that compositions were predicted in this case. $Q_{11}$ and $Q_{10,10}$ means $Q(1,1)$ and $Q(10,10)$ element of the $Q$ matrix. For a single composition control only $Q(1,1)$ is required therefore, a blank is placed under $Q(10,10)$. 
Table 6.1: Summary of Various Simulated Control Studies

<table>
<thead>
<tr>
<th>Case</th>
<th>Q11 (Q_{10,10})</th>
<th>R11 (R_{22})</th>
<th>Set point</th>
<th>Us</th>
<th>Tc</th>
<th>Fig #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.0</td>
<td>0.00001</td>
<td>0.9092 (U_f)</td>
<td>0.03</td>
<td>8.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>5.0</td>
<td>0.0001</td>
<td>0.9092 (U_f)</td>
<td>0.03</td>
<td>8.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0001</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>5.0</td>
<td>0.0001</td>
<td>0.9092 (U_{in})</td>
<td>0.03</td>
<td>8.4</td>
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</tr>
<tr>
<td>4</td>
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<td>0.00000</td>
<td>0.9092 (U_{in})</td>
<td>0.03</td>
<td>8.5</td>
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<tr>
<td>6</td>
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<td>0.928 (U_{in})</td>
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</tr>
<tr>
<td>7</td>
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<td>0.0001</td>
<td>0.928 (U_f)</td>
<td>0.03</td>
<td>8.8</td>
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<td></td>
<td></td>
<td>0.0001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>5.0</td>
<td>0.00003</td>
<td>0.928 (U_f)</td>
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<tr>
<td></td>
<td></td>
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<tr>
<td>9</td>
<td>1.0</td>
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<td>0.9092 (U_f)</td>
<td>0.03</td>
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<td></td>
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<td>11</td>
<td>100.</td>
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<td>0.9092 (U_f)</td>
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<td></td>
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<td>0.0001</td>
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</tr>
<tr>
<td>12</td>
<td>1.0</td>
<td>0.00001</td>
<td>0.9092 (U_{in})</td>
<td>0.03</td>
<td>8.13</td>
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<td></td>
<td></td>
<td>0.0001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>10.0</td>
<td>0.00001</td>
<td>0.9092 (U_{in})</td>
<td>0.03</td>
<td>8.14</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>100.0</td>
<td>0.00001</td>
<td>0.9092 (U_{in})</td>
<td>0.03</td>
<td>8.15</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.0001</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 8.1 (continued): Summary of Various Simulated Control Studies

<table>
<thead>
<tr>
<th>Case#</th>
<th>Q11 Q10,10</th>
<th>R11 R22</th>
<th>Set point</th>
<th>Uf</th>
<th>Tc</th>
<th>Fig #</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>5.0 0.0001</td>
<td>0.0001</td>
<td>0.9092</td>
<td>0.09</td>
<td>8.16</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>5.0 0.0001</td>
<td>0.0001</td>
<td>0.9092</td>
<td>0.12</td>
<td>8.17</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>5.0 0.0001</td>
<td>0.0001</td>
<td>0.9092</td>
<td>Uin</td>
<td>0.09</td>
<td>8.18</td>
</tr>
<tr>
<td>18</td>
<td>5.0 0.0001</td>
<td>0.0001</td>
<td>0.9092</td>
<td>Uin</td>
<td>0.09</td>
<td>8.19</td>
</tr>
<tr>
<td>19</td>
<td>5.0 0.0001</td>
<td>0.0001</td>
<td>0.9092</td>
<td>Uin</td>
<td>0.12</td>
<td>8.20</td>
</tr>
<tr>
<td>20</td>
<td>10.0 0.0003</td>
<td>0.1613</td>
<td>0.9213</td>
<td>Uf</td>
<td>0.12</td>
<td>8.21</td>
</tr>
<tr>
<td>21</td>
<td>10.0 0.0001</td>
<td>0.1613</td>
<td>0.9213</td>
<td>Uin</td>
<td>0.12</td>
<td>8.22</td>
</tr>
<tr>
<td>22</td>
<td>5.0 0.0002</td>
<td>0.1221</td>
<td>0.7971</td>
<td>Uf</td>
<td>0.12</td>
<td>8.23</td>
</tr>
<tr>
<td>23</td>
<td>10.0 0.0003</td>
<td>0.1613</td>
<td>0.9213</td>
<td>Uf</td>
<td>0.12</td>
<td>8.24</td>
</tr>
<tr>
<td>24</td>
<td>5.0 0.0002</td>
<td>0.1221</td>
<td>0.7971</td>
<td>Uf</td>
<td>0.12</td>
<td>8.25</td>
</tr>
</tbody>
</table>

8.3 SINGLE COMPOSITION CONTROL (SIMULATION STUDY):

In this section, only acetone in the top product is controlled. The initial operating conditions of the column are given in Table 8.2. The system equations for these
operating conditions are presented in Appendix D. For the simulation studies two different cases are considered. In one case \( U_s = U_f \), where \( U_f \) corresponds to the final value of the manipulated variable required to get the final states. This is obtained from the steady state simulation. In the second case \( U_s \) is kept at the initial steady state values of the manipulated variables and this is denoted by \( U_{in} \).

**CASE 1:**

In this simulation it was required to move the acetone composition from its initial value of 0.8938 to 0.9092 mole percent. From the steady state program it was found that this final state corresponds to the reflux flow rate of 190.0 ml/min. Since only the acetone composition is controlled, 5 state variables are required. The initial state vector is given in appendix D. The elements of the final state vector are obtained from the acetone composition profile corresponding to the final acetone composition required; i.e., 0.9092. This profile is obtained from the steady state simulation and is given below:

\[
X^T = [ \begin{array}{c} 0.9092, 0.7401, 0.2675, 0.1621, 0.0466 \end{array} ]
\]
Table 5.2: Initial Operating Conditions

Feed = 110.0 ml/min at 43°C
Solvent = 45.0 ml/min at 60°C
Feed Composition: Acetone = 0.6429
                   Methanol = 0.3312
                   Water = 0.0258
Reflux = 165.0 ml/min, Steam Pressure = 144.8 kPa (gauge)
Steam flow = 144.9 ml/min, Room Temperature = 24°C

Product Compositions (mole fraction):

<table>
<thead>
<tr>
<th></th>
<th>Top Product</th>
<th>Bottoms Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone</td>
<td>0.8938</td>
<td>0.033</td>
</tr>
<tr>
<td>Methanol</td>
<td>0.0713</td>
<td>0.1599</td>
</tr>
<tr>
<td>Water</td>
<td>0.0349</td>
<td>0.8069</td>
</tr>
</tbody>
</table>

Since only the acetone in the top product is the main variable, Q selected as:

\[
Q = \begin{bmatrix}
5.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
\end{bmatrix}
\]

The nature of the Q matrix is the same in all the subsequent runs. Therefore, it is written as Q_{11} = 5.0, which means that only the Q_{11} element of the Q matrix is nonzero, all
the other elements are zero. The $S$ matrix corresponding to $Q_{11} = 5.0$ is given in part 1 of Appendix D. The $R$ matrix used in this case is:

$$
R = \begin{bmatrix}
0.00001 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}
$$

The control action is taken after every $T_C = 0.03$ hrs. The results are shown in Figure 8.1. There is no offset in the acetone composition, but the reflux flow rate is not smooth. Due to the fact that the largest difference in the acetone composition occurs at the time the controller was implemented, a large initial control action (i.e., from 165.0 to 220.0 ml/min) is required. But as the composition moves closer to the setpoint, the reflux flow approaches 190.0 ml/min and fluctuates around this value. The slight fluctuations are due to the small value of $R_{11}$. The control law involves the term $R^{-1}$, which becomes very large, and so small changes in the acetone composition from setpoint produce appreciable control action. In this case, the magnitude of the fluctuations is approximately 2.0 ml/min.

The open loop test for the step in the reflux flow rate from 165 ml/min to 190.0 ml/min was also performed on the dynamic simulation. The response of the open loop test is shown in Figure 8.2. It can be seen that closed loop
configuration reaches the final state approximately 30 minutes earlier than the for open loop strategy.

**CASE 2:**

This simulation run is similar to Case 1, except that the $R$ matrix is changed to get a smooth reflux flow response. The following $R$ matrix is selected:

$$
R = 
\begin{bmatrix}
0.0001 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}
$$

$Q_{11} = 5.0$ is the same as in Case 1. The effect of changing the $R$ matrix can be seen in the responses shown in Figure 8.3. The controller behavior is smooth and the reflux flow rate finally settles down at 190.0 ml/min. The acetone in the top product shows no offset, however, it takes slightly longer to get to the setpoint. Thus, the $R$ matrix can be used to get smooth controller behavior and to change the time to get to the final state.

**CASE 3:**

The control problem is the same as of Case 2 but Us
\[ U_{\text{in}} \]. The \( R \) and \( Q \) matrices are the same as for Case 2. The simulated response is shown in Figure 8.4. There is an offset in the acetone composition. The controller behaviour is satisfactory but the final value of the reflux flow rate is 182.0 ml/min. Since the final \( \Delta U \approx 0.0 \), the Hamiltonian is not zero along the optimal trajectory. The final offset depends upon the \( R \) and \( Q \) matrices.

**CASE 4:**

The Case 3 problem is re-evaluated in order to reduce the final offset. In this case \( R_{11} \) is decreased, which means less penalty on the control action. The matrix used in this case is:

\[
R = \begin{bmatrix}
0.00001 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}
\]

The \( Q \) matrix remains unchanged. The response is shown in Figure 8.5. The magnitude of the offset is negligible and the reflux flow rate settles down around 190.0 ml/min. The controller performance is acceptable.

**CASE 5:**

In the above cases, the change in the reboiler steam
pressure was negligible. It may be due to the detuned value of $R_{22}$ or because the controller selects only the most important variable to manipulate in order to achieve the single composition control objective. In this case, the problem of Case 4 is repeated with the following $R$ matrix:

$$R = \begin{bmatrix} 0.00001 & 0.0 \\ 0.0 & 0.00001 \end{bmatrix}$$

The simulated response is shown in Figure 8.6. Initially the reboller steam pressure changes but finally comes back to its original value of 144.8 kPa (gauge). The effect of initial change in the steam pressure can also be seen in the reflux flow rate behavior. The minimum value of the reflux flow rate is 140.0 ml/min as compared to 148.0 ml/min in Case 4. This is due to the interaction effect. The multivariable nature of the controller takes these interaction effects into account. The final controller values are reflux flow rate, 190.0 ml/min, and steam pressure, 144.8 kPa (gauge). This should be the case since the final state vector corresponds to a change in the reflux flow rate and not to steam pressure. A robust controller should only select the most pertinent variables, and a bilinear optimal controller exhibits this characteristic.
CASE 6:

A different servo problem was simulated. In this case, the system was moved from acetone composition of 0.8938 to 0.9280. From the steady state program it was found that this value corresponds to a reflux value of 195 ml/min and steam pressure of 127.5 kPa(gauge). The following $R$ and $Q$ matrices were selected:

$$
R = \begin{bmatrix}
0.00001 & 0.0 \\
0.0 & 0.00001
\end{bmatrix}
$$

$Q_{11} = 5.0$

The $U_S$ was selected as $U_{in}$. The response is shown in Figure 8.7. There is very little offset in the acetone composition, however, the reflux flow reaches its maximum value and saturates. The final steam pressure is 141.3 kPa(gauge).

CASES 7 and 8

Figure 8.8 for Case 7, shows the response of the Case 6 problem but with the following $R$ matrix:

$$
R = \begin{bmatrix}
0.00001 & 0.0 \\
0.0 & 0.00001
\end{bmatrix}
$$
Q_{11} = 5.0

The controller was activated with \( U_s = U_f \). The performance is acceptable. There is no ringing in the manipulated variables. The final value of reflux flow rate is 195 ml/min and the steam pressure 127.5 kPa(gauge). The bottoms product was not controlled but it finally returns to its initial value.

In case 8, the elements of \( R \) matrix are decreased in order to decrease the response time. The following \( R \) matrix is used:

\[
R = \begin{bmatrix}
0.00003 & 0.0 \\
0.0 & 0.00003
\end{bmatrix}
\]

All the rest of the parameters are the same as in Case 7. The controller performance is given in Figure 8.9. The reflux flow rate shows a ringing behaviour and the top product and the bottoms product compositions also show fluctuations. The controller behaviour is unsatisfactory for this \( R \) matrix.

From these results, it is clear that if \( U_s = U_{in} \) the elements of the \( R \) matrix should be small so that the controller can take larger actions to track the setpoint. On the other hand if \( U_s = U_f \), and the elements of \( R \) matrix are lowered, then the response time may be shorter but the
performance may be unacceptable due to possible large fluctuations or ringing of the manipulated variable. In cases when $U_S = U_f$ there is no offset, whereas, when $U_S = U_{in}$ the offset depends on the controller gain.

In order to study the effect of the $Q$ matrix choice (penalty on the states), the Case 2 and Case 4 problems were re-solved for three different $Q$ matrices: (1) $Q_{11} = 1.0$, (2) $Q_{11} = 10.0$, (3) $Q_{11} = 100.0$. Case 2 corresponds to $U_S = U_f$ and in Case 4 $U_S = U_{in}$ and both were seen to produce acceptable results.

**CASES 9, 10, and 11:**

Figure 8.10, corresponding to Case 9, shows the simulated response of the system for the problem of Case 2, but with $Q_{11} = 1.0$. The time to reach the setpoint is larger than for Case 2. This is due to the initial small change in the reflux flow rate from 165.0 to 200.0 ml/min, as compared with 165.0 to 220.0 ml/min in Case 2. There is no offset in both cases. In Case 10, $Q_{11}$ is changed to 10.0. The performance is shown in Figure 8.11. There is no appreciable difference in the performance as compared to Case 2. It should be noted that each time the $Q$ matrix is changed, equation (7.15) has to be re-solved to get new parameters for the $S$ matrix. A heavy penalty on the states was made in Case 11. $Q_{11} = 100.0$ is selected for this case and the
response is given in Figure 8.12. Due to the heavy penalty, the reflux flow controller shows high fluctuations and does not settle to a final value. There is no apparent offset in the acetone in the top product. Since there is a higher penalty on the states, any small change in composition results in a larger control action, thus producing fluctuations in the reflux flow rate. If $Q_{11}$ is increased further it may result in ringing. The $R$ matrix in all three cases (Case 9, 10, and 11) was the same as for Case 2. Compared with the previous cases where ringing was observed when $R$ was decreased, here ringing is seen if the elements of $Q$ are increased. Thus, for the proper and smooth operation, it is necessary to select the proper combination of both the $Q$ and $R$ matrices.

**CASES 12, 13, and 14**

The problem of Case 4 is re-investigated in these cases. The $R$ matrix for all three cases is the same as in Case 4, and $U_s = U_{in}$. $Q_{11}$ is equal to 1.0 in Case 12. The response shown in Figure 8.13 shows appreciable offset. The initial rise in the system behavior is slower when compared to Case 4. The value of $Q_{11}$ is increased to 10.0 and 100.0 in Case 13 and 14, respectively. The responses are given in Figure 8.14 and 8.15. The final offset in the state is decreased, but at the expense of larger control actions.
Case 14 results in ringing control action.

From these results, it can be concluded that the controller performance depends on both the $Q$ and the $R$ matrices. Also, if $u_s = u_f$ then the system shows no offset whereas for $u_s = u_{in}$, the final steady state depends on the values of $Q$ and $R$ matrices.

The main objective of this study is to apply a bilinear optimal controller on the pilot plant distillation column. As stated earlier, the particular gas chromatograph installed on the column takes around 7 minutes to analyse the sample and to communicate to the VAX. Therefore, the fastest control action is only possible after 7 min, if compositions are to be used as the state variables. Hence, the controller performance was checked at the following two control intervals $T_c = 0.09$ and $T_c = 0.12$ hr. The control time of $T_c = 0.12$ hr corresponds to the actual situation, when the gas chromatograph data is available. Again Case 2 and Case 4 were re-solved with above control times.

