THE APPLICATION OF OPTIMAL CONTROL

TO A PILOT SCALE DISTILLATION COLUMN

by

P J King
This work is concerned with the application of optimal control methods to a pilot scale distillation column. A dynamic model of the column is derived from physical equations and the model results are verified by comparison with those obtained in practice. A reduced order model of the column was also obtained by calculating model frequency responses.

Optimal control systems to regulate the column are designed using Kalman's formulation of Bellman's dynamic programming principle. A quadratic cost function and a linearised plant model are used to obtain a state feedback and feedforward control system. Methods of reducing the number of measurements required for optimal control are investigated, including the use of an observer system and the elimination of control coefficients using a penalty function.

The optimal control was tested using computer simulation and online to the distillation column under direct digital computer control. The results were compared with those obtained using discrete-time two-term control systems. An approximate method of achieving time optimal control was also investigated.
ACKNOWLEDGEMENTS

I wish to thank my supervisor Dr B Reasor of the University of Surrey for his guidance during the period of this work. I also wish to thank Mr P H Hamond and his staff at both the National Physical Laboratory and Warren Spring Laboratory for their assistance, and especially to G Jackson, R Malsall, I Leitch and K Wilkinson for maintaining the experimental system. I am also indebted to R Weekes and M Sunderland who have contributed freely to this work in informal discussions.

Finally I would like to thank the Science Research Council for supporting me financially while working on this project.
# LIST OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract</td>
<td>2</td>
</tr>
<tr>
<td>Acknowledgements</td>
<td>3</td>
</tr>
<tr>
<td>List of Contents</td>
<td>4</td>
</tr>
<tr>
<td>List of Symbols</td>
<td>7</td>
</tr>
<tr>
<td>Chapter 1. The Computer Control of Distillation Columns</td>
<td></td>
</tr>
<tr>
<td>1.1 Introduction</td>
<td>15</td>
</tr>
<tr>
<td>1.2 Outline of this Work</td>
<td>16</td>
</tr>
<tr>
<td>1.3 Original Contributions</td>
<td>17</td>
</tr>
<tr>
<td>Chapter 2. The Control Scheme of Grethlein and Lapidus</td>
<td></td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>19</td>
</tr>
<tr>
<td>2.2 Control Strategy</td>
<td>20</td>
</tr>
<tr>
<td>2.3 Theoretical Results</td>
<td>20</td>
</tr>
<tr>
<td>2.4 Simulated Results</td>
<td>21</td>
</tr>
<tr>
<td>2.5 Conclusions</td>
<td>21</td>
</tr>
<tr>
<td>Chapter 3. A Dynamic Model of a Distillation Column</td>
<td></td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>23</td>
</tr>
<tr>
<td>3.2 General Considerations</td>
<td>23</td>
</tr>
<tr>
<td>3.3 Analogue Computer Solutions</td>
<td>27</td>
</tr>
<tr>
<td>3.4 Digital Computer Solutions</td>
<td>28</td>
</tr>
<tr>
<td>3.5 The Pilot Scale Distillation Column</td>
<td>30</td>
</tr>
<tr>
<td>3.6 A Model of the N.P.L. Column</td>
<td>31</td>
</tr>
<tr>
<td>3.7 Linearising the Equations</td>
<td>37</td>
</tr>
<tr>
<td>3.8 Conclusions</td>
<td>38</td>
</tr>
</tbody>
</table>
Chapter 4. The Solution of the Equations

4.1 Introduction 40
4.2 General Considerations 40
4.3 The Steady State Programme 44
4.4 Transient Response Programme 45
4.5 Solution of the Linearised Equations 46
4.6 Comparison of the Programmes 49
4.7 Conclusions 50

Chapter 5. Model Performance

5.1 Introduction 52
5.2 Steady State Results 52
5.3 Step Responses 58
5.4 Comparison of Linear and Non-linear Models 66
5.5 Model Frequency Responses 71
5.6 Conclusions 79

Chapter 6. The Control of Distillation Columns - Theory

6.1 Introduction 85
6.2 General Considerations 85
6.3 Digital Control System Design Methods 89
6.4 The Design of Integrated Control Systems 94
6.5 Optimal Linear Regulator Theory 96
6.6 Reducing the Number of Measurements 99
6.7 Conclusions 109

Chapter 7. The Control of Distillation Columns - Design and Simulation
### LIST OF SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>a matrix</td>
<td>37</td>
</tr>
<tr>
<td>$A_0(k)$</td>
<td>a matrix chosen to minimise the estimate error covariance</td>
<td>105</td>
</tr>
<tr>
<td>$A_r$</td>
<td>a matrix</td>
<td>104</td>
</tr>
<tr>
<td>$a_{ij}$</td>
<td>an element of $A$</td>
<td>37</td>
</tr>
<tr>
<td>$a$</td>
<td>coefficient in the enthalpy equation</td>
<td>35</td>
</tr>
<tr>
<td>$a_i$</td>
<td>control equation coefficient</td>
<td>147</td>
</tr>
<tr>
<td>$B$</td>
<td>a matrix</td>
<td>37</td>
</tr>
<tr>
<td>$B(z)$</td>
<td>adjoint matrix polynomial, a function of $z$</td>
<td>136</td>
</tr>
<tr>
<td>$B_K$</td>
<td>$K$th matrix of $B(z)$</td>
<td>136</td>
</tr>
<tr>
<td>$b_{ij}$</td>
<td>an element of $B$</td>
<td>37</td>
</tr>
<tr>
<td>$b$</td>
<td>coefficient in the enthalpy equation</td>
<td>35</td>
</tr>
<tr>
<td>$b_i$</td>
<td>control equation coefficient</td>
<td>147</td>
</tr>
<tr>
<td>$C$</td>
<td>a matrix</td>
<td>73</td>
</tr>
<tr>
<td>$C_r$</td>
<td>control matrix evaluated over $r$ stages</td>
<td>98</td>
</tr>
<tr>
<td>$C_{Er}$</td>
<td>control matrix with zero elements</td>
<td>100</td>
</tr>
<tr>
<td>$C_{pj}$</td>
<td>specific heat of liquid of composition $x_j$</td>
<td>33</td>
</tr>
<tr>
<td>$c$</td>
<td>coefficient in the enthalpy equation</td>
<td>35</td>
</tr>
<tr>
<td>$D$</td>
<td>distillate flow rate ($\text{gm-moles/min}$)</td>
<td>33</td>
</tr>
<tr>
<td>$D$</td>
<td>state vector weighting matrix</td>
<td>96</td>
</tr>
<tr>
<td>$D(z)$</td>
<td>sampled data control system transfer function</td>
<td>91</td>
</tr>
<tr>
<td>$d$</td>
<td>coefficient in the enthalpy equation</td>
<td>35</td>
</tr>
<tr>
<td>$d(k)$</td>
<td>vector of random disturbances</td>
<td>105</td>
</tr>
<tr>
<td>$d(z)$</td>
<td>determinant of $z$ transform matrix</td>
<td>136</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>d_k</td>
<td>coefficient of d(z)</td>
<td>136</td>
</tr>
<tr>
<td>E</td>
<td>a matrix</td>
<td>73</td>
</tr>
<tr>
<td>E_j</td>
<td>plate efficiency factor for plate j</td>
<td>26</td>
</tr>
<tr>
<td>E(z)</td>
<td>system error z-transformed</td>
<td>91</td>
</tr>
<tr>
<td>e_i</td>
<td>past value of error</td>
<td>147</td>
</tr>
<tr>
<td>F_j</td>
<td>feed flow rate to plate; (gm-moles/min)</td>
<td>25</td>
</tr>
<tr>
<td>F(z)</td>
<td>z-transform of column feed flow rate</td>
<td>89</td>
</tr>
<tr>
<td>G</td>
<td>a matrix</td>
<td>73</td>
</tr>
<tr>
<td>G</td>
<td>process gain</td>
<td>77</td>
</tr>
<tr>
<td>G_j</td>
<td>coefficient of the jth equation</td>
<td>45</td>
</tr>
<tr>
<td>G_r</td>
<td>a symmetric matrix for the rth stage</td>
<td>97</td>
</tr>
<tr>
<td>G(z)</td>
<td>process z transfer function</td>
<td>89</td>
</tr>
<tr>
<td>g(x,t)</td>
<td>a function</td>
<td>41</td>
</tr>
<tr>
<td>H</td>
<td>forcing function weighting matrix</td>
<td>96</td>
</tr>
<tr>
<td>H_j</td>
<td>liquid holdup on plate j (gm-moles)</td>
<td>25</td>
</tr>
<tr>
<td>h_j</td>
<td>vapour holdup on plate j (gm-moles)</td>
<td>25</td>
</tr>
<tr>
<td>I</td>
<td>the identity matrix</td>
<td>46</td>
</tr>
<tr>
<td>I_1</td>
<td>a matrix</td>
<td>100</td>
</tr>
<tr>
<td>I_j</td>
<td>enthalpy of saturated liquid of composition x_j (cals/gm-mole)</td>
<td>25</td>
</tr>
<tr>
<td>I_j</td>
<td>enthalpy of liquid of composition x_j cooled below its boiling point (cals/gm-mole)</td>
<td>25</td>
</tr>
<tr>
<td>i</td>
<td>an index</td>
<td>37</td>
</tr>
<tr>
<td>J_j</td>
<td>enthalpy of saturated vapour of composition y_j (cals/gm-mole)</td>
<td>25</td>
</tr>
<tr>
<td>j</td>
<td>an index</td>
<td>37</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>j</td>
<td>( \sqrt{-1} ), complex operator</td>
<td>73</td>
</tr>
<tr>
<td>K</td>
<td>a constant</td>
<td>53</td>
</tr>
<tr>
<td>( K_j )</td>
<td>slope of vapour-liquid curve at composition ( x_j )</td>
<td>70</td>
</tr>
<tr>
<td>( K(z) )</td>
<td>sampled data closed loop transfer function</td>
<td>91</td>
</tr>
<tr>
<td>( K(k) )</td>
<td>estimate error covariance matrix</td>
<td>105</td>
</tr>
<tr>
<td>k</td>
<td>an index</td>
<td>46</td>
</tr>
<tr>
<td>L</td>
<td>sampled data time constant of open loop system</td>
<td>91</td>
</tr>
<tr>
<td>( L_j )</td>
<td>liquid flow rate from plate ( j ) (g mole/min)</td>
<td>25</td>
</tr>
<tr>
<td>l</td>
<td>number of available measurements</td>
<td>101</td>
</tr>
<tr>
<td>( l )</td>
<td>perturbation of flow from steady state</td>
<td>70</td>
</tr>
<tr>
<td>M</td>
<td>approximation matrix</td>
<td>47</td>
</tr>
<tr>
<td>( M )</td>
<td>system measurement matrix</td>
<td>101</td>
</tr>
<tr>
<td>N</td>
<td>number of column plates</td>
<td>35</td>
</tr>
<tr>
<td>( N )</td>
<td>number of sampling intervals in time delay</td>
<td>91</td>
</tr>
<tr>
<td>P</td>
<td>system state transition matrix</td>
<td>46</td>
</tr>
<tr>
<td>( p(\cdot) )</td>
<td>a function</td>
<td>99</td>
</tr>
<tr>
<td>Q</td>
<td>sampled data time constant of closed loop system</td>
<td>92</td>
</tr>
<tr>
<td>( Q_j )</td>
<td>heat supplied to plate ( j ) (cals/min)</td>
<td>25</td>
</tr>
<tr>
<td>( Q_{Lj} )</td>
<td>heat lost from plate ( j ) (cals/min)</td>
<td>35</td>
</tr>
<tr>
<td>( Q_o )</td>
<td>heat supplied to the column reboiler (cals/min)</td>
<td>33</td>
</tr>
<tr>
<td>( Q_o )</td>
<td>heat removed by the condenser (cals/min)</td>
<td>33</td>
</tr>
<tr>
<td>( Q(z) )</td>
<td>( z )-transform of column heat input</td>
<td>89</td>
</tr>
<tr>
<td>R</td>
<td>reflux ratio</td>
<td>35</td>
</tr>
<tr>
<td>R</td>
<td>remainder matrix</td>
<td>47</td>
</tr>
<tr>
<td>R</td>
<td>number of performance criterion terms summed</td>
<td>88</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td></td>
</tr>
<tr>
<td>$R$</td>
<td>a matrix</td>
<td></td>
</tr>
<tr>
<td>$R(z)$</td>
<td>$z$-transform of the reflux ratio</td>
<td></td>
</tr>
<tr>
<td>$r_{ij}$</td>
<td>element of the remainder matrix</td>
<td></td>
</tr>
<tr>
<td>$r$</td>
<td>an index</td>
<td></td>
</tr>
<tr>
<td>$S_j$</td>
<td>coefficient in equation $j$</td>
<td></td>
</tr>
<tr>
<td>$S$</td>
<td>discrete forcing function matrix</td>
<td></td>
</tr>
<tr>
<td>$SP(z)$</td>
<td>$z$-transform of set point value</td>
<td></td>
</tr>
<tr>
<td>$s$</td>
<td>laplace operator</td>
<td></td>
</tr>
<tr>
<td>$T$</td>
<td>linear transformation matrix</td>
<td></td>
</tr>
<tr>
<td>$T_j$</td>
<td>temperature of liquid on plate $j$ ($°C$)</td>
<td></td>
</tr>
<tr>
<td>$T_{Bj}$</td>
<td>boiling temperature of liquid on plate $j$ ($°C$)</td>
<td></td>
</tr>
<tr>
<td>$T_j$</td>
<td>coefficient in equation $j$</td>
<td></td>
</tr>
<tr>
<td>$T_d$</td>
<td>time delay matrix or time delay for a simple process</td>
<td></td>
</tr>
<tr>
<td>$T_c$</td>
<td>time constant of first order process</td>
<td></td>
</tr>
<tr>
<td>$t$</td>
<td>time</td>
<td></td>
</tr>
<tr>
<td>$U$</td>
<td>column forcing function vector</td>
<td></td>
</tr>
<tr>
<td>$U_j$</td>
<td>coefficient in equation $j$</td>
<td></td>
</tr>
<tr>
<td>$U(s)$</td>
<td>laplace transform of system input</td>
<td></td>
</tr>
<tr>
<td>$u$</td>
<td>perturbation of column forcing function vector</td>
<td></td>
</tr>
<tr>
<td>$u(k)$</td>
<td>value of forcing function vector at time $k$</td>
<td></td>
</tr>
<tr>
<td>$V$</td>
<td>steady state vapour flow rate</td>
<td></td>
</tr>
<tr>
<td>$V_j$</td>
<td>vapour flow rate from plate $j$ (gm moles/min)</td>
<td></td>
</tr>
<tr>
<td>$V_o$</td>
<td>covariance matrix of state vector noise corruption</td>
<td></td>
</tr>
<tr>
<td>$v$</td>
<td>perturbation of vapour flow rate</td>
<td></td>
</tr>
<tr>
<td>$W$</td>
<td>column bottom flow rate (gm moles/min)</td>
<td></td>
</tr>
<tr>
<td>$W_o$</td>
<td>covariance matrix of measurement noise</td>
<td></td>
</tr>
</tbody>
</table>
\( x(k) \) \hspace{1cm} \text{vector of measurement noise corruptions} \\
\( x \) \hspace{1cm} \text{column composition state vector} \\
\( x_j \) \hspace{1cm} \text{steady state composition on plate } j \\
\( x(s) \) \hspace{1cm} \text{system open-loop transfer function} \\
\( x(z) \) \hspace{1cm} \text{system open-loop z-transfer function} \\
\( x \) \hspace{1cm} \text{column composition perturbation vector} \\
\( x_j \) \hspace{1cm} \text{composition of liquid on plate } j \\
\( x(t) \) \hspace{1cm} \text{value of } x \text{ at time } t \\
\( x(k) \) \hspace{1cm} \text{discrete system state vector at time } kT \\
\( y_j \) \hspace{1cm} \text{steady state vapour composition} \\
\( y(k) \) \hspace{1cm} \text{vector space of vectors } y(i) \text{ to } y(k) \\
\( y_j \) \hspace{1cm} \text{composition of vapour on plate } j \\
\( y_j^\circ \) \hspace{1cm} \text{composition of vapour in equilibrium with liquid of composition } x_j \\
\( y(k) \) \hspace{1cm} \text{vector of available measurements} \\
\( z(z) \) \hspace{1cm} \text{z transform of feed composition} \\
\( z \) \hspace{1cm} \text{forward shift operator} \\
\( z_j \) \hspace{1cm} \text{feed composition to plate } j \\
\( z(k) \) \hspace{1cm} \text{observer state vector at time } kT \\

**Greek Symbols** \\
\( \alpha \) \hspace{1cm} \text{enthalpy factor } (d-c)/(b-a) \\
\( \beta \) \hspace{1cm} \text{enthalpy factor } (b-c) \\
\( \Delta \) \hspace{1cm} \text{increase in cost due to use of an observer} \\
\( e \) \hspace{1cm} \text{error ratio} \\
\( \theta \) \hspace{1cm} \text{a coefficient}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta_r )</td>
<td>cost calculated over ( r ) stages</td>
<td>97</td>
</tr>
<tr>
<td>( \lambda )</td>
<td>performance criterion weighting coefficient</td>
<td>96</td>
</tr>
<tr>
<td>( \mu )</td>
<td>an eigen value</td>
<td>106</td>
</tr>
<tr>
<td>( \sigma )</td>
<td>lagrange multiplier</td>
<td>99</td>
</tr>
<tr>
<td>( \tau )</td>
<td>sampling interval</td>
<td>44</td>
</tr>
<tr>
<td>( \omega )</td>
<td>angular frequency</td>
<td>75</td>
</tr>
</tbody>
</table>

**Prefix**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta )</td>
<td>change in a variable</td>
<td>41</td>
</tr>
</tbody>
</table>

**Superscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>( o )</td>
<td>optimal value</td>
<td>104</td>
</tr>
<tr>
<td>( A )</td>
<td>estimated value or component resolved in a</td>
<td>104</td>
</tr>
<tr>
<td></td>
<td>vector space</td>
<td></td>
</tr>
<tr>
<td>( \nu )</td>
<td>orthogonal component</td>
<td>104</td>
</tr>
</tbody>
</table>

**Subscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>( j )</td>
<td>column plate number ( j )</td>
<td>25</td>
</tr>
<tr>
<td>( n )</td>
<td>enriching section plate</td>
<td>36</td>
</tr>
<tr>
<td>( n )</td>
<td>stripping section plate</td>
<td>39</td>
</tr>
<tr>
<td>( f )</td>
<td>feed plate</td>
<td>39</td>
</tr>
<tr>
<td>( O )</td>
<td>condenser</td>
<td>33</td>
</tr>
<tr>
<td>( N+1 )</td>
<td>reboiler</td>
<td>39</td>
</tr>
<tr>
<td>( s )</td>
<td>steady state value</td>
<td>37</td>
</tr>
<tr>
<td>( T )</td>
<td>transfer function relating to column upper</td>
<td>89</td>
</tr>
<tr>
<td></td>
<td>measurement point</td>
<td></td>
</tr>
<tr>
<td>( B )</td>
<td>transfer function relating to column lower</td>
<td>89</td>
</tr>
<tr>
<td></td>
<td>measurement point</td>
<td></td>
</tr>
</tbody>
</table>
1) Introduction

The work described here covers the following fields:

i) Distillation Column Control

Distillation columns have received a great deal of attention in the last 20 years. Much of the effort has been devoted to developing improved dynamic models, based on the physical equations of the process, which have been used to predict column behaviour over a wide range of operating conditions. The use of these models in control system design has been limited as a model in matrix form is obtained rather than in transfer function form.

Column feedback control has in general been restricted to single-variable two or three term control of pressures, temperatures and flows. Interaction between control loops has been reported but industrial users have avoided this problem by leaving "difficult" (interacting) loops under manual control.

The most significant recent development has been the widespread use of feedforward control. Disturbances are sensed before entering the column and control variables are manipulated, according to a mathematical
model of the plant, to compensate for their effect. This type of predictive control has obvious advantages when long process time delays occur, and successful applications have been reported.

ii) Computer Control

In the last decade considerable progress has been made in the use of digital computers to control chemical plant. This has stimulated interest in sampled-data control theory and much work has been done on the design of digital control systems.

Computer control systems have not been responsible for any great improvement in process control for the following reasons:

a) No significant improvements in control have been achieved, in most installations digital control systems are designed to reproduce the functions of analogue control systems.

b) The effort required to prepare computer control programmes is large, systems programme development time ranges from fifty to one hundred man-years and applications programming for a specific plant can take a further twenty man-years.

c) In most applications the computer is used to monitor plant measurements and prepare data logs.
iii) Optimal Control Theory

In the last decade a great deal of effort has been devoted to optimal control theory. A control system is designed to optimise a performance criterion to achieve control yielding minimum cost in some sense. While many mathematical results and optimising techniques have been developed little of this work has been applied in practice. This is due to several factors:-

a) The optimal control design calculations are complex and the results are not usually obtained in closed form, and an open loop control strategy results.

b) It has proved extremely difficult to formulate a realistic performance criterion for most practical control problems.

c) Plant models used in the chemical industry are based on simple tests, e.g. step function inputs, whereas optimal control problems are usually formulated in terms of matrices. The optimal solution often requires more measurements than are generally available.

Optimal control theory has been of use in indicating what the best control solution is likely to be and in suggesting suboptimal solutions which can yield improved control.
2) Outline of this Work

The increasing "gap" between control theory and practice, and the lack of success in using the full power of the digital computer in process control are serious problems. In this work an attempt has been made to close the "gap" by designing optimal digital control systems for a pilot scale distillation column and comparing the results obtained with current industrial practice. Distillation column control presents two main problems:-

i) To change the columns state in minimum time, the start-up and shut-down problem.

ii) To regulate the column at steady state in the presence of disturbances.

When applying optimal control theory to a practical plant approximations must be made to simplify the problem. This is particularly true in the start-up case where:-

i) The column behaviour is non-linear

ii) To obtain the complete optimal solution a two point boundary value problem must be solved.

An approximate method of obtaining time optimal control suggested by Grethlein and Lapidus\(^1\), described in Chapter 2, was tested on simple second order systems. It was found to be unsuitable and further effort was devoted to the problem of column regulation.
In Chapter 3 a plant model based on the physical equations of the process is described. The model is in matrix form and is well suited to use in optimal controller design. In Chapter 4 the solution of the model equations using a digital computer is discussed, and in Chapter 5 the model is compared with observed results to check its validity. A method of reducing the model order is also presented.

In Chapter 6 methods of designing multi-variable feedforward and feedback control systems using optimal control theory are presented. Two methods of reducing the number of measurements required by these control systems are also discussed. In Chapter 7, the control systems designed for the N.P.L. column are tested by digital computer simulation. Finally, in Chapter 8 these control methods are applied on-line to the N.P.L. column under digital computer control. The results obtained are compared with those obtained using discrete-time two-term control systems.

The results show that the optimal control system does not offer any significant improvement in column control in this case. Since contrary claims have been made in the published literature on the theory of optimal control, the present work should provide a more realistic assessment of the potential advantages of this type of control.

3) Original Contributions

These are considered to be:
a) A critical assessment of the control scheme of Grethlein and Lapidus.
b) The use of heat losses in the column model instead of the plate efficiency factor.
c) The use of a frequency response programme to reduce the order of a column model.
d) The practical application of multivariable controllers designed using the optimal linear regulator method.
e) The use of an observer in a practical control situation to estimate plant measurements.
f) A practical comparison between an optimal linear control system and discrete-time two-term control.
CHAPTER 2

THE CONTROL SCHEME OF GRETHLEIN AND LAPIDUS

1) Introduction

The optimal on-off control of distillation columns, offers the following advantages:

i) Column start up can be optimised by making large state changes in minimum time.

ii) Regulation can be improved by correcting deviations from a desired state in minimum time.

iii) Batch distillation can be optimised by distilling a batch in the shortest possible time.