CASES 15 and 16:

The Case 2 problem, where $u_s = u_f$, was investigated in these cases. The $Q$ and $R$ matrices were the same as in Case 2. Case 15 corresponds to $T_c = 0.09$ hr and its response is given in Figure 8.16. The system behavior is nearly the same as for Case 2. The controller behavior is acceptable and
there is no apparent offset. $T_C=0.12$ hr was used in Case 17 and the performance is shown in Figure 8.17. Again, there is no offset and the controller behaves satisfactorily.

**CASES 17, 18 and 19:**

In these cases, $U_s=U_{in}$ and the $Q$ and $R$ matrices were selected from the Case 4 problem. Case 17 is for $T_C=0.09$ and Figure 8.18 shows its response. Large fluctuations in the reflux controller were obtained. In Case 18 the controller was implemented with the following $R$ matrix:

$$R = \begin{bmatrix}
0.0001 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}$$

The response is shown in Figure 8.19. The controller shows no large fluctuations. However, a final offset from the setpoint exists in the system behavior, suggesting that the $R$ should be retuned. Case 19 corresponds to $T_C=0.12$ hr and the $R$ matrix of Case 18. There are no large fluctuations in the controller behavior, but the offset is larger than for the previous case. The response is shown in Figure 8.20.

From the above cases it can be concluded that the controller performance depends upon the $Q$ and $R$ matrices and the $T_C$ used. For the cases where $U_s=U_f$, the system shows
no offset and the $Q$ and $R$ matrices are less sensitive to the $T_C$ used. In contrast, if $U_s = U_{in}$ is used, the amount of offset depends upon $Q$, $R$ and $T_C$. The system is sensitive to the $Q$ and $R$ parameters as different $T_C$ values are used, and an optimum value of $Q$ and $R$ are needed for satisfactory performance. The sensitivity of the parameters in this case is because $\Delta U$ is not zero, and the final Hamiltonian is not zero. It does attain a constant value, however.

8.4 Dual Composition Control (Simulation Study):

In this section, both the acetone in the top product and the methanol in the bottoms product were controlled. Rewriting equation (8.7) for the acetone and the methanol:

$$ \dot{X}_a = A_a X_a + U_1 B_{1a} X_a + U_2 B_{2a} X_a + C_{1a} U \quad (8.24) $$

$$ \dot{X}_m = A_m X_m + U_1 B_{1m} X_m + U_2 B_{2m} X_m + C_{1m} U \quad (8.25) $$

where $X_a$ is the deviation state vector for acetone, $X_m$ is the deviation state vector for methanol. The subscript 'a' is for the acetone and 'm' is for the methanol. Combining equations (8.24) and (8.25) to get:
\[
\begin{align*}
\ddot{X}_a &= \begin{bmatrix}
X_a \\
-\dot{X}_m
\end{bmatrix} = \begin{bmatrix}
\dot{A}_a & 0 \\
0 & \dot{A}_m
\end{bmatrix} \begin{bmatrix}
\dot{X}_a \\
-\dot{X}_m
\end{bmatrix} + U_1 \begin{bmatrix}
B_{1a} & 0 \\
0 & B_{1m}
\end{bmatrix} \begin{bmatrix}
\dot{X}_a \\
-\dot{X}_m
\end{bmatrix} \\
&\quad + U_2 \begin{bmatrix}
0 & B_{2a} \\
0 & B_{2m}
\end{bmatrix} \begin{bmatrix}
\dot{X}_a \\
-\dot{X}_m
\end{bmatrix} + \begin{bmatrix}
C_A \\
C_m
\end{bmatrix} U
\end{align*}
\]

Matrices \(A_m, B_{1m}, B_{2m}\) and \(C_m\) for the methanol composition vector are evaluated in the same way as for the acetone composition explained earlier. The complete order of the system is \(10 \times 10\) for the 5 compartmental model. The Liapunov equation should be solved for the complete \(A\) matrix (whose dimensions are \(10 \times 10\)), and so \(Q\) and \(S\) should both be \(10 \times 10\). Since only acetone in the top product and methanol in the bottoms product are being controlled, only these two states are penalized. Thus, all the elements of \(Q\) matrix are zero except \(Q_{11}\) and \(Q_{10,10}\); these correspond to the acetone in the top product and the methanol in the bottoms product.

The initial operating conditions are the same as those given in Table 8.1. The system equations are given in Part 2 of Appendix D. The steady state program was used to calculate the final values of the manipulated variables for the servo problem and the composition profile obtained was given as the final specified states. Different \(Q\) and \(R\) matrices were tried, but only those which gave acceptable performance are reported.
CASE 201

In this case the desired acetone composition in the top product and methanol composition in the bottoms product are 0.9213 and 0.1613. Their initial values were 0.8938 and 0.1599, respectively. The magnitude of the reflux flow rate and the steam pressure, as obtained from the steady state simulation, are 190.0 ml/min and 131.0 kPa(gauge). The control time is $T_C = 0.12$ hrs. The following $Q$ and $R$ matrices were used:

$$Q_{11} = 10.0, \quad Q_{10,10} = 10.0$$

All the rest of the elements of the $Q$ matrix are zero.

$$R = \begin{bmatrix} 0.0003 & 0.0 \\ 0.0 & 0.0001 \end{bmatrix}$$

The response is shown in Figure 8.21. The $U_f$ is used as the $U_g$ vector. Both compositions reach their respective setpoints and the control actions are acceptable. Both manipulated variables settle down at their final values. The bottoms product methanol composition response is slower than the top product response. To increase the response of the
bottoms product the controller was also implemented with \[ R_{11} = 0.0003 \] and \[ R_{22} = 0.00001 \]. The response showed ringing in both control actions. The ringing is the result of interactions present in the system. The controller tries to cancel the interactions by taking large control actions, and these result in ringing. The controller also gave large fluctuations when \( Q_{11} \) was changed to 100.0 from 10.0 while keeping \( Q_{10,10} = 10.0 \). However, when \( Q_{10,10} \) was changed to 100.0 and \( Q_{11} = 10.0 \), the controller performance was acceptable. However, the maximum deviation in the methanol composition form the desired setpoint was larger than for the case where \( Q_{11} \) and \( Q_{10,10} \) were equal to 10.0.

**CASE 21:**

The problem in this case is the same as in Case 20 except that \( U_S \) is taken as \( U_{in} \). The initial \( Q \) and \( R \) matrices were:

\[ Q_{11} = 10.0, \quad Q_{10,10} = 10.0 \]

\[
R = \begin{bmatrix}
0.0003 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}
\]

It was observed that the simulated response showed offset in both compositions. Therefore the control problem was re-
evaluated with the following $Q$ and $R$ matrices:

$$Q = \begin{bmatrix} 10.0 & 0.0 \\ 0.0 & 10.0 \end{bmatrix}$$

$$R = \begin{bmatrix} 0.0001 & 0.0 \\ 0.0 & 0.000001 \end{bmatrix}$$

The response for this study is shown in Figure 8.22. From the response it is seen that the system still shows a slight offset for the acetone in the top product. This result is similar to a single composition control case, where the $R$ matrix needed to be tuned. Also, the final values of the reflux flow rate and the steam pressure are approximately 205 ml/min and 141.4 kPa(gauge) which are different from the values attained in Case 19. This shows that the $U_S = U_f$ system is more robust than $U_S = U_{in}$ for the dual composition control problem.

CASE 22:

In this case the acetone composition in the top product and the methanol composition in the bottoms product were changed from their initial values of 0.8938 and 0.1599 to 0.7971 and 0.1221, respectively. From the steady state simulation the final state corresponds to a reflux flow rate of 130.0 ml/min and a steam pressure of 158.6
kPa(gauge). The following Q and R matrices were used:

\[
Q_{11} = 5.0, \quad Q_{10,10} = 5.0
\]

\[
R = \begin{bmatrix}
0.0002 & 0.0 \\
0.0 & 0.00005
\end{bmatrix}
\]

The response is shown in Figure 8.23. The performance of the controller is acceptable as there is no offset and no ringing in the control action.

In both cases discussed above, the controller performance is acceptable for dual composition control. It was found that dual composition control with \( U_S = U_f \) gives more robust results than \( U_S = U_{in} \). As was the case for a single composition control with \( U_S = U_{in} \), the final offset depends upon the \( R \) matrix.

### 8.5 Prediction of Composition Using Temperatures:

In the above analysis it was assumed that all compositions are available at each control interval. For dual composition control a total of 10 states are required at each control interval for the controller to calculate the optimum control action. As explained in Chapter 2, the online gas chromatograph used to analyse the product quality
can only calculate the composition of one stream at a time. This means that analysis of either top or bottoms product is available each control interval. Furthermore, compositions of the streams leaving the three compartments, i.e., compartments 2, 3 and 4 (refer to Chapter 4 for the compartment configuration), are not measured. Since temperature measurements are available at each tray, these are used to predict those states which are not available through composition measurement.

For the application of the bilinear optimal controller described in the previous section, one needs to know the liquid composition leaving each compartment. For the dual composition control with a 5 compartment model a total of 10 composition values (five for the acetone and five for the methanol) are required at each control interval. Only composition analysis of one stream either top or bottom is available through the gas chromatograph analyses. The other eight compositions must be predicted using temperature measurements. The linear predictor theory of Joseph and Brosilow (1978) was used. In brief the theory is given below.

The unmeasured composition vector $\mathbf{y}$ and the temperature measurement vector $\mathbf{g}$ can be related to the input disturbance $\mathbf{u}$ as follow:
\[ \theta = \mathbf{a}^T \mathbf{u} \] (8.27)
\[ \chi = \mathbf{b}^T \mathbf{u} \] (8.28)

The variables in equations (8.27) and (8.28) are deviation variables. Using least squares estimation theory, the estimate \( \hat{\chi} \) of the composition leaving the compartments are obtained as a linear combination of the temperature measurements. The equation relating \( \hat{\chi} \) and \( \theta \) is:
\[ \hat{\chi} = \Omega^T \theta \] (8.29)

where \( \Omega^T \) is the steady state estimator which is given as:
\[ \Omega^T = (\mathbf{a}^T \mathbf{a})^{-1} \mathbf{a} \mathbf{b} \] (8.30)

The accuracy of the estimation is measured by the projection error \( P_0 \) and the condition number \( Z \) of the matrix \( (\mathbf{a}^T \mathbf{a}) \) which measures the sensitivity. The projection error is defined as:
\[ P_0 = (|| \mathbf{r} || / || \mathbf{b} ||) \times 100.0 \] (8.31)

where \( \mathbf{r} = \text{Residual vector} \mathbf{b} - \mathbf{a} \Omega \)
\[ || . || = \text{norm of the vector} \]

The condition number is defined as:
\[ Z = (\pi_{\text{max}} / \pi_{\text{min}}) \] (8.32)
where $\pi_{\max}$ and $\pi_{\min}$ are the maximum and the minimum singular values of the matrix $\mathbf{a}$.

Temperatures can be measured at various stages of the distillation column. From this set of temperatures, an adequate number of temperatures must be selected such that the matrix $\mathbf{a}$ has a low projection error and a low condition number. In general, more than one temperature measurement is required for inferential composition prediction in a multicomponent system; see Yu and Luyben (1981). Joseph and Brosilow (1976) suggest that the conditions for an acceptable measurement set are that the projection error $P_0 \leq 5.0$ and condition number $Z \leq 100.0$. Shah and Luyben (1979) proposed using static nonlinear rigorous estimators for a binary system based on the tray to tray equations. However, the computation time required for these estimators is large and the method is not considered practicable for nonideal, multicomponent systems.

In the above analysis, a dynamic compensator is added to include the dynamics of the system. For this analysis, the temperature and composition responses to step inputs are approximated as first order systems. From these approximated transfer functions, a lead-lag type of model is used for the dynamic compensator. With the dynamic compensation equation (8.29) becomes:
\[ \hat{\mathbf{Y}}(s) = \Omega^T(s) \Phi(s) \]  

where

\[ \Omega(s) = \Omega(0) \frac{T_2 s + 1}{T_1 s + 1} e^{-T_s} \]  

\[ T_d = T_{d1} - T_{d2} \]  

\[ T_2, T_{d2} = \text{Average time constant and time delay, respectively, for the temperature transfer for all steps.} \]

\[ T_1, T_{d1} = \text{Average time constant and time delay, respectively, for the composition transfer function for all steps.} \]

\[ \Omega(0) = \text{Steady state Estimator given by equation (8.30)} \]

\[ s = \text{Laplace variable} \]

The composition transfer function \( b(s) \) and temperature transfer function \( a(s) \) can be calculated using the dynamic simulation for the various steps. For the case under study, \( b(s) \) and \( a(s) \) were determined for steps in the reflux rate and the reboiler steam pressure.

Substituting equation (8.34) into (8.33) the following expression is obtained:

\[ \hat{\mathbf{Y}}(s) = K g e^{-T_s} \frac{(T_2 s + 1)}{(T_1 s + 1)} \Phi(s) \]  

\[ (8.35) \]
\[ \dot{Y}(t) = \sum_{0}^{\infty} K_g \left( \frac{T_2}{T_1} - \frac{1}{T_1} \right) e^{-(t-T_d)/T_1} \left( \frac{T_2}{T_1} - 1 \right) \Theta(t) \cdot t \]

In equation (8.36) \( \dot{Y}(t) \) and \( \Theta(t) \) are deviation variables in composition and temperature, respectively. These deviation variables are calculated from the steady state values. The variable, \( t \), is the time elapsed from the steady state time.

The parameters for the first order transfer functions were calculated using a dynamic simulation. Eleven different steps in the reflux and the reboiler steam pressure were given and a nonlinear regression program was used to estimate the time constants, gains, and the delay times. The transfer functions for the acetone and the methanol compositions leaving each compartment and temperatures leaving each tray were obtained. Simple first order transfer functions were fitted although it was found that in some cases use of a second order transfer function resulted in a lower residual variance. Use of the second order temperature dynamics with the first order composition dynamics would result in an unrealizable transfer function.
It was also observed that the temperature dynamics for the top three trays could not be expressed as a simple first order transfer function. This is due to the nonlinearity of the column near the top where the acetone composition was high. Therefore, for the inferential calculations these trays were excluded. The composition transfer function, the temperature transfer function and the type of input steps used in obtaining the transfer function are given in Tables 8.3 to 8.7.

The data were split into two sets. One set correspond to temperature down dynamics (Table 8.5) and the other set for the temperature up (Table 8.6) dynamics. In Table 8.7, input types from 1 to 6 produce temperature down dynamic and input types 7 to 11 resulted in temperature up dynamics. It was observed that there was a considerable difference in the time constants for up and down dynamics. Therefore, the analysis was broken into two parts. The projection error and condition number criterion were used to select the temperature points for the inferential calculation.

Tables 8.8a and 8.8b list the projection error and condition number for the various temperature measurements selected for each compartment. Table 8.8a is for the acetone analysis and Table 8.8b is for the methanol. The last row in these tables shows the temperature points selected for each compartment. Keeping in mind the constraint on the
projection error < 5.0 and condition number < 100.0, an attempt was made to select the same measurement points for the up and down dynamics. The same combination was obtained in only some cases.

The gain estimators in each case were calculated using equation (8.30). The dynamic compensation was added using the average time constant and average time delay as described earlier. The results are shown in Table 8.9a for the acetone and in Table 8.9b for the methanol composition. For the methanol composition leaving compartments 3 and 4, the average temperature time delays were greater than average composition delay. This would require forecasting. To avoid this, all delay terms \(-T_d\) s which were positive were forced to be zero. This introduced some model mismatch for the controller. The transfer function in Tables 8.9a and 8.9b were converted into the time domain using equation (8.35) to allow the calculation of composition data to be used with the bilinear optimal controller.