However, time optimal control is difficult to apply as a two-point boundary value problem has to be solved to calculate the correct switching times. This requires a great deal of computer time and is not suitable for on-line control applications.

Sub-optimal on-off control strategies which require limited on-line calculation, but give only a small degradation in performance can be used. Rees suggested that a scheme devised by Grethlein and Lapidus, to obtain approximate time optimal control, was suitable for the N.P.L. column. The scheme was assessed by computer simulation when controlling a simple second order system. The results obtained were compared with theory and were published as an N.P.L. report, which is included in this
volume as Appendix 1. The results of that investigation are summarised briefly here.

2) Control Strategy

The control scheme was based on a sampled data approach, and the assumption that time optimal control is on-off for most physical systems. At each sampling interval a plant model was used to predict the system state if three possible input values were applied, the two limit values and some intermediate value. These predicted values were used to evaluate a quadratic cost function of the system state, for the next sampling interval and the value of control which minimised it was applied to the system. If the intermediate value was used, a second order curve was fitted to the three values and the control which minimised this curve was applied to the system.

3) Theoretical Results

The time optimal control of a simple second order system was calculated using Pontryagins maximum principle, and it was shown that an on-off control resulted. The optimal control with a state error quadratic performance criterion, similar to that used by Grethlein and Lapidus was also calculated. The optimal control was on-off, but with singular intervals, where the Hamiltonian function is not an explicit function of the control. The singular control gave linear phase plane trajectories.
4) **Simulated Results**

The simple second order system was simulated on a digital computer under the control of the Grethlein and Lapidus scheme. The results obtained showed that:

i) System performance depended on the values assigned to performance criterion weighting coefficients.

ii) With the correct weighting coefficient values approximate time optimal control could result but the control also depended on the initial error value.

iii) The intermediate control also gave linear phase plane trajectories but these were not related to the optimal singular trajectories.

iv) The performance criterion for the whole trajectory was not minimised using a one sampling interval prediction.

5) **Conclusions**

The results obtained show that approximately time optimal control can result using the Grethlein and Lapidus strategy. However the control schemes performance depends entirely on the values assigned to performance criterion weighting coefficients and the magnitude of the error. A theoretical analysis shows that the assumption of "on-off" control is not always justified.
It was concluded that the method is too sensitive to these effects to be used in practice. As the column is highly non-linear it was felt that any approximate method of time optimal control for large state changes will be difficult to implement in practice. In the next chapter the problems of column modelling are discussed in more detail.
CHAPTER 3

A DYNAMIC MODEL OF A DISTILLATION COLUMN

1) Introduction

In this chapter equations describing the dynamic behaviour of a plate distillation column are presented. The equations are derived from the plate material and enthalpy balances to give a set of non-linear differential equations describing the column composition dynamics. The validity of the simplifying assumptions involved are discussed, and attention is given to the problems encountered in modelling the six plate column at N.P.L. Finally the equations are presented in linearised form suitable for the design of linear control systems.

2) General Considerations

The basic differential equations describing distillation column dynamics were first presented by Marshall and Pigford in 1947. They consist of the light component, material and enthalpy differential balances for each plate and are briefly presented here for a binary system.

Fig. (3.1) shows the conditions at three adjacent plates $j+1$, $j$, and $j-1$ in a binary distillation column. On plate $j$ quantities of liquid
FIG. 3.1. THREE COLUMN PLATES.
H_1 of composition x_j, and vapour h_j of composition y_j, are held up. Liquid of composition z_j is fed onto plate j with a flow rate F_j. A vapour stream of composition y_j with a flow rate V_j and a liquid stream of composition x_j with a flow rate L_j leave plate j; while vapour of composition y_{j+1} and liquid of composition x_{j-1} with flow rates of V_{j+1} and L_{j-1} arrive at plate j from the plates below and above respectively.

Then for plate j the following balance equations can be written:

a) Total material balance

\[ \frac{dH_j}{dt} + \frac{dh_j}{dt} = L_{j-1} - L_j + V_{j+1} - V_j + F_j. \]  \hspace{1cm} (1)

b) Light component material balance

\[ \frac{d(h_j x_j + h_j y_j)}{dt} = L_{j-1} x_{j-1} - L_j x_j + V_{j+1} y_{j+1} - V_j y_j + F_j z_j. \]  \hspace{1cm} (2)

c) Enthalpy balance

\[ \frac{d}{dt} (H_j I_j + h_j J_j) = L_{j-1} I_{j-1} - L_j I_j + V_{j+1} J_{j+1} - V_j J_j + Q_j + F_j I_j^e. \]  \hspace{1cm} (3)

Where I_j is the enthalpy of saturated liquid with composition x_j,

J_j is the enthalpy of saturated vapour with composition y_j,

I_j^e is the enthalpy of liquid with composition z_j, which may not be boiling,

and Q_j is the heat transfer to plate j.

The composition of vapour leaving plate j, under ideal conditions will be in equilibrium with that of the boiling liquid and is defined by the vapour-liquid equilibrium relationship for the mixture,
In practice, equilibrium may not be attained and the vapour composition \( y_j \) will differ from the equilibrium vapour composition \( y_j^* \). The extent of this deviation is defined by the plate efficiency factor,

\[
y_j = f(x_j) \quad (4)
\]

\[
E_j = \frac{y_j^* - y_{j-1}}{y_j^* - y_j} \quad (5)
\]

The balance equations (1) to (3) are exact and have formed the basis of all physical models proposed for distillation columns. However, they do not define a solution to the problem unless further equations based on suitable simplifying assumptions are specified. Common assumptions are as follows:

a) Binary mixture.

b) The liquid and vapour in each column stage are perfectly mixed.

c) The column consists of ideal plates, \( E_j = 1 \). This usually includes the reboiler.

d) The column operates at constant pressure.

e) Vapour holdup \( h_j \) is negligible. This assumption means that composition dynamics due to vapour holdup and vapour flow dynamics are neglected.

f) Column operation is adiabatic.

g) The components have similar latent heats. This together with assumption (f) means that the enthalpy balance is ignored and \( V_j = V_{j-1} \) and \( L_j = L_{j-1} \), except at the feed plate.
h) The liquid holdup $H_j$ is independent of time and liquid flow dynamics are neglected.

i) Only small changes in operating conditions are of interest and the equations can be linearised.

j) $E_j$ is independent of time.

k) The column is in overall steady state balance.

All or some of these assumptions have been used to derive dynamic models of distillation columns. In general the choice of assumptions depends in part on the way in which the equations are to be solved. These methods can be divided into two main types, described in the next two sections.

3) Analogue computer solutions

The use of an analogue computer normally means that the distillation column equations must be linearised. A non-linear model would require at least one multiplier and one function generator for each plate. This limits the order of a non-linear problem and makes setting up difficult.

The model developed by Lamb, Pigford and Rippin is typical of this group. They use all the assumptions except (c) and (h) to derive a linearised model describing liquid flow and composition dynamics, the change in liquid flow rate transmitted from one plate to the next is described by a first order lag. Gerster et al. compared this model with practical results and reported good agreement for small changes in operating conditions.
Rijnsdorp\textsuperscript{7} proposed a linearised model using assumptions (a), (b), (c), (e), (f), (g), (i), (j) and (k) and solved the equations on an analogue computer in which a large number of passive networks were used. The model included pressure, liquid flow and composition dynamics and included the effect of vapour flow rate changes on the liquid flow dynamics. Following a change in vapour flow rate the plate liquid holdup was found to decrease causing a temporary increase in liquid flow rate to the plate below. This effect could cause a column to exhibit an inverse response under certain circumstances and by adjusting a coefficient Rijnsdorp was able to reproduce this effect with his model.

4) \textit{Digital computer solutions}

Numerical solutions can be obtained by solving the equations using a digital computer. This approach is not confined to linearised models but the problem arises of finding a stable and accurate numerical integration method.

Rosenbrock\textsuperscript{8} used assumptions (a), (b), (c), (d), (e), (f), (g), (h), (j) and (k) to develop a non-linear dynamic model based on the mass balance equations. He paid particular attention to the numerical difficulties encountered in solving the equations on a digital computer and suggested means of overcoming them. The model was extended\textsuperscript{9} to include multicomponent mixtures and was compared with practical results from an eight plate three-component column.
Huckaba, May and Franke\textsuperscript{10} used assumptions\,(a),\,(b),\,(c),\,(d),\,(e),\,(f),\,(h),\,(j)\,and\,(k)\,to\,derive\,a\,model\,describing\,composition\,dynamics,\,by\,assuming\,linear\,enthalpy-concentration\,relationships\,they\,eliminated\,some\,dependent\,variables\,from\,the\,equations\,so\,that\,separate\,enthalpy\,balance\,equations\,were\,not\,required.\,The\,model\,results\,were\,compared\,with\,those\,obtained\,in\,practice\,from\,a\,12\,plate\,binary\,column.

Pieser\,and\,Grover\textsuperscript{11} presented\,a\,model\,using\,assumptions\,(b),\,(c),\,(e),\,(f)\,and\,(k)\,for\,a\,multicomponent\,column.\,The\,model\,included\,liquid\,flow\,dynamics\,and\,the\,effect\,of\,pressure\,drop\,across\,plates.\,The\,model\,was\,used\,to\,study\,"flooding"\,effects\,in\,a\,column\,which\,were\,causing\,control\,difficulties.\,The\,numerical\,methods\,used\,were\,not\,stated,\,and\,Rijnsdorp's\,linearised\,approach\,would\,probably\,have\,been\,equally\,revealing.

Williams\textsuperscript{12} used\,a\,model\,similar\,to\,that\,derived\,by\,Rosenbrock\,to\,describe\,the\,composition\,dynamics\,of\,the\,N.P.L.\,column.\,He\,also\,included\,the\,effect\,of\,vapour\,condensing\,in\,the\,column\,by\,assuming\,that\,at\,each\,plate\,the\,vapour\,flow\,rate\,is\,reduced\,by\,a\,factor\,(1-k)\,and\,the\,liquid\,flow\,rate\,is\,correspondingly\,increased.\,The\,factor\,k\,was\,chosen\,to\,match\,the\,model\,top\,product\,flow\,rate\,to\,values\,obtained\,in\,practice.\,The\,model\,was\,compared\,with\,practical\,step\,responses\,and\,was\,found\,to\,agree\,well\,except\,that\,the\,top\,product\,composition\,was\,usually\,3\%\,low,\,Williams\,suggested\,that\,this\,was\,due\,to\,feed\,flow\,rate\,errors.\,The\,equations\,were\,solved\,using\,Michaelson,\,Mah\,and\,Sargent's\textsuperscript{13} method\,which\,will\,be\,discussed\,in\,Chapter\,4.
Sunderland simulated Williams non-linear model using the FIFI digital simulation programme. He studied the effect of introducing hydrodynamics in the model as:

i) A pure time delay in the propagation of liquid flow changes from plate to plate.

ii) A pure time delay in the propagation of composition changes from plate to plate.

The dynamic effect described by (i) caused the model to exhibit a non-minimum phase response, while (ii) caused a general slowing in the model step response. Sunderland concluded that delays of type (ii) were more likely to occur in the N.P.L. column, but the effects were of little significance in this case.

5) The pilot scale distillation column

The pilot scale distillation column at N.P.L. separates a mixture of water and ethyl alcohol, whose physical data is given in Appendix 2. The vapour-liquid equilibrium curve exhibits a pronounced "knee" in the region about 20% molar liquid composition. Above 75% molar liquid composition the mixture enters an azeotropic region where the vapour composition is the same as that of the boiling liquid and further separation by distillation is not possible.
The column, which is constructed of glass, has six bubble-cap plates and is well-lagged. Feed is supplied to the column at the fourth plate from the top by a constant volume delivery pump. Thermistor probes measure plate liquid temperature and the column is open to the atmosphere. The reboiler is heated by electric elements and the liquid level in it is held constant.

The condenser consists of a vertical spiral tube through which cold water flows at a constant rate. Liquid hold-up in the condenser is negligible as condensate falls directly into a pivoted funnel which determines the reflux ratio. The funnel is moved by a solenoid and has two positions; in one position condensate flows out of the column as product and in the other it is returned to the top plate as reflux. The relative times in each position within a 32 sec. cycle determines the reflux ratio. The top product passes through a composition meter which measures its dielectric constant.

Sixteen variables can be scanned every 32 secs. and their values recorded on paper tape in binary coded decimal. The column ceased operation in 1969 when the experimental work described here was completed.

6) A Model of the N.B.L. Column

All distillation column models are based on the basic balance equations (1), (2) and (3). The assumptions used in a particular model depends on the method of solution and the particular physical effects
exhibited by the column of interest.

The N.P.L. column model was required in a linearised form for control system design, but a non-linear model was developed because:

i) The FIFI digital simulation language was available.

ii) The non-linear model allowed comparison between model and plant step responses.

iii) The non-linear model could be used to determine the range of validity of the linearised model.

Practical results obtained from the column indicated that vapour flow and composition dynamics and liquid flow dynamics were negligible and the column operated at constant (atmospheric) pressure, so assumptions (a), (d), (e) and (h) were used. The N.P.L. column is small so perfect mixing assumption (b) and unity plate efficiency assumptions (d) and (j) were used. Steady state heat balances showed a loss of about 30% and to include this effect in the equations it was assumed that heat loss occurs at each plate but column operation between plates is adiabatic. The enthalpy-composition relationships for water and ethyl alcohol were assumed to be linear and the column was assumed to be in overall balance, assumption (k).

The assumptions, apart from the inclusion of heat losses, are similar to those used by Huckaba, May and Franke and their approach is used to obtain the model equations. The assumptions are used to simplify the general plate equations (1), (2) and (3) derived for the column
plates shown in Fig. (3.1) and are as follows:

i) Total material balance

\[ V_{j+1} - V_j + L_{j-1} - L_j + F_j = 0 \]  \hspace{1cm} (6)

ii) Light component balance

\[ \frac{dx_j}{dt} = V_{j+1}x_{j+1} - V_jx_j + L_{j-1}x_{j-1} - L_jx_j + F_jz_j \]  \hspace{1cm} (7)

iii) Enthalpy balance

\[ \frac{dI_j}{dt} = L_{j-1}I_{j-1} - L_jI_j + V_{j+1}I_{j+1} - V_jI_j + F_jI_j + Q_j. \]  \hspace{1cm} (8)

The equations are for any plate \( j \), but in each column section shown in Fig. (3.2) they differ in detail and the restrictions and end conditions are listed in Table 3.1. All flows are in g\(\text{m-moles}/\text{min} \) and compositions are the molar proportion of ethyl alcohol.

These basic equations are now simplified further by eliminating some of the dependent variables. First we consider the condenser which has no liquid holdup and hence no dynamic effect. However it implies certain algebraic relationships and the balance equations including end conditions are:

Material balance, \( V_1 = L_0 + D \) \hspace{1cm} (9)

Light component balance, \( x_0 = y_1 \) \hspace{1cm} (10)

Enthalpy balance, \( V_1J_1 = (L_0 + D) (I_0 - C_{p0}(T_{BO} - T_0)) + Q_0. \) \hspace{1cm} (11)

Now as the enthalpy–composition relationships are assumed to be linear, then at plate \( j \), for saturated liquid,
FIG. 3.2. DIAGRAM OF COLUMN SECTIONS
I_j = ax_j + c, \quad (12)

and for saturated vapour, \quad J_j = y_j + d \quad (13)

Substituting equations (9), (12) and (13) into equation (11) gives,

$$L_0 + D = \frac{Q_o}{y_1(b-a) + (a-c) + C_{p0}(T_{BO} - T_0)}.$$ \quad (14)

As the reflux ratio R is defined so that \( L_0 = RD \), which is substituted into equation (14) to give,

$$D = \frac{Q_o}{(R+1) \left[ \beta(y_1 + a) + C_{p0}(T_{BO} - T_0) \right]}.$$ \quad (15)

Where \( \alpha = \frac{d-c}{b-a} \) and \( \beta = b-a \). To obtain an expression for \( Q_o \) the overall column enthalpy balance is used,

$$F(I_z - C_{pz}(T_{Bz} - T_z)) + Q_s = Q_o + \sum_{j=1}^{N+1} Q_{Lj} + W(T_{N+1} + D(I_o - C_{p0}(T_{BO} - T_0))). \quad (16)$$

Substituting equation (12) and the column overall material balance,

$$F = W + D, \quad (17)$$

and the overall light component balance,

$$Fz = Wx_{N+1} + Dx_o, \quad (18)$$

in equation (16) gives,

$$Q_o = Q_s - \sum_{j=1}^{N+1} Q_{Lj} - F C_{pz}(T_{Bz} - T_z) + D C_{p0}(T_{BO} - T_0). \quad (19)$$

Now substituting for \( Q_o \) in equation (15) gives,

$$D = \frac{Q_s + \sum_{j=1}^{N+1} Q_{Lj} - F C_{pz}(T_{Bz} - T_z)}{\beta (R+1)(y_1 + \alpha) + R C_{p0}(T_{BO} - T_0)}. \quad (20)$$
In the enriching section a total material balance about the whole of the column above each plate is taken, then for a plate \( m \)

\[
V_{m+1} = L_m + D. \tag{21}
\]

Substituting for vapour flow rate terms in equation (7) gives,

\[
\frac{dx}{dt}_m = L_m (y_{m+1} - x_m) + L_{m-1} (x_{m-1} - y_m) + D(y_{m+1} - y_m). \tag{22}
\]

Similarly in equation (8),

\[
\frac{dI}{dt}_m = L_m (I_{m+1} - I_m) + L_{m-1} (I_{m-1} - I_m) + D(J_{m+1} - J_m) - Q_{LM}. \tag{23}
\]

Differentiating the liquid enthalpy-composition equation (12) gives

\[
\frac{dI}{dt}_m = \frac{dI_m}{dx_m} \frac{dx}{dt}_m, \text{ which with equations (12) and (13) is substituted into equation (23) and using equation (22) gives,}
\]

\[
I_m = \frac{L_{m-1} (y_m + \alpha) + D(y_m - y_{m+1}) + Q_{LM}/\beta}{(y_{m+1} + \alpha)}. \tag{24}
\]

As \( L_0 = RD \) this is used to work down the column from the condenser using equation (24) to obtain \( L_1, L_2 \) etc., thus

\[
L_m = D \frac{(R+1) (y_1 + \alpha) + RC_{P0} (m_{BO} - m_0)}{(y_{m+1} + \alpha)} - 1 + \sum_{r=1}^{m} Q_{LR} \frac{\beta(y_{m+1} + \alpha)}{\beta(y_{m+1} + \alpha)} \tag{25}
\]

When equations (20) and (25) are used to replace the liquid and distillate flow rates in equation (22) an equation results which describes the plate composition dynamics in terms of independent variables (plate holdups and column inputs) and compositions.
Similar equations can be derived for the other parts of the column and with the vapour-liquid equilibrium relationship, equation (4), they give a set of non-linear differential equations which describe the column dynamics.

7) Linearising the Equations

The equations were linearised by expanding them in a Taylor series and neglecting terms of greater than first order for small perturbations. The set of equations may be written as,

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

(26)

where \( X \) is a vector of plate compositions and \( U \) is a vector of forcing functions. If \( X, U \) are steady state values then \( f(X_s, U_s) = 0 \). Writing \( X = X_s + x, U = U_s + u \), where \( x \) and \( u \) are perturbations from steady state values, then,

\[ x = f(X_s + x, U_s + u) \approx \frac{\partial f_x}{\partial x} + \frac{\partial f_u}{\partial u} + \text{higher order terms}, \]

Thus the linearised equations are

\[ \dot{x} = Ax + Bu \text{ say,} \]

(27)

where \( a_{ij} = \frac{\partial f}{\partial x_j}, b_{ij} = \frac{\partial f}{\partial u_j} \), evaluated at \( (X_s, U_s) \).

The expressions for the coefficients were determined by partial differentiation of the non-linear equations for each column section.
6) **Conclusions**

A dynamic model of the N.P.L. column has been derived. It is based on the usual balance equations but an original feature of the model is the inclusion of heat loss terms. The model can be used on any binary distillation column and is not restricted to columns with negligible condenser holdup. The extension to multi-component columns is not straight-forward as the elimination of the enthalpy balances becomes more complicated. In the next chapter methods of solving the equations are discussed.
TABLE 3.1 Column Section Details

1) End Conditions

\[ L_{-1} = V_0 = L_{N+1} = V_{N+2} = F_m = F_n = 0 \]

\[ X_{-1} = y_0 = y_{N+2} = z_m = z_n = 0 \]

\[ I_{-1} = J_0 = J_{N+2} = I_m = I_n = 0 \]

\[ H_0 = 0 \]

2) Feed and Product Streams

Bottom product, \( F_{N+1} = -W, z_{N+1} = x_{N+1} \)

Distillate, \( F_0 = D, z_0 = x_0, I_0 = C_p (T_{BO} - T_0) \).

Feed, \( F_f = F, z_f = z, I_f = T_{Bz} - C_p (T_{Bz} - T_z) \).

Where \( C_{pj} \) = specific heat of liquid of composition \( x_j \).

\( T_{BO} \) = boiling point temperature of distillate.

\( T_0 \) = temperature of distillate.

\( T_{Bz} \) = boiling point temperature of feed.

\( T_z \) = temperature of feed.

3) Heat supplied to column

\[ Q_m = -Q_{Ln}, Q_n = -Q_{Ln}, Q_f = -Q_{Lf} \]

where \( Q_{Lj} \) = heat lost from plate \( j \).

\( Q_{N+1} = Q_S - Q_{LN+1} \), where \( Q_S \) is heat supplied to the reboiler.

\( Q_{L0} = Q_o \), heat removed by the condenser.

4) Suffixes

0 = condenser

m = enriching section

n = stripping section

\( N+1 = \) reboiler

f = feed plate
CHAPTER 4

THE SOLUTION OF THE EQUATIONS

1) Introduction

In this chapter methods of solving the non-linear differential equations describing the N.P.L. column, using a digital computer, are considered.

First the general problems encountered in solving such equations are discussed. Three computer programmes were written to solve the N.P.L. column equations:

i) A programme to calculate steady states rapidly and evaluate the coefficients of the linearised equations.

ii) The FIFI digital simulation programme was used to calculate transient responses of the non-linear equations.

iii) A programme designed to calculate transient responses of the linearised equations.

2) General Considerations

To solve differential equations using a digital computer a numerical integration algorithm is required. A large number of algorithms are
available but the one chosen for a particular application must be:

i) Numerically stable.

ii) Accurate.

iii) Reasonably fast in operation.

Many authors have discussed the solution of distillation column equations using a digital computer and several have reported problems due to numerical instability. This is due to two factors:

a) The large difference between reboiler and plate holdup gives the linearised equations a large range of time constants.

b) A distillation column is a very stable physical system and if an exact solution is perturbed the effect is rapidly damped out.

When a numerical approximation to the solution is made, small errors in the value of plate composition \( x_j \), can cause large errors in the calculated values of \( \frac{dx_j}{dt} \), and hence can lead to instability.

Consider the first order differential equation, \( \dot{x} = g(x,t) \), (1) which represents one plate in a distillation column. Rosenbrock \(^8\) investigated the solution of such an equation using Euler's method, where the value of \( x \), at time \( t_1 + \delta t \), is approximated by,

\[
x(t_1 + \delta t) = x(t_1) + \delta t \; g[x(t_1), t_1].
\] (2)

He showed how instability, due to (b) above, could occur and that prohibitively small time steps were required to obtain a stable solution. As an alternative he suggested an implicit method,

\[
x(t_1 + \delta t) = x(t_1) + \delta t \left\{ (1 - \theta) \; g[x(t_1), t_1] + \theta g[x(t_1 + \delta t), t_1 + \delta t] \right\}
\] (3)
where $0 < \theta < 1$. Rosenbrock and Storey investigated the accuracy and stability of this method and showed that:

i) When $\theta = 0$ the formula is Euler's method which has been discussed, they also showed that the more accurate Runge-Kutta method offered very little advantage from a stability point of view.

ii) When $\theta = \frac{1}{2}$ the method is the trapezoidal rule and the truncation error is $O(\delta t^3)$, where $\delta t$ is the magnitude of the time step. The stability is improved, because solutions are locally approximated by rational functions (Pade approximation) instead of approximating by polynomials (Taylor expansion).

iii) When $\theta = 1$ the truncation error is $O(\delta t^2)$, but the polynomial in $\delta t$ which approximates to the exponential function tends to zero as $\delta t \to \infty$, so that the stability in a linear problem is high. This algorithm was used to calculate steady state values of the N.P.L. column equations by taking large time steps.

In general, when an implicit method is used to solve a set of differential equations a set of algebraic equations must be solved at each time step. By linearising the equations and using the column end conditions the resulting set of simultaneous equations can be solved by substitution. Details of the computer programme are given in the next section.

Several authors have used predictor-corrector methods to solve distillation equations. An explicit formula is used to predict a value of $x(t + \delta t)$ and a second implicit formula, the corrector, is used
iteratively with previous values to improve an approximation to $x(t + \delta t)$.

These methods have several disadvantages:

a) The iterative process may not converge unless $\delta t$ is small.

b) The corrector often uses several past values and requires another integration method to provide starting values.

c) The use of several past values makes the order of the difference equation higher than that of the differential equation and parasitic solutions are generated in addition to the required solution. These parasitic solutions are often unstable.

The FIFI digital simulation programme uses a predictor-corrector algorithm which has been studied by FIFI's author Sumner\textsuperscript{15} and by Sunderland\textsuperscript{11} who used it to solve the N.P.L. column equations. It is a second order method, the predictor equation being $x(t + \delta t) = 2x(t) - x(t - \delta t)$, \quad \quad \quad (4)

and the corrector being $3x(t + \delta t) = 2\delta tx(t + \delta t) + \frac{1}{3}x(t) - x(t - \delta t)$. \quad \quad \quad (5)

It can be shown that this formula has very good stability characteristics when solving linear equations, also the corrector is of a fairly low order.

The programme has automatic convergence and truncation error checking which adjusts the step length. When using FIFI to solve non-linear equations it seems unlikely that instability would pass undetected and it was therefore used to solve the column equations to obtain transient responses.

Mah, Michaelson and Sargent\textsuperscript{13} suggested a method which avoids the problem of replacing differential equations with difference equations.

Instead they linearise the non-linear equations $3(26)$ and obtain equation
3(27) and assume that the matrices $A$ and $B$ are constant over a time step. The solution of equation 3(27) is well known to be,

$$x(t) = e^{At} x(0) + e^{At} \int_0^t e^{-A\phi} Bu(\phi) d\phi$$

(6)

where $u(\phi)$ is assumed constant over the time step. For a distillation column the $A$ matrix can be shown to have real eigen-values which can be calculated and used to evaluate the matrix $e^{(At)}$. The $A$ and $B$ matrices are updated at the end of each time step and the method is completely stable over each step. To obtain accurate results the time interval must be short enough to ensure that the approximation is good over the whole step. In this work a similar method was used to calculate the response of the linearised equations. The state transition matrix $e^{(At)}$, where $\tau$ is the sampling interval, was computed by summing its defining series instead of using equation (6).

3) The Steady State Programme

When the steady state only, is of interest then large time steps can be taken to speed up the approach to the steady state values. Rosenbrocks implicit method with $\theta = 1$ was used because of its high stability.

Writing $\delta g[x(t_1), t_1] = g[x(t_1 + \delta t), t_1 + \delta t] - g[x(t_1), t_1]$, and $\delta x = x(t_1 + \delta t) - x(t_1)$ in equation (3) gives,

$$\delta x = \delta t \ g[x(t_1), t_1] + \theta \ \delta t \ \delta g[x(t_1), t_1].$$

(7)

Now for one plate $j$ in a distillation column,
Now assuming that the liquid and vapour flow rates are constant over a
time step and substituting equation (8) in equation (7) gives,

\[
- \theta L_{j-1} \delta x_{j-1} + (\theta L_j + \frac{H_j}{\delta t} + \theta V_j f'(x_j)) \delta x_j - \theta V_{j+1} f'(x_{j+1}) \delta x_{j+1} = S_j [x(t_1), t_1],
\]

where \( y_j = f(x_j) \) and \( f'(x_j) = \frac{df(x_j)}{dx_j} \). Equation (9) has the form,

\[
S_j \delta x_{j-1} + T_j \delta x_j + U_j \delta x_{j+1} = G_j,
\]

where \( S_j, T_j, U_j \) and \( G_j \) are coefficients. For a distillation column
\( S_0 = U_{N+1} = 0 \) which allows the equation to be solved by substitution.

A computer programme was written using this method of solution,
with \( \theta = 1 \), to calculate column steady state values and the linearised
A and B matrix coefficients. The solution was started from arbitrary
initial conditions and the time step \( \delta t \) was doubled every r steps. Both
\( r \) and \( \delta t \) were chosen by trial and error and the equations were integrated
until \( \sum_{j=0}^{N+1} (\delta x_j)^2 \leq 10^{-8} \).

4) The Transient Response Programme

The FIFI digital simulation programme developed by the UKAEA was
available on the N.P.L. KDF9 computer and was used to calculate the column
transient response. To use FIFI certain subroutines have to be written:-
i) SPEC; This contains the system differential equations, which have been described in Chapter 3.

ii) SEQU; this routine reads in the data and sequences the calculation, the numerical integration routine being initiated by calling the FIFI subroutine CALC. In addition the following were written for the distillation programme,

iii) HEAT; calculates the enthalpy of feed and distillate at temperatures below boiling point as a function of composition and temperature.

iv) HOLDUP; converts volumetric holdups into molar terms as a function of composition.

The vapour-liquid equilibrium relationship was specified as a look-up table with linear interpolation between points, which means that the equations are linearised before each time step.

5) Solution of the Linearised Equations

The general solution of equation (3.27) was stated in equation (6), over a time interval $\tau$ with initial values set at time $k\tau$, the solution is,

$$x(k + 1\tau) = P x(k\tau) + S u(k\tau). \quad (11)$$

It can be shown that the state transition matrix $P = e^{A\tau}$ and the forcing matrix $S = (e^{A\tau} - I) A^{-1} B$, where $u(k\tau)$ is constant over the time interval
and I is the identity matrix. Equation (11) can be used to calculate transient responses from initial values by matrix multiplication.

Matrices P and S were evaluated, using a method suggested by Liou\textsuperscript{17}, to a prescribed accuracy. Expressing the transition matrix P as an infinite series gives,

\[ e^{At} = \sum_{k=0}^{\infty} \frac{A^k t^k}{k!}, \]

where \( A^0 = I \), the identity matrix. Now let

\[ e^{At} = M + R, \]

where, \( M = \sum_{k=0}^{K} \frac{A^k t^k}{k!} \), is an approximation to \( e^{At} \) and \( R = \sum_{k=K+1}^{\infty} \frac{A^k t^k}{k!} \), is the remainder. If each element of \( M \) is required to an accuracy of \( d \) significant digits then,

\[ |r_{ij}| \leq 10^{-d} |m_{ij}|, \]

where \( r_{ij} \) and \( m_{ij} \) are elements of \( R \) and \( M \). The norm of matrix \( A \) is defined as,

\[ ||A|| = \sum_{i,j=1}^{m} |a_{ij}|, \]

and it can be shown that

\[ ||A^k|| \leq ||A||^k, \quad k = 1, 2, \ldots. \]

Hence each element of \( A^k \leq ||A||^k \) and it follows that,

\[ |r_{ij}| \leq \sum_{k=K+1}^{\infty} \frac{||A||^k t^k}{k!}. \]
Taking the ratio of the first to the second term in the series (17) to be \( \varepsilon = \frac{||A||_2}{K+2} \), and when \( k \geq K + 2 \), then \( \frac{||A||_2}{K} \leq \varepsilon \). Substituting \( \varepsilon \) in equation (17) gives,

\[
|r_{ij}| \leq \frac{||A||_{K+1}}{(K+1)!} \frac{r_{K+1}}{1 + \varepsilon + \varepsilon^2 + \cdots},
\]

\( (18) \)

Equation (18) gives the maximum value of any element in the remainder matrix and the state transition matrix can then be calculated by the following procedure:

i) A value of \( K \) is chosen arbitrarily.

ii) The approximation matrix \( M \) is then evaluated.

iii) Then \( \varepsilon \) is determined.

iv) Then the upper bound of \( r_{ij} \) is calculated from equation (18).

v) The value of each element of \( M \) is compared with \( r_{ij} \times 10^a \), if this test is not satisfied \( K \) is increased and the process is continued.

The forcing matrix \( S \) is calculated at the same time by evaluating the following series which avoids the need for matrix inversion,

\[
S = (e^A - I) A^{-1} B = \left( \sum_{k=1}^{\infty} \frac{A^k}{k!} \right) A^{-1} B
\]

\( (19) \)

This simplifies to give \( S = \tau \left( \sum_{k=0}^{\infty} \frac{k^k}{(k+1)!} \right) B \), this series converges
faster than that of $e^{At}$ and the value of $K$ which satisfied $e^{At}$ will also satisfy equation (19).

The discrete system equations were used to calculate step response from the steady state values by matrix multiplication. A computer programme in KDF9 Algol, using the matrix package, was written to calculate the discrete equations and the transient response. The programme also includes an option to simulate the response of digital control systems of the state feedback type. FIFI could also have been used to solve the linearised equations but as the state transition matrix was required to design digital controllers it was computationally more efficient to use the discrete equations.

6) A Comparison of the Programmes

The model and practical results are compared and discussed fully in the next Chapter. A brief discussion of the use of each computer programme is given here.

The steady state and FIFI programmes were tested by calculating a steady state with test data. A linear vapour-liquid equilibrium relationship was used and the column was at total reflux. The equations were also solved by hand and the three sets of results compared well, showing that the programmes were working correctly.
When used on non-linear data the steady state programme took about 12 sec. to calculate a steady state and integrated the equations over 1700 mins of simulated time. The step length was initially set to 1.0 min and was doubled every 2 steps. Tests with smaller initial step lengths and doubling less frequently gave similar results with longer computing times. No attempt was made to make the results become unstable.

To calculate a transient response lasting 320 mins FIFI took about 3 mins and no sign of instability was detected. The results obtained from FIFI and the steady state programme with similar data differed by up to 0.5% on top product composition. This is probably due to the larger truncation error in the steady state programme and, using FIFI, after 320 mins the equations were still approaching their steady state values.

The programme to solve the linearised equations was tested solving a first order equation. It took about 30 sec. to calculate the column transition matrix and a further 20 sec. to calculate each 320 min transient response. To satisfy an error bound of four significant figures 80 terms of the expansion of $e^{At}$ had to be summed. Williams summed the defining series to solve his non-linear equations and updated the matrix values after each time step. He summed about 15 terms and did not test the accuracy of his results.

7) Conclusions

In this Chapter methods of solving the equations have been discussed. Three methods of solving the equations were studied in detail,
though one was only used to solve the linearised equations. No problems of numerical instability were encountered in solving the N.P.L. column equations. The writing of additional computer programmes to solve the linearised equations and to obtain steady states was justified by savings in computer time.
CHAPTER 5

MODEL PERFORMANCE

1) Introduction

In this Chapter results obtained from the mathematical model derived in Chapter 3 are compared with those obtained from the N.P.L. column. The model is compared with the plant in three ways:

i) At steady state. An original study of the effect of heat losses is made and methods of matching the model to the plant results are discussed.

ii) Step responses. Model step responses are compared with observed results to assess the validity of the model.

iii) In the frequency domain. The linearised column equations are Fourier transformed using a computer programme to yield frequency responses.

A comparison of step responses from the non-linear and linearised equations is also made.

2) Steady State Results

The practical results were obtained by running the column to steady
state and recording all the instrument readings. All external flow rates, temperatures and compositions were measured to check heat and mass balances. The steady state heat balance usually showed a heat loss of about 25%. Samples of plate liquid were not taken as this upset the steady state.

Many of the results quoted here were taken by Weeks who gives a full description of experimental technique.

At steady state, if constant latent heat of vaporisation with composition is assumed, then the vapour flow rate from plate $j$ becomes,

$$V_j = V = KQ_S, \; j = 1, N + 1,$$

(1)

where $K$ is a constant (gm-moles/min/watt). From the condenser mass balance equation 3(9) and the definition of reflux ratio $R$, the distillate flow rate $D$ in gm-moles/min is,

$$D = \frac{KQ_S}{R+1}.$$  

(2)

The reflux ratio on the N.P.L. column is set up as a binary number $R_K$, which defines the mark-space ratio of the tipping funnel reflux device such that,

$$R + 1 = \frac{256}{R_K},$$

(3)

also for the water-ethanol mixture $K = 1.433 \times 10^{-5}$ gm-moles/min/watt.

Substituting the values into equation (2) gives,

$$D = 5.6 \times 10^{-6} Q_S R_K.$$ 

(4)
From a large series of column steady state runs at different heat input and reflux values Weeks obtained the following expression for distillate flow rate,

\[ D = 5.6 \times 10^{-6} (0.764 Q_S - 167) (B_K + 7.83) - 8.35 \times 10^{-3}. \]  (5)

Comparison of equations (4) and (5) indicate that:

a) Not all the heat supplied to the reboiler was used to create vapour, some heat was lost through the column walls. The total heat loss being,

\[ Q_L = 0.236 Q_S + 167 \text{ watts} \]  (6)

b) The reflux ratio device was subject to a constant error equivalent to binary 7.83 and the distillate flow rate was greater than that predicted by equation (4) i.e. a nominal reflux of 7:1 is in fact 5.4:1. This can be accounted for as a constant error in the mark-space ratio of the reflux device.

c) The assumption of constant latent heat of vapourisation is only an approximation, and the results do not account for the effect of cold feed to the column. These however, are minor effects and the primary causes of the discrepancy are due to a) and b) above.

To test the effect of these factors on the model a steady state was calculated with and without reflux correction, the total heat loss value was chosen to obtain the same value of top product composition. The results are given in Table 5.1 and are compared with the observed results.
The calculated results give similar external flow rates and composition profiles though there is some discrepancy between measured and calculated profiles. The internal flow rates, which cannot be measured, are quite different, as are the total heat losses required, in the corrected case 495 W, and in the uncorrected case 270 W. These compare with a measured heat loss of 437 W and a heat loss predicted from equation (6) of 499 W after taking feed cooling into account. The model with corrected data requires a heat loss close to the observed one and is probably a better approximation to the column.

The value of total heat loss also affects the model results. Fig. (5.1) shows composition profiles calculated with different total heat loss values for the steady state described in Table (5.1). When the total heat loss is increased, the column compositions also increase but the distillate flow rate decreases. The top product composition value obtained in run D agrees with the measured value but the plate composition values agree with those of run E which has a higher top product composition value. This is due to errors in the thermistor calibrations and in converting the temperature readings to compositions. The distillate flow rate is approximately correct for both these runs.

In Fig. (5.1) the observed profile shows that below plate three the liquid composition is very low; this is due to the steep slope of the vapour-liquid equilibrium curve in this region, the column has too many plates for separating the water-ethanol mixture. To avoid forcing the column top product composition into the azeotropic region, which would damp out dynamic change the column bottoms have to be run in a condition of
FIG. 5.1. STEADY STATE PROFILES WITH DIFFERENT HEAT LOSS VALUES.

<table>
<thead>
<tr>
<th>RUN</th>
<th>TOTAL HEAT LOSS (ft² sf)</th>
<th>TOP PRODUCT COMP. %</th>
<th>TOP PRODUCT FLOW (MMOLES/HR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>47.6</td>
<td>0.321</td>
</tr>
<tr>
<td>B</td>
<td>198</td>
<td>63.8</td>
<td>0.319</td>
</tr>
<tr>
<td>C</td>
<td>377</td>
<td>61.9</td>
<td>0.276</td>
</tr>
<tr>
<td>D</td>
<td>4.95</td>
<td>68.5</td>
<td>0.249</td>
</tr>
<tr>
<td>E</td>
<td>522</td>
<td>70.1</td>
<td>0.243</td>
</tr>
<tr>
<td>F</td>
<td>557</td>
<td>72.1</td>
<td>0.235</td>
</tr>
<tr>
<td>G</td>
<td>74.5</td>
<td>75.6</td>
<td>0.191</td>
</tr>
<tr>
<td>COLUMN</td>
<td>437</td>
<td>68.6</td>
<td>0.244</td>
</tr>
</tbody>
</table>
almost total separation.

The heat loss distribution up the column was found to have only a small effect on the column composition profile. A distribution in which 60% of the heat loss was attributed to the reboiler, with each plate losing an equal amount of the remainder was used, as this was believed to be a reasonable approximation to the practical situation.

The results of several steady states are given in Table (5.2) and are compared with the model results. The distillate flow rate values often differ because the model equations assume that the overall steady state balance equations 3(16) to 3(18) are satisfied. In practice steady state balances are often in error, due to measurement errors and the comparatively short time period used to determine flows.

The total heat loss value for the model was chosen to match the model top product composition to the observed value. This is justified because the model describes composition dynamics and the top product value is checked by a density measurement. The model heat loss differed from the value obtained from equation (6) by 5% of the total heat input, which was within the margin of experimental error.

At steady state the column was subject to continual small changes in operating conditions, which appear at the column outputs as noise and low frequency drift. The drift is mainly due to ambient temperature changes and changes of ± 50 Watts in the reboiler heater power due to
mains voltage fluctuations and resistance changes in the heater elements. Reflux and heat loss corrections according to equation (6) did assist in obtaining a model which agreed with observed results. These corrections were therefore included in the model equations and used in all subsequent work concerned with column dynamics.

3) **Step Responses**

The column was run to steady state and instrument readings were recorded as described in section 2. A step change was made in an input variable and the instrument readings were recorded on paper tape until steady state was again reached. If the measured top product composition differs from the composition meter readings, the meters calibration was adjusted.

The FIFI programme generated step responses by integrating the equations from initial conditions, calculated by the steady state programme, to the final steady state. The programme required the following data:

- i) Initial plate composition values.
- ii) The values of input variables corresponding to the final steady state.
- iii) The heat loss value, calculated from equation (6).
- iv) Volumetric holdups which were estimated at 70cc on each plate and 5800cc in the reboiler.
The top product composition response to step changes in reflux, heat and feed conditions are shown in Figs (5.2) to (5.13). Table (5.3) gives the data for the step responses, comparing the observed and model results shows that:

i) The model and column both have predominantly first order responses to step changes and there is a reasonable agreement between the results.

ii) Several observed results show evidence of time delays. For feed changes these represent delays in the feed pipe before the change enters the column. Delays of about 3 mins in the columns response to heat and reflux changes (Figs 5.4, 5.5 and 5.7) are due to liquid holdup in the composition meter. The top plate temperature response did not reveal any corresponding delay, in fact any delay due to column hydraulic effects was less than the minimum 32 sec. sampling period and was probably about 10 sec., the value estimated by Sunderland.

iii) The model and observed initial and final steady states differ by up to 1% in composition in some cases. This is due to the use of the general heat loss correction value determined from equation (6) rather than choosing a particular value of heat loss for each steady state.

iv) The column responses show the effects of non-linearity, the magnitude and speed of response depends on the direction of the step change and the initial composition value. The model gives generally similar results indicating that the only non-
FIG. 5.2. STEP RESPONSE TO A CHANGE IN REFLUX RATIO.

**TOP PRODUCT COMPOSITION**

% MOLES

- COMPUTED RESULT
- COLUMN RESULT

TIME: 1 UNIT = 1.6 MIN.

FIG. 5.3. STEP RESPONSE TO A CHANGE IN REFLUX RATIO.

**TOP PRODUCT COMPOSITION**

% MOLES

- COMPUTED RESULT
- COLUMN RESULT

TIME: 1 UNIT = 1.6 MIN.
FIG. 5.4. STEP RESPONSE TO A CHANGE IN REFUX RATIO.

Top product composition % moles.

- Computed result
- Column result

TIME: 1 UNIT = 1.6 MIN.

FIG. 5.5. STEP RESPONSE TO A CHANGE IN REFUX RATIO.

Top product composition % moles.

- Computed result
- Column result

TIME: 1 UNIT = 1.6 MIN.
FIG. 5.6 STEP RESPONSE TO A CHANGE IN HEAT INPUT.

**TOP PRODUCT COMPOSITION**

\% MOLES.

- **Computed Result**
- **Column Result**

TIME: 1 UNIT = 1.6 MIN.

FIG. 5.7 STEP RESPONSE TO A CHANGE IN HEAT INPUT.

**TOP PRODUCT COMPOSITION**

\% MOLES.

- **Computed Result**
- **Column Result**

TIME: 1 UNIT = 1.6 MIN.
Fig. 5.9. Step response to a change in heat input.
**Fig. 5.10. Step Response to a Change in Feed Flow Rate.**

**Fig. 5.11. Step Response to a Change in Feed Flow Rate.**
**FIG. 5.12. STEP RESPONSE TO A CHANGE IN FEED FLOW RATE.**

**FIG. 5.13. STEP RESPONSE TO A CHANGE IN FEED COMPOSITION.**
linearity present in the column is the vapour-liquid equilibrium relationship.

v) The models responses are slightly slower than those obtained from the column. This is due to the plate holdup value of 70cc used, this value was obtained experimentally but was subject to large errors.

4) Comparison of Linear and Non-linear Models

Several step responses about a steady state (Table 5.3 run 9) were computed to find the range over which the linearised and non-linear models agreed. Top plate composition changes about a steady value of 39% are shown for reflux (Fig. 5.14), heat input (Fig. 5.15), and feed composition (Fig. 5.16) changes of ± 3%, ± 10% and for feed composition ± 20%.

The results show that the two model responses are very similar for top product composition changes of less than 8%. The non-linear model is a quasi-linearisation as it uses a table look-up representation of the vapour-liquid equilibrium curve with linear interpolation.

For negative going steps the non-linear model has a slightly faster response but the composition value saturates at about -23% deviation from the initial value. Some information about the effect of non-linearity can be obtained from the plate light component and overall balance equations 3(1) and 3(2). Rewriting the equations in terms of perturbations
FIG. 5.14. STEP RESPONSES OF LINEAR AND NON-LINEAR MODELS TO REFLUX RATIO

TIME; UNIT = 1-6 MIN.

NON-LINEAR MODEL
LINEAR MODEL
FIG. 5.15. STEP RESPONSES OF LINEAR AND NON-LINEAR MODELS TO HEAT INPUT.

TOP PLATE COMPOSITION, 24% MOLES, DEVIATION FROM STEADY STATE VALUE.
FIG. 5.16. STEP RESPONSES OF LINEAR AND NON-LINEAR MODELS TO FEED COMPOSITION.

TOP PLATE COMPOSITION
% MOLES
DEVIATION FROM STEADY STATE VALUE.