**CASE 23:**

A simulation of a bilinear optimal controller designed for dual composition control using predicted compositions was performed so that Case 20 was re-evaluated. The \(Q\) and \(R\) matrices were the same as in Case 20 with \(U_s = U_f\) and \(T_c = 0.12\) hr. It was assumed that at each control interval,
either the top product or the bottoms product analysis was available. Other state elements were predicted using the method discussed above. The above assumptions were made so that the simulation would conform to the application of the controller on the pilot plant where one gas chromatograph is used to alternatively analyse the top product and bottoms product streams. In inferring the compositions from temperatures, only gain terms were used. Comparison with a complete inferentiatior is also discussed later. The controller was implemented with the following Q and R matrices:

\[
Q_{11}=10.0 \quad Q_{10,10}=10.0
\]

\[
R = \begin{bmatrix}
0.0003 & 0.0 \\
0.0 & 0.0001
\end{bmatrix}
\]

The responses are given in Figure 8.24. There is no offset in the acetone or methanol composition. The final small oscillations in the reflux flow rate are due to the errors in composition predictions. The magnitude of the oscillations is of the order of 2.0 ml/min. The accuracy of the prediction depends upon the region of application and it should be kept in mind that a linear predictor was used for this nonlinear process. In the above calculations, the inferential points used for the prediction of acetone
composition leaving the second compartment were temperatures of the 6th, and 13th trays, this corresponds to the temperature down dynamics. The inferential points corresponding to temperatures on the 4th, and 19th trays could have also be used as the condition number for this set is 3.5. When this set was used, however, it was found that the response was not very different from Figure 8.24, but that the final fluctuations in the reflux flow rate were of the order of 3 ml/min. The increase in the magnitude of the fluctuations was due to a larger error in predicting the composition. This also suggests that for better performance for this column, optimum inferential points corresponding to the particular type of dynamics (i.e., temperature up or temperature down) should be used.

Another simulation was performed using a predictor with a dynamic compensator and gain terms. It was observed that including the dynamic compensator did not alter the control behavior significantly, but a slight offset was observed in the top product acetone composition. This may be due to the delay terms which were approximated to avoid forecasting. Therefore, it was decided to use only gain terms for inferring the composition using tray temperatures. The use of the only gain terms also requires less computational time than a complete dynamic predictor.
CASE 24:

In Case 23 the changes in the compositions were small. The problem defined in Case 22 required composition changes for acetone of 12% and for methanol composition a change of 23%. This was resolved in Case 24 using inferential points. The \( Q \) and \( R \) matrices were the same as for Case 22 with \( T_c=0.12 \) hr and \( U_s=U_f \). There were large fluctuations due to large errors in predicting the top and bottoms product compositions whenever these were not measured. This was due to the fixed parameter linear predictor. As the system moves over a wide operating range, the gain terms change. To overcome this limitation, the recursive least squares (RLS) method (Taylor, 1984) was used to update the gains for the top and bottoms product analysis. The gains are updated whenever the composition analysis is available and these gains are used to predict the compositions at the next control interval (i.e., when that composition analysis is not available). Thus, parameters are updated at every alternate control interval. The controller was implemented using this method of inferring the composition with the same \( Q \) and \( R \) matrices; the results are shown in Figure 8.25. The controller performance is acceptable and the final offset is quite small. Comparing this result with Case 22, it is observed that there is a slight fluctuations in reflux flow rate.
Thus, it can be concluded that for this nonlinear system, gain terms should be updated continuously to cover the wider operating zone.

In the next chapter, the validity of the predictor with and without the RLS algorithm will be tested against experimental data.

8.6 REMARKS ON THE BILINEAR CONTROLLER DESIGN:

The bilinear optimal controller designed here is a fixed parameter controller. In the real situation the controller parameters (i.e., \( A, B_1, B_2, \) and \( C \) matrices) should change as the operating point changes since this is a nonlinear system. Even if the system parameters are not changed at every control interval, they should be changed after few control intervals if the system is moving from one operating point to a significantly different operating point. This, however, will make the system matrices time variant and the complete control problem will change. The mathematics of even the linear time varying optimal controller are quite complicated, and those for the time varying bilinear case are not well understood at this time. Therefore, a fixed parameter controller was used.

The controller was designed for unconstrained manipulated variables, but it can be seen from the simulations that the maximum and minimum values of the
manipulated variables were used to clamp the inputs to the column. These limits are the same as those discussed in Chapter 6. This contradiction between the design and implementation did not cause problems in the application of the controller.

The performance of the controller depends upon the performance index used to obtain the controller design. If the performance index is different than the one presented in Chapter 7, the controller will behave differently.

8.7 CONCLUSIONS:

A bilinear optimal controller designed in Chapter 7 was simulated to study the system performance for single and dual composition control. The performance depends upon the \( Q \) and \( R \) matrices, and for satisfactory performance the optimum \( Q \) and \( R \) matrix should be selected. It was found that for the conditions when \( U_s = U_f \) the controller gives no offset and it is more robust than when \( U_s = U_{in} \). For \( U_s = U_{in} \), the offset in the final state depends upon the values of the \( Q \) and \( R \) matrices and an optimum value of these is required for satisfactory performance. For different values of \( T_c \) (i.e., control action) the system behavior is more sensitive for \( U_s = U_{in} \) than for \( U_s = U_f \). For \( U_s = U_f \), the system showed no offset. Therefore, it is recommended that \( U_s = U_f \) be used. To apply the designed controller on the pilot plant the
prediction of a few states is required. These states were predicted by a linear predictor using tray temperatures. The gain parameters and the dynamic compensator terms were calculated using a complete dynamic simulator. Different tray numbers were recommended depending upon the column dynamics. The controller with inferred composition performs well for the case where the required changes in states were not large. However, for a larger operating range the gain parameters needed to be updated for the top and bottoms product predictor alternatively using a recursive least square method. It was found that the addition of a dynamic compensator did not alter the performance significantly. Therefore, the predictor was implemented with gain terms only. The design procedure using the predictor will be applied to an experimental equipment for dual composition control in the next chapter.
NOMENCLATURE

\[ A = n \times n \text{ System Matrix for the bilinear state equation (8.1)} \]
\[ \Delta = \text{A matrix for deviation variables defined in equation (8.8)} \]
\[ \Delta a = \text{A matrix for acetone} \]
\[ \Delta m = \text{A matrix for methanol} \]
\[ a = \text{Matrix used in equation (8.26) to relate temperatures and inputs} \]
\[ b = \text{Matrix used in equation (8.27) to relate composition and inputs} \]
\[ B_1 = \text{Matrix of dimension } n \times n \text{ for the state equation (8.1) for first manipulated variable} \]
\[ B_{1a} = \text{B}_1 \text{ matrix for acetone} \]
\[ B_{1m} = \text{B}_1 \text{ matrix for methanol} \]
\[ B_2 = \text{Matrix of dimension } n \times n \text{ for the state equation for the second manipulated variable} \]
\[ B_{2a} = \text{B}_2 \text{ matrix for acetone} \]
\[ B_{2m} = \text{B}_2 \text{ matrix for methanol} \]
\[ C = \text{Matrix of dimension } n \times m \text{ for the state equation (8.7) and defined by equation (8.9)} \]
\[ C^* = \text{Matrix of dimension } n \times m \text{ whose } i^{\text{th}} \text{ column is equal to } B_i \times X + C_i \]
\[ C_a = C \text{ for acetone} \]
\[ x_m = \text{C for methanol} \]

\[ D = \text{Disturbance vector of 1 x n} \]

\[ F_1 = \text{Solvent flow rate} \]

\[ F_2 = \text{Feed Flow rate} \]

\[ J = \text{performance function given by equation (8.14)} \]

\[ K_g = \text{Gain vector for equation (8.35)} \]

\[ K_{ji} = \text{Compartmental Kk-value for the jth compartment and ith component} \]

\[ M_j = \text{Molar holdup for the jth compartment} \]

\[ m = \text{Number of manipulated variables} \]

\[ n = \text{Number of state variables} \]

\[ P_0 = \text{Projection error} \]

\[ Q = \text{State penalty matrix of dimension n x n} \]

\[ r = \text{Residual vector b - a C} \]

\[ R = \text{Penalty Matrix for the manipulated variables m x m} \]

\[ S = \text{Matrix of dimension n X n satisfying equation (8.16)} \]

\[ s = \text{Laplace variable} \]

\[ s = \text{Represents steady state if used as subscript} \]

\[ T_c = \text{Control time hrs} \]

\[ t = \text{Time variable} \]

\[ T_1 = \text{Time constant for composition transfer function in equation (8.34)} \]

\[ T_2 = \text{Time constant for temperature transfer} \]
function in equation (8.34)

\[ T_d = \text{Average Time delay} \]

\[ T_{d2} = \text{Average time delay for temperature dynamics} \]

\[ T_{d1} = \text{Average time delay for composition dynamics} \]

\[ U = \text{Vector of manipulated variables of dimension m x 1} \]

\[ u = \text{Input disturbance vector of equation (8.27)} \]

\[ U_1 = \text{1st Manipulated variable, i.e., Reflux flow rate} \]

\[ U_1 = \text{1st manipulated variable in deviation form} \]

\[ U_{1s} = \text{Steady state value of the 1st manipulated variable} \]

\[ U_2 = \text{2nd Manipulated variable i.e., Steam pressure} \]

\[ U_2 = \text{2nd manipulated variable in deviation form} \]

\[ U_{2s} = \text{Steady State value of the 2nd manipulated variable} \]

\[ \bar{U} = \text{Vector of Manipulated variables in deviation form of m x 1} \]

\[ \bar{U}^* = \text{Optimal manipulated variables vector in deviation form defined by equation (8.15)} \]

\[ \bar{U}_f = \bar{U} \text{ vector corresponding to the final state} \]

\[ \bar{U}_{in} = \bar{U} \text{ vector corresponding to the initial state} \]

\[ \bar{U}_s = \text{Steady state value of the } \bar{U} \text{ vector} \]

\[ X_{jis} = \text{Liquid composition of component i leaving jth compartment at the steady state} \]

\[ X = \text{State Vector of dimension n x 1} \]

\[ \bar{X} = \text{State vector in the deviation form} \]
\[ \dot{X}_a = \text{Deviation state vector for acetone} \]
\[ \dot{X}_m = \text{Deviation State vector for methanol} \]
\[ X_S = \text{Steady state value of the state vector} \]
\[ Y = \text{Composition vector for inferential calculations equation (8.28)} \]
\[ \hat{Y} = \text{Estimated value of the } Y \text{ vector} \]
\[ Z = \text{Condition number of the } (a^T a) \text{ matrix} \]

**GREEK SYMBOLS:**

\[ \alpha = \text{Constants for equation (5.12)} \]
\[ \beta = \text{Constants for equations (5.13)} \]
\[ \gamma = \text{Constant for equation (5.13)} \]
\[ \Theta = \text{Vector of Temperature values at trays} \]
\[ \Omega = \text{Vector defined by equation (8.30)} \]
\[ \pi_{\text{max}} = \text{Maximum singular value of the } a \text{ matrix} \]
\[ \pi_{\text{min}} = \text{Minimum Singular value of the } a \text{ matrix} \]

**SUBSCRIPTS:**

\[ a = \text{Acetone} \]
\[ f = \text{Corresponding to final states} \]
\[ \text{in} = \text{Corresponding to initial states} \]
\[ j = \text{Compartment number} \]
\[ k = \text{kth column of the matrix} \]
\[ m = \text{when used as subscript is for methanol} \]
\[ s = \text{when used as subscript is steady state} \]
<table>
<thead>
<tr>
<th>INPUT TYPE</th>
<th>TOP PRODUCT</th>
<th>COMPT # 2</th>
<th>COMPT # 3</th>
<th>COMPT # 4</th>
<th>BOTTOM PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01200 exp (-0.41 s)</td>
<td>0.03010 exp (-0.12 s)</td>
<td>0.02590 exp (-0.47 s)</td>
<td>0.02920 exp (-0.35 s)</td>
<td>0.00975 exp (-0.28 s)</td>
<td></td>
</tr>
<tr>
<td>(0.3730 s + 1.0)</td>
<td>(0.1455 s + 1.0)</td>
<td>(0.2034 s + 1.0)</td>
<td>(0.3395 s + 1.0)</td>
<td>(0.4350 s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>0.02300 exp (-0.40 s)</td>
<td>0.05790 exp (-0.12 s)</td>
<td>0.05940 exp (-0.25 s)</td>
<td>0.06940 exp (-0.32 s)</td>
<td>0.02523 exp (-0.36 s)</td>
<td></td>
</tr>
<tr>
<td>(0.3360 s + 1.0)</td>
<td>(0.1153 s + 1.0)</td>
<td>(0.1583 s + 1.0)</td>
<td>(0.3178 s + 1.0)</td>
<td>(0.3920 s + 1.0)</td>
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</tr>
<tr>
<td>0.03700 exp (-0.38 s)</td>
<td>0.02970 exp (-0.12 s)</td>
<td>0.02100 exp (-0.21 s)</td>
<td>0.06910 exp (-0.11 s)</td>
<td>0.02807 exp (-0.12 s)</td>
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</tr>
<tr>
<td>(0.3380 s + 1.0)</td>
<td>(0.0750 s + 1.0)</td>
<td>(0.1490 s + 1.0)</td>
<td>(0.3558 s + 1.0)</td>
<td>(0.3637 s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>0.00900 exp (-0.38 s)</td>
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<td>0.01130 exp (-0.23 s)</td>
<td>0.03460 exp (-0.10 s)</td>
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<tr>
<td>(0.3615 s + 1.0)</td>
<td>(0.0860 s + 1.0)</td>
<td>(0.1712 s + 1.0)</td>
<td>(0.3633 s + 1.0)</td>
<td>(0.3506 s + 1.0)</td>
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<tr>
<td>0.01870 exp (-0.30 s)</td>
<td>0.04390 exp (-0.11 s)</td>
<td>0.04010 exp (-0.24 s)</td>
<td>0.05740 exp (-0.10 s)</td>
<td>0.02100 exp (-0.13 s)</td>
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<td>(0.1217 s + 1.0)</td>
<td>(0.1773 s + 1.0)</td>
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<td>(0.5217 s + 1.0)</td>
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</tr>
<tr>
<td>0.01630 exp (-0.38 s)</td>
<td>0.03440 exp (-0.12 s)</td>
<td>0.02830 exp (-0.23 s)</td>
<td>0.05490 exp (-0.10 s)</td>
<td>0.02063 exp (-0.14 s)</td>
<td></td>
</tr>
<tr>
<td>(0.3660 s + 1.0)</td>
<td>(0.1108 s + 1.0)</td>
<td>(0.1792 s + 1.0)</td>
<td>(0.4263 s + 1.0)</td>
<td>(0.4320 s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>-0.05210 exp (-0.35 s)</td>
<td>-0.15260 exp (-0.12 s)</td>
<td>-0.05770 exp (-0.23 s)</td>
<td>-0.05080 exp (-0.21 s)</td>
<td>-0.01570 exp (-0.20 s)</td>
<td></td>
</tr>
<tr>
<td>(0.5290 s + 1.0)</td>
<td>(0.3148 s + 1.0)</td>
<td>(0.3440 s + 1.0)</td>
<td>(0.4890 s + 1.0)</td>
<td>(0.6080 s + 1.0)</td>
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<td>-0.02640 exp (-0.23 s)</td>
<td>-0.02420 exp (-0.24 s)</td>
<td>-0.00800 exp (-0.18 s)</td>
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<td>(0.4675 s + 1.0)</td>
<td>(0.2306 s + 1.0)</td>
<td>(0.2900 s + 1.0)</td>
<td>(0.4137 s + 1.0)</td>
<td>(0.6041 s + 1.0)</td>
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</tr>
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<td>0.01280 exp (-0.27 s)</td>
<td>-0.02060 exp (-0.12 s)</td>
<td>-0.01490 exp (-0.24 s)</td>
<td>-0.03620 exp (-0.14 s)</td>
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<td></td>
</tr>
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<td>(0.6233 s + 1.0)</td>
<td>(0.1970 s + 1.0)</td>
<td>(0.3222 s + 1.0)</td>
<td>(0.3623 s + 1.0)</td>
<td>(0.3282 s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>-0.03270 exp (-0.22 s)</td>
<td>-0.05200 exp (-0.09 s)</td>
<td>-0.03440 exp (-0.20 s)</td>
<td>-0.06800 exp (-0.16 s)</td>
<td>-0.01822 exp (-0.19 s)</td>
<td></td>
</tr>
<tr>
<td>(0.6093 s + 1.0)</td>
<td>(0.3910 s + 1.0)</td>
<td>(0.3868 s + 1.0)</td>
<td>(0.3544 s + 1.0)</td>
<td>(0.3264 s + 1.0)</td>
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<td>-0.02720 exp (-0.30 s)</td>
<td>-0.05640 exp (-0.11 s)</td>
<td>-0.03320 exp (-0.24 s)</td>
<td>-0.04700 exp (-0.14 s)</td>
<td>-0.01472 exp (-0.19 s)</td>
<td></td>
</tr>
<tr>
<td>(0.5682 s + 1.0)</td>
<td>(0.2720 s + 1.0)</td>
<td>(0.3228 s + 1.0)</td>
<td>(0.4400 s + 1.0)</td>
<td>(0.4200 s + 1.0)</td>
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</tr>
</tbody>
</table>
### Table 8.4: Methanol Composition Transfer Functions