TIME: 1 UNIT = 1.6 MIN

- - - - NON-LINEAR MODELS
- - - - - - - - LINEAR MODELS.
(lower case letters) about steady state values (upper case letters) gives

\[ (L_{j+1} \cdot V_{j+1}) - (L_j \cdot V_j) + (V_{j-1} + V_{j+1}) - (V_j + V_{j-1}) = 0, \]  
(7)

and

\[ \frac{dx_j}{dt} = (L_{j+1} + L_{j+1}) (x_{j+1} + x_j) - (L_j + L_j) (x_j + x_{j-1}) \]
\[ + (V_{j-1} + V_{j-1}) (y_j - y_{j-1}) - (V_j + V_{j-1}) (y_j + y_{j-1}). \]  
(8)

Assuming equal latent heats gives \( L_j = L_{j+1} = L \) and \( V_j = V \) and from equation (7) \( l_j = l_{j+1} = 1 \) and \( v_j = v \). Then equation (8) becomes, neglecting second order terms and steady state values,

\[ \frac{dx_j}{dt} = Lx_{j+1} - Lx_j + (x_{j+1} - x_j) + (y_{j-1} - y_j) \]
\[ + v (y_{j-1} - y_j). \]  
(9)

Setting \( y_j = k_j x_j \) where \( k_j = \frac{\frac{dx}{dx_j}}{j} \) and Laplace transforming with zero initial conditions gives, after rearrangement,

\[ \left( \frac{H_j}{L + VK_j} + 1 \right) x_j (s) = \frac{L}{L + VK_j} x_{j+1} (s) + \frac{(x_{j+1} - x_j) L (s)}{L + VK_j} \]
\[ + \frac{VK_j - 1}{L + VK_j} x_{j-1} (s) + \frac{Y_{j-1} - Y_j}{L + VK_j} v (s). \]  
(10)

Equation (10) describes the composition dynamics of a plate to composition, liquid flow rate (reflux) and vapour flow rate (heat input) changes. The plate time constant and steady state gains, except for that of \( x_{j-1} \), are inversely proportional to the vapour-liquid equilibrium.
curve slope $K_j$. The vapour-liquid equilibrium curve and its slope are shown in Fig. (5.17). At low composition the slope is steep (9.0), so with decreasing composition the N.P.L. column plates should have shorter time constants and lower gains. The overall column dynamics are described by $N$ equations of the style of equation (10), modified at the feed plate, reboiler and condenser, which are difficult to reduce. However the effect of changes on one plate should indicate the likely effects of non-linearity on the overall dynamics.

For large positive disturbances the non-linear model has a slower time response and its gain is reduced as the azeotropic region is approached. Equation (10) shows that when $K_j = 1$ the gain and time constant of a plate depend on the liquid and vapour flow rates and the composition on all plates in the azeotropic region tend to the same value when $y_j = x_j$. However composition changes on the plates below which are not working at the azeotrope are transmitted to the top of the column.

5) Model Frequency Responses

A computer programme was used to calculate model frequency responses from the linearised model equations, the programme was written by Milsom$^{19}$ of UKAEA for the KDF9 computer using the EGDON (Fortran) language. This programme was run on the N.P.L. KDF9 after some initial debugging.
FIG. 5.17 VAPOUR-LIQUID EQUILIBRIUM CURVE AND SLOPE FOR WATER AND ETHYL ALCOHOL.
Frequency responses are calculated from the general set of linear differential equations,

$$Gx + Ax + Cx(t - T_d) = Bu + Eu,$$  \hspace{1cm} (11)

where \(x\) is the state vector, \(u\) is a vector of forcing functions. The values of time delay \(T_d\) and the matrices \(G, A, B, C\) and \(E\) are supplied as data. The Fourier Transform of equation (11) is written as,

$$\left[ (A + C \cos \omega T_d) + j(\omega G - C \sin \omega T_d) \right] x(j\omega) = (B + j\omega E) u(j\omega).$$  \hspace{1cm} (12)

Equation (12) is evaluated for several values of angular frequency \(\omega\), by equating real and imaginary parts at each value and by performing some simple matrix operations the complex matrices are inverted using real arithmetic. The result being the real and imaginary parts of \(x\) at each frequency, the frequency response in cartesian coordinates. A short extra section of programme was written to calculate the results in log gain (dB) and phase form. The amount of core storage used by the programme depends on the square of the equations order and the programme is limited to calculating 30 frequencies for up to 65 state variables. It would not be possible to calculate the frequency response of large distillation columns \(u\) using this method.

A transfer function block diagram of a plate, as described by equation (10) is shown in Fig. (5.22). The plate composition response depends on that of the surrounding plates, any change in composition is transmitted to the plates above and below and these are returned to the original plates as changes in \(x_{j+1}\) and \(x_{j-1}\). Each column plate, in this model, adding a further first order lag.
The frequency response programme was used to analyse the linearised differential equation obtained from Table (5.3) run 9. Frequency responses of the top plate composition to reflux, heat and feed changes are shown in Figs (5.18) to (5.23).

All the responses show a dominant time constant of about 40 minutes, though there is some evidence of higher order response with all additional time constants being less than 2 minutes. The dominant time constant is due to interaction between plates and compares with values, calculated from equation (10), of about 1 minute for a single plate and 82 minutes for the reboiler. The input changes considered act on the model in different ways:

i) The model ignores fluid flow dynamics and a reflux change (l) causes an immediate composition change on all plates. The top plate response however is of first order.

ii) Heat changes (v) also cause an immediate composition change on all plates, but this change is counteracted by a corresponding increase in liquid flow rate due to reflux. This effect is shown in the frequency response, which is of third order, where a higher order response would otherwise be expected.

iii) The feed composition response shows the effect of the composition response on the feed plate propagating up and down the column. The response is of fourth order as there are four plates from the feed point to the top of the column.

iv) Feed flow only changes the flows in the stripping section, where its effect is highly attenuated due to the low gain in
FIG. 5.18. TOP PLATE COMPOSITION FREQUENCY RESPONSE TO REFLUX RATIO.

FIG. 5.19. TOP PLATE COMPOSITION FREQUENCY RESPONSE TO HEAT INPUT.
FIG. 5.20. TOP PLATE COMPOSITION FREQUENCY RESPONSE TO FEED FLOW.

FIG. 5.21. TOP PLATE COMPOSITION FREQUENCY RESPONSE TO FEED COMPOSITION.
this region. The frequency response is very similar to that obtained for feed composition.

In practice, information obtained at high frequency is not valid as the reflux cycle has a frequency of about 1.9 cycles/min and will cause false readings in this region.

The dominant first order time constant and gain values obtained from the frequency response programme were compared with those estimated from column step responses. The transfer function was assumed to be

$$\frac{X(s)}{U(s)} = \frac{G e^{-T_d s}}{T_c s + 1}$$  \hspace{1cm} (13)

and the parameters are estimated from step responses as shown in Fig. (5.23) where \(G\) is the system gain, \(T_d\) is the delay time, \(T_c = t_o - T_d\) is the time constant, \(X(s)\) is the Laplace transform of the top plate composition, and \(U(s)\) is the Laplace transform of the input.

The comparative results for gain and time constant values are given in Table 5.4. In all the practical results for top plate temperature the values of pure time delay were very small and were neglected. The practical and model time constant values agree well, the model results could yield further short time constant values but the practical results were close to first order and it was not possible to extract more than one value. These model gain values were larger than those obtained in practice. This is due to heat loss errors and non-linearities in the distillation column, the gain and time constant values differing depending on the direction and magnitude of the step. The practical results given here are the average
FIG. 5.22. TRANSFER FUNCTION BLOCK DIAGRAM
OF A COLUMN PLATE.

\[ \frac{X_{j+1} - X_j}{Y_{j-1} - Y_j} \]

\[ \frac{1}{1 + V K_j} \]

\[ \frac{1}{V K_j} \]

\[ \left( \frac{K}{\gamma_j s + 1} \right)^n \]

PLATES ABOVE

PLATES BELOW

FIG. 5.23. RESPONSE TO A UNIT STEP.

\[ \text{TRANSFER FUNCTION} = \frac{G e^{-t_0 s}}{(t_1 - t_0) s + 1} \]
of several steps made in the operating region, the range of time constant values being from 33 to 51 mins before averaging.

6) Conclusions

In this chapter model results have been compared with those obtained from the column. The results indicate that the steady state and step response results agree well when observed factors like heat loss and balance errors are taken into account. In practice such effects are bound to occur and experimentally observed relationships have to be used to make the model a reasonable representation of the process.

The inclusion of heat loss terms in the model proved most useful especially when equation (6) was included in the model. The use of a plate efficiency factor was not necessary when heat losses were taken into account. Plate efficiency is usually measured at one steady state and an efficiency against composition relationship is obtained. It is unlikely that such a relationship is valid over all column operating conditions, the heat loss equation (6) was determined from a large number of steady states.

The linearised model gave a good agreement with the non-linear model for small changes in composition. The analysis of the linearised model in the frequency domain is a useful technique, which could be applied to medium sized distillation columns. The gains and time constants obtained from the frequency responses did show differences from
results predicted from column step responses. These errors are due to column non-linearities and errors in the heat loss relationship.

The model developed here is similar to those described in Chapter 3. Such detailed models based on the plate balances including plate hydraulics, if necessary, give an adequate representation of the column transient response. However further work is needed to find simpler methods of predicting distillation column transient responses. The use of a frequency response programme described here is a useful start but more work is required so that the detailed equations need not be formulated initially. The other difficulty with reduced order transfer functions of greater than first order, is that state variables are introduced which may not be measurable in practice.
### TABLE 5.1
Comparison of Corrected and Uncorrected Steady States

Operating Conditions.

**Holdups** Plate 70cc. Reboiler 5800cc.
- Feed Flow Rate 3.06 moles/min.
- Feed composition 5.6% moles of ethanol
- Feed temperature 77°C.
- Distillate temperature 79.8°C.
- Heat supplied 1650W.
- Reflux ratio, nominally 7:1

<table>
<thead>
<tr>
<th></th>
<th>Practical Results</th>
<th>Corrected Data</th>
<th>Uncorrected Data</th>
<th>moles/min.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top product flow</td>
<td>0.244</td>
<td>0.249</td>
<td>0.248</td>
<td></td>
</tr>
<tr>
<td>Bottom</td>
<td>2.82</td>
<td>2.81</td>
<td>2.81</td>
<td></td>
</tr>
<tr>
<td>Top product compn.</td>
<td>68.5%</td>
<td>68.48%</td>
<td>68.9%</td>
<td>moles of ethanol</td>
</tr>
<tr>
<td>Plate 1</td>
<td>60.0%</td>
<td>57.5%</td>
<td>58.4%</td>
<td></td>
</tr>
<tr>
<td>Plate 2</td>
<td>43.0%</td>
<td>34.7%</td>
<td>36.3%</td>
<td></td>
</tr>
<tr>
<td>Plate 3</td>
<td>11.5%</td>
<td>7.5%</td>
<td>7.9%</td>
<td></td>
</tr>
<tr>
<td>Heat loss</td>
<td>437W.</td>
<td>495W.</td>
<td>270W.</td>
<td></td>
</tr>
<tr>
<td>Mass balance error</td>
<td>-2.8%</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Heat loss</td>
<td>26.5%</td>
<td>30.0%</td>
<td>16.4%</td>
<td>% of heat input</td>
</tr>
<tr>
<td>Reflux ratio</td>
<td>7:1 Nom.</td>
<td>5.44:1</td>
<td>7:1</td>
<td></td>
</tr>
<tr>
<td>Liquid $L_1$</td>
<td>-</td>
<td>1.34</td>
<td>1.73</td>
<td>Moles/min.</td>
</tr>
<tr>
<td>Flow $L_2$</td>
<td>-</td>
<td>1.32</td>
<td>1.70</td>
<td></td>
</tr>
<tr>
<td>Rates $L_3$</td>
<td>-</td>
<td>1.29</td>
<td>1.67</td>
<td></td>
</tr>
<tr>
<td>$L_4$</td>
<td>-</td>
<td>1.48</td>
<td>1.48</td>
<td></td>
</tr>
<tr>
<td>$L_5$</td>
<td>-</td>
<td>4.48</td>
<td>4.805</td>
<td></td>
</tr>
<tr>
<td>$L_6$</td>
<td>-</td>
<td>4.48</td>
<td>4.804</td>
<td></td>
</tr>
</tbody>
</table>
TABLE 5.2

SEVERAL STEADY STATES

<table>
<thead>
<tr>
<th>Run No.</th>
<th>Feed Comp. %</th>
<th>Feed Flow Rate (Nom.)</th>
<th>Reflux Ratio</th>
<th>Heat Loss Rate</th>
<th>Calculated Heat Balance</th>
<th>Measured &amp; Calculated Compn.</th>
<th>Measured &amp; Calculated Flow Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.25</td>
<td>2.26</td>
<td>7:1</td>
<td>1650</td>
<td>557</td>
<td>2.1</td>
<td>61.2</td>
</tr>
<tr>
<td>2</td>
<td>6.25</td>
<td>1.96</td>
<td>7:1</td>
<td>1650</td>
<td>557</td>
<td>0</td>
<td>55.3</td>
</tr>
<tr>
<td>3</td>
<td>6.25</td>
<td>2.56</td>
<td>7:1</td>
<td>1650</td>
<td>557</td>
<td>2.5</td>
<td>68.0</td>
</tr>
<tr>
<td>4</td>
<td>7.0</td>
<td>1.88</td>
<td>7:1</td>
<td>1460</td>
<td>511</td>
<td>3.8</td>
<td>64.0</td>
</tr>
<tr>
<td>5</td>
<td>7.0</td>
<td>1.88</td>
<td>5.9:1</td>
<td>1460</td>
<td>511</td>
<td>5.3</td>
<td>58.7</td>
</tr>
<tr>
<td>6</td>
<td>7.0</td>
<td>1.88</td>
<td>8.2:1</td>
<td>1435</td>
<td>506</td>
<td>6.0</td>
<td>69.6</td>
</tr>
<tr>
<td>7</td>
<td>7.0</td>
<td>1.88</td>
<td>7:1</td>
<td>1600</td>
<td>535</td>
<td>4.5</td>
<td>59.5</td>
</tr>
<tr>
<td>8</td>
<td>7.0</td>
<td>1.88</td>
<td>7:1</td>
<td>1290</td>
<td>471</td>
<td>6.0</td>
<td>70.4</td>
</tr>
<tr>
<td>9</td>
<td>7.15</td>
<td>2.02</td>
<td>7:1</td>
<td>1730</td>
<td>575</td>
<td>2.1</td>
<td>59.5</td>
</tr>
<tr>
<td>10</td>
<td>7.15</td>
<td>2.02</td>
<td>5.7:1</td>
<td>1730</td>
<td>575</td>
<td>-7.0</td>
<td>56.0</td>
</tr>
<tr>
<td>11</td>
<td>7.15</td>
<td>2.02</td>
<td>8.85:1</td>
<td>1730</td>
<td>575</td>
<td>9.0</td>
<td>65.5</td>
</tr>
<tr>
<td>12</td>
<td>7.15</td>
<td>1.45</td>
<td>7:1</td>
<td>1810</td>
<td>594</td>
<td>1.8</td>
<td>59.0</td>
</tr>
</tbody>
</table>
### TABLE 5.3

**STEP RESPONSE GRAPHS**

<table>
<thead>
<tr>
<th>Figure No.</th>
<th>Heat W.</th>
<th>Reflux Ratio</th>
<th>Comp. Flow Ml</th>
<th>Temp. C.</th>
<th>Variable changed</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.2</td>
<td>1450</td>
<td>8.2:1</td>
<td>0.07</td>
<td>1.88</td>
<td>Reflux to 7:1</td>
</tr>
<tr>
<td>5.3</td>
<td>1730</td>
<td>7.0:1</td>
<td>0.072</td>
<td>2.02</td>
<td>Reflux to 5.7:1</td>
</tr>
<tr>
<td>5.4</td>
<td>1730</td>
<td>7.0:1</td>
<td>0.072</td>
<td>2.02</td>
<td>Reflux to 8.85:1</td>
</tr>
<tr>
<td>5.5</td>
<td>1730</td>
<td>8.85:1</td>
<td>0.072</td>
<td>2.02</td>
<td>Reflux to 7:1</td>
</tr>
<tr>
<td>5.6</td>
<td>1600</td>
<td>7.0:1</td>
<td>0.07</td>
<td>1.88</td>
<td>Heat to 1430W</td>
</tr>
<tr>
<td>5.7</td>
<td>1430</td>
<td>7.0:1</td>
<td>0.07</td>
<td>1.88</td>
<td>Heat to 1290W</td>
</tr>
<tr>
<td>5.8</td>
<td>1450</td>
<td>7.0:1</td>
<td>0.07</td>
<td>1.88</td>
<td>Heat to 1600W</td>
</tr>
<tr>
<td>5.9</td>
<td>1650</td>
<td>7.0:1</td>
<td>0.056</td>
<td>3.06</td>
<td>Heat to 1450W</td>
</tr>
<tr>
<td>5.10</td>
<td>1650</td>
<td>7.0:1</td>
<td>0.063</td>
<td>2.26</td>
<td>Feed flow to 1.96</td>
</tr>
<tr>
<td>5.11</td>
<td>1650</td>
<td>7.0:1</td>
<td>0.063</td>
<td>1.96</td>
<td>Feed flow to 2.26</td>
</tr>
<tr>
<td>5.12</td>
<td>1650</td>
<td>7.0:1</td>
<td>0.063</td>
<td>2.26</td>
<td>Feed flow to 2.56</td>
</tr>
<tr>
<td>5.13</td>
<td>1440</td>
<td>7.0:1</td>
<td>0.054</td>
<td>2.20</td>
<td>Feed comp. to 0.082</td>
</tr>
</tbody>
</table>
TABLE 5.4

COMPARISON OF MODEL AND PRACTICAL FIRST ORDER TIME CONSTANTS AND STEADY STATE GAIN

Column operating region Table 5.2 Run 1

<table>
<thead>
<tr>
<th>Input Variable</th>
<th>Model Results</th>
<th>Column Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Steady State Gain</td>
<td>Time Constant</td>
</tr>
<tr>
<td>Heat</td>
<td>+6.53</td>
<td>43.1</td>
</tr>
<tr>
<td>Reflux</td>
<td>-8.1</td>
<td>40.8</td>
</tr>
<tr>
<td>Feed Flow</td>
<td>-3.5</td>
<td>39.8</td>
</tr>
</tbody>
</table>

Units. Gain top plate temp. change °C/Binary keyboard Volt.
Time constant. Minutes
1) Introduction

In this chapter the theory of distillation column control is presented and the effects of control loop interaction and feed disturbances on the quality of control are discussed.

The design of conventional two-term digital control systems is outlined and an alternative control strategy based on optimal control theory is presented. It is shown that the optimal control method allows the design of feedforward and feedback control systems, by the same calculation, in an integrated fashion. This is an original application of existing theory. Methods of reducing the number of available measurements required are considered and the relevant theory is presented. Again this work is original in the context of distillation column applications.

2) General Considerations

A distillation column control system has to maintain desired product composition values in the presence of disturbances. In general only small changes about a particular steady state are of interest and a linear model is adequate for control system design. A typical feedback control scheme
is shown in Fig. (6.1), plate temperatures near the top and bottom of the column are controlled by manipulation of reflux ratio and reboiler heat input respectively.

This control configuration has not always given satisfactory control of product compositions for the following reasons:

a) Poor Correction of Feed Disturbances

There is often a considerable time lag before the results of feed disturbances are sensed as errors at the measurement points and until this happens a feedback controller cannot take corrective action. By this time a large disturbance will be present in the column and off-specification product will be produced.

Bollinger and Lamb suggested the use of feedforward control to overcome this problem. Feed disturbances are sensed in the feed pipe before entering the column and immediate control action is taken to cancel the effect of the disturbance on the controlled variables. A feedforward control system requires a plant model which will predict responses to changes in uncontrolled and manipulated variables. They simulated the controllers on an analogue computer model of a five plate column, and reported an improvement in control.

Applications on industrial columns have been described by:

i) McCullen and Shinskey who used a "static" controller designed using plant steady state gains which still gave a considerable improvement in performance.
FIG. 6.1. A TYPICAL TWO PRODUCT COMPOSITION CONTROL SYSTEM.
ii) Lupfer and Parsons\textsuperscript{22} who used a dynamic model obtained by fitting transfer functions to column step responses. Feedback control is always required in addition to feedforward control, to compensate for inaccuracies in the plant model and unmeasured disturbances.

b) Interaction

Changes in heat input and reflux ratio cause composition changes at both ends of the column. This causes interaction between the two control loops shown in Fig. (6.1) and can cause severe control problems.

Rosenbrock\textsuperscript{23} has studied these effects and concluded that, in the absence of interaction, column control will be satisfactory if secondary time lags are small. However when interaction does occur control will depend on the primary mass-transfer effects in the column. He suggested a method of achieving non-interacting control by using the sum and difference of the measurements shown in Fig. (6.1) as controlled variables. Analogue computer simulation showed that this approach did improve column control to a certain degree. Rijnsdorp\textsuperscript{24} also considered the problem and overcame interaction by controlling heat input to keep the ratio of reflux flow rate to top vapour flow rate constant. Top product composition control then changed this ratio. The approach overcomes interaction by avoiding it rather than by using control theory to improve matters.

In general the design of interacting control systems remains a major problem. The control system can be designed to make the loops non-
interacting, but this is a rather arbitrary approach to control and controlled variable constraints are not taken into account. In many industrial applications the problem is avoided by leaving some variables under manual control.

Control studies on the N.P.L. column have been conducted by Williams, he compared several methods of designing digital controllers to control top product composition by manipulating reflux ratio. He concluded that the best results were given by control systems designed to minimise the sum of squared errors obtained by evaluating residues in the z-plane. He compared these controllers with three term controllers and optimal linear regulators.

3) Digital Control System Design Methods

i) Feedforward Control

To design a digital feedforward controller for the column in Fig. (6.1) the linearised mathematical model is expressed in terms of z transfer functions. The response of the upper measurement point $x_T$ to input changes in z-transform form is,

$$X_T(z) = G_{T1}(z)R(z) + G_{T2}(z)Q(z) + G_{T3}(z)F(z) + G_{T4}(z)Z(z). \quad (1)$$

Similarly the response of the lower measurement point $x_B$ is,

$$X_B(z) = G_{B1}(z)R(z) + G_{B2}(z)Q(z) + G_{B3}(z)F(z) + G_{B4}(z)Z(z). \quad (2)$$

Where $R(z)$, $Q(z)$, $F(z)$ and $Z(z)$ are the z-transforms of the reflux, heat
input, feed flow rate and feed composition respectively. \( G_{T_1} \) to \( G_{T_4} \) and \( G_{B_1} \) to \( G_{B_4} \) are the appropriate open loop z-transfer functions.

Now for the perfect feedforward control the change in the measured variables due to feed changes will be zero. So setting \( x_B = x_T = 0 \) in equations (1) and (2) gives two simultaneous equations which can be solved for \( R(z) \) and \( Q(z) \) to give,

\[
R(z) = \frac{(G_{B_2} G_{T_3} - G_{T_2} G_{B_3}) F(z) + (G_{B_2} G_{T_4} - G_{T_2} G_{B_4}) Z(z)}{(G_{T_2} G_{B_1} - G_{B_2} G_{T_1})}, \tag{3}
\]

and

\[
Q(z) = \frac{(G_{B_1} G_{T_3} - G_{T_1} G_{B_3}) F(z) + (G_{B_1} G_{T_4} - G_{T_1} G_{B_4}) Z(z)}{(G_{T_2} G_{B_2} - G_{B_1} G_{T_2})}. \tag{4}
\]

These equations fully define the feedforward control, when only a "static" control is required the transfer functions are replaced by steady state gain terms. The feedforward controllers will be stable unless the plant exhibits non-minimum phase response, in which case the controller has a pole outside the unit circle in the z-plane and is unstable.

ii) Feedback Control System Design

Continuous controllers used for process control are usually two or three term pneumatic or electronic devices. In most applications the controller design is done empirically and then tuned on-site to give good control. Computer control studies have shown that satisfactory digital control can be obtained by using difference approximations to these simple control functions.
The design method described here is one used by Higham to control first order processes with time delay. When it is applied to a process without time delay a discrete-time proportional plus integral controller is obtained.