<table>
<thead>
<tr>
<th>INPUT TYPE</th>
<th>TOP PRODUCT</th>
<th>COMPT # 2</th>
<th>COMPT # 3</th>
<th>COMPT # 4</th>
<th>BOTTOM PRODUCT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.01120 exp (-0.60 s)</td>
<td>-0.01150 exp (-0.22 s)</td>
<td>-0.00300 exp (0.00 s)</td>
<td>-0.00860 exp (-0.08 s)</td>
<td>0.00820 exp (-0.12 s)</td>
</tr>
</tbody>
</table>
<pre><code>| (0.3170 s + 1.0) | (0.3145 s + 1.0) | (0.6330 s + 1.0) | (0.7709 s + 1.0) | (0.4588 s + 1.0) |
</code></pre>
<p>| 2          | -0.02070 exp (-0.60 s) | -0.02174 exp (-0.20 s) | -0.01100 exp (-0.03 s) | -0.02430 exp (-0.09 s) | -0.00480 exp (-0.11 s) |
| (0.2817 s + 1.0) | (0.2880 s + 1.0) | (0.5460 s + 1.0) | (0.7634 s + 1.0) | (0.2500 s + 1.0) |
| 3          | -0.01765 exp (-0.50 s) | -0.01725 exp (-0.15 s) | -0.01740 exp (-0.06 s) | -0.03350 exp (-0.11 s) | 0.00540 exp (-0.14 s) |
| (0.3070 s + 1.0) | (0.2931 s + 1.0) | (0.3069 s + 1.0) | (0.4933 s + 1.0) | (0.2850 s + 1.0) |
| 4          | -0.00950 exp (-0.50 s) | -0.00900 exp (-0.15 s) | -0.00960 exp (-0.08 s) | -0.01620 exp (-0.12 s) | 0.00350 exp (-0.15 s) |
| (0.3480 s + 1.0) | (0.3150 s + 1.0) | (0.3805 s + 1.0) | (0.5270 s + 1.0) | (0.5330 s + 1.0) |
| 5          | -0.01760 exp (-0.57 s) | -0.01820 exp (-0.18 s) | -0.01000 exp (-0.03 s) | -0.02120 exp (-0.13 s) | 0.00460 exp (-0.14 s) |
| (0.3020 s + 1.0) | (0.3092 s + 1.0) | (0.4908 s + 1.0) | (0.6685 s + 1.0) | (0.1548 s + 1.0) |
| 6          | -0.01600 exp (-0.54 s) | -0.01650 exp (-0.17 s) | -0.01190 exp (-0.04 s) | -0.02300 exp (-0.12 s) | 0.00450 exp (-0.16 s) |
| (0.3300 s + 1.0) | (0.3097 s + 1.0) | (0.4007 s + 1.0) | (0.5742 s + 1.0) | (0.0558 s + 1.0) |
| 7          | 0.04990 exp (-0.49 s) | 0.05780 exp (-0.23 s) | -0.00650 exp (-0.02 s) | 0.00590 exp (-0.15 s) | -0.01590 exp (-0.17 s) |
| (0.5205 s + 1.0) | (0.4815 s + 1.0) | (0.2338 s + 1.0) | (0.0518 s + 1.0) | (1.4200 s + 1.0) |
| 8          | 0.01690 exp (-0.55 s) | 0.01871 exp (-0.23 s) | 0.00450 exp (0.00 s) | 0.00390 exp (-0.15 s) | -0.00550 exp (-0.15 s) |
| (0.4240 s + 1.0) | (0.4028 s + 1.0) | (0.2338 s + 1.0) | (0.0518 s + 1.0) | (0.8854 s + 1.0) |
| 9          | 0.01370 exp (-0.41 s) | 0.01432 exp (-0.10 s) | 0.01340 exp (-0.03 s) | 0.01350 exp (-0.11 s) | -0.00520 exp (-0.12 s) |
| (0.5890 s + 1.0) | (0.5502 s + 1.0) | (0.5850 s + 1.0) | (0.5729 s + 1.0) | (0.1148 s + 1.0) |
| 10         | 0.03520 exp (-0.35 s) | 0.03821 exp (-0.10 s) | 0.03800 exp (-0.04 s) | 0.02000 exp (-0.10 s) | -0.01175 exp (-0.11 s) |
| (0.7910 s + 1.0) | (0.7365 s + 1.0) | (0.6318 s + 1.0) | (0.5979 s + 1.0) | (0.1996 s + 1.0) |
| 11         | 0.02800 exp (-0.44 s) | 0.03097 exp (-0.15 s) | 0.01650 exp (-0.10 s) | 0.01270 exp (-0.09 s) | -0.00990 exp (-0.08 s) |
| (0.5670 s + 1.0) | (0.5560 s + 1.0) | (0.6340 s + 1.0) | (0.3700 s + 1.0) | (0.3770 s + 1.0) |</p>
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<th>INPUT TYPE 3</th>
<th>INPUT TYPE 4</th>
<th>INPUT TYPE 5</th>
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<td>( 0.0194 s + 1.0 )</td>
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<td>-1.23909 exp (-0.09 s)</td>
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<td>-2.78434 exp (-0.20 s)</td>
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<td>-1.48190 exp (-0.08 s)</td>
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<td>0.29435 exp (-0.11 s)</td>
<td>0.07355 exp (-0.10 s)</td>
<td>0.17701 exp (-0.12 s)</td>
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<td>( 0.3729 s + 1.0 )</td>
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<td>0.39780 exp (-0.21 s)</td>
<td>0.32059 exp (-0.13 s)</td>
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<td>( 0.4636 s + 1.0 )</td>
<td>( 0.4235 s + 1.0 )</td>
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<td>( 0.4037 s + 1.0 )</td>
<td>( 0.3678 s + 1.0 )</td>
<td>( 0.3774 s + 1.0 )</td>
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<td>1.74 exp (-0.10 s)</td>
<td>3.41 exp (-0.10 s)</td>
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<td>( 0.2900 s + 1.0 )</td>
<td>( 0.3130 s + 1.0 )</td>
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### TABLE 8.7: MAGNITUDE AND TYPE OF INPUTS FOR CALCULATING THE ESTIMATOR FUNCTIONS

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<td>1</td>
<td>Reflux flow rate</td>
<td>165.0 --- 180.0 ml/min</td>
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<td>Reflux flow rate</td>
<td>165.0 --- 200.0 ml/min</td>
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<td>3</td>
<td>Reboiler steam pressure</td>
<td>144.8 --- 131.0 kPa</td>
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<tr>
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<td>Reboiler steam pressure</td>
<td>144.8 --- 137.8 kPa</td>
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<td>5</td>
<td>Reflux rate</td>
<td>165.0 --- 185.0 ml/min</td>
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<td>144.8 --- 141.3 kPa</td>
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<td>Reflux rate</td>
<td>165.0 --- 175.0 ml/min</td>
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<td>Reboiler steam pressure</td>
<td>144.8 --- 137.9 kPa</td>
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<td>Reflux rate</td>
<td>165.0 --- 150.0 ml/min</td>
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<td>Reboiler steam pressure</td>
<td>144.8 --- 151.7 kPa</td>
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<td>Reboiler steam pressure</td>
<td>144.8 --- 158.6 kPa</td>
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<td>144.8 --- 151.7 kPa</td>
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<td></td>
<td>Reflux rate</td>
<td>165.0 --- 155.0 ml/min</td>
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<td>COMPARTMENT # 3</td>
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Table 8.8b: Selection of Temperature Measurements for Methanol Composition

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<td>-0.936E-02</td>
<td>(0.4201E+1.0) * \exp(-0.13)</td>
<td>-0.972E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.6035E+1.0)</td>
<td>(0.3593E+1.0)</td>
</tr>
<tr>
<td>COMPT # 2</td>
<td>4, 10</td>
<td>-0.101E00</td>
<td>(0.0915E+1.0) * \exp(-0.03)</td>
<td>-0.128E-01</td>
</tr>
<tr>
<td></td>
<td>Down = 6, 13</td>
<td></td>
<td>(0.2811E+1.0)</td>
<td>(0.1214E+1.0) * \exp(0.00)</td>
</tr>
<tr>
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<td></td>
<td>-0.983E-02</td>
<td>(0.3625E+1.0) * \exp(0.00)</td>
<td>-0.524E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.2811E+1.0)</td>
<td>(0.4193E+1.0) * \exp(0.01)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.3330E+1.0)</td>
<td>(0.1094E+1.0)</td>
</tr>
<tr>
<td>COMPT # 3</td>
<td>6, 9</td>
<td>0.109E01</td>
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<td>0.376E-01</td>
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<td>(0.1214E+1.0) * \exp(-0.15)</td>
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<td>-0.483E-01</td>
<td>(0.3216E+1.0) * \exp(-0.11)</td>
<td>-0.817E-01</td>
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<tr>
<td></td>
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<td>(0.3330E+1.0)</td>
<td>(0.1637E+1.0) * \exp(-0.14)</td>
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<tr>
<td></td>
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<td></td>
<td>(0.4098E+1.0) * \exp(-0.01)</td>
<td>(0.1731E+1.0)</td>
</tr>
<tr>
<td>COMPT # 4</td>
<td>11, 13</td>
<td>0.221E-01</td>
<td>(0.4098E+1.0) * \exp(-0.01)</td>
<td>-0.537E-02</td>
</tr>
<tr>
<td></td>
<td>Down = 9, 14</td>
<td></td>
<td>(0.4193E+1.0) * \exp(-0.05)</td>
<td>(0.1637E+1.0) * \exp(-0.05)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.270E-01</td>
<td>(0.4193E+1.0) * \exp(-0.05)</td>
<td>-0.192E-01</td>
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<td></td>
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<td></td>
<td>(0.4193E+1.0)</td>
<td>(0.3707E+1.0)</td>
</tr>
<tr>
<td>BOT PRODUCT</td>
<td>12, 13</td>
<td>-0.132E-01</td>
<td>(0.4201E+1.0) * \exp(-0.02)</td>
<td>0.449E-02</td>
</tr>
<tr>
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<td>Down = 13, 14</td>
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<td>(0.4573E+1.0)</td>
<td>(0.4556E+1.0) * \exp(-0.06)</td>
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<td>-0.153E-01</td>
<td>(0.4193E+1.0) * \exp(-0.06)</td>
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<td></td>
<td></td>
<td>(0.4573E+1.0)</td>
<td>(0.4158E+1.0)</td>
</tr>
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<td>STREAM NAME</td>
<td>SET</td>
<td>TUF</td>
<td>ESTIMATOR</td>
<td>TDOWN</td>
</tr>
<tr>
<td>-------------</td>
<td>-----</td>
<td>-----</td>
<td>-----------</td>
<td>-------</td>
</tr>
<tr>
<td>TOP PRODUCT</td>
<td>6, 9.12.</td>
<td>0.1150E-01</td>
<td>(0.2843s + 1.0) exp(-0.34)</td>
<td>0.1436E+01</td>
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<tr>
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<td></td>
<td>(0.5783s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.1145E-01</td>
<td>(0.3216s + 1.0) exp(-0.33)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5783s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.1147E-01</td>
<td>(0.4201s + 1.0) exp(-0.26)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5783s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>COMPT # 2</td>
<td>4.10.</td>
<td>0.1465E-01</td>
<td>(0.0915s + 1.0) exp(-0.05)</td>
<td>0.4618E-02</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5454s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.4284E-01</td>
<td>(0.3635s + 1.0) exp(0.01)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5454s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>COMPT # 3</td>
<td>7.11.</td>
<td>-0.8613E-02</td>
<td>(0.2974s + 1.0) exp(0.11)</td>
<td>-0.1645E-01</td>
</tr>
<tr>
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<td></td>
<td>(0.4637s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.2494E-01</td>
<td>(0.4098s + 1.0) exp(0.09)</td>
<td></td>
</tr>
<tr>
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<td></td>
<td></td>
<td>(0.4637s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>COMPT # 4</td>
<td>10.13.</td>
<td>-0.4476E-01</td>
<td>(0.3635s + 1.0) exp(0.05)</td>
<td>-0.3011E-01</td>
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<td></td>
<td>(0.3289s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.1533E-01</td>
<td>(0.4193s + 1.0) exp(0.01)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.3289s + 1.0)</td>
<td></td>
</tr>
<tr>
<td>BOT PRODUCT</td>
<td>6, 9.11.</td>
<td>-0.8413E-02</td>
<td>(0.2843s + 1.0) exp(-0.01)</td>
<td>-0.1053E-01</td>
</tr>
<tr>
<td></td>
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<td></td>
<td>(0.5998s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.1481E-01</td>
<td>(0.3216s + 1.0) exp(-0.01)</td>
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</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5998s + 1.0)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.1086E-01</td>
<td>(0.4098s + 1.0) exp(0.00)</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>(0.5998s + 1.0)</td>
<td></td>
</tr>
</tbody>
</table>
Figure 8.1: Single Composition Control for Case 1
Parameters are: $Q_{11} = 5.0, R_{11} = 0.00001$
$R_{22} = 0.0001, U_s = U_f$, Set Point
Acetone = 0.9092, $T = 0.03$
Figure 8.2: Open Loop Response for the Reflux Flow
Step from 165.0 to 190.0 ml/min
Figure 8.3: Single Composition Control for Case 2
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.0001$
$R_{22} = 0.0001$, $U_s = U_f$, Set Point Acetone $= 0.9092$, $T = 0.03$
Figure 8.4: Single Composition Control for Case 3
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.0001$
$R_{22} = 0.0001$, $U_s = U_{in}$, Set Point Acetone 0.9092, $T = 0.03$
Figure 8.5: Single Composition Control for Case 4
Parameters are: $Q_{\text{in}} = 5.0$, $R_{\text{in}} = 0.00001$,
$R_{\text{out}} = 0.0001$, $U_s = U_{\text{in}}$, Set Point Acetone.
$= 0.9092$, $T = 0.03$
Figure 8.6: Single Composition Control for Case 5
Parameters are: \( Q_{11} = 5.0 \), \( R_{11} = 0.00001 \),
\( R_{22} = 0.00001 \), \( U_s = U_{in} \), Set Point Acetone
0.9092, \( T = 0.03 \)
Figure 8.7: Single Composition Control for Case 6
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.00001$
$R_{22} = 0.00001$, $U_s = U_{in}$, Set Point Acetone
= 0.928, $T = 0.03$
Figure 8.8: Single Composition Control for Case 7

Parameters are: \( Q_{11} = 5.0, R_{11} = 0.0001, \)
\( \theta_{22} = 0.0001, U_S = U_T, \) Set Point Acetone
\( = 0.928, T = 0.03 \)
Figure 8.9: Single Composition Control for Case 8.
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.00003$, $R_{22} = 0.00003$, $U_s = U_f$, Set Point Acetone = 0.928, $T = 0.03$.
Figure 8.10: Single Composition Control for Case 9
Parameters are: $Q_{11} = 1.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_S = U_F$, Set Point Acetone
= 0.9092, $T = 0.03$
Figure 8.11: Single Composition Control for Case 10

Parameters are: $Q_{11} = 10.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_s = U_f$, Set Point Acetone