The control loop configuration is shown in Fig. (6.2). The process transfer function $G(s)$ is preceded by a sample: and hold element which represents the computer interface. The plant output $X(z)$ is compared with the set point $SP(z)$ to form an error $E(z)$ which is fed into the digital controller $D(z)$.

The closed loop z-transfer function $K(z)$ is given by,

$$K(z) = \frac{D(z) G(z)}{1 + D(z) G(z)}. \quad (5)$$

Then $D(z)$ can be expressed as

$$D(z) = \frac{1}{G(z). (1-K(z))}. \quad (6)$$

Now the plant transfer function is assumed to be,

$$G(s) = \frac{Ge^{-sN\tau}}{1 + sT_c}, \quad (7)$$

where $G$ is the steady state gain, $\tau$ is the sampling interval, $N\tau$ is the delay ($N$ is an integer), and $T_c$ is the process time constant. Combining $G(s)$ with a zero-order hold and z-transforming gives,

$$G(z) = \frac{GL z^{(N + 1)}}{1 - (1-L) z^{-1}}, \quad (8)$$

where $L = (1 - e^{-\tau/T_c})$. 
FIG. 6.2. A SAMPLED-DATA CONTROL SYSTEM.
By specifying the required closed loop response the control equation $D(z)$ can be calculated using equation (6). A suitable form of closed loop transfer function is

$$K(z) = \frac{z^{-[(N+1)Q]}}{1- (1- Q)z^{-1}},$$

so that following a step change in set point, after the delay, the system follows an exponential curve of time constant $T_c$ where $Q = 1 - e^{-\tau/T_c}$. Substituting this equation into equation (6) gives,

$$D(z) = \frac{1}{G(z)} \frac{Q z^{-(N+1)}}{(1-(1-Q)z^{-1} - Qz^{-(N+1)})}$$

$$= \frac{1}{G} \frac{(Q/L - z^{-1} Q/L(1-L))}{(1-(1-Q)z^{-1} - Qz^{-(N+1)})}.$$  

The parameter $Q$ can be tuned "on line" to obtain the best speed of response and to compensate for model inaccuracies. For equation (9) to be stable $Q \leq 1$, and when $Q = L$ the closed loop response is the same as the open loop response.

When the plant has no delay ($N = 0$) equation (10) becomes,

$$D(z) = \frac{Q}{GL} \left(1 + \frac{Lz^{-1}}{1-z^{-1}}\right)$$

which is the discrete-time form of a proportional integral controller with a gain of $Q/GL$ and a reset time of $\tau/L$. 
4) The Design of Integrated Control Systems

The design method described in section 3 are typical of the best industrial practice and do not take interaction or control variable constraints into account. It is desirable to investigate methods of designing control systems in an integrated manner, treating the column as a multi-variable system and designing feedforward and feedback controllers with the same calculation.

In recent years methods of design have been suggested which seek to optimise plant performance with respect to a performance criterion. These methods design control systems in an integrated fashion, and while recognising the existence of interaction, do not attempt to achieve non-interacting control.

The optimal control system which results depends on the performance criterion and plant model equations and may be difficult to apply successfully. To obtain a linear control system the optimisation problem has to be subject to the following restrictions:

i) The plant model is linear.

ii) An integral of error squared performance criterion is used.

When control variable constraints are not included in the performance criterion the linear control system has an infinite gain. This poses problems in implementation as control variable constraints can cause poor control or instability.
To overcome this problem constraints must be included in the optimisation calculation. Two methods of doing this have been suggested:

i) Kalman and Bertram used a sub-optimal method when the control variable \( u \) is specified as \( |u| \leq a \) constant. Then for a system described by equation 3(27) the sub-optimal control is on-off. The control is chosen to minimise the performance criterion and make the time derivative of the system Lyapunov function as negative as possible.

Brosilow and Handley applied this type of control to a column enriching section, controlling top plate temperature using reflux flow manipulation. Their application was successful but the method suffers from the following disadvantages:

a) To manipulate both heat and reflux ratio using on-off control could aggravate the secondary hydrodynamic effects in the column and could cause instability

b) For large state changes where constraint control would be an advantage a linearised plant model may not be adequate.

c) Some evidence of cycling about steady state could be observed in Brosilow and Handley's results.

ii) The other approach suggested by Kalman and Koepke is to include a quadratic penalty on the control variables in the performance criterion. The result is a linear state feedback controller which has a limited gain. This controller is often termed the optimal linear regulator.

This method has received much attention, and text-books by Tou.
Noton and Athens and Fall are available. However few attempts to apply these methods in practice have been made, though some simulation studies in aerospace and power boiler applications have been reported.

Williams is the only person to have applied these methods to distillation columns. He designed a single loop controller for the N.P.L. column, he did not consider the implications of choosing suitable weighting coefficients in the performance criterion and much remains to be done in applying this technique.

5) Optimal Linear Regulator Theory

To design digital controllers the system differential equation must be expressed in discrete time form,

$$x(k+1) = Px(k) + Su(k). \quad (12)$$

Where, if equation 3(27) represents the continuous system, $x(k)$ is the state vector at time $k\tau$, $u(k)$ is the forcing function vector at time $k\tau$, $\tau$ is the sampling interval, $P = e^{A\tau}$ and $S = (s^{A\tau} - I) A^{-1}B$ as described in section 4.5.

The performance criterion is expressed as a series summation over $r$ stages,

$$\sum_{k=0}^{r-1} [x'(k) Dx(k) + u'(k) \lambda Hu(k)]\tau. \quad (13)$$

where ' indicates transposition and $D$ is a symmetric (pxp) matrix, $H$ is
a diagonal (sxs) matrix and $\lambda$ is a positive scalar.

The cost function $\theta_r$ is defined, for an $r$ stage process, as,

$$\theta_r(x(0)) = \min_{u(0), \ldots, u(r-1)} \sum_{k=0}^{r-1} [x'(k) D x(k) + u'(k) \lambda H u(k)] \tau. \quad (14)$$

Equation (14) is a function of the initial state $x(0)$ only, as when all the values of $u(k)$ have been chosen, each value of $x(k)$ can be calculated from the values of $x(k-1)$ using equation (12). Equation (14) can be rewritten as,

$$\theta_r(x(0)) = \min_{u(0)} [x'(0) D x(0) + u'(0) \lambda H u(0)] \tau + \min_{u(1), \ldots, u(r-1)} \sum_{k=1}^{r-1} [x'(k) D x(k) + u'(k) \lambda H u(k)] \tau. \quad (15)$$

The second term on the r.h.s. of equation (15) is a minimisation starting at $x(1)$ over $r-1$ stages so rewriting,

$$\theta_r(x(0)) = \min_{u(0)} [x'(0) D x(0) + u'(0) \lambda H u(0)] \tau + \theta_{r-1}(x(1)). \quad (16)$$

Now assuming that $\theta_r$ can be expressed as a quadratic form in $x(0)$,

$$\theta_r(x(0)) = x'(0) G_r x(0), \quad (17)$$

where $G_r$ is a symmetric (pxp) matrix. Substituting equations (17) and (12) into equation (16) gives,

$$x'(0) G_r x(0) = \min_{u(0)} [x'(0) D x(0) + u'(0) \lambda H u(0)] \tau + [Fx(0) + Su(0)]' G_{r-1} [Fx(0) + Su(0)]. \quad (18)$$

Equation (18) is minimised by differentiating w.r.t. the forcing functions and then collecting the s equations gives,

$$u'(0) \lambda H = -[Fx(0) + Su(0)]' G_{r-1} S. \quad (19)$$
Transposing and solving for u(0),

\[ u(0) = -(\lambda H + S'G_{r-1}S)^{-1}S'G_{r-1}Px(0), \]  \hspace{1cm} (20)

\[ = -C_r x(0), \]  \hspace{1cm} (21)

where \( C_r \) is an \((sxp)\) matrix. Substituting equation (21) into equation (18) gives,

\[ G_r = (D + C_r \lambda H C_r') + (P - SC_r)'G_{r-1} (P - SC_r). \]  \hspace{1cm} (22)

This equation is symmetric if \( G_{r-1} \) is symmetric which proves the assumption of a quadratic form for \( \theta_r \). Equations (21) and (23) provide a relationship to calculate \( C_r \) and \( G_r \) from values of \( G_{r-1} \). When \( r = 1 \) and assuming a free end point problem, \( x(r) \) unspecified, then \( u(0) \) must minimise \( [x'(0) Dx(0) + u'(0) \lambda Hu(0)] \), giving \( u(0) = 0 \). Then

\[ C_1 = 0 \text{ and } G_1 = D_r. \]  \hspace{1cm} (23)

These values start an iterative process using equations (21) and (23) from \( r = 1 \) to \( R \) where \( R \) is the interval of interest.

The resulting optimal control described by equation (21) is linear and all the state variables are fed back. The \( R \) values of the \( C_r \) matrix are time varying over the \( R \) stages. However when \( R \) is greater than the process settling time, \( C_r \) tends to a constant value which is the optimal control at time \( kr = 0 \) to regulate the plant for an unspecified period.

When disturbances are included in the state vector as extra state variables, the minimisation calculation leads additionally to the design of the best feedforward control.
6) Reducing the Number of Measurements

The control equation (21) requires measurements of all the system state variables. In practice this may not be possible as state variables may be inaccessible, or useless due to noise.

In binary distillation columns, using the model derived in Chapter 3, one measurement on each plate is required. With multi-component mixtures the situation is even worse, for \( m \) components, \( m-1 \) measurements are required on each plate. For large columns this is obviously not practicable.

Several methods of reducing the number of measurements required by the controller were studied and their theory is outlined here.

i) Introducing a Penalty Function in the Performance Criterion

This method was suggested by Hoskins\(^{33}\) for use with continuous systems and the theory presented here is adapted for application to discrete time systems.

An additional constraint \( \sum_{k=0}^{r} p[x(k), u(k), k] \tau = 0 \) is included in the performance criterion equation (13) which is rewritten as,

\[
\sum_{k=0}^{r} [x'(k) Dx(k) + u'(k) \lambda Hu(k) + p'(k)\sigma] \tau \tag{21}
\]

where \( \sigma \) is a Lagrange multiplier. This equation can then be expressed in
the form of equation (16) and the assumption of a quadratic form, equation (17) is also made. So equation (18) is rewritten as,

\[ x'(0)G_r x(0) = \min_{u(0)} \left( x'(0) D x(0) + u'(0) \lambda H u(0) + p'(0) \sigma \tau \right) \]

\[ + (P x(0) + S u(0))^T G_{r-1} (P x(0) + S u(0)), \tag{25} \]

Minimising by differentiating w.r.t. the forcing functions gives,

\[ \tau \lambda H u(0) + S' G_{r-1} S u(0) = -\frac{1}{2} \frac{3}{\delta u(0)} [p'(0) \sigma] - S' G_{r-1} P x(0) \tag{26} \]

Now choosing

\[ \frac{3}{\delta u(0)} [p'(0) \sigma] = \frac{2}{\tau} Q x(0), \tag{27} \]

where Q is an sxp matrix, and substituting in equation (26), gives

\[ (\lambda H + S' G_{r-1} S) u(0) = -(Q + S' G_{r-1} P) x(0). \tag{28} \]

State variable measurements can be reduced if Q is chosen to set coefficients of the control matrix to zero. This is done by writing \( Q = S' G_{r-1} P I_1 \)

where \( I_1 \) is a diagonal matrix with diagonal elements zero if the state variable is to be present in the control and -1 if the state variable is to be eliminated. Re-arranging equation (28) gives the control matrix with null coefficients, \( C_{Er} \) as,

\[ C_{Er} = (\tau \lambda H + S' G_{r-1} S)^{-1} [S' G_{r-1} P (I + I_1)]. \tag{29} \]

Substituting equation (29) into equation (25) gives the following expression for \( G_r \),

\[ G_r = (D + C_{Er}' \lambda H C_{Er}) \tau + (P - S C_{Er})' G_{r-1} (P - S C_{Er}). \tag{30} \]

Equations (29) and (30) define an iterative relationship similar to the one obtained in section 5. By considering a one stage process the starting values for this relationship are obtained and are the same as those obtained in section 5.
ii) Introducing Dynamics into the Control

If the process model was fed with the input values, then the model state vector could be used to calculate the control. This procedure is susceptible to model inaccuracies and the plant outputs are not controlled directly. However, the model equations can be rearranged to obtain a dynamic system whose inputs are plant inputs and available plant outputs (measurements), this system's output being an estimate of the plant's state vector. In general, initial condition errors and disturbance effects will only die away at the speed of the plant model and the estimate will not be suitable for control.

Luenberger\(^3\) has shown how a suitable dynamic system, which is not directly based on a plant model, can provide an estimate of a plant's state vector. Such systems, called observers, are driven by available plant inputs and outputs. Consider the discrete system, equation (12) of order \(p\),

\[
x(k+1) = Px(k) + Su(k)
\]

(31)

with a limited number of output measurements

\[
y(k) = Mx(k),
\]

(32)

where \(y(k)\) is a vector of order \(1 < p\) and \(M\) is an \(1 \times p\) matrix. The equation of a second dynamic system driven by \(y(k)\) and \(u(k)\) is,

\[
z(k+1) = Bz(k) + Dy(k+1) + Gu(k),
\]

(33)

where \(z(k)\) is the system's state vector of order \(p\) and \(B\) (\(p \times p\)), \(D\) (\(p \times 1\)) and \(G\) (\(p \times s\)) are matrices.
If \( z(k) \) is to provide an estimate of \( x(k) \) then they must be related by a constant linear transformation \( T \). Assuming that such a transformation exists then,

\[
z(k) = Tx(k). \tag{34}
\]

Substituting equations (31), (32) and (34) in equation (33) gives,

\[
Tx(k+1) = BTx(k) + DMPx(k) + CMSu(k) + Gu(k). \tag{35}
\]

Then multiplying equation (31) by \( T \) gives,

\[
Tx(k+1) = TPx(k) + TSu(k). \tag{36}
\]

Equating the r.h.s. of equations (35) and (36) gives,

\[
BTx(k) + DMPx(k) + DMSu(k) + Gu(k) = TPx(k) + TSu(k). \tag{37}
\]

Setting \( G = TS - DMS \) for convenience gives,

\[
TP = BT. \tag{38}
\]

Equation (38) is well known and has a unique solution \( T \) if \( P \) and \( B \) have no common eigen values. The system equations (31) give values for \( P \) and \( M \), and \( B \) and \( D \) are chosen to give an observer with suitable dynamics.

Subtracting equation (36) from equation (33) with equations (31) and (32) substituted for \( y(k+1) \) gives,

\[
z(k+1) - Tx(k+1) = Bz(k) + (DMP-T)x(k) + (G+DMS-TS)u(k). \tag{39}
\]

As \( G = TS - DMS \) and substituting equation (38) gives,

\[
z(k+1) - Tx(k+1) = B \left[ z(k) - Tx(k) \right]. \tag{40}
\]

This is a first order difference equation in \( z-Tx \) and solves to give,

\[
z(k) = Tx(k) + B^k (z(0) - Tx(0)). \tag{41}
\]

Where \( z(0) \) and \( x(0) \) are initial values at time \( kT = 0 \). Equation (41) shows that \( z(k) \) will be linearly related to \( x(k) \) and will give an exact estimate of \( x(k) \) for all values of \( k > 0 \) if the initial conditions are properly set.
To obtain the estimated state vector from \( z(k) \) then \( T \) must be non-singular and in this work was chosen to be the identity matrix. Then equation (38) becomes

\[
P - B = DMF
\]  

(42)

The matrices \( P \) and \( M \) are defined by the system of interest, if a value for \( D \) is specified equation (42) gives a value for \( B \). No straightforward method exists for choosing \( B \) and \( D \) in a particular application. However a method which approaches the same problem in a different manner can be used to design the observer.

iii) Kalman Filtering

Tuo\textsuperscript{30} and Noton\textsuperscript{31} have applied theory originally developed by Kalman\textsuperscript{35} to design an observer which gives the best estimate of a linear systems state vector, when the measurements are corrupted by Gaussian noise. The system equation (12) is modified to include noise disturbances,

\[
x(k+1) = Fx(k) + Su(k) + E_kd(k)
\]  

(43)

where \( d(k) \) is a vector of \( p \) random disturbances and \( E_k \) is an \((pxp)\) matrix. The available measurement vector \( y(k) \) is also corrupted by noise and equation (32) becomes,

\[
y(k) = Mx(k) + w(k).
\]  

(44)

where \( w(k) \) is a vector of \( 1 \) random disturbances.

The optimal control law derived in section (5) was obtained for a deterministic system. Tuo\textsuperscript{30} has shown that, when Gaussian disturbances are present, a similar control law is obtained when the expected value of
the performance criterion is minimised. Equation (21) gives the optimum control value \( u^O(k) \), when \( x(k) \) is not available for measurement then some sub-optimal control \( u(k) \) will be realised. This control will increase the cost over the optimum by a factor \( \Delta \), where

\[
\Delta = \theta_k(u,x) - \theta_k(u^O,x),
\]

and \( \theta_k \) is the cost for a \( k \) stage process. Substituting for \( \theta_k \) from equation (18) and simplifying gives,

\[
\Delta = [u(0) - u^O(0)]^T [R + \sum_{i=1}^{k-1} \phi_i^{-1} \phi_i^T] [u(0) - u^O(0)].
\]

Assuming that \( u(k) \) is a linear combination of present and past measurements then

\[
u(k) = \sum_{r=1}^{n} A_r y(r),
\]

where \( A_r \) is an \((p \times 1)\) matrix and \( u(k) \) is in the vector space \( Y(k) \) made up of vectors \( y(1) \) to \( y(k) \). Resolving \( u^O(k) \) in terms of \( Y(k) \) gives \( u^O(k) = \hat{u}^O(k) + \bar{u}^O(k) \), where \( \hat{u}^O(k) \) is in the space and \( \bar{u}^O(k) \) is orthogonal to it. By substituting into equation (46) it can be shown that the value of \( u(k) \) which minimises \( \Delta \) is,

\[
u(k) = \hat{u}^O(k) = -C \hat{x}(k).
\]

Where \( \hat{x}(k) \) is the component of \( x(k) \) in \( Y(k) \) and is the best linear estimate of \( x(k) \) in a least squares sense. The problem of determining the best sub-optimal control is then reduced to the problem of determining \( \hat{x}(k) \).

Kalman\(^{35}\) has presented the complete solution to this problem and the results are fully described in his work. Using the theory of linear vector spaces and the properties of orthogonal vectors he obtained a
dynamic system, which determines the value of $\hat{x}(k)$ from the measured values. The equation for the estimator is,

$$\hat{x}(k+1) = [I - A_o(k)M] [P - SC] \hat{x}(k) + A_o(k) y(k+1)$$

(49)

$A_o(k)$ is an $(p \times 1)$ matrix determined to minimise the estimate error covariance matrix,

$$K(k) = E_x [\hat{x}(k|k-1) \hat{x}'(k|k-1)]$$

where $E_x$ is expected value and $\hat{x}(k|k-1)$ is the component of $x(k)$ orthogonal to $Y(k-1)$. The minimisation is achieved by an interactive procedure described by the following equations,

$$A_o(k) = K(k)M^{-1} (MK(k)M^{-1} + W^{-1})$$

(50)

and

$$K(k+1) = P [I - A_o(k)M] K(k) [I - A_o(k)M]'P' + PA_o(k)W_oA_o'(k)P'$$

$$+ E_1V_0E_1'$$

(51)

Where $W_o = E_x \{w(k)w'(k)\}$ and $V_o = E_x \{d(k)d'(k)\}$.

These relations were first obtained by Kalman who also showed that the estimation problem is the dual of the control problem: there is a correspondence between equations (50) and (51), and equations (20) and (22) which is listed in Table 6.1. The statistical steady state solution

$$\lim_{k \to \infty} A_o(k)$$

where $A_o(k)$ tends to a constant value, was used in this work.

Substituting $u(k) = -C \hat{x}(k)$ in equation (49) gives,

$$\hat{x}(k+1) = (I - A_oM) P \hat{x}(k) + (I - A_oM) Su(k) + A_o y(k+1)$$

(52)

This is an observer equation with $T = I$, $G = (I - A_oM)S$, $D = A_o$ and $B = (I - A_oM)P$ which satisfies equation (42). Hence the optimal
estimator has all the properties of an observer for a deterministic system with its pole locations and gain chosen according to the noise statistics. A diagram of the closed loop system is shown in Fig. (6.3).

When \( T = I \) the observer state vector \( z(k) \) equals \( \hat{x}(k) \) the estimated state vector. The control based on \( \hat{x}(k) \) can be expressed as \( u(k) = -Cz(k) \) and the closed loop system equations are,

\[
\begin{align*}
  x(k+1) &= P - SC x(k) \\
  z(k+1) &= A_0 MP (I - A_0 M)P - SC z(k)
\end{align*}
\]

Then for an eigen value \( \mu \),

\[
P x(k) - SC z(k) = \mu x(k)
\]

and

\[
A_0 MP x(k) + [I - A_0 M]P - SC z(k) = \mu z(k)
\]

Subtracting equation (55) from equation (54) gives,

\[
(I - A_0 M)P [x(k) - z(k)] = \mu [x(k) - z(k)].
\]

This equation is satisfied if \( \mu \) is an eigen value of \([I - A_0 M]P \) or when \( x(k) = z(k) \). When \( x(k) = z(k) \) then equation (54) becomes,

\[
(P - SC) x(k) = \mu x(k)
\]

which is satisfied if \( \mu \) is an eigen-value of \( P - SC \). Equations (56) and (57) show that the closed loop system eigen-values are those of \( P - SC \) and \( (I - A_0 M)P \). The presence of an observer does not change the closed loop poles of the system, but it adds to its own poles which for the observer designed here are the eigen-values of \( (I - A_0 M)P \).

The observer poles could be assigned quite arbitrarily but the observer was designed as a Kalman estimator for two reasons:
FIG. 6.3. CONTROL OF THE COLUMN USING AN OPTIMAL CONTROL SYSTEM AND AN OBSERVER
a) The design method took account of noise disturbances present in practice.

b) As the calculation of the $A_0$ matrix is a dual of the optimum controller calculation, the same computer programme can be used, with minor changes, to perform both sets of calculations.

The observer with the control law included, equation (49), defines the calculations needed to determine $\hat{x}(k)$. However this is not in a suitable form for implementing as a control law on a digital computer. So $z$-transforming equation (49) gives,

$$z\hat{x}(z) - z\hat{x}(0) = (I - A_0M)(P - SC)\hat{x}(z) + zA_0Y(z) - zA_0y(0), \quad (58)$$

where $\hat{x}(z)$ and $Y(z)$ are the $z$-transforms of $\hat{x}(k)$ and $y(k)$ and $\hat{x}(0)$ and $y(0)$ are their initial values. Putting $(I - A_0M)(P - SC) = R$ and rearranging gives,

$$(zI - R) \hat{x}(z) = zA_0Y(z) + z(\hat{x}(0) - A_0\hat{y}(0)). \quad (59)$$

Now assuming that the observer initial conditions are properly set and $\hat{x}(0) = A_0\hat{y}(0)$, then equation (59) becomes,

$$\hat{x}(z) = (zI - R)^{-1} zA_0Y(z). \quad (60)$$

The $z$-transform of the control equation is $U(z) = -C\hat{x}(z)$ and so the control equation becomes,

$$U(z) = -C(zI - R)^{-1} zA_0Y(z). \quad (61)$$

As $y(k)$ represents deviations from a desired measurement value and as $(zI - R)^{-1}$ is a rational function in $z$ equation (61) is the equation of a sampled data controller using past values of $u(k)$ and $y(k)$. The assumption of initial-condition equality will usually be justified as control
will commence from a set-point of zero and \( y(0) = 0 \) and \( x(0) \) is set as zero in the computer.