$= 0.9092$, $T = 0.03$
Figure 8.12: Single Composition Control for Case 11

Parameters are: $Q_{11} = 100.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_s = U_f$, Set Point Acetone = 0.9092, $T = 0.03$
Figure 8.13: Single Composition Control for Case 12
Parameters are: $Q_{11} = 1.0$, $R_{11} = 0.00001$, $R_{22} = 0.0001$, $U_s = U_{in}$, Set Point Acetone = 0.9092, $T = 0.03$
Figure 8.14: Single Composition Control for Case 13
Parameters are: $Q_{11} = 10.0$, $R_{11} = 0.00001$,
$R_{22} = 0.0001$, $U_s = U_{in}$, Set point Acetone
$= 0.9092$, $T = 0.03$
Figure 8.15: Single Composition Control for Case 14
Parameters are: $Q_{11} = 100.0$, $R_{ll} = 0.00001$,
$R_{22} = 0.0001$, $U = U_{in}$, Set Point Acetone
= 0.9092, $T = 0.03$
Figure 8.16: Single Composition Control for case 15
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_s = U_f$, Set Point Acetone = 0.9092, $T = 0.09$.
Figure 8.17: Single Composition Control for Case 16
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_s = U_f$, Set Point Acetone 0.9092, $T = 0.12$
Figure 8.18: Single Composition Control for Case 17
Parameters are: \( Q_{11} = 5.0, R_{11} = 0.00001, R_{21} = 0.0001, \) \( U = U_{in}, \) Set Point Acetone = 0.9092, \( T = 0.09 \)
Figure 8.19: Single Composition Control for Case 18
Parameters are: $Q_{\text{in}} = 5.0$, $R_{\text{in}} = 0.0001$, $R_{\text{22}} = 0.0001$, $U_S = U_{\text{in}}$, Set Point Acetone = 0.9092, $T = 0.09$
Figure 8.20: Single Composition Control for Case 19
Parameters are: $Q_{11} = 5.0$, $R_{11} = 0.0001$, $R_{22} = 0.0001$, $U_S = U_{in}$, Set Point Acetone = 0.9092, $T = 0.12$
Figure 8.21: Dual Composition Control for Case 20
Parameters are: $Q_{11} = 10.0$, $Q_{10,10} = 10.0$
$R_{11} = 0.0003$, $R_{22} = 0.001$, $U_s = U_f$
Set Points Acetone = 0.9213, Methanol = 0.1613
$T = 0.12$
Figure 8.22: Dual Composition Control for Case 21

Parameters are: \( Q_{11} = 10.0 \), \( Q_{10,10} = 10.0 \)
\( R_{11} = 0.0001 \), \( R_{22} = 0.000001 \), \( U_s \approx U_f \),
Set Points Acetone = 0.9213, Methanol = 0.1613
\( T = 0.12 \)
Figure 8.23: Dual Composition Control for Case 22

Parameters are: \( Q_{11} = 5.0 \), \( Q_{10,10} = 5.0 \),
\( R_{11} = 0.0002 \), \( R_{22} = 0.00005 \), \( U_s = U_f \)
Set Points Acetone = 0.7971, Methanol = 0.1221, \( T = 0.12 \)
Figure 8.24: Dual Composition Control for Case 23
Parameters are: \( Q_{11} = 10.0 \), \( Q_{10,10} = 10.0 \)
\( R_{11} = 0.0003 \), \( R_{22} = 0.0001 \), \( U_s = U_f \)
Set Points Acetone= 0.9213, Methanol= 0.1613, \( T = 0.12 \), Compositions Predicted
Figure 8.25: Dual Composition Control for Case 24
Parameters are: \( Q_{11} = 5.0 \), \( Q_{10,10} = 5.0 \)
\( R_{11} = 0.0002 \), \( R_{22} = 0.00005 \), \( U_s = U_{in} \)
Set Points Acetone = 0.7921, Methanol = 0.1221, \( T = 0.12 \), Compositions Predicted
Chapter - 9

APPLICATION OF CONTROLLERS TO THE PILOT SCALE EXTRACTIVE DISTILLATION COLUMN

9.1 INTRODUCTION:

One of the criticisms of advanced control theory is that it is typically applied on simulation studies. There are very few papers in the literature where advanced controllers have been applied on experimental equipment. In this chapter, the bilinear optimal controller developed in the previous chapters is applied to a pilot scale extractive distillation column. The configuration and the set-up of the pilot plant are given in Chapter 2. Section 9.2 details the procedure for applying the controller to an extractive distillation column. The reflux flow rate and the steam pressure are considered as the manipulated variables. Results and discussions on Servo Runs 1, 2, and 3 are given in Section 9.3. The estimation of composition using the linear predictor theory and its comparison with experimental data is also discussed in Section 9.3. In Section 9.4, the regulatory control problem is considered. Results are shown for a bilinear optimal controller in Run 4 and 5. Section
9.4 would also show the inadequacy of the bilinear optimal controller designed for reflux and steam. To show the performance of water and steam pressure as manipulated variables, on the pilot plant in Run 6, a PI controller with a steady state decoupler is applied for the regulatory problem. Results of replacing reflux flow rate by the solvent (water) flow rate is also discussed. In Section 9.5, the bilinear optimal controller is redesigned for water flow rate and steam pressure as manipulated variables and applied on the simulation study. This is done as a natural extension of the work to compare two bilinear optimal controllers. Conclusions are presented in Section 9.6.

9.2 PROCEDURE FOR IMPLEMENTING THE CONTROLLER:

To implement a bilinear optimal controller (BOC) a real time program TROLL.FOR was developed. This program operates in the main computer (i.e., VAX 11/750) and sends appropriate data to the extractive distillation column via a DPM-28 front-end. Another program, KILL.FOR, developed by Yashchenko (1988) was used to abort the operation of the plant. It can be used to shutdown the plant in an orderly fashion at the end of the experiment or should any abnormal situation develops. It only takes 1-2 minutes to shutdown the column.

The column takes approximately 5-6 hours to reach
its initial steady state from a cold start. The following points in the database were used for the identification of different stages of the experiments. The structure and details of the database is given in Wong(1984).

<table>
<thead>
<tr>
<th>Point</th>
<th>0 state Description</th>
<th>1 state Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SP(5,66)</td>
<td>Activate Initialization</td>
<td>Bypass Initialization</td>
</tr>
<tr>
<td>SP(5,67)</td>
<td>Transient State</td>
<td>Steady State</td>
</tr>
<tr>
<td>SP(5,68)</td>
<td>Controller OFF</td>
<td>Controller ON</td>
</tr>
<tr>
<td>SP(5,69)</td>
<td>Predictor OFF</td>
<td>Predictor OFF</td>
</tr>
</tbody>
</table>

Once the system has reached the steady state, a steady state simulation is run off-line to get the composition profile. The steady state temperature profile, along with the composition profile from the simulation, is stored in a data file which is used by the predictor once it is activated. When the recursive least squares (RLS) algorithm is used to update the parameters, updated parameters are stored in a separate data file such that the most recent values are available.

Depending upon the type of control run (i.e., servo or regulatory) the \( U_s \) vector is calculated for the final desired compositions for the servo problem. For the regulatory run \( U_s \) was not changed. This was done off-line using the compartmental steady state program and the final parameters are written on the file which is used by the
controller. When the controller is activated, the initial parameters (deviation variable form) are calculated and stored. These parameters are only calculated at the first control step; thereafter they remain constant. They are based on the $Q$ and $A$ matrix since the Liapunov equation is solved to get the $\mathcal{G}$ matrix of equation (7.15) and the elements of the $\mathcal{G}$ matrix are kept constant for the complete control run.

For prediction of the compositions using temperatures, a temperature profile is taken at the same time that the gas chromatograph (G.C.) takes the sample for the analysis. As soon as the G.C. analysis is available, it is passed to the TROLL program. Refer to Chapter 2 for the different communication programs. If the predictor is on, compositions are predicted using the updated parameters as soon as the G.C. analysis is available. The compositions of those streams which are not available through G.C. analysis are predicted; i.e., if G.C. analysis is for the top product stream then the bottoms product compositions are predicted and vice versa. For the stream for which the G.C. analysis is available the predictor parameters are updated using the RLS algorithm.

These steps are summarised below:

1) Select the initial operating conditions of the experiment; i.e., feed composition, flow rates, temperatures, etc.
2) Run the column and wait for 1 to 2 hours and then start the G.C.

3) Set SP(5,66) = 0 (on-line) to activate the initialization routine when TROLL starts to run. The main objective of the initialization routine is to set all previous points to be zero.

4) Start The TROLL program.

5) Check whether SP(5,67), SP(5,68), SP(5,69) are all zero. The initialization routine should have set these points to zero if it was activated properly. If not, set these points to zero manually. As soon as the initialization routine is completed SP(5,66) is set to 1 by the routine to bypass the initialization the next interval. At this stage G.C. analysis data appear on the screen.

6) Wait for 5 to 6 hours from the start to get to the initial steady state.

7) Run the steady state simulation off-line with the particular experimental conditions to get the initial composition profile.

8) Set SP(5,67) = 1 and SP(5,69) = 1 to let the TROLL know about the steady state and to activate the predictor.

9) Run the system at the initial conditions for at least 4-5 more G.C. points. The predictor will also give the predicted data at this time.

10) Select the type of control run. For a Servo run, select the final setpoints and run the steady state program off-
line to calculate $U_g$. Store this vector and the final compositions in a data file used by the controller.

11) Activate the controller by setting $SP(5, 68) = 1$

12) If the regulatory problem is being considered, insert the disturbance after the controller is activated. Both the disturbance and the controller can be activated at the same time.

13) Run the controller for the appropriate time and use the KILL program to terminate the experiment.

A summary of control runs reported in this chapter is given Table 9.1.

**Table 9.1: Summary of Control Runs**

<table>
<thead>
<tr>
<th>RUN #</th>
<th>Type of Run</th>
<th>Set Points (Acetone, Methanol)</th>
<th>Figure #</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Servo BOC</td>
<td>0.9036, 0.1614</td>
<td>9.3</td>
</tr>
<tr>
<td>2</td>
<td>Servo BOC</td>
<td>0.9175, 0.1700</td>
<td>9.6</td>
</tr>
<tr>
<td>3</td>
<td>Servo BOC</td>
<td>0.8675, 0.1200</td>
<td>9.7</td>
</tr>
<tr>
<td>4</td>
<td>Regulatory BOC</td>
<td>0.8895, 0.1525</td>
<td>9.8</td>
</tr>
<tr>
<td>5</td>
<td>Regulatory BOC</td>
<td>0.8988, 0.1598</td>
<td>9.9</td>
</tr>
<tr>
<td>6</td>
<td>Regulatory PI+ Decoupler</td>
<td>0.8955, 0.1600</td>
<td>9.10</td>
</tr>
</tbody>
</table>
9.3 SERVO CONTROL PROBLEM:

In this section an experimental servo control for dual composition control is discussed. The compositions being controlled are the acetone in the top product and the methanol in the bottoms product. As explained in the previous chapter, top product and bottoms product compositions are predicted alternately. The experimental verification of the predictor is discussed first.

To test the predictor against the experimental data, the reflux flow rate was changed from 165.0 to 155.0 ml/min. A small change was selected to observe the performance of the predictor near the steady state, before applying a larger change. The acetone and methanol compositions in the top and bottoms product were predicted using the fixed linear predictor developed in Chapter 8. The performance of the predictor, whose parameters are given in Tables 8.9a and 8.9b, is shown in Figures 9.1 and 9.2. The tray numbers where the temperature measurements are taken for the predictor are given in Tables 8.8a and 8.8b. Figures 9.1 and 9.2 compare the acetone and methanol compositions in the top product and the bottoms product respectively from the gas chromatograph and the predictor. The compositions are predicted only when the gas chromatograph takes the sample
Figure 9.1: Comparison of Experimental and Predicted Data for Top Product

Figure 9.2: Comparison of Experimental and Predicted Data for Bottoms Product
for the analysis. The difference between the observed and the predicted data is very small. The maximum difference is for the acetone composition in the top product at 975 minutes. This difference is equal to 0.006 mole percent, which is acceptable, knowing that the G.C. analysis at times can result in such noise levels. From these data it can be concluded that a fixed parameter linear predictor can be used, if the system operates in the close neighborhood of the initial steady state.

RUN # 1:

Based on the above results, the first experiment was performed in the neighborhood of the initial operating conditions. The operating conditions of Run 1 along with the experimental initial steady state composition is given in Table 9.2. The Q and R matrices selected for this experiment are given below:

\[
R = \begin{bmatrix}
0.00015 & 0.0 \\
0.0 & 0.00001
\end{bmatrix}
\]

\[Q_{11} = 5.0, \ Q_{10,10} = 5.0\]

All the rest of the elements of the Q matrix are zero.
The desired setpoints for the acetone composition in the top product and the methanol composition in the bottoms product are:

\[ \text{Acetone} = 0.9036 \quad \text{Methanol} = 0.1614 \]

The system performance for the bilinear optimal controller is shown in Figure 9.3. From the steady state program the following values of the manipulated variables were obtained for the desired setpoint conditions:

- Reflux flow rate = 192 ml/min
- Steam pressure = 144.8 kPa (gauge)

The acetone composition in the top product and methanol in the bottoms product are predicted whenever G.C. analysis is not available. The dark points in the figures are the predicted points.

Methanol in the bottoms product shows a slight oscillatory behavior and produces a small offset from the desired setpoint. The offset in the top product is almost negligible. The system performance is satisfactory. Both the reflux flow rate and the steam pressure converge to new levels and are stable. The final change in the reflux flow rate is from 165.0 to 193.0 ml/min. There are small oscillations in the reflux flow rate and in the steam.
<table>
<thead>
<tr>
<th>RUN NUMBER</th>
<th>1</th>
<th>2</th>
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<tr>
<td>FLOW ML/MIN</td>
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<td>110.0</td>
<td>110.0</td>
<td>110.0</td>
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<td>41.99</td>
<td>43.15</td>
<td>45.28</td>
<td>43.68</td>
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<td>0.6316</td>
<td>0.6794</td>
<td>0.6523</td>
<td>0.6586</td>
<td>0.6588</td>
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<td>0.3470</td>
<td>0.2788</td>
<td>0.3132</td>
<td>0.3044</td>
<td>0.3027</td>
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<td>0.0416</td>
<td>0.0335</td>
<td>0.0368</td>
<td>0.0384</td>
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<td>170.0</td>
<td>165.0</td>
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<td></td>
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<tr>
<td>PRESSURE kPa</td>
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<td>0.8955</td>
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<td>0.0382</td>
<td>0.0380</td>
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<td></td>
<td></td>
<td></td>
<td></td>
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</tr>
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<td>0.1525</td>
<td>0.1577</td>
<td>0.1600</td>
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<td>0.8001</td>
<td>0.8214</td>
<td>0.8011</td>
<td>0.8071</td>
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</tbody>
</table>

pressure. These are due to the error in predicting the composition. The magnitude of the oscillation is around 3-4 ml/min for the reflux flow rate and about 0.69 kPa for the steam pressure.

The experiment shows the acceptable performance of the controller and the predictor when the desired setpoint
Figure 9.3: Dual Composition Control using BOC for Servo Problem, $Q_{11} = 5.0$, $Q_{10,10} = 5.0$, $R_{11} = 0.00015$, $R_{22} = 0.00001$, (Experimental, Run 1)
is in the close vicinity of the initial steady state.

To test the controller performance for a wider operating region, an experiment was performed in which it was required to change the acetone and methanol compositions from 0.7558 and 0.1211 to 0.9115 and 0.1675, respectively. A fixed parameter linear predictor was used. It was found that the controller resulted in ringing. This was due to the fixed parameter linear predictor failing to produce correct compositions. The predicted compositions were lower than the G.C. analysis. Thus, at alternate points the difference in the composition from the setpoints was large. This difference was sufficient to move the manipulated variable from 220.0 ml/min to 120.0 ml/min, which are the physical limits on the reflux flow rate. Ringing was also observed in the steam pressure. Therefore, it was confirmed that a fixed parameter linear predictor is not sufficient for the extractive distillation column for a wide range of operation. To improve this method, a RLS algorithm was implemented to update the parameters whenever a G.C. analysis is available.