7) Conclusions

In this chapter the theoretical basis of certain control system design methods has been presented. Some of these methods have not been used in distillation column control before, and few applications in other fields have been reported. The use of the linear optimal regulator theory to design controllers in an integrated fashion is believed to be a new departure in distillation column control; both feedforward and feedback controllers are designed using the same calculation. It is hoped that integrated design may give better control when interaction occurs.

As well as this new method, conventional design techniques have been presented for purposes of comparison. The sampled data two-term controller relies on canceling a pole in the z-plane and on-line tuning of controller gain to achieve good performance. This method has been used with considerable success\(^{33}\) and is typical of the best industrial practice.

Finally two methods of reducing the number of measurements required by the integrated controller have been studied. The first method is rather artificial as a mathematical device is used to set controller coefficients to zero. The use of observers has also been studied and the properties of these dynamic systems have been presented. The problem of observer pole
allocation has been overcome by making the observer a Kalman estimator. Again the application of both these methods to distillation columns is believed to be original.

In the next chapter the application of these methods to designing controllers for the N.F.L. distillation column will be described.

TABLE 6.1
DUAL RELATIONS FOR CONTROL AND ESTIMATION

<table>
<thead>
<tr>
<th>Control</th>
<th>Estimation</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>P'</td>
</tr>
<tr>
<td>S</td>
<td>M'</td>
</tr>
<tr>
<td>D\tau</td>
<td>E_1 V_0 E_1'</td>
</tr>
<tr>
<td>\times H</td>
<td>W_0</td>
</tr>
<tr>
<td>C</td>
<td>A_0 'P'</td>
</tr>
<tr>
<td>G</td>
<td>K</td>
</tr>
</tbody>
</table>
1) **Introduction**

In this chapter the control problems encountered on the N.P.L. column are discussed and a two loop control configuration is suggested. The control theory presented in Chapter 6 is used to design control systems for this column.

The design of discrete-time two-term controllers is straightforward, but the application of optimal control theory is complicated by the following problems:

a) The large number of measurements required by this type of control system.
b) The lack of integral action which causes steady state errors.

Techniques are presented which overcome these problems and a systematic design procedure is developed. This work is an original application of existing theory.

The control schemes are assessed by simulating their performance on a digital computer model of the column. The results obtained in practice are described in Chapter 8.
2) **Control of the N.P.L. Column**

Control studies on the N.P.L. column were limited to some extent by the physical behaviour of the process and the instrumentation available. No measurement of feed flow or composition was available on-line so feed-forward control could only be tested in computer simulations.

As already stated in Chapter 5 the column gain, at low compositions, is very small and at high composition the azeotrope tends to damp out dynamic change. To obtain top product composition changes of a reasonable magnitude (top product composition of 60%), the bottom of the column was run in a condition of total separation. Therefore the full effects of interaction on control could not be tested and an alternative control strategy was used in which heat and reflux ratio were used to control the top plate composition.

The column is still a useful test bed for comparative control studies because:—

i) It is non-linear.

ii) Hydrodynamic delays occur to a limited extent.

iii) It is subject to drift and noise disturbances.

The sampling interval was fixed by hardware to be a multiple of 32 secs and a value of 96 secs, was chosen. This value was also used by Williams.¹²
3) The Design of Conventional Control Systems

i) Feedforward Control

A "static" feedforward control was designed for comparison with the feedforward control designed by the optimum control calculation. The steady state gains were calculated from the transfer functions given in Table (5.4). These values were substituted in equation (6.3) and the following control equations were obtained,

\[ R(z) = -0.876 F(z) + 58.2 Z(z). \]  \hspace{1cm} (1)
\[ Q(z) = -8,650 F(z) + 95,800 Z(z). \]  \hspace{1cm} (2)

ii) Feedback Control

The first order transfer functions obtained from the frequency response programme were z-transformed using a sampling interval of 1.6 mins to give the following top plate composition responses:

\[ \frac{X(z)}{R(z)} = \frac{0.35z^{-1}}{1 - 0.962z^{-1}}, \text{ where } L = 0.038. \]  \hspace{1cm} (3)
\[ \frac{X(z)}{Q(z)} = \frac{-0.0263z^{-1}}{1 - 0.964z^{-1}}, \text{ and } L = 0.036. \]  \hspace{1cm} (4)

Substituting these transfer functions into equation (6.11) gives the following controller transfer functions for the two loops,

\[ \frac{R(z)}{R(z)} = \frac{Q (2.86 - 2.75z^{-1})}{(1 - z^{-1})}, \]  \hspace{1cm} (5)
\[ \frac{Q(z)}{Q(z)} = \frac{-Q (3.80 - 3.66z^{-1})}{(1 - z^{-1})}, \]  \hspace{1cm} (6)
where the time constant of the closed loop response is $\frac{1}{\log_e(1-Q)}$ and is adjusted by "on-line" tuning of the controller gain $Q$.

The control equations were simulated on the linearised model. Fig. (7.1) shows the top plate composition response to a step change in set point, when reflux only is manipulated. The following effects were observed:

i) As predicted when $Q=1$ the closed loop response is the same as the open loop response.

ii) As $Q$ is increased the column follows an exponential response whose time constant is governed by the value of $Q$.

iii) When $Q=1$ the closed loop response should be "deadbeat", the system settling in one sampling interval. The simulated response overshoots by 13% due to mismeasurement of the process parameters and because the first order model is an approximation to a seventh order system. Control difficulties of this type are overcome by reducing $Q$, making the control less "tight".

A general criticism of cancellation compensation design methods is that imperfect cancellation can allow undesirable lightly damped terms in the closed loop response. In this particular application this does not present a serious problem because:

i) When $\tau = 1.6$ mins and $T_c = 40$ then $(1-L) = 0.96$, if $T_c = 20$ then $(1-L)$ = 0.951 and if $T_c = 60$, $(1-L) = 0.968$. So errors of 50% in estimating $T_c$ only cause errors of 1% in $(1-L)$.

ii) If, the model has a pole in the z-plane at $(1-L')$ and the process has
FIG. 7.1. COLUMN MODEL RESPONSE TO A SET POINT CHANGE WITH TWO-TERM CONTROL OF REFLUX

FIG. 7.2. Z-PLANE POLE-ZERO PLOTS FOR TWO-TERM CONTROL SYSTEMS WITH PARAMETER ERRORS.

1) \( L = L' \) PERFECT CANCELLATION

2) \( L > L' \)

3) \( L < L' \)

X OPEN LOOP POLE.
O OPEN LOOP ZERO.
X CLOSED LOOP POLE.
a pole at \((1-L)\) then using equations 6(8) and 6(11) the open loop transfer function is,

\[
\frac{L Q z^{-1} (1 - (1 - L) z^{-1})}{L' (1 - (1 - L) z^{-1}) (1 - z^{-1})}
\]

Depending on the relative magnitudes of \(L'\) and \(L\) three different root-locus plots, shown in Fig. (7.2), are obtained:

a) \(L = L'\) giving perfect cancellation with the remaining closed loop pole on the real axis inside the unit circle.

b) \(L > L'\) and two real closed loop poles result within the unit circle.

c) \(L < L'\) gives complex closed loop poles for certain values of \(Q\).

As the difference between \(L\) and \(L'\) should be small, both these poles should be inside the unit circle and close to the real axis.

These arguments only apply when the system transfer function is of first order, additional poles and zeros present in the column transfer function can still cause control problems.

When both heat and reflux are used to control top plate composition the two loops are not independent. A block diagram of the system is shown in Fig. (7.3) and the closed loop z-transfer function is,

\[
K(z) = \frac{G_1(z) D_1(z) + G_2(z) D_2(z)}{1 + G_1(z) D_1(z) + G_2(z) D_2(z)},
\]

(7)

where \(G_1(z)\) and \(G_2(z)\) are the process z-transfer functions including sample and hold elements and \(D_1(z)\) and \(D_2(z)\) are the respective control equation transfer functions.
FIG. 7.3. Z-TRANSFER FUNCTION BLOCK DIAGRAM OF THE COLUMN TWO-LOOP CONTROL SYSTEM.

FIG. 7.4. COLUMN MODEL RESPONSE TO A SET POINT CHANGE WITH TWO TERM CONTROL OF HEAT AND REFLUX.
If the control systems are designed using Higham's method as single loops and the process transfer functions are of first order, then using symbols defined in Chapter 6,

\[ q_1(z) n_1(z) = \frac{a_1 L_1 z^{-1}}{1 - (1 - L_1) z^{-1}} \cdot \frac{Q_1 [1 - (1 - L_1) z^{-1}]}{Q_1 L_1 (1 - z^{-1})} \]

\[ q_1 z^{-1} \]

and similarly,

\[ q_2(z) n_2(z) = \frac{q_2 z^{-1}}{1 - z^{-1}} \]

Substituting equations (9) and (10) into equation (8) gives,

\[ K(z) = \frac{(q_1 + q_2) z^{-1}}{1 - (1 - [q_1 + q_2]) z^{-1}}. \]

If \( q_1 = q_2 = 0 \) then equation (11) becomes,

\[ K(z) = \frac{2q z^{-1}}{1 - (1 - 2q) z^{-1}}. \]

which is an exponential response (\( Q \leq 0.5 \)) with a time constant of \( \tau/\log_2(1-2Q) \). Equation (12) shows that in terms of response two loop control offers no advantage over single-loop control and this agrees with the simulated results shown in Fig. (7,5) for \( Q = 0.019, 0.038, 0.1 \) and 0.2. However a distinct advantage of two loop control is that fast responses for a single loop, i.e. \( Q = 0.5 \), which cause excessive control variable excursions can be achieved using two loops with acceptable levels of control action.
The control system described by equation (6.21) is shown applied to a distillation column in Fig. (7.5). The "set point" is the desired column composition profile and heat and reflux are manipulated according to equation (6.22) to correct for deviations from this desired state. Feedforward control is also shown and feed disturbances were included in the column equations as step changes. If random disturbances occur, they can be included if a suitable noise model is specified.

A computer programme was written in KDF9 Algol using the matrix library procedures to perform the iterative minimisation calculations, equations (6.20) and (6.22). The continuous system equations calculated using the steady state programme and the performance criterion weighting matrices were given as data. The programme converted the system equations to discrete time form, as described in section 4.5, and then performed the minimisation over a preset number of stages. All the \( G_r \) matrices were printed out to check that the solution had reached a constant value and the final \( G_r \) matrix was printed to check for symmetry. The programme was tested on examples quoted in textbooks and reproduced the results satisfactorily.

Fig. (7.5) also, illustrates the effect of the performance criterion weighting matrices on the control. The control system C matrix and hence the controller performance depend on the value assigned to these matrices which can be specified quite arbitrarily. This is a serious logical flaw in the design method, but if a systematic method of choosing these coefficients can be established, this is not a serious drawback to an
FIG. 7.5. OPTIMAL CONTROL OF A DISTILLATION COLUMN.
engineer concerned with applications. The procedure used in this work is as follows:-

i) The A matrix penalises offsets from the desired composition profile. As only product compositions are of interest, the top plate \( x_1 \) and reboiler \( x_r \) compositions were equally weighted with unity value. As the reboiler composition is much smaller than that of the top plate the ratio of \( x_1^2 : x_r^2 \) was about \( 1:10^{-10} \) and the reboiler weighting had little effect on control.

ii) The B matrix weights the relative amounts of correcting action provided by the heat and reflux. The B matrix coefficients were chosen in the ratio of the inverse squares of the steady state gains of top plate composition to each control variable. This meant that each control variable had the same correcting action on top plate composition changes.

iii) The value of \( \lambda \) is used to weight the relative effects of the A and B matrices in the performance criterion. It was chosen by simulating the system performance with several controllers designed using different values of \( \lambda \) and choosing the control which gave the best performance from an engineering point of view.

The column equations were linearised about a composition profile which was used as the control "set point". Fig. (7.6) shows the control matrix (C) coefficients for the most useful range of \( \lambda \) plotted against column plate number, the results show that:-

a) As \( \lambda \) decreases the control gain increases.
Fig. 7.6. Plot of optimal control matrix feed-forward and feedback coefficients against plate number for several values of λ.

λ values:

- $4 \times 10^{-6}$
- $2.8 \times 10^{-4}$
- $2.8 \times 10^{-3}$

Reflux coefficients:

Feedforward coefficients:

Plate number:

Reboiler feed flow feed compn.
b) The reboiler feedback coefficient is much larger than any of the others.

c) The controller coefficients exhibit a peak in the region of plate 3.

This shows that the coefficient values depend on the relative magnitude of changes on each plate as well as the performance criterion weighting.

The feedforward coefficients calculated in section (7.3) are larger than those shown in Fig. (7.6) as control variable changes are not penalised in the conventional design method.

Figs (7.7) and (7.8) show the control system response to set point changes and feed changes respectively, when simulated on the linearised model. The responses are faster with small values of $\lambda$ as larger control variable changes are permitted. The response to feed changes show that:

i) The system always exhibits a steady state offset following a step change in feed. This is characteristic of systems controlled in this fashion, the plant does not contain any form of integration in its open-loop response and the optimum controller has no integral action. When a feed change occurs, there is a shift in the column composition profile which is sensed by the controller and used to generate a correcting signal, if the offset is brought to zero the correcting signal will also go to zero, hence this type of control must allow some steady state offset. In practice this will not be serious if the controller can reduce the offset to a reasonably small value, and simulations indicate that for the smaller values of $\lambda$ this will be so.
FIG. 7.7. SIMULATED RESPONSES TO A SET POINT CHANGE WITH OPTIMAL CONTROL FOR SEVERAL VALUES OF $\lambda$.

**λ VALUE**
- $4 \times 10^{-6}$
- $2.8 \times 10^{-5}$
- $2.8 \times 10^{-4}$
- $2.8 \times 10^{-3}$
- $2.8 \times 10^{-2}$
- OPEN LOOP

TIME UNIT = 1.6 MIN.

TOP PLATE COMPOSITION CHANGE:
% MOLES
FIG. 7.8 SIMULATED RESPONSE TO A 0.5% MOLES COMPOSITION IN FEED COMPOSITION WITH OPTIMAL CONTROL FOR SEVERAL VALUES OF $\lambda$. 

**TOP PLATE COMPOSITION OFFSET**

% MOLES

$\lambda$ VALUE

- OPEN LOOP
- $2.8 \times 10^{-3}$
- $2.8 \times 10^{-4}$
- $2.8 \times 10^{-5}$ (NO FEED FORWARD)

**TIME: 1 UNIT = 1.6 MIN.**

**TOP PLATE COMPOSITION OFFSET**

% MOLES x 10^{-4}

$\lambda$ VALUE

- $2.8 \times 10^{-4}$
- $2.8 \times 10^{-5}$
- $4.0 \times 10^{-6}$

**TIME: 1 UNIT = 1.6 MIN.**
ii) When $\lambda$ is large the system response to disturbances is exponential, but as $\lambda$ decreases the system exhibits a pronounced spike in the opposite direction to the disturbance. This is characteristic of "static" feedforward control, because the change in control variables cause overcompensation initially.

The response of a feedback only controller is shown in Fig. (7.8) and the steady state offset is much greater than when feedforward is also included.

The control system performance was also simulated on the non-linear model to test:

i) The effect of control variable limits.

ii) The effect of non-linearity on control system stability.

The control system obtained when $\lambda = 2.8 \times 10^{-5}$ gave a good response with acceptable control variable changes. Two other control systems with lower gains, $\lambda = 2.8 \times 10^{-3}$ and $2.8 \times 10^{-4}$ were also studied, in case the high gain control system was unstable in practice.

Sunderland modified the FI FI programme so that it could simulate digital control systems. Two extra subroutines were written, EVY in which a sum of squared errors was calculated and STEP in which the control equations were specified. The results obtained for set point changes of $\pm 14\%$ in top plate composition and a feed composition change of $1.25\%$ are shown in Figs (7.9), (7.10) and (7.11).

The graphs show top plate composition responses which are very
FIG. 7.9. NON-LINEAR MODEL RESPONSE TO A SET POINT CHANGE UNDER OPTIMAL CONTROL.

FIG. 7.10. NON-LINEAR MODEL RESPONSE TO A SET POINT CHANGE UNDER OPTIMAL CONTROL.
Fig. 7.11. Non-linear model response with optimally controlled feed composition change of \(-1.25\%\) moles.
similar to those obtained from the linearised model. The results showed that:

i) The reboiler composition was about 0.1%, and was not affected by control action.

ii) The response with increasing composition, Fig. (7.9), is slower than those with decreasing composition, Fig. (7.10).

iii) The set point change, Fig. (7.10) with decreasing composition exhibit some overshoot due to reflux saturation and column non-linearity.

iv) The steady state offset following a feed change is larger on the non-linear model, but is not excessive with the higher gain controllers.

v) The spike caused by the static feedforward controller is not present because FIFI has to integrate the equations for one sampling interval before control is applied. When control is applied both feedforward and feedback elements contribute to the correction and the spike does not occur.

5) Control with Integral Action

Steady state offsets following changes in the feed can be eliminated when control with integral action is used. An additional state variable which is the integral of the top plate composition was added to the model and to include it in the control equation it was assigned weighting values of 1.0 and 0.1 in the performance criterion. The optimal control calculation was then repeated for the same values of \( \lambda \).
The simulated results for this control system to set point and feed changes are shown in Figs (7.12), (7.13) and (7.14). The response to a set point change now overshoots, because the integrator acts as a memory of the large initial offset which is brought to zero by overshooting. Following a feed change the steady state offset is brought to zero, the speed of response depending on the performance criterion weighting. Including an extra state variable has little effect on the other control equation coefficient values.

6) The Performance of the Reduced Optimal Controller

The computer programme written to calculate the controller C matrix included a facility to allow it to also calculate the iterative relationship given by equations 6(29) and 6(30). The resulting control system has a C matrix with selected elements set to zero.

In distillation column applications a large number of state variables have to be eliminated. Two control systems were designed for the N.P.L. column, one with only top and bottom plate compositions feedback and the other with the feedplate composition feedback as well, when \( \lambda = 2.8 \times 10^{-5} \).

These controllers were simulated on the linearised model, and were compared with the full optimal controller. Fig. (7.15) shows the top plate response to a set point offset. The reduced controllers give poorer
FIG. 7.12. NON-LINEAR MODEL RESPONSE WITH OPTIMAL INTEGRAL (WEIGHTING OF 0.1) CONTROL TO A SET POINT CHANGE.

FIG. 7.13. NON-LINEAR MODEL RESPONSE WITH OPTIMAL INTEGRAL (WEIGHTING OF 1.0) CONTROL TO A SET POINT CHANGE.
FIG. 7.14. NON-LINEAR MODEL RESPONSE TO A FEED COMPOSITION CHANGE OF -1.25% WITH OPTIMAL INTEGRAL CONTROL.

A) INTEGRAL WEIGHTING = 1.0.

TIME: 1 UNIT = 1.6 MIN.

B) INTEGRAL WEIGHTING = 0.1.

TIME: 1 UNIT = 1.6 MIN.
responses than the full controller but they are still satisfactory.

Fig. (7.16) compares the controller's response to a feed change of 0.5% B.M. with feedforward and feedback control. The steady state offset with the eliminated controllers is greater than that of the full controller by a factor of more than twenty.

While the reduced controllers gave reasonable results, it was decided that an excessive number of state variables had to be eliminated. Although Hoskins theory is sound the changes in the C matrix were such that similar results could be obtained by ignoring selected coefficients in the full control C matrix.

7) Control with Observers

To design a Kalman estimator as described in section 6.6 the noise statistics of the column have to be specified. This presented certain difficulties because:-

i) The N.P.L. column was being rebuilt at Warren Spring Laboratory and was not available to obtain the necessary operating records.

ii) The noise was composed of a limited range of frequencies and would have to be represented by Gaussian noise passed through suitable first order filters.

To avoid these difficulties the noise was assumed to be "white".
FIG. 7.15 MODEL RESPONSE TO A SET POINT CHANGE WITH OPTIMAL CONTROL WITH SOME STATE VARIABLES ELIMINATED.

TIME: 1 UNIT = 1.6 MIN.

FIG. 7.16. MODEL RESPONSE TO A FEED COMPOSITION CHANGE OF 1.25% MOLES WITH OPTIMAL CONTROL WITH SOME STATE VARIABLES ELIMINATED.

TIME: 1 UNIT = 1.6 MIN.
This is a gross assumption, but the theory of observers shows that the observer dynamics, if stable, are not critical. The noise levels present still have to be calculated, and several short steady state operating records obtained at N.P.L. were used for this purpose. The mean and variance of the records were calculated using a computer programme. The r.m.s. value of noise level was found to vary on all plates between 3.0% and 5% of the mean value depending on the record. The observer was designed with a noise level corresponding to an r.m.s. value of 4% on all plates to calculate the process noise covariance. \( (E) \) is taken to be the unit matrix. The separation of process noise from measurement noise is more difficult and the ratio of the two decides the estimator calculation value of \( \lambda \) (Table 6.1) and hence the magnitude of \( \lambda \). The measurement noise covariance was calculated assuming an r.m.s. measurement noise of 1% of the mean value of top plate composition.

The noise bandwidth was estimated from the short operating records to test the assumption of "white" noise. The number of mean value crossings were counted and using the approximate formula given by Goff\(^{35} \) the lowpass noise bandwidth \( f_n = \beta/2\pi \times 0.8 \). Where \( \beta \) is the average number of mean value crossings/unit time. This gives a lowpass noise bandwidth (counted over 100 mean value crossings) of \( 8.0 \times 10^{-2} \) cycles/min compared with the column bandwidth of \( 4 \times 10^{-3} \) cycles/min. While the "white" noise Kalman estimator will not be optimum for signals corrupted by lowpass noise, the bandwidths are such that satisfactory results should be obtained.
The feedforward control was not included in the estimator design as no on-line measurements of feed conditions were available and feedforward control could not be implemented with the existing control programme.

The programme used to calculate the control matrix $C$, was modified so that it could calculate the observer $A_0$ matrix. The data input section was rewritten so that the matrices in the iterative minimisation were assigned according to Table 6.1. The initial covariance matrix $K(0)$ was assumed to be zero and iterations were continued until the value of the $A_0$ matrix in the statistical steady state was obtained.

To obtain control equations which could be implemented using the Hermes control programme equation 6(6) must be evaluated,

$$U(z) = -C \ (zI - R)^{-1} \ zA_0Y(z)$$

Zadeh and Desoer\textsuperscript{37} have shown that,

$$(zI - R)^{-1} = B(z)/d(z),$$

where $d(z) = \det(zI - R) = z^m + d_1z^{m-1} + \cdots + d_{m-1}z + d_m$, \hspace{1cm} (15)

and $B(z) = \text{adj}(zI - R) = B_0z^{m-1} + B_1z^{m-2} + \cdots + B_{m-2}z + B_{m-1}$. \hspace{1cm} (16)

$B_0$ to $B_{m-1}$ are $(m \times m)$ matrices. The following-iterative relationship can be used to evaluate the coefficients,

$$B_k = B_{k-1}R + d_kI \text{ and } \hat{d}_k = \frac{-1}{k} \text{ trace } (B_{k-1}R),$$

where $k = 1, \ldots, m$ and $B_0 = I$ and $\hat{d}_0 = 1$. 


A computer programme was written to calculate the values of $B_k$ and $d_{k0}$. The null matrix,

$$ B_m = 0 = B_{m-1}R + d_m I $$

was evaluated and used to determine the magnitude of rounding errors.

The $B$ matrices were pre-multiplied by $C$ and post multiplied by $zA_0$ to yield the control equation (13).

When integral control is introduced the measured value $Y(z)$ was integrated using the rectangular approximation by extending equation (13), thus,

$$ U(z) = -C_1(zI - R)^{-1} A_0 Y(z) - C_2(zI - I)^{-1} zY(z). $$

The control matrix $C$ is partitioned into the state feedback matrix $C_1$ and the integrated feedback matrix $C_2$. The first term was evaluated using the computer programme and the second term was added to it.