To test the ability of the RLS algorithm to update the parameters, a step change in the reflux flow rate from 170.0 to 130.0 ml/min was given. Figures 9.4 and 9.5 show the comparison of the experimental and the predicted data using RLS algorithm for the top product and the bottoms product analysis, respectively. The updated predictor
parameters overwrite the last updated parameters in a separate file. From the figures it can be concluded that RLS method for updating the gains of the predictor results in better composition predictions than a fixed parameter predictor. It should be kept in mind that the set of tray temperature measurements used in the prediction remain unchanged. Due to the nonlinearity of the system it is possible that for the operating point which is not in the close neighborhood of the initial conditions, a different set of tray measurements may produce a lower condition number and projection error. This however, would require a large computation time. Therefore, the original set of tray measurements were used over the entire operating region.

**RUN #2:**

The RLS algorithm was used with a bilinear optimal controller in Run 2. Compositions of the top and the bottoms product are estimated alternately using the updated parameters. The initial operating conditions for this run are given in Table 9.2. The following $R$ and $Q$ matrices are used:

$$
R = egin{bmatrix}
0.00015 & 0.0 \\
0.0 & 0.00001
\end{bmatrix}
$$
Figure 9.4: Comparison of Experimental and Predicted Data using RLS method for Top Product

Figure 9.5: Comparison of Experimental and Predicted Data using RLS method for Bottoms Product
\( Q_{11} = 5.0, \quad Q_{10,10} = 5.0 \)

The objective of this experiment was to move the system from the initial steady state of acetone composition of 0.8195 and methanol composition of 0.1417 to 0.9175 and 0.1700, respectively. The following values of the manipulated variables were calculated using the steady state program:

Reflux flow rate = 180 ml/min

Steam pressure = 132.4 kPa(gauge)

The system performance is given in Figure 9.6. The predictor was started at 753 minutes and the controller was started at 851 minutes. The data plotted in Figure 9.6 are from 798 minutes. Between 753 minutes and 851 minutes the process was at initial steady state, and RLS was updating the parameters. After 851 minutes both controllers start to take action such that both compositions reach their desired setpoints. The reflux flow rate and the steam pressure exhibit satisfactory behavior. One data point at 949 minutes was missed due to a disk space quota problem. Therefore, no control action was taken (i.e., the manipulated variables were kept at the previous level). This was possible only because the controller was working in the main VAX 11/750 computer, whereas the system parameters, once passed from
the main computer, stay in the memory of the front-end DPM-23. So when the disk quota problem occurred, it stopped the controller program in the VAX, but did not effect the front-end. This is the main advantage of this kind of distributed configuration. The problem was soon rectified and the controller and the predictor were restarted with the parameters the same as those before the problem. After restarting the controller the system finally reaches the desired setpoints. The final values of the reflux flow rate is 178ml/min and the steam pressure is 131.0 kPa(gauge).

**RUN 3:**

In the above two runs it was shown that a bilinear optimal controller can be used to move the acetone and methanol compositions upward from their initial steady state values. In this run an opposite case is desired, where the requirement is to move the acetone and methanol compositions below their initial values. The initial operating conditions with the experimental steady state are given in Table 9.2. The $R$ and $Q$ matrices used are the same as in run 2. The desired setpoints are:

\[
\text{Acetone} = 0.8675 \quad ; \quad \text{Methanol} = 0.1200
\]

The initial operating point is:
Figure 9.6: Dual Composition Control using BOC for
Servo Problem, $Q_{11} = 5.0, Q_{10,10} = 5.0$
$k_{11} = 0.00015, R_{22} = 0.00001, \text{(Experimental Run 2)}$
Acetone = 0.9155; Methanol = 0.1400

The calculated values of the manipulated variables are:

Reflux flow rate = 140.0 ml/min
Steam Pressure = 155.1 kPa (gauge)

The system performance is shown in Figure 9.7. Both acetone and methanol compositions reach their setpoints. The manipulated variable responses are also acceptable. In this case the RLS algorithm is used to update the predictor parameters. The predictor was started at 758 minutes and the controller was started at 811 minutes. On an average, the methanol in the bottoms product shows an offset with a trend moving toward the setpoint. It should be noted that the controller parameters are the same in all runs. Actually, these parameters should change with the operating conditions. However, the results show that even the constant parameter controller works well for these cases. This also indicates that the controller is not very sensitive to the operating conditions.

From these servo control runs it can be concluded that a bilinear optimal controller works satisfactorily for upward and downward dynamics. When the system is required to move over a wider range, the predictor with a RLS algorithm to update its parameters gives better composition values
Figure 9.7: Dual Composition Control using BOC for Servo Problem, $Q_{11} = 5.0$, $Q_{10,10} = 5.0$
$R_{11} = 0.00015$, $R_{22} = 0.00001$, (Experimental Run 3)
than a fixed parameter predictor. If the predictor is not predicting the intermediate compositions properly the controller may produce in ringing in the manipulated variable. Although the controller parameters should be changed, it was found that a constant parameter controller worked well for these tests.

9.4 REGULATORY CONTROL PROBLEM:

**Rungs 4 and 5:**

In the previous section a bilinear optimal controller was applied to a servo problem. In this section the same controller is used for a regulatory problem. The disturbance considered is a change in the feed flow rate. For this problem the $U_s$ was kept at the original operating condition. The following values of $R$ and $Q$ matrices were used:

$$R = \begin{bmatrix} 0.00008 & 0.0 \\ 0.0 & 0.00001 \end{bmatrix}$$

$$Q_{11} = 5.0 \quad Q_{10,10} = 5.0$$

Lower $R$ values were used because it was observed in Chapter 8, that when $U_s$ is kept at the original conditions,
the $R$ values should be lowered to reduce the offset.

The operating conditions for this Run 4 are given in Table 9.2. The top product acetone and the bottoms product methanol compositions were required to stay at the initial steady state values of 0.8895 and 0.1525 during and after the feed flow rate disturbance from 110.0 to 135.0 ml/min. The RLS algorithm is used to update the predictor parameters.

Due to a constantly changing temperature in the pilot plant area a good initial steady state could not be achieved. The controller and the feed flow disturbance were started simultaneously at 851 minutes and the predictor was implemented at 830 minutes. The system response is given in Figure 9.8. Although the change in the acetone and methanol composition were not very large, there is no evidence in the data showing that these would finally come back to the setpoints. Both controller outputs kept on increasing. It should be realized that in this case $\Delta U \neq 0.0$. Also the optimal controller is designed for impulse disturbances. For the step disturbances a performance index where the rate of change of the manipulated variable is penalized should be used as compared to penalizing the manipulated variable only. In addition to this consideration, internal interactions have driven the controller to keep on increasing the manipulated variables. Similar results were obtained for PI controllers when reflux and steam pressure.
Figure 9.8: Dual Composition Control using BOC for
Regulatory Control, 20% Feed Flow Disturbance, \( Q_{11} = 5.0 \), \( Q_{10,10} = 5.0 \)
\( R_{11} = 0.00008 \), \( R_{22} = 0.00001 \), (Experimental Run 4)
were used as manipulated variables in Chapter 6 and the independent experimental work of Mayer (1985) and Latosinsky (1988). From these results it is clear that the feed flow disturbance can not be controlled efficiently, even with a bilinear optimal controller when reflux flow rate and steam pressure is used as manipulated variables.

A bilinear controller was tested for a 5% feed flow rate disturbance in Run 5. The operating conditions for this run are given in Table 9.2 and the performance is shown in Figure 9.9. The Q and R matrices were the same as in the previous case. The setpoints are 0.8988 for the acetone compositions and 0.1598 for the methanol compositions. The feed disturbance is from 110.0 to 115.5 ml/min. The predictor was started at time 720 minutes and the controller started and feed flow disturbance introduced at 764 and 780 minutes, respectively. The responses show that the compositions are near the setpoints with acetone moving downward and methanol upward from their setpoints. However, even for this small disturbance the reflux flow rate changed from 165 to 185.0 ml/min and the steam pressure moved from 144.8 to 158.6 kPa(gauge). Similar results were reported in Chapter 6 where it was shown that for a small feed flow disturbance, when reflux flow rate and steam pressure were selected as manipulated variables, large control actions were required for PI controller. In this experiment, although it seems that the controller has worked well from
Figure 9.9: Dual Composition Control using BOC for Regulatory Problem. 5% Feed Flow Disturbance, $Q_{i1} = 5.0$, $Q_{10,10} = 5.0$, $R_{11} = 0.00008$, $R_{22} = 0.00001$ (Experimental Run 5)
the composition point of view, it can be said that for such a small disturbance the compositions would not move very far away from their initial values under open loop conditions. Therefore, looking at the changes in the manipulated variables, it can be concluded that a bilinear optimal controller designed for the reflux flow rate and steam pressure is not adequate for feed flow disturbances.

To test whether or not the constant controller matrix was the cause of this poor performance the average value of the controller matrix was determined by solving the Liapunov equation off line at different operating points. It was found that the average matrix was not significantly different from the original matrix.

RUN 6:

In Chapter 6, it was concluded that Solvent (water) flow rate is a better choice of manipulated variable than the reflux flow rate. In this run a PI controller with a steady state decoupler, which uses the water flow rate and steam pressure as manipulated variables, is implemented on the experimental extractive distillation column for a feed flow disturbance. The operating conditions for Run 6 are given in Table 9.2. The following parameters were used for the two PI controllers with a decoupler:
<table>
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<th></th>
<th>Gain</th>
<th>Reset Time</th>
<th>Decoupler Gain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water Flow rate</td>
<td>140.0</td>
<td>1.2</td>
<td>1.25</td>
</tr>
<tr>
<td>Steam Pressure</td>
<td>-40.0</td>
<td>2.0</td>
<td>-0.4</td>
</tr>
</tbody>
</table>

The feed flow rate was changed from 110.0 to 130.0 ml/min. It was desired to keep the acetone and methanol compositions at 0.8365 and 0.1424, respectively. The predictor was started at 785 minutes and the controller and feed flow rate disturbance were introduced at 808 minutes. The system performance is given in Figure 9.10. Initially the top product acetone composition starts to deviate from the initial setpoint due to the feed flow disturbance effect, but the controller brings it back to its setpoint. In the methanol composition, the controller takes longer to get back to its setpoint. Both water flow rate and steam pressure are stable. The response of the bottoms product can be improved with better tuning parameters. The main objective of this experiment was to confirm the result of Chapter 6, that water and steam pressure can be used for feed flow disturbances.

From the above experiments it can be concluded that for feed flow disturbances, water flow rate and steam pressure are a better choice of manipulated variables than reflux flow rate and steam pressure for dual composition control. The bilinear controller designed in Chapter 7 does
Figure 9.10: Dual Composition Control using PI + Decoupler for 20% Feed Flow Disturbance (Experimental Run 6)
not perform well for feed flow disturbances and it is recommended that the design should be changed to water and steam pressure from reflux flow and steam pressure.

9.5 DESIGN OF THE BILINEAR OPTIMAL CONTROLLER

USING WATER AND STEAM PRESSURE:

Based on the conclusions of Section 9.4, the bilinear optimal controller is redesigned for water and steam pressure. This is a natural extension of the work. This would also compare the results of two bilinear optimal controllers. To change the manipulated variables in the controller design, the first step is to change the form of the bilinear state model so that water flow rate is the manipulated variable in place of reflux flow rate. A method similar to the one used in Chapter 5 is used to derive the system matrices for the state space model of equation (5.25). The only change is that $U_1$ now refers to the water flow rate. The resulting system matrices are given in Appendix E. In the second step, the variables are changed to deviation variables. Equations (8.4) to (8.6) and equations (8.8) and (8.9) are used to get a bilinear state space model of equation (8.7). The form of the bilinear optimal controller remains the same as equation (7.24). The resulting bilinear controller is applied to the dynamic simulation of the extractive distillation column.
For the simulation studies the operating conditions of Run 4 are selected. The objective of this study is to check the system performance for a feed flow disturbance. The feed flow rate was changed from 110.0 to 130 ml/min. In the previous design of the predictor, the trays were selected for reflux flow rate and steam pressure disturbances. For this case the number of trays to be used for the prediction would be different. Since this study is being performed on the simulation it can therefore be assumed that all the compositions are available. Thus, the predictor was not used in this case and all compositions were provided by the dynamic simulator. If the design has to be implemented on the experimental equipment then a suitable set of trays for the prediction should be calculated. The following $Q$ and $R$ matrices are selected:

$$
R = \begin{bmatrix}
0.00002 & 0.0 \\
0.0 & 0.000001
\end{bmatrix}
$$

$$
Q_{11} = 10.0,
Q_{10,10} = 10.0
$$

The simulated system performance is shown in Figure 9.11. The controller performance is acceptable. The feed flow disturbance and the controller were started at 3.0 hours. The $U_g$ vector was kept at its initial values. The major effect of the feed flow disturbance is in the methanol composition in the bottoms product. The methanol composition
Figure 9.11: Dual Composition Control using BOC for Regulatory Control, 20% Feed Flow Disturbance, $Q_{11}=10.0$, $Q_{10,10} = 10.0$, $R_{11} = 0.00002$, $R_{22} = 0.00001$ (Simulation)
starts to deviate earlier than the acetone composition. The controller responds by changing the water flow rate and by making slight changes in steam pressure to bring the compositions back to their desired values. The acetone composition starts to move from its initial setpoint but the increased water flow rate in the system brings it back. Figure 9.12, shows a similar study, but in this case a feedforward controller was also used. The feedforward controller element was the water flow rate. Thus, water flow rate is used in the feedforward and feedback loops. As soon as the system sees the feed flow change it changes the water flow rate. For the feed flow disturbance from 110.0 to 130.0 ml/min the water flow rate changes from 45.0 to 49.5 ml/min. The performance is better than the previous case since the maximum deviation in the methanol composition in the bottoms product is smaller than in the previous case.

From these simulation studies it can be concluded that a bilinear optimal controller designed for water flow rate and steam pressure could be used for feed flow rate disturbances.

9.6 CONCLUSIONS:

A bilinear optimal controller was implemented on a pilot plant extractive distillation column for dual composition control. In the first part a servo problem was
Figure 9.12: Dual Composition Control using BOC + Feedforward Controller for Regulatory Control, 20% Feed Flow Disturbance, \( Q_{11} = 10.0 \), \( Q_{10,10} = 10.0 \), \( R_{11} = 0.00002 \), \( R_{22} = 0.000001 \), (Simulation)
considered. To implement a controller, composition predictions were required. It was found experimentally that a fixed parameter linear predictor is good only in the neighborhood of the initial operating conditions. For a wider range of operation it was shown experimentally that an RLS algorithm can be used to update the predictor parameters. A bilinear controller with the RLS algorithm to update predictor parameters was implemented successfully for the servo control problem of driving the system towards more purity in the acetone composition, and in the other case towards less purity, from the initial operating conditions.

A bilinear controller was also evaluated for the regulatory problem during a feed flow disturbance. A controller based on reflux flow rate and the steam pressure did not produce favorable results. Even for a small disturbance, the reflux flow rate and steam pressure changed by a large amount suggesting that a controller will reach saturation if a larger disturbance was applied. Similar results were shown with the PI controller in Chapter 6 and in the experiments of Mayer (1985) and Latosinsky (1988). To control the system against the feed flow disturbances a PI controller with a steady state decoupler based on water flow rate and steam pressure as manipulated variables was implemented on the column. It was found that this controller structure produces a acceptable system performance. The changes in the water flow rate and steam pressure were not
large even for a feed flow rate disturbance of 20%. This suggests that this pair is a better choice of manipulated variables. The reason that water performs better than the reflux flow rate lies in the thermodynamics of the system. As the feed flowrate is increased, acetone in the top product decreases while methanol in the bottoms product increases. To keep these compositions at their initial steady state points, the controller increases the reflux flow rate to increase the acetone composition in the top product. This however, also increases the methanol composition in the bottoms product taking it further away from the setpoint. The reboiler steam pressure is increased to boil off more methanol which results in a decrease in the acetone composition in the top product. This sequence continues so that compositions which may not be very far away from their setpoints cause large changes in the manipulated variables. This type of performance makes the controller unacceptable. If water is manipulated, the acetone composition in the top product increases and methanol composition in the bottoms product decrease simultaneously as the water flow rate is increased. This is due to the high boiling point and large density of water as compared to acetone and methanol. As the water flow rate is increased it flows down the column, increasing the amount of water in the reboiler, and thus decreasing the methanol composition. Since methanol has more affinity for water than
for acetone an increasing water flowrate increases the acetone composition in the top product. Changes in the steam pressure help in this case and also increase the rate of recovery of the compositions. Therefore, this combination works better than a combination of reflux flow rate and steam pressure.