The $A_0$ matrix value calculated was used to compute the following three sets of observer and control equations for the three $\lambda$ values:

a) Estimated state feedback control.

b) Estimated state feedback control with integral action calculated with 0.1 weighting.

c) Estimated state feedback control with integral action calculated with a weighting of 1.0.

The control equations obtained showed that:
i) Coefficients of terms of order greater than $z^{-3}$ were small relative to the $z^0$ coefficient and were neglected. This shows that a lower order column model could have been used.

ii) The elements of the $B_m$ matrix were $0 (10^{-13})$ as was the coefficient of $z^{-7}$. Hence rounding errors were as large as the smallest coefficient and the method of matrix inversion is not particularly accurate.

The optimal control equations with state estimation were tested by computer simulation with the non-linear model. The control systems without integral action were subject to larger steady state offsets than those of the equivalent simulated state feedback system. The magnitude of the offset depended on the value of $\lambda$ and was between 1% and 2% in composition for a 14% set point change.

When the final value theorem for z-transforms is applied to the closed loop transfer function, equation (7), for a unit step set point change then,

$$X(z) = \lim_{z \to 1} (z - 1) \frac{D_1(z) G_1(z) + D_2(z) G_2(z)}{1 + D_1(z) G_1(z) + D_2(z) G_2(z)} \frac{z}{(z - 1)} \quad (20)$$

This was evaluated with the calculated control z-transfer functions and the approximate first order column z-transfer functions, equations (3) and (4), to give a value for the steady state offset. The values obtained showed that the increased offsets were due to the control equations and are therefore introduced in the evaluation of the observer and control polynomials. Fadeeva's algorithm used to invert $(zI - R)$ is well known.
for its lack of numerical accuracy but no alternative method is available. When integral action is included the control equations have a pole at \( z = 1 \) and the offsets are forced to zero in spite of observer errors.

These results show that observer systems are extremely sensitive to errors, this is due to the following reasons:

a) The observers desirable properties of state estimation and adding its own poles to those of the closed loop system are only obtained when equation 6(38) is satisfied. Any error such as a difference between a plant and its model which is very likely to occur in practice, especially in process applications, will cause state vector estimate errors and change the system closed loop pole configuration.

b) A second relationship also has to be satisfied, the observer is driven by \( Gu(k) \) to account for system inputs, where \( G = TS - DMS \), any errors in \( T \) or \( S \) will again cause state estimate errors.

The simulated responses obtained when integral action is included are shown in Fig. (7.17) for set point changes and Fig. (7.18) for feed composition changes. The steady state offset has been eliminated and the results are similar to those in Figs (7.12), (7.13) and (7.14) with complete state feedback but the speed of response is slower. The observer errors are the same with and without integral action and the degradation of performance mentioned is due to these observer errors. Integration improves control compared with estimated state feedback control because:

a) Long term offsets due to observer errors and proportional control are reduced to zero.
FIG. 7.7 NON-LINEAR MODEL RESPONSE TO A SET-POINT CHANGE WITH OPTIMAL INTEGRAL CONTROL AND AN OBSERVER.
FIG. 7.18 NON-LINEAR MODEL RESPONSE TO A FEED
COMPOSITION CHANGE OF 1.25% MOLES WITH OPTIMAL
INTEGRAL CONTROL AND AN OBSERVER.

A) INTEGRAL WEIGHTING = 0.1

B) INTEGRAL WEIGHTING = 1.0
b) The integral is generated directly from the measured value and is added to the estimated state feedback according to equation (19). Hence the integral term is not subject to any observation error.

The Kalman estimator design method with \( T = I \) estimates the entire state vector including the values available as measurements. Hence any errors introduced by the observer are added to the values available as measurements. Luenberger has also developed reduced order observers where available measurements are used directly and only unmeasured variables are estimated, which should reduce the effect of observer errors.

The large steady state offsets obtained when no integral action was included were unacceptable for practical application and no attempt was made to implement these control systems on the N.P.L. column.

8) Conclusions

In this chapter control systems for the N.P.L. distillation column have been designed and tested by computer simulation. The results obtained show that the linearised column equations represent only mass transfer effects and in theory the column can be controlled with any desired speed of response. The discrete time two-term control system gave good results, was easy to design and could be tuned on-line to obtain the best performance.
The application of optimal linear control to distillation columns is original, the results obtained show that:

i) A great deal of computation is required to obtain an optimal control system which offers only marginal improvements in performance compared with two-term control.

ii) The optimal control system performance depends on the values of the performance criterion coefficients, which are usually chosen by trial and error. In this work this problem was reduced to choosing a value for one coefficient which determined the control system gain.

iii) The optimal system obtained does not have integral action although it is clear that this is required when a range of operating conditions have to be achieved. It was found that steady state offsets could be reduced to acceptable levels with high gain control systems, and could be eliminated by introducing integration as an additional system state variable.

iv) The optimal control system requires measurements of all the column state variables.

Two methods of reducing the number of measurements required were studied, a method of state variable elimination which sets any desired control coefficient to zero and the use of observers to estimate the system state vector.

The observer introduces dynamics into the control and is an original application of existing theory. In this work the observer was
designed to minimise the estimate error in the presence of noise using Kalman's method. It was shown that this system has the same properties as an observer and when the noise statistics are known only approximately a state vector estimate will still be obtained. The observer was found to be very sensitive to model errors and dynamic changes due to non-linearity, which caused offsets in the estimated state vector. When the observer was used with integral control good control was obtained because long term offsets caused by errors were reduced to zero.

It is important to note that the optimal control calculation reveals no information on the best control structure. In order to obtain good control the problem must be formulated so that desirable control functions, e.g. integral action, will result. In the next chapter the optimal integral control systems will be compared with two-term control systems on the N.P.L. column under direct digital control.
CHAPTER 8

THE CONTROL OF DISTILLATION COLUMNS — PRACTICAL RESULTS

1) Introduction

In this chapter the controllers designed in Chapters 6 and 7 are applied to the N.P.L. column under computer control. This work was the first in which the column was controlled by more than one loop.

The performance of the digital two-term control is compared with the optimum control with integral action and an observer for set point changes and feed changes. No practical applications of optimal linear regulators have been reported and this work is original.

Although only a limited number of results are presented, they represent a considerable amount of effort spent in maintaining the column instrumentation and in observing the control experiments.

2) The Computer Control System

The N.P.L. column was connected to the Ferranti Hermes digital computer to perform computer control experiments, a schematic diagram of the system is shown in Fig. (8.1).

Every 96 seconds a crystal controlled clock initiates a scan of 16
FIG. 8.1 COMPUTER CONTROL SYSTEM FOR THE
N.P.L. COLUMN.

COLUMN INSTRUMENTATION  COMPUTER INTERFACE  COMPUTER PROGRAM

- 96 SEC. CLOCK PULSE -

SCAN 16 ANALOGUE VALUES.

DIGITISE IN BCD FORM

HESITATION INPUT TO HERMES

CHANGE HEAT AND REFLUX

PROGRAM INTERRUPT ENTRY

CONVERT BCD DIGITS TO FLOATING POINT FORM.

CALCULATE CONTROL VALUES

SCALE AND TRANSMIT CONTROL OUTPUTS

UPDATE LOG LISTS.

DISPLAY GRAPH/LOGS ON CRT.

DISTILLATION COLUMN.
variables, as analogue voltages in the range -20V to +20V, at a one second sampling rate. These variables include column inputs, plate temperatures, composition meter readings, control set point value and a master channel which specified which control loops are in use. These voltages are digitised by a digital voltmeter and are sent in parallel to a binary coded decimal (B.C.D.) encoder and are converted into 6 digit B.C.D. numbers. These 8 bit digits are sent to Hermes serially and are "hesitated" into the computer core store. Hesitation is a process where a computer cycle (6μ sec) is "stolen" by the interface and used to place a number in a chosen store location. In this case one of the top 96 locations of the store. Each B.C.D. digit is counted and when 96 (16 x 6) digits have been received the counter interrupts the computer and forces it to obey the control programme.

The control programme was written by K. Wilkinson of N.P.L. for use in computer control experiments. On entry the B.C.D. numbers are converted into binary number form and column logs are updated. Up to six control equations of the following form are evaluated,

\[ u_0 = \sum_{i=0}^{n} a_i e_i + \sum_{i=1}^{n} b_i u_i, \]

where \( u_i \) are the past values of input, \( e_i \) are past error values, \( n \) is the number of past terms (less than 12) and \( a_i, b_i \) are coefficients. The coefficients are specified on a small data tape which can be changed at any time during an experiment. The calculated output values are sent to the column as three 8-bit binary numbers, from the Hermes 24 bit digital output, and are stored in buffer stores and used to set the new values of
control variable.

When the control programme is completed the computer returns to a programme which displays a log of the values last read in or a graph of 100 past values of any logged variable. This programme is suspended when an interrupt occurs at the end of the next input scan.

3) Experimental Technique

The column model used for control system design was obtained at the operating conditions given in Table 5.2, run 1. The column was set to reproduce these conditions, with a top product composition of 61% BM and a top plate composition of 37.5% BM, for the control experiments. The control equations were scaled in terms of column hardware; details of the scaling factors used are given in Appendix (2). Top plate temperature, read as a thermistor voltage was used as the controlled variable. Drift in the thermistor reference voltage was large enough to cause erroneous readings during a control response. To overcome this problem the following relationship was deduced.,

\[ T_1 = 3.8V_1 + 4.29V_R + 2.925, \]

where \( T_1 \) is the plate temperature (°C) deviation from 80°C, \( V_1 \) is the top plate thermistor voltage, and \( V_R \) is the thermistor reference voltage. The coefficient values were determined from measurements taken at constant reference voltage values.
In Hermes this correction was applied before the control equation was calculated and the set point was specified as a temperature. The temperature levels and equivalent compositions used for control are given in Table (8.1).

To perform a control experiment the column was first run to steady state, then the computer was connected with the master channel set to data logging only. The set point voltage was set to the same value as the top plate temperature reading and the column values were logged for at least \( n \) scans (where \( n \) is the number of control equation terms). When the master channel was set to control (negative) a "bumpless" transfer was achieved, and control experiments could begin. If the control equations were changed in mid-experiment a period of logging was again required before initiating control.

h) Two Term Control

The values of \( Q \) which gave good results when simulated were used, so that the two design methods could be compared. When \( Q = 0.2 \) unstable responses were obtained, for both single and two-loop control, with decreasing composition (increasing temperature) set point changes. The instability is caused by the vapour-liquid equilibrium curve non-linearity, which is shown in Fig. (5.18). Instability commences as the vapour-liquid equilibrium curve "knee" is approached, the column time constants shorten and the gain decreases. The response overshoots into the low gain region and takes a long time to recover.
When \( Q = 0.1 \) both heat and reflux responses to set point changes are stable, and are shown in Figs (8.2) and (8.3). The responses are exponential and are the same as the simulated results. The control settles with a steady state offset which is due to coarse control variable quantisation levels.

The steady state temperature change following a one bit input change is \( 0.461^\circ C \) for reflux and \( 0.366^\circ C \) for heat. The worst case error due to quantisation of the output should be half these values and the steady state offsets observe agree with this. While the input variable range is 8 bit (1 part in 256) a range of 15 covered the control region of interest. The heat control gain was adjusted to give the finest possible quantisation but the reflux control was preset and could not be altered.

Two loop control with \( Q = 0.1 \) gave unstable results, but after tuning on-line stable results were obtained with \( Q = 0.09 \). These are shown in Fig. (8.4), a faster exponential response is obtained and quantisation errors are reduced. The column shows a quicker response with increasing temperature than with decreasing temperature, which is further evidence of the columns non-linearity.

The effect of column time constant changes, due to non-linearity on control performance was discussed in Chapter 7, gain errors however were not considered. The effect of gain errors on the control can be seen from the closed loop transfer function (equation 6(5)) evaluated with different plant and model gains,
FIG. 8.2. COLUMN RESPONSE TO SET POINT CHANGES WITH TWO-TERM CONTROL OF REFLUX \((Q=0.1)\).

FIG. 8.3. COLUMN RESPONSE TO SET POINT CHANGES WITH TWO-TERM CONTROL OF HEAT \((Q=0.1)\).
**Figure 8.4.** Column response to set point change with two-term control of heat and reflux.

**Figure 8.5.** Column response to set point changes with optimal integral control.

Controller No. 3, $\lambda = 2.0 \times 10^{-3}$, integral weighting = 1.0.
\[ K(z) = \frac{Q G' z^{-1}/G}{1 - z^{-1} (1 - Q G'/G)}. \]

Where \( G' \) is the actual gain of the plant and \( G \) is the estimated gain used in controller design. So the sampled time constant becomes \( Q' = QG'/G \) and in this case \( G' < G \) and hence \( Q' < Q \) and the effect of the gain error is to slow the closed loop response observed. If \( G' > G \) the closed loop response would be faster than expected and instability could result in the worst cases.

5) **Optimal Control**

The optimal control system with integral action and an observer were tested on-line to the N.P.L. column. The control equations and the corresponding values of \( \lambda \) and integral weighting are given in Table 8.2.

a) **Control with 1.0 Integral Weighting**

Control systems 1 and 2 in Table 8.2 gave unstable responses to set point changes with decreasing composition (increasing temperature). The observed results indicated that instability commenced as the vapour-liquid equilibrium curve "knee" was approached and large overshoots into the low gain region resulted.

Control system 3 which has a lower gain was stable and its response to a set point change is shown in Fig. (8.5). The results are similar to those obtained by computer simulation and have the same speed of response and overshoot.
b) Control with 0.1 Integral Weighting

Control systems 4 to 6 in Table 8.2 were stable and several responses to set point changes are given in Figs (8.6) to (8.12) which show that:

i) The responses are similar to the simulation results.

ii) Controller 6 is much slower than controllers 4 and 5 which have similar response speeds.

iii) The responses to decreasing temperature (increasing composition) set point changes are very slow due to the azeotropic region being approached.

iv) The non-linearity of the process is clearly shown in Fig (8.10) and (8.11), the column behaviour differs for each set point change in a different direction.

Only one regulation experiment was conducted and the results are shown in Fig. (8.13), the response of controllers 4 and 5 to 13% changes in feed flow rate. The two controllers give similar responses, with small final offsets due to control signal quantisation. The disturbance takes between 30 and 40 sampling intervals to die away, and the maximum deviation from the set point is ±0.4°C equivalent to a top plate composition offset of ±1.2%. Without control the feed changes would cause a steady state offset of 1.7°C or about ±5.4% in top product composition.

All the optimal control responses have steady state offsets due to control variable quantisation, however no additional offsets following feed changes were observed. Any observer errors caused by errors in the
FIG. 8.6. COLUMN RESPONSE TO SET POINT CHANGES
WITH OPTIMAL INTEGRAL CONTROL.

CONTROLLER NO. 4. \( \lambda = 2.8 \times 10^{-5} \) INTEGRAL WEIGHTING = 0.1

FIG. 8.7. COLUMN RESPONSE TO SET POINT CHANGES
WITH OPTIMAL INTEGRAL CONTROL.

CONTROLLER NO. 4. \( \lambda = 2.8 \times 10^{-5} \) INTEGRAL WEIGHTING = 0.1
FIG. 8.8. COLUMN RESPONSE TO SET POINT CHANGES WITH OPTIMAL INTEGRAL CONTROL.

CONTROLLER NO. 4 \( \lambda = 2.8 \times 10^{-5} \) INTEGRAL WEIGHTING = 0.1

![Graph showing the response of a column to set point changes with optimal integral control. The graph plots temperature on the y-axis against time on the x-axis. The graph shows a set point and observed response with a time unit of 1.6 minutes.]

FIG. 8.9. COLUMN RESPONSE TO SET POINT CHANGES WITH OPTIMAL INTEGRAL CONTROL.

CONTROLLER NO. 5 \( \lambda = 2.8 \times 10^{-4} \) INTEGRAL WEIGHTING = 0.1

![Graph showing the response of a column to set point changes with optimal integral control. The graph plots temperature on the y-axis against time on the x-axis. The graph shows a set point and observed response with a time unit of 1.6 minutes.]

TIME: 1 UNIT = 1.6 MIN.
WITH OPTIMAL INTEGRAL CONTROL

CONTROLLER NO. 5  \( \lambda = 2.8 \times 10^{-4} \)  INTEGRAL WEIGHTING = 0.1

FIG. 8.10. COLUMN RESPONSE TO SET POINT

TOP PLATE TEMPERATURE °C.

- SET POINT
- OBSERVED RESPONSE

FIG. 8.11. COLUMN RESPONSE TO SET POINT CHANGES WITH OPTIMAL INTEGRAL CONTROL

CONTROLLER NO. 5  \( \lambda = 2.8 \times 10^{-4} \)  INTEGRAL WEIGHTING = 0.1

TOP PLATE TEMPERATURE °C.

- SET POINT
- OBSERVED RESPONSE
FIG. 8.12. COLUMN RESPONSE TO SET POINT CHANGES WITH OPTIMAL INTEGRAL CONTROL. CONTROLLER NO. 6  λ = 2.8 \times 10^{-3}  INTEGRAL WEIGHTING = 0.1

TOP PLATE TEMPERATURE °C.

- SET POINT
- - OBSERVED RESPONSE.

TIME: 1 UNIT = 1.6 MIN.
FIG. 9.13. COLUMN RESPONSE TO FEED FLOW CHANGES WITH OPTIMAL INTEGRAL CONTROL

A) CONTROLLER S  \[ \lambda = 2.6 \times 10^{-4} \] INTEGRAL WEIGHTING = 0.1

B) CONTROLLER H  \[ \lambda = 2.6 \times 10^{-5} \] INTEGRAL WEIGHTING = 0.1

--- OBSERVED RESPONSES
--- SET POINT

FEED FLOW RATE CHANGE ± 13%

FEED FLOW RATE MOLES/MIN.

0  20  40  60  80  100
TIME 1 UNIT = 1.6 MIN.
plant model were compensated for by the integral term. When control commences \( y(k) = 0 \) and \( x(k) \) are set to zero in the computer so that observer initial condition errors are eliminated.

6) Discussion of Results

Unstable responses caused by non-linearity is the major control problem encountered on the N.P.L. column. The effect of the vapour-liquid equilibrium curve shape on column dynamics is described in Chapter 5, as the slope of the curve increases plate time constants become shorter and the gain decreases.

Table 8.3 gives the plate compositions and vapour-liquid equilibrium curve slope, obtained from the steady state programme, for the three control conditions given in Table 8.1. The following changes can be observed:

i) At 61% top product composition the top two plates are working outside the high slope region.

ii) As composition increases the slope of plates 2 and 3 decrease by a factor of 4 causing a much slower response.

iii) With decreasing composition the slope at plate 2 doubles but that at plate 1 increases by only 6%, but the composition is 25% BM just above the "knee" and if the control overshoots the slope increases rapidly.

When the high slope region is entered, control becomes ineffective and large offsets are corrected for very slowly, due to the low gain. Both
linear design methods showed instability with control systems designed for fast responses, due to non-linearity. However the two-term control coefficients could easily be adjusted to obtain good, stable results.

Secondary dynamic effects also occur which contribute to instability in that they increase column phase lag or change the column dynamics. These include:-

i) Referring to equation 5(10), the plate gains and time constants depend on liquid and vapour flow rates as well as the vapour-liquid equilibrium curve shape. The control action changes these flows and therefore for large changes alters the column dynamics.

ii) For changes which decrease composition, control causes increased vapour flow and reduced liquid flow. This will decrease the liquid holdup on the plates and in severe cases could cause "flooding" on the lower plates.

iii) Hydrodynamic delays, though of only a few seconds duration, do occur and will increase the columns phase lag and contribute to instability.

Comparing the results obtained from the two control system design methods shows that:-

i) Control systems which gave rapid responses became unstable due to column non-linearity, in both cases this problem was overcome by using control systems with lower gains.
ii) Both methods gave good results, with the tuned two-term controller giving the best performance. This is not a comparison of similar cases, which should both be based on the plant model, but the optimal control system could not be tuned on-line.

iii) On-line tuning of two-term control systems is a means of eliminating errors caused by model inaccuracies. The optimal control system could not be tuned and therefore a more accurate plant model is required.

iv) No problems were encountered with interaction using the two loop single output control configuration.

v) Offsets caused by coarse control variable quantisation effected both control systems equally.

vi) The results indicate that a tuned two-term control system could not be improved on, though an optimal control system with a similar performance could probably be designed by a careful choice of the performance criterion. In this case the additional effort required to design the optimal system was not justified.

7) General Conclusions

This work has concentrated on applying optimal control theory to a distillation column and comparing the results obtained with those of simpler control methods. Several points have emerged in the course of the work:-
i) The non-linear model developed gave a good representation of the column dynamics.

ii) A linearised version of the model was suitable for linear optimal regulator design.

iii) This model could be reduced using a frequency response programme to give an approximate first order model which was successfully used to design two-term controllers.

iv) The optimal controller performance was not significantly better than that of the two term controller when simulated or when it was applied in practice.

v) An optimal controller will usually require some form of state vector estimation to reduce the number of available measurements required.

vi) Column non-linearity was a major control problem in this case.

vii) An observer system can be included in a state feedback controller but it is very sensitive to errors in the plant model.

The lack of improved control with the optimal method is due to several reasons which have not been stated clearly in the literature:

i) The performance of the optimal controller depends on the value assigned to the performance criterion weighting coefficients.

ii) Steady state offsets occur following feed changes.

iii) The design method depends on an accurate plant model.

iv) The controllers require a large number of measurements.

v) A large amount of computing is required.
vi) Simple control systems can be adjusted on-line to compensate for model errors, this cannot be done with optimal control systems.

vii) In most practical applications integral action must be included.

viii) Errors in state estimation can degrade the performance of the optimal control system.

In most applications the extra effort required to design optimal linear control systems is not justified in terms of improved performance.

Further work in the column modelling field should be devoted to obtaining less detailed models from the large sets of equations used here. Some progress can be made by reducing full linearised models using a frequency response programme and lumping column sections together.