Based on the results of the PI controller, the bilinear controller was redesigned for water and steam pressure. The controller was implemented successfully on the simulation for 20% feed flow disturbance. A feedforward controller, which uses water flowrate as its manipulated variable, was implemented in conjunction with a bilinear optimal controller. The simulations indicate that this structure performs slightly better than the bilinear optimal controller used alone.

It should be noticed that the initial controller parameters were not changed during the control runs. For a nonlinear system such as the extractive distillation column a time varying model would result in better control strategies. However, the servo control runs show that the controller parameters are not very sensitive to the operating condition used. Also, the performance of the bilinear optimal controller depends upon the performance criterion selected for the optimality. Results in this chapter and in the previous chapter are based on the
performance index selected in Chapter 7.
Chapter - 10

CONCLUSIONS AND RECOMMENDATIONS

A pilot scale distillation column was built to study the separation of an azeotropic mixture of acetone and methanol. The construction of the column was a joint effort with other students. The extractive distillation process is used to break and azeotrope using water as a solvent. This is a non-ideal, non-linear, multicomponent system. The column is controlled by VAX 11/750 computer via DPM-23 industrial front-end system. This is a distributed control configuration in which data archiving and advanced multivariable composition control are performed on the VAX and low level loop controllers of the proportional-integral (PI) type executing in the front-end. An on-line Varian-6000 gas chromatograph (G.C.) is used for the top and bottoms product analysis. These streams are analysed alternately and the results are transmitted to VAX via a VISTA-401 data station.

To understand the system behaviour, steady state and dynamic mass and energy balance models were developed. The validity of these models has been explored using experimental data over a wide operating region. The simulated behaviour from the dynamic model was compared with
the experimental column behaviour for various open loop steps in the reflux flow rate, feed flow rate, feed composition and reboiler duty. The non-linear behaviour of the system was simulated by the models. A simple model for vapour liquid equilibrium (VLE) calculations was developed and its validity was proven.

In order to get a reduced order model of the extractive distillation column, a compartmental technique was used. After comparing 3, 4 and 5 compartment models of this column, it was found that a 5 compartment model shows good agreement with the experimental data and with a tray to tray model. A saving of 70% in the computation time was achieved over the tray to tray model. The 5 compartment model was used to develop a reduced order bilinear model of the system using the reflux flow rate and the reboiler duty as manipulated variables. In the experimental and simulation studies steam pressure to the reboiler was used to change the reboiler duty of the column. The dynamics of the column were investigated for steps in steam pressure, reflux flow rate and feed flow rate. The system behaviour using the bilinear model and a complete tray to tray model were similar to the actual plant data. The difference between the bilinear model and the experimental data is due to the assumption of constant factors to represent flows. In the actual process, these change with time and the region of application.
PI control strategies were simulated for single and dual composition control for four different kinds of disturbances. From the simulation studies it was found that the control strategy with two single loops and the conventional pairing of the reflux flow rate and reboiler duty is suitable for only certain kinds of disturbances. Selection of the water flow rate and reboiler duty (steam pressure) as a manipulated variable pairing showed better performance. The performance of the PI+decoupler was better than PI controller alone. It was also observed that PI+decoupler along with feed forward controller, where the feed forward element is the water flow rate, further improves the system performance for feed forward disturbances. To understand the feasibility of the manipulated variable pairing, a simple method based on a linear system assumption was developed to calculate the control action required to compensate for the changes in the composition produced by the various disturbances. The required action was compared to the operating limits of the manipulated variables to find out if the pairing can be used for that kind of disturbance.

In order to implement an advanced multivariable controller, a bilinear optimal controller design was developed which would result in an asymptotically stable system. The optimal controller for a bilinear system is nonlinear in nature, but the control law depends upon the
objective function selected. The proof of optimality is
given. It was also shown that an optimal controller based on
a bilinear equation has a larger region of application than
a controller designed from a linearized model. The optimal
controller, along with a reduced order bilinear model, was
applied to a simulation and on the pilot plant for dual
composition control. Reflux flow rate and reboiler duty were
used as the manipulated variable pair. The weighting
matrices from the objective function and the constant system
matrices from the model were used to solve a Liapunov
equation to obtained the matrix used in the control law.
This matrix was determined when the controller was first
implemented and then held constant.

To apply the controller on the pilot plant a few of
the states needed to be predicted since the online gas
chromatograph analyses the top product and the bottoms
product streams alternately. These states are predicted by a
linear predictor using tray temperatures. The parameters
were calculated using a complete dynamic simulator. For the
operation of the controller over a wide operating region,
predictor parameters were updated for the top and bottoms
product alternately using a recursive least squares (RLS)
method when the G.C. analyses were available. An optimal
controller with the RLS algorithm was implemented
successfully on the pilot scale extractive distillation
column for the servo control problem of driving the system
toward higher purity in the acetone composition; and also for the other case driving towards lower purity.

A bilinear controller was also applied to the regulatory problem of a feed flow disturbance. It was found that even a multivariable controller based on the reflux flow rate and reboiler duty did not perform well. To test whether or not the constant controller matrix was the cause of this poor performance, the average value of the controller matrix was determined by solving the Liapunov equation off line at different operating points. It was found that the average matrix was not significantly different from the original matrix. The cause of this poor performance could be the fact that a step disturbance is a non-stationary disturbance and the optimal controller designed to minimize the selected objective function is optimal for stationary disturbances. However, it was previously concluded that the two single loop controller configuration based on this pairing also resulted in the poor system performance. It was shown through simulation that the performance was improved by replacing the reflux flow rate by water flow rate as a manipulated variable. Therefore, it is concluded that the conventional pairing of reflux flow rate and the reboiler duty is not an appropriate choice for this disturbance. Consequently, an experiment was performed to control the feed flow rate disturbance using two PI controllers and a steady state decoupler using water
flow rate and reboiler duty (steam pressure) as manipulated variables. This controller structure resulted in acceptable performance. Subsequently, bilinear model for the extractive distillation was changed to use water flow rate and reboiler duty as manipulated variables. The controller resulting from this model was implemented successfully on the simulation for 20% feed flow disturbance. It should be noted that the system performance depends upon the performance index used in the design of the bilinear controller and that the conclusions in thesis are based on the performance index given in Chapter 7.

**Contribution Of the Thesis:**

The followings contributions follow from this work:

1. Complete Models of an Extractive Distillation:

   Complete tray to tray models to predict the steady state and dynamic behaviour of an extractive distillation were developed. Experimental data were used to prove the validity of these models. This also contributes experimental data on an extractive distillation to the open literature.
2. Development of Compartmental Technique:

Development of the compartmental technique to obtain a reduced order model for the non-linear system. The existing techniques for near ideal system were modified for this non-linear system. Criterion for selection of a compartment were presented and it was shown that for a non-linear, non-ideal system like an extractive distillation column, increasing a compartment size produces inaccurate predictions of dynamic behaviour.

3. Reduced Order Bilinear Model:

Development of a reduced order bilinear model of an extractive distillation column. The developed model shows good agreement with a complete tray to tray model and an experimental data.

4. Solvent is a Better Manipulated Variable:

Solvent is a better manipulated variable for the control studies as compared to reflux flow rate. Both for a simple control strategy (i.e., PI type controllers) and advanced controller, it was shown that paring of solvent and reboiler duty can handle almost any kind of disturbance, whereas the reflux flow rate and reboiler duty pair
(conventional paring) is good only for a certain kinds of disturbance.

5. Application of Bilinear Optimal Controller:

A bilinear optimal controller and its proof was developed. The proof of optimality was derived from the first principles. The developed controller was successfully implemented in conjunction with a predictor to predict compositions on a pilot scale distillation column, and on a complete tray to tray simulation.

6. Experimental Data on Extractive Distillation:

As it is stated in the first chapter that there is little data on an extractive distillation columns in the open literature; most of the work is hidden in the patent literature. This work presents data on the steady state, dynamic and closed loop behaviour of an extractive distillation column. The experimental data presented is in a wide operating zone can be used by other researchers into better model and control techniques.

Recommendations:

The followings recommendations follow from this
work:

1. Since this was the first experimental application of bilinear optimal control to an extractive distillation process which is both a non-linear and a non-ideal system, only one kind of performance index was used. Different kinds of performance indices, particularly ones for non-stationary disturbances (in which the rate of change of manipulated variable is penalised in the quadratic function as compared to penalising the manipulating variable only), should be investigated to determine if the reflux flow rate and steam pressure pairing could be used for regulation and servo responses. In the meantime, the experience gained in this study leads to the recommendation that water flow rate and reboiler duty be used as manipulated variables. It is also recommended that time varying bilinear controllers be developed and implemented. In this method, the Liapunov equation should be re-solved at each control interval depending on the column conditions. The theory of such methods for bilinear systems is not very well understood, but such a development would be a contribution to non-linear process control.

2. Time series models (dynamic transfer function and noise models) of the column have not been obtained because of difficulties with the G.C. and the feed inventory. With
only one G.C., each stream (either the top product or the bottoms product) is analysed every 15 minutes. Considering that a good model requires at least 100 switching periods, time series modelling requires approximately 48 hours of continuous operations. More data points could be obtained during this time by using two G.C.s for the analysis. Both linear and bilinear time series models should be identified and both linear and bilinear stochastic controllers designed and implemented.

3. Two things which effect the experiments very significantly are variations of the ambient temperature and the quality of the gas chromatograph analysis. The temperature in the pilot plant area was not properly controlled, and since the apparatus was not perfectly insulated the column performance changed significantly as these ambient conditions changed. A constant ambient temperature would help in comparing different experimental runs. The gas chromatograph analysis needs some improvement. Since two polar compounds are being analysed there is a overlap in the peak areas of the methanol and water. Temperature programming on the G.C. is one way of improving the G.C. performance. Another way is to use a predictor. It was shown that a linear predictor with the RLS algorithm gives satisfactory composition predictions using tray temperatures. Use of an extended Kalman filter is another
method of predicting composition using temperatures (due to nonlinearities in the system, an extended Kalman filter would perform better than a regular Kalman filter). It would be interesting to see how this method compares with the RLS method and then to use the best one to augment the gas chromatograph measurements during the control studies.

4. This study has focussed mainly on manipulated variables such as water flow rate, reflux flow rate, and reboiler duty (steam pressure). Controllers which utilize ratios of these process inputs should also be examined. These can be chosen in concert with a mechanistic understanding of the thermodynamic equilibria and mass transfer in the column.
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APPENDIX-- A

Derivation of the Effective \( A_j \).

A method of induction is used to derive a general expression for \( A_j \) for a compartment with \( N \) trays.

Case #1

\( N = 1 \)

\[
\begin{align*}
V_{ij} & \quad \downarrow l_{i, j-1} \\
V_{i j+1} & \quad \downarrow l_{ij} \\
V_{i 1} & \quad \downarrow l_{i 0} \\
V_{i 2} & \quad \downarrow l_{i 1}
\end{align*}
\]

compartmental variables \quad tray variables

Relationship between compartmental and tray variables (Note: Subscript for the component is dropped)

\[
V_{j-1}' = V_0 \quad V_j' = V_1 \quad V_{j+1}' = V_2
\]

The compartmental component balance is equation (4.8)

\[
A_{j-1}'' V_{j-1}' - (A_j' + 1) V_j' + V_{j+1}' = 0 \quad (A.1)
\]

The tray equation

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\begin{align*}
A_0 V_0 - (A_1 + 1) V_1 + V_2 &= 0 \quad (A.2)
\end{align*}

Relationship between and $A'$ and $A$ is
\begin{align*}
A''_{j-1} &= A_0 \quad (A.3a) \\
A'_j &= A_1 \quad (A.3b)
\end{align*}

Case \#2 $N = 2$ (compartment with two trays)

\[
\begin{array}{c}
V_1 \\
1 \\
2 \\
V_3 \\
1_2 \\
\end{array}
\]

Relationship between compartmental and tray variables.
\begin{align*}
V'_{j-1} &= V_0 \quad ; \quad V'_j = V_1 \quad ; \quad V'_{j+1} = V_3
\end{align*}

Tray equations are:
\begin{align*}
A_0 V_0 - (A_1 + 1) V_1 + V_2 &= 0 \quad (A.4) \\
A_1 V_1 - (A_2 + 1) V_2 + V_3 &= 0 \quad (A.5)
\end{align*}

Calculate $V_2$ from equation (A.4) and substitute in equation (A.5) to get:
\begin{align*}
A_1 V_1 - (A_2 + 1) [(A_1 + 1) V_1 - A_0 V_0] + V_3 &= 0 \quad (A.6)
\end{align*}

Simplifying
\begin{align*}
(A_2 + 1) A_0 V_0 - [A_2 A_1 + A_2 + 1] V_1 + V_3 &= 0 \quad (A.7)
\end{align*}
Relationship between $A'$ and $A$:

\[ A_{j-1}' = (A_2 + 1) \frac{A_0}{A_1} \]  \hspace{1cm} (A.8a)

\[ A_j' = (A_2 A_1 + A_2) \]  \hspace{1cm} (A.8b)

**Case 3**  \hspace{1cm} $N = 3$ (compartment with 3 trays)

\[ \begin{array}{c}
V_1 \\
1 \\
2 \\
V_4 \\
V_3 \\
1_3 \\
1_0
\end{array} \]

Relationship between compartmental and tray variables:

\[ V_{j-1}' = V_0 \hspace{.5cm} V_j' = V_1 \hspace{.5cm} V_{j+1}' = V_4 \]

The additional equation for the third tray is:

\[ A_2 V_2 - (A_3 + 1) V_3 + V_4 = 0 \]  \hspace{1cm} (A.9)

Substitute for $V_3$ from equation (A.7) and $V_2$ from equation (A.4) into equation (A.9) to get:

\[ A_2[(A_1 + 1) V_1 - A_0 V_0] - [(A_3 + 1) [-A_2 + 1] A_0 V_0 + [A_2 A_1 + A_2 + 1] V_1] + V_4 = 0 \]  \hspace{1cm} (A.10)

Simplifying will result in:

\[ [A_3 A_2 + A_3 + 1] A_0 V_0 - [A_3 A_2 A_1 + A_3 A_2 + A_3 + 1] V_1 + V_4 = 0 \]  \hspace{1cm} (A.11)
Relationship between $A'$ and $A$

\[ A''_{j-1} = [A_3A_2 + A_3 + 1]A_0 \]  
\[ A'_{j} = [A_3A_2A_1 + A_3A_2 + A_3] \]  

Case 4  \( N = 4 \) (compartment with 4 trays):

\[ \begin{array}{c}
V_1 \\
1 \\
2 \\
3 \\
4 \\
V_5 \\
\end{array} \]

Relationship between compartmental and tray variables

\[ V'_{j-1} = V_0 \; ; \; V'_{j} = V_1 \; ; \; V'_{j+1} = V_5 \]

Equation for the fourth tray is:

\[ A_3V_3 - (A_4 + 1)V_4 + V_5 = 0 \]  
\[ (A.13) \]

Substitute for $V_4$ from equation (A.10) and $V_3$ from (A.7) into equation (A.13) and simplify to get:

\[ [A_4A_3A_2 + A_4A_3 + A_4 + 1]A_0V_0 - [A_4A_3A_2A_1 + A_4A_3A_2 + A_4A_3 + A_4 + 1]V_1 + V_5 = 0 \]  
\[ (A.14) \]
Relationship between $A'$ and $A$

\[ A''_{j-1} = \{ A_4 A_3 A_2 + A_4 A_3 + A_4 \} A_0 \]  \hspace{1cm} (A.15a)

\[ A'_j = [ A_4 A_3 A_2 A_1 + A_4 A_3 A_2 + A_4 A_3 + A_4 ] \]  \hspace{1cm} (A.15b)

These results are summarised in Table 4.1 and general expressions for a compartment with $N$ trays are given in equations (4.10) and (4.11).
APPENDIX—B

DEVELOPMENT OF BILINEAR MODEL FOR
A DISTILLATION COLUMN

In Chapter 5, a bilinear model was developed for a representation, where flows were replaced by the linear combination of manipulated variables. In this section, equations are developed for the second set of representation of flows.

Since the vapours are initiated from the reboiler and liquid flows from the reflux flow rate, therefore one can write:

\[ V'_j = nU_2 + a'_j \quad (B.1) \]
\[ L'_j = U_1 + \beta'_j \quad (B.2) \]

where \( n \) is a constant such that at a steady state vapours generated from the reboiler are given as:

\[ V'_b = nU_2 \quad (B.3) \]

In equation (B.3) and in equation (B.1), \( U_2 \) is equal to:

\[ U_2 = U'_2 - H_{ls} \quad (B.4) \]
where \( U'_2 \) is the actual heat supplied. In the case where the column is insulated \( U_2 = U'_2 \).

The dynamic component material balance for the \( j \)th compartment is given as:

\[
M_j \dot{X}_{ij} = \delta F_j (X_{iF} - X_{ij}) + v_{j+1}(Y_{ij+1} - X_{ij}) \\
+ L_{j-1}(X_{ij-1} - X_{ij}) - v_{j}'(Y_{ij} - X_{ij}) \tag{B.5}
\]

Variable nomenclatures is the same as in Chapter 5.

Substitute equation (B.1) and (B.2) along with equation (5.14) into equation (B.5) to get:

\[
M_j \dot{X}_{ij} = \delta F_j (X_{iF} - X_{ij}) + (\eta U_2 + \alpha'_{j+1}) \\
* (K'_{ij+1}X_{ij+1} - X_{ij}) \tag{B.6}
\]

\[
+ (U_1 + \beta'_{j-1}) \\
* (X_{ij-1} - X_{ij}) - (\eta U_2 + \alpha'_{j}) \\
* (K'_{ij}X_{ij} - X_{ij})
\]

Simplify equation (B.6) and rearrange in the vector form, the equation obtained is:
\[ M_j \dot{x}_{ij} = \]
\[ [\beta'_{j+1} - (\delta F_j + \alpha'_j + \beta'_{j-1} + \alpha'_j (K'_{ij} - 1)), \alpha'_{j+1} K'_{ij+1}] \]
\[ \begin{bmatrix} x_{ij-1} \\ x_{ij} \\ x_{ij+1} \end{bmatrix} \]
\[ + u_1 \begin{bmatrix} 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} x_{ij-1} \\ x_{ij} \\ x_{ij+1} \end{bmatrix} \]
\[ + u_2 \begin{bmatrix} 0 & -n K'_{ij} & n K'_{ij+1} \end{bmatrix} \begin{bmatrix} x_{ij-1} \\ x_{ij} \\ x_{ij+1} \end{bmatrix} \]
\[ + \delta F_j x_{iF} \quad (B.7) \]
Equation (B.7) can be written for all 5 compartments for an extractive distillation column to get equation (5.18) with the following parameters, which completely defines a bilinear state space model.
\[
A = \begin{bmatrix}
\frac{\alpha'}{M_1} & \sqrt{\frac{\alpha'}{M_1}} K_{y2} & 0 & 0 & 0 \\
\frac{\beta'}{M_2} & (\frac{\alpha'}{M_2} + \frac{\beta'}{M_2} + \frac{\alpha'}{M_2} (K_{y2} - 1)) & \frac{\alpha'}{M_2} K_{y3} & 0 & 0 \\
0 & \frac{\beta'}{M_3} & (F_1 + \frac{\alpha'}{M_3} + \frac{\beta'}{M_3} + \frac{\alpha'}{M_3} (K_{y3} - 1)) & \frac{\alpha'}{M_3} K_{y4} & 0 \\
0 & 0 & \frac{\beta'}{M_4} & (F_2 + \frac{\alpha'}{M_4} + \frac{\beta'}{M_4} + \frac{\alpha'}{M_4} (K_{y4} - 1)) & 0 \\
0 & 0 & 0 & \frac{\beta'}{M_5} & -\frac{\beta'}{M_5}
\end{bmatrix}
\]
\[ B_1 = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{M_2} & \frac{-1}{M_2} & 0 & 0 & 0 \\
0 & \frac{1}{M_3} & \frac{-1}{M_3} & 0 & 0 \\
0 & 0 & \frac{1}{M_4} & \frac{-1}{M_4} & 0 \\
0 & 0 & 0 & \frac{1}{M_5} & \frac{-1}{M_5}
\end{bmatrix} \]

\[ B_2 = \begin{bmatrix}
\frac{-n}{M_1} & \frac{nK'_{i2}}{M_1} & 0 & 0 & 0 \\
0 & \frac{-nK'_{i2}}{M_2} & \frac{nK'_{i3}}{M_2} & 0 & 0 \\
0 & 0 & \frac{-nK'_{i3}}{M_3} & \frac{nK'_{i4}}{M_3} & 0 \\
0 & 0 & 0 & \frac{-nK'_{i4}}{M_4} & \frac{nK'_{i5}}{M_4} \\
0 & 0 & 0 & 0 & \frac{-(nK'_{i5} - 1)}{M_5}
\end{bmatrix} \]

\[ E = \begin{bmatrix}
0 & 0 & \frac{F_1 X_{1f}'}{M_3} & \frac{F_2 X_{2f}'}{M_4} & 0
\end{bmatrix} \]

\[ D = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix} \]
Appendix-C

Proof of a selection of $\mu$ in Section 7.3

Condition (c) of section 7.3 regarding the selection of $\mu = S X$ being consistent with the costate equation (7.19) is given here.

Rewriting the Hamiltonian equation (7.16)

$$H = \frac{1}{2} X^T Q X + \frac{1}{2} X^T S C^* R^{-1} C^T S X + \frac{1}{2} U^T R U + \mu^T [A X + C^* U]$$

The costate equation is:

$$\dot{\mu} = \frac{\partial H}{\partial X}$$

(7.19)  

(7.19)

$\mu$ is selected as:

$$\mu = S X$$

Differentiate the Hamiltonian wrt. the state vector $X$, and use equation (C.1) to get:

$$\dot{\mu} = - \frac{\partial H}{\partial X} = - \left[ \frac{\partial X}{\partial X} Q X + \frac{\partial X}{\partial X} (Q X) \right] - \frac{\partial}{\partial X} \left[ \frac{1}{2} X^T S C^* R^{-1} C^T S X \right]$$

$$- \left( \frac{\partial X}{\partial X} A^T \mu \right) - \frac{\partial}{\partial X} [\mu^T C^* U]$$

(C.3)

$$\dot{\mu} = - Q X - \frac{\partial}{\partial X} \left[ \frac{1}{2} X^T S C^* R^{-1} C^T S X \right] - A^T \mu - \frac{\partial}{\partial X} (\mu^T C^* U)$$

(C.4)

Differentiate (C.2) wrt. time and use the system
equation (7.3) to get;
\[ \dot{\mu} = S \dot{x} = S(Ax + C^*U) \]  
(C.5)

Take the difference of equations (C.4) and (C.5) and rearrange results in:

\[ -QX - (A^TS + SA)x - SC^*U - \frac{d}{\hat{\delta}x} \left[ \frac{1}{2} x^T S C^* R^{-1} C^* T S x \right] \]

\[ \frac{d}{\hat{\delta}x} (\mu^T C^* U) = 0 \]  
(C.6)

The requirement is to show that equations (C.6) is correct. Using the equation (7.15)

\[ A^TS + SA = -Q \]  
(7.15)

The L.H.S. of (C.6) becomes:

\[ -QX + QX - SC^*U - \frac{d}{\hat{\delta}x} \left( \frac{1}{2} x^T S C^* R^{-1} C^* T S x \right) - \frac{d}{\hat{\delta}x} (\mu^T C^* U) \]

Term 1  Term 2  Term 3  
(C.7)

Simplify each term in (C.7) separately:

Term 3:

\[ \frac{d}{\hat{\delta}x} (\mu^T C^* U) = \frac{d}{\hat{\delta}x} \left( U^T C^T U \right) \]

since \( \mu^T C^* U \) is a scalar quantity

\[ \frac{d}{\hat{\delta}x} (\mu^T C^* U) = U^T \left( \frac{\partial C^*}{\partial x} \right) \mu \]  
(C.8)

Term 2:

\[ \frac{1}{2} \frac{d}{\hat{\delta}x} \left[ x^T S C^* R^{-1} C^* T S x \right] \]
Define the following terms

\[ X^T S = A_1^T \quad \text{(C.9)} \]

\[ C^* P^{-1} C^{*T} = A_2 \quad \text{(C.10)} \]

then term 2 of (C.7) becomes

\[
\frac{1}{2} \frac{\partial}{\partial X} \left[ A_1^T A_2 A_1^T \right] = \frac{1}{2} \left[ \frac{\partial A_1^T}{\partial X} \right] A_2 A_1 + \frac{1}{2} \left[ \frac{\partial A_1^T}{\partial X} \right] A_2 A_1 + \frac{1}{2} A_1^T \left[ \frac{\partial A_2}{\partial X} \right] A_1
\]

where

\[
\left[ \frac{\partial A_1^T}{\partial X} \right] = \frac{\partial}{\partial X} \left[ X^T S \right] = S
\]

\[ A_2 = A_2^T \quad \text{since } R \text{ is a diagonal matrix thus equation (C.11) becomes:} \]

\[
\frac{1}{2} \frac{\partial}{\partial X} \left[ A_1^T A_2 A_1^T \right] = \frac{1}{2} S A_2 A_1 + \frac{1}{2} S A_2 A_1 + \frac{1}{2} A_1^T \left[ \frac{\partial A_2}{\partial X} \right] A_1
\]

\[
= S A_2 A_1 + \frac{1}{2} A_1^T \left[ \frac{\partial A_2}{\partial X} \right] A_1 \quad \text{(C.12)}
\]

where \( S A_2 A_1 = S C^* R^{-1} C^{*T} S X \)

using equation (7.24) \( S A_2 A_1 = -S C^* U \)

Substitute for \( S A_2 A_1 \) equation (C.12) becomes:

\[
\frac{1}{2} \frac{\partial}{\partial X} \left[ A_1^T A_2 A_1^T \right] = -S C^* U + \frac{1}{2} A_1^T \left[ \frac{\partial A_2}{\partial X} \right] A_1 \quad \text{(C.13)}
\]

Consider
\[
A_1^T \left[ \frac{\partial A_2}{\partial X} \right] A_1 = A_1^T \left[ \frac{\partial}{\partial X} \left( C^{*T} R^{-1} C^* \right) \right] A_1
\]

\[
= A_1^T \left[ C^* R^{-1} \frac{\partial C^*}{\partial X} + \left( \frac{\partial C^{*T}}{\partial X} \right) R^{-1} C^{*T} \right] A_1
\]

Substitute for \( A_1 \) to get:

\[
= X^T S C^* R^{-1} \frac{\partial C^*}{\partial X} SX + X^T S \left( \frac{\partial C^{*T}}{\partial X} \right) \bar{R}^{-1} C^{*T} SX
\]

using equation (7.24)

\[
= - U^T \left( \frac{\partial C^*}{\partial X} \right) \mu - U^T \left( \frac{\partial C^{*T}}{\partial X} \right) U
\]

\[
= -2 U^T \left( \frac{\partial C^*}{\partial X} \right) \mu
\]

or term 2 of equation (C.7) is equal to:

\[
\frac{1}{2} \frac{\partial}{\partial X} \left( X^T S C^* R^{-1} C^{*T} SX \right) = - U^T C^* \frac{\partial \mu}{\partial X} - S C^* U
\]

Substitute the values of term 2 and term 3 in equation (C.7) to get:

\[
- S C^* U + S C^* U + U^T \frac{\partial C^*}{\partial X} \mu - U^T \frac{\partial C^*}{\partial X} U = 0
\]

This proves the validity of the selection of \( \mu = SX \).
Appendix --D

System Matrices for Bilinear Model

Part 1

The following are the system matrices for the bilinear state equation for the 5 compartment model. Only the acetone composition in the top product is being controlled.

****** A Matrix ******

\[
\begin{array}{cccccc}
-59.07 & 73.31 & 0.0 & 0.0 & 0.0 \\
5.11 & -14.21 & 26.49 & 0.0 & 0.0 \\
0.0 & 1.93 & -14.99 & 12.50 & 0.0 \\
0.0 & 0.0 & 5.51 & -24.00 & 23.88 \\
0.0 & 0.0 & 0.0 & 2.49 & -9.14 \\
\end{array}
\]

****** B1 Matrix ******

\[
\begin{array}{cccccc}
-0.433 & 0.537 & 0.0 & 0.0 & 0.0 \\
0.037 & -0.051 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0152 & -0.0152 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.042 & -0.042 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0194 & -0.0194 \\
\end{array}
\]

****** B2 Matrix ******

\[
\begin{array}{cccccc}
0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & -0.004 & 0.016 & 0.0 & 0.0 \\
0.0 & -0.0001 & -0.006 & 0.008 & 0.0 \\
0.0 & 0.0 & -0.0001 & -0.009 & 0.0145 \\
0.0 & 0.0 & 0.0 & -0.0001 & -0.0039 \\
\end{array}
\]
**** C Matrix *****

\[
\begin{array}{cccccccccc}
0.0 & 0.0 \\
0.071 & 0.004 \\
0.0142 & 0.002 \\
0.0151 & 0.001 \\
0.0021 & -0.0001 \\
\end{array}
\]

Part 2

System matrices for dual composition control cases.

**** A Matrix *****

\[
\begin{array}{cccccccccc}
-59.07 & 73.31 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
5.11 & -14.21 & 26.49 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 1.93 & -14.99 & 12.5 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 5.51 & -24.0 & 23.88 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 2.49 & -9.15 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -59.07 & 99.50 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 5.11 & -17.60 & 3.02 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.93 & -5.43 & 2.18 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 5.51 & -10.45 & 8.88 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.49 & -4.22 & 0.0 \\
\end{array}
\]

**** B_1 Matrix *****

\[
\begin{array}{cccccccccc}
-0.29 & 0.36 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.03 & -0.03 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.01 & -0.01 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.02 & -0.02 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.01 & -0.01 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -0.29 & 0.48 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.04 & -0.04 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.02 & -0.02 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.02 & -0.02 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.01 & -0.01 & 0.0 \\
\end{array}
\]
**Matrix B**

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**Matrix C**

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</table>
Appendix E

System Matrices for Water/Steam Configuration

System matrices for the bilinear model of the extractive distillation column for the water flow rate and steam pressure as the manipulated variables. The bilinear model is given below:

\[
\dot{X} = A \dot{X} + U_1 B_1 X + U_2 B_2 X + C U + D
\]

where

- \( U_1 = \text{Water flow Rate} \)
- \( U_2 = \text{Steam pressure} \)

other variables are defined in Chapter 8 nomenclature

Matrices \( A, B_1, B_2, C \) are given below:

\[
A = \begin{bmatrix}
\frac{-\alpha_2}{M_1} & \frac{\alpha_2 K_{2i}^d}{M_1} & 0 & 0 & 0 \\
\frac{\beta_1}{M_2} & \frac{-(\alpha_3 + \beta_1 + \alpha_2 (K_{2i}^d - 1))}{M_2} & \frac{\alpha_3 K_{3i}^d}{M_2} & 0 & 0 \\
0 & \frac{\beta_2}{M_3} & \frac{-(\alpha_4 + \beta_2 + \alpha_3 (K_{3i}^d - 1))}{M_3} & \frac{\alpha_4 K_{4i}^d}{M_3} & 0 \\
0 & 0 & \frac{\beta_3}{M_4} & \frac{-(\alpha_5 + \beta_3 + \alpha_4 (K_{4i}^d - 1))}{M_4} & 0 \\
0 & 0 & 0 & \frac{\beta_4}{M_5} & \frac{-\beta_4}{M_5}
\end{bmatrix}
\]