Further studies of optimal linear regulators on interacting systems should be made, preferably using reduced order models. The main problem being to obtain reduced models which have state variables available for measurement. More attention should also be given to observer systems to establish methods of designing the best observer in a given deterministic situation. Design methods which reduce the observers sensitivity to plant model errors are required in view of the results which were obtained here.
### TABLE 8.1

**SET POINTS FOR COMPUTER CONTROL**

<table>
<thead>
<tr>
<th>Set Point</th>
<th>Top Plate logged value</th>
<th>Top Plate Temperature °C</th>
<th>Top Plate Composition % BM</th>
<th>Top Product Composition % BM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>79.5</td>
<td>57.0</td>
<td>67.0</td>
</tr>
<tr>
<td>2</td>
<td>2.4</td>
<td>81.4</td>
<td>39.2</td>
<td>60.8</td>
</tr>
<tr>
<td>3</td>
<td>4.3</td>
<td>83.3</td>
<td>24.9</td>
<td>54.9</td>
</tr>
</tbody>
</table>

### TABLE 8.3

**PLATE COMPOSITIONS AND SLOPES AT THE CONTROL SET POINTS**

<table>
<thead>
<tr>
<th>Plate No.</th>
<th>Plate Composition % BM</th>
<th>Equilibrium Curve Slope</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set Point 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>57.0</td>
<td>0.475</td>
</tr>
<tr>
<td>2</td>
<td>35.8</td>
<td>0.400</td>
</tr>
<tr>
<td>3</td>
<td>7.9</td>
<td>2.520</td>
</tr>
<tr>
<td>4</td>
<td>1.8</td>
<td>8.950</td>
</tr>
<tr>
<td>Set Point 2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>39.0</td>
<td>0.400</td>
</tr>
<tr>
<td>2</td>
<td>8.9</td>
<td>1.725</td>
</tr>
<tr>
<td>3</td>
<td>1.8</td>
<td>8.950</td>
</tr>
<tr>
<td>4</td>
<td>1.1</td>
<td>8.950</td>
</tr>
<tr>
<td>Set Point 3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>24.9</td>
<td>0.425</td>
</tr>
<tr>
<td>2</td>
<td>4.2</td>
<td>3.450</td>
</tr>
<tr>
<td>3</td>
<td>1.3</td>
<td>8.950</td>
</tr>
<tr>
<td>4</td>
<td>0.9</td>
<td>6.950</td>
</tr>
</tbody>
</table>
Control equations are scaled for column hardware and are in the form

\[ \frac{u(s)}{e(s)} = \frac{-1.16 + 1.27s^{-1} - 0.206s^{-2} + 0.025s^{-3}}{1.0 - 1.1s^{-1} + 0.137s^{-2} - 0.041s^{-3}} \]

**Heat loop**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -1.16 + 1.27s^{-1} - 0.206s^{-2} + 0.025s^{-3} )</td>
<td>1 2.8 ( \times 10^{-5} )</td>
</tr>
</tbody>
</table>

\[ \frac{-2.0i + 2.16s^{-1} - 0.296s^{-2} + 0.036s^{-3}}{1.0 - 1.1s^{-1} + 0.137s^{-2} - 0.041s^{-3}} \]

**Reflux loop**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -0.768 + 0.88s^{-1} - 0.107s^{-2} + 0.002s^{-3} )</td>
<td>2 2.8 ( \times 10^{-4} )</td>
</tr>
</tbody>
</table>

\[ \frac{-0.895 + 0.989s^{-1} - 0.12s^{-2} + 0.002s^{-3}}{1.0 - 1.447s^{-1} + 0.504s^{-2} - 0.057s^{-3}} \]

**Reflux loop**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -0.30 + 0.318s^{-1} - 0.041s^{-2} + 0.001s^{-3} )</td>
<td>3 2.8 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

\[ \frac{-0.282 + 0.299s^{-1} - 0.038s^{-2} + 0.001s^{-3}}{1.0 - 1.677s^{-1} + 0.656s^{-2} - 0.0807s^{-3}} \]

**Heat loop**

**ii) 0.1 Integral weighting**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -0.584 + 0.637s^{-1} - 0.087s^{-2} + 0.002s^{-3} )</td>
<td>4 2.8 ( \times 10^{-5} )</td>
</tr>
</tbody>
</table>

\[ \frac{-1.02 + 1.07s^{-1} - 0.12s^{-2} + 0.003s^{-3}}{1.0 - 1.137s^{-1} + 0.163s^{-2} - 0.031s^{-3}} \]

**Reflux loop**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -0.364 + 0.41s^{-1} - 0.055s^{-2} + 0.001s^{-3} )</td>
<td>5 2.8 ( \times 10^{-4} )</td>
</tr>
</tbody>
</table>

\[ \frac{-0.444 + 0.474s^{-1} - 0.058s^{-2} + 0.001s^{-3}}{1.0 - 1.532s^{-1} + 0.599s^{-2} - 0.068s^{-3}} \]

**Reflux loop**

<table>
<thead>
<tr>
<th>Control Equation</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -0.15 + 0.159s^{-1} - 0.02s^{-2} + 0.001s^{-3} )</td>
<td>6 2.8 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

\[ \frac{-0.141 + 0.150s^{-1} - 0.018s^{-2} + 0.001s^{-3}}{1.0 - 1.784s^{-1} + 0.879s^{-2} - 0.097s^{-3}} \]

**Reflux loop**
REFERENCES


APPENDIX 1

H.P.L. Report

A Critical Study of a Proposed Method of Optimal Control
Critical Study of a Proposed Method of Optimal Control

by

P.J. King
(Guest worker from University of Surrey)

Introduction

This report is the result of an investigation into a computer control scheme, proposed by Grethlein and Lapidus\(^1\) to give approximately time-optimal control of constrained systems.

The scheme is based on the assumptions that deviations from a desired state must be corrected as quickly as possible, that the optimal control is an instantaneous function of system input and output, and that time-optimal control will be "bang-bang". A mathematical model of the system is used to predict values of a performance criterion, for various control values over each sampling interval. The control value which minimises the criterion is applied to the system.

It has been proposed to apply the scheme to the control of a distillation column\(^2\). As a preliminary step it has been applied to second order linear systems, simulated on a digital computer. The results of this work show that approximate time optimal control can result. However the control scheme's performance depends on the relative weighting of the terms in the performance criterion and the magnitude of the error. It is concluded that the scheme is too sensitive to these effects to give an adequate approximation to time-optimal control.

A theoretical analysis of a second order linear system shows that the assumption of "bang-bang" optimal control is not always justified.

Control Scheme

If a process is being maintained at a desired state (e.g. product composition) deviations from this state must be corrected as soon as possible. Also it is economically sound to achieve desired changes in state (e.g. process start-up) in the shortest possible time. If the cost of control (e.g. heating or cooling) is small the optimal control problem becomes one of minimising response time.

The full solution to the time-optimal control problem for a process requires a great deal of computation and is unsuitable for direct computer control. The computer control scheme of Grethlein and Lapidus\(^1\) makes certain assumptions which are stated to give approximately time optimal control with simple and rapid computation. An outline of their assumptions and of the proposed control scheme is as follows.
In the diagram $X$ is the process input vector with phase components $x_1, x_2, \ldots, x_m$; it describes the desired state of the system. The main process has an output vector $Y$ with phase components $y_1, y_2, \ldots, y_n$. The control $u$ is chosen to optimise the system response; in most practical systems this input will be bounded.

The process is described by the set of equations

$$\frac{dY}{dt} = F(Y, u, t).$$

To optimise the system by choice of control $u$ a performance criterion must be chosen. A general one for this particular application is

$$Q = \int_0^\infty q(X, Y) \, dt.$$

It has been shown by Fuller\(^{(3)}\) that the control $u(t)$ which minimises $Q$ is given by

$$u_{opt}(t) = U(X, Y)$$

that is an instantaneous function of the process input and output. In practice this function may be difficult to determine.

If the control is bounded then for a linear process true time optimal control is achieved when the control input is "bang-bang". The control magnitude then lies on its boundaries and switches at computable instants. For non-linear systems it is not in general possible to make such a statement\(^{(4)}\), each process has to be considered specifically. However when "bang-bang" control does give an optimal response in a non-linear process it can be controlled by this scheme.

In order to avoid the determination of the function $U$, Grethlein and Lapidus\(^{(1)}\) predict forwards over one sampling interval and use a discrete mathematical process model. At each sampling instant the process response to the maximum and minimum control values and to an intermediate value are computed. Then by evaluating the performance function for the predicted responses, the
control input which minimises the performance function over the next sampling interval is chosen as the optimum.

The sampled data representation of the system equation, with sampling interval $T$, at time $kT$ is

$$Y(k+1,T) = \Phi[Y(kT), u(kT), T]$$

Choose a quadratic performance criterion so that

$$q(x, y) = a_1(y_1-x_1)^2 + a_2(y_2-x_2)^2 + \ldots + a_m(y_m-x_m)^2.$$

The performance function integral then becomes a summation

$$Q(N) = \sum_{k=1}^{N} q(kT) \times T$$

where $NT$ is greater than the settling time of the process.

Then at time $kT$, using the process model equations and the measured values of $Y(kT)$ from the process, the values of $Y(k+1,T)$ are calculated for three values of control, the minimum $u_1$, the maximum $u_3$ and an intermediate value $u_2$.

With each predicted value of $Y(k+1,T)$ a value for the $k$th term in the performance criterion summation can be calculated. The smallest of the three predicted values is then chosen. If this value corresponds to either the maximum or minimum control value, this value is applied to the system. If however the intermediate control gives the smallest cost value a second order curve is fitted to the three values, and the control input which corresponds to the minimum of the second order curve is applied to the system. At the end of the sampling interval the procedure is repeated to select the next control value.

Grethlein and Lapidus\(^1\) state that this control scheme gives an approximation to time optimal control over most of the system transient, the intermediate control only coming into action near the steady state value at the end of the transient.

The procedure can easily be extended to systems with uncontrolled disturbances.

**Theoretical Analysis of a Second Order System**

As Cotter\(^4\) has pointed out, for some non-linear systems the time-optimal control is not "bang-bang" but of a "singular" form\(^5\).
"Singular" control occurs when a system and index of performance are such that after applying Pontryagin's Maximum Principle, the Hamiltonian function $H$ has the form

$$H = I(t) + u.F(t)$$

where $I(t)$ is the collection of terms which are not explicit functions of $u$
$F(t)$ is the collected coefficients of $u$
$u$ is the control variable

Then the control input which maximises $H$ and gives optimal control is

$$u^*(t) = M \text{sgn} P(t).$$

Now if $F(t)$ becomes identically zero over some finite time interval, $H$ ceases to be an explicit function of $u$. Then the usual procedure of choosing $u^*$ the optimum value of $u$ which maximises $H$, breaks down. The nature of the control is then referred to as "singular" and is fully discussed by Johnson and Gibson.

As the computer control scheme proposed uses a quadratic-error integral performance criterion the second order system is analysed for both this and the true minimum settling time form.

a) Minimal Time Solution

Consider the second order differential equation

$$\frac{d^2y}{dt^2} + a \frac{dy}{dt} + by = u$$

and the performance index $J = \int_0^T dt$.

Let $y_1 = y$, $y_2 = y$.

Let the desired system state coordinates be $y_1 = y_2 = 0$.

Choose as an auxiliary state variable

$$y_0 = \int_0^T dt.$$ 

Then the system state equations are

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = u - ay_2 - by_1$$
$$\dot{y}_0 = 1$$
Using Pontryagin's Maximum Principle the Hamiltonian function $H$ is given by:

$$H = p_1 y_2 + p_2 (u - a y_2 - b y_1) + p_0$$

where $p_1$, $p_2$ and $p_0$ are Lagrange multiplier functions.

$p_1$ and $p_2$ cannot be identically zero.

Now

$$\frac{dp_0}{dt} = -\frac{\partial H}{\partial y_0} = 0$$

so $p_0$ is a constant and it can be shown that $p_0 = -1$.

Also

$$\frac{dp_1}{dt} = -\frac{\partial H}{\partial y_1} = b p_2$$

and

$$\frac{dp_2}{dt} = -\frac{\partial H}{\partial y_2} = -p_1 + a p_2$$

Now the optimal control input is that which maximises $H$ at all times.

$$\frac{\partial H}{\partial u} = p_2$$

which cannot be identically zero.

Hence $H$ has no extremum value and is limited by the value of $u$.

So the control input must be $u = \text{sgn} \ p_2$.

If $p_2$ and $\dot{p}_2$ both go to zero together a singular solution may exist.

However, if $p_2 = 0$ then $\dot{p}_1 = 0$

and if $\dot{p}_2 = 0$ then $a p_2 = p_1$.

This means that $p_1$ would have to go to zero with $p_2$ which it cannot do.

Hence a singular solution does not exist and the time-optimal control is "bang-bang".

b) Solution with a quadratic performance index

Taking the same system equations, but with the performance index,

$$y_0 = \int_0^T (\xi_1 y_1^2 + \xi_2 y_2^2) \, dt$$

where $T$ is a free terminal time, the state
equations become

\[ \begin{align*}
\dot{y}_1 &= y_2 \\
\dot{y}_2 &= u - a y_2 - b y_1
\end{align*} \]

Forming the Hamiltonian functions as before and taking \( p_0 = -1 \) as before gives:

\[ H = -g_1 y_1^2 - g_2 y_2^2 + p_1 y_2 + p_2 u - a p_2 y_2 - b p_2 y_1 \]

and

\[ \begin{align*}
\dot{p}_1 &= -\frac{\partial H}{\partial y_1} = +2g_1 y_1 + b p_2 \\
\dot{p}_2 &= -\frac{\partial H}{\partial y_2} = +2g_2 y_2 - p_1 + a p_2
\end{align*} \]

Now for the control input to maximise the Hamiltonian at all times

\[ \frac{\partial H}{\partial u} = p_2 \]

so \( u = \text{sgn} \ p_2 \), as before.

When \( p_2 = 0 \), \( \dot{p}_2 = 2g_2 y_2 - p_1 \), so when \( 2g_2 y_2 = p_1 \) a singular solution can exist.

Now rearranging the Hamiltonian gives

\[ H = p_2 u + \left[ -g_1 y_1^2 - g_2 y_2^2 + p_1 y_2 - a p_2 y_2 - b p_2 y_1 \right] \]

Then the maximised Hamiltonian \( H^* \) with the optimal control input \( u^* \) has the form

\[ H^* = I + u^* F = 0 \]

because the problem is explicitly independent of time and has a free terminal time.

(Johnson and Gibson(5)).

To test for a singular solution

\[ I = I = 0 \quad F = F = 0 \]
so that

\[ I = -g_1 y_1^2 - g_2 y_2^2 + p_1 y_2 - a p_2 y_2 - b p_2 y_1 = 0 \]

and

\[ \dot{I} = -2g_1 y_1 - 2g_2 y_2 + \dot{p}_1 y_2 + p_1 \dot{y}_2 - a p_2 \dot{y}_2 - a p_1 y_1 - b p_2 y_1 - b p_1 \dot{y}_1 = 0 \]

so that

\[ F = p_2 = 0 \]

\[ \dot{F} = \dot{p}_2 = 0 \]

so that

\[ -g_1 y_1^2 - g_2 y_2^2 + p_1 y_2 = 0 \quad (A) \]

and

\[ -2g_1 y_1 \dot{y}_1 - 2g_2 y_2 \dot{y}_2 + \dot{p}_1 y_2 + p_1 \dot{y}_2 = 0 \quad (B) \]

Now \( p_1 = 2g_2 y_2 \) and \( \dot{p}_1 = 2g_2 \dot{y}_2 \)

so solving (A) and (B)

\[ g_2 y_2^2 - g_1 y_1^2 = 0 \]

This gives the equation of the singular trajectory as

\[ (y_2 + \frac{g_1}{g_2} y_1)(y_2 - \frac{g_1}{g_2} y_1) = 0. \]

Solving (B) to obtain the value of control \( u \) along this trajectory

\[ g_1 y_1 \dot{y}_1 = g_2 y_2 \dot{y}_2 \]

so from the system state equations

\[ g_1 y_1 y_2 = g_2 y_2 (u - ay_2 - by_1) \]

so when \( y_2 \neq 0 \) the control \( u \) along the singular trajectory is

\[ u = -\frac{g_1}{g_2} y_1 + by_1 + ay_2, \quad |u| < 1. \]

The optimal control is "bang-bang" except along the singular trajectory. The control input along this trajectory decreases as \( y_1 \) and \( y_2 \) decrease and the settling time is greater than the minimum settling time \( (C) \).
The trajectories for a double integrator system are shown in figure 1(6). In this case $a = b = 0$ and the equation of the singular trajectory is

$$y_2 = \pm \sqrt{\frac{\varepsilon_1}{\varepsilon_2}} y_1$$

and the control on this trajectory is

$$u = \frac{\varepsilon_1}{\varepsilon_2} y_1, \quad |u| < 1$$

The minimal time example can be extended to any linear system with real roots and the optimal control is "bang-bang". The quadratic performance criterion example can also be extended to any linear system with real roots and provided that the performance criterion contains more than one state variable (i.e., $\varepsilon_1$ and $\varepsilon_2 \neq 0$) singular trajectories or surfaces will exist. It has been shown(5) that in most cases, including that of the linear system, the singular trajectory is part of the complete optimal trajectory.

The assumption that for a linear system time optimal control is "bang-bang" is correct. When time is replaced by a quadratic error criterion it has been shown that the control is no longer wholly "bang-bang" but exhibits singular intervals. So the artifice of replacing the criterion of time by an error penalty criterion and assuming that the performance will approximate to minimal time is not justified.

**Application of the control scheme to second order systems**

To test the proposed control scheme it was applied to two linear second order systems with input saturation using a digital computer simulation shown below.

$$\frac{d^2y}{dt^2} = u, \quad |u| < 1 \quad \text{System A}$$
and
\[ \frac{d^2y}{dt^2} + \frac{dy}{dt} = u, \quad |u| \leq 1 \]........................................ System B

The time-optimal trajectories for both these systems are well known, to aid comparison with the computed results. The discrete forms were used with a high sampling rate so that the results approximated closely those of a continuous system.

The performance criteria chosen for both systems was, in sampled form

\[ q(N) = \sum_{k=1}^{N} \left[ \left( y_1(kT) - x_1(kT) \right)^2 + g_2 \left( y_2(kT) - x_2(kT) \right)^2 \right] \times T \]

\[ g_2 = \text{a weighting coefficient (} g_1 = 1 \) \]

The control scheme already outlined was applied to both systems with initial condition errors in output position and \( x_i = x_2 = 0 \). The three values of control input used in calculation were

\[ \begin{align*}
  u \text{ maximum} &= +1 \\
  u \text{ intermediate} &= 0 \\
  u \text{ minimum} &= -1
\end{align*} \]

The phase plane diagrams plotted in figures 2 and 3 for both systems show that the relative weighting of the terms in the performance criteria determines, to a large extent, the nature of the system response.

Starting from an initial position error of \(-1.0\), the systems start on a positive value of control input, which is the positive limit if \( g_2 \) is small enough (\( g_1 = 1 \)). Some time after motion has commenced the system switches from the positive limit input either to the negative control input limit or the intermediate mode depending on the value of \( g_2 \). If the system switches to the negative limit, then at a point near the zero error it switches into the intermediate control mode.

For any particular value of \( g_2 \) (\( g_1 = 1 \)) the intermediate control mode trajectory is a straight line on the phase plane passing through the zero error position. When the "bang-bang" trajectory crosses this line the system switches into intermediate mode and down the line trajectory with the value of control input decreasing as the error gets smaller. When the value of control input required to follow the intermediate trajectory is greater than the limit value the system behaves in a "bang-bang" fashion. The intermediate mode of control was suppressed in some tests by allowing the control input to take maximum and minimum values only. Then the system enters a "sliding" mode switching rapidly from one control limit to the other so that it jitters down the intermediate mode line.

It was found that for one particular value of \( g_2 \), 0.005 for system A and 0.003 for system B, the switching from positive to negative control input limits occurs at the correct point for theoretical time optimal control. Switching to
the intermediate mode occurs very near the origin and a good approximation to
time optimal control is achieved.

If the values of $g$ are less than these "optimum" values the controller
switches too late and the systems overshoot, causing an increase in settling
time.

If $g_2 = 0$ the system behaves as though $u = \text{sgn} (e)$ where $e$ is system
position error. Then the undamped system A does not converge to the zero error
point, system B with damping converges slowly. The trajectories followed in
these cases are not the same as the optimal ones given by Fuller(6) using the
same performance criterion. This shows that piece-wise minisation of integrals
does not approximate to actual integral minisation.

When $g_2$ is too large, the system enters the intermediate control mode too
early and the effect is that of putting a velocity constraint on the system.

The times for the two systems to reach a region near the zero error point
on the phase plane were plotted against $g_2$ (graph 4). There is a well defined
minimum in both graphs at the time-optimal $g_2$ value.

The time optimal value of $g_2$ was determined with an initial position
error of -1.0. If the magnitude of this initial error is changed and $g_2$ is
kept the same, the system switched from positive control limit to negative limit
at points rather before or after the theoretical optimal switching point
depending on whether the initial error is less than or greater than -1.0. An
example of this is shown in figure 5 for system B for initial position errors of
-1.0 and -0.5. The effect is small on the two systems tested as system A has
symmetrical trajectories and system B exhibits velocity saturation which limits
the size of this effect. However in some systems with highly "curved"
switching trajectories this effect could be much more pronounced.

Discussion

From figures 1, 2 and 3 it is clear that singular trajectories and
intermediate node trajectories are both linear. Comparison of the slopes of the
two types of trajectory and comparison of the control values along them in
terms of phase space coordinates has revealed no simple correspondence between
them (Tables 1 and 2).

The shape of the intermediate node trajectories is evidently inherent in
the control scheme. It depends on the relative performance criterion weightings,
the positions of the system in the phase space, the nature of the system and its
mathematical model.

Variation in switching point with initial error magnitude is inherent in
the control scheme. The switching point occurs when the predicted values of
position and velocity and the weighting of the performance criteria are all such
that a sudden shift of the criterion minimum occurs. The position in the phase
space and the predicted values decide when this occurs, and the weighting
coefficients can be adjusted to make this shift occur at a point near the true
time optimal. Starting from a particular initial condition the weighting
coefficients can be suitably chosen, however if the initial error value differs
from the one selected the system travels along a different trajectory in the
phase space and a different relative weighting would be required to achieve time-optimal switching.

The assumptions made by Grethlein and Lapidus are correct, in so far as time optimal control of a linear system is "bang-bang" and the optimal control input is an instantaneous function of process input and output. It has been shown here however that when the performance criterion is a quadratic error integral, the optimal trajectories are not normally "bang-bang" as assumed for a linear system. Also the results show that when $g_2 = 0$ and control is "bang-bang" the piece-wise minimisation of the criterion does not approximate to the trajectory given by Fuller(6) which minimises the time integral of position error squared.

The difficulties with the method are due to the assumption that by using "bang-bang" control and attempting, erroneously, to minimise a function which penalises system state errors, an approximation to time optimal control results. Certainly, using a relay control input moves the system about the phase space as rapidly as possible, but unless a method of predicting the correct switching instants is used, minimum response time control will not result.

To apply the scheme to high order systems a search procedure to find the minimum settling time weighting coefficients is necessary. In most practical problems this is not a suitable form of control.

It is unlikely that a linear system with complex poles and hence a complicated time-optimal switching curve could be controlled by this scheme. Extension of the controller to systems with more than one control input is also not practicable as the number of predictions for such a system is $3^r$ where $r$ is the number of inputs and the curve fitting and minimising for intermediate control inputs becomes very complex.
References

1. Grethlein, H. and Lapidus, L.
"Time Optimal Control of Non-Linear Systems with Constraints".

2. Rees, N.
"An approximately time optimal control scheme for a distillation tower".

3. Fuller, A.T.

4. Cotter, J.E.
"Evaluation of Optimal Control Strategies".

5. Johnson, C.D. and Gibson, J.E.
"Singular solutions in Problems of Optimal Control".

6. Fuller, A.T.
"Relay Control Systems Optimised for Various Performance Criteria".

7. Pontryagin, L., Boltyanskii, V., Gankrelidge, R. and Mishchenko, E.
"The Mathematical Theory of Optimal Processes".
(InterScience Publishers 1962).

8. Wonham and Jonson
"Optimal Bang-Bang Control with Quadratic Performance Indices".
Trans A.S.M.E. Journal of Basic Engineering. Vol.86, Series D, No.1,
Page 107, March 1964.
Comparison of the equations of singular and intermediate trajectories for both systems

### Table 1

System A, \( \frac{d^2y}{dt^2} = u \), \(|u| \leq 1\)

Along the singular trajectory \( u = \frac{S_1}{S_2}, y_2 = \pm \sqrt[3]{\frac{S_1}{S_2}} \cdot y_1 \)

\( S_1 = 1 \)

<table>
<thead>
<tr>
<th>( S_2 )</th>
<th>Singular Trajectory</th>
<th>Intermediate Trajectory</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Trajectory equation</td>
<td>Control Input (</td>
</tr>
<tr>
<td>0.1</td>
<td>( y_2 = \pm 3.16y_1 )</td>
<td>( u = 10y_1 )</td>
</tr>
<tr>
<td>0.01</td>
<td>( y_2 = \pm 0.9y_1 )</td>
<td>( u = 100y_1 )</td>
</tr>
<tr>
<td>0.007</td>
<td>( y_2 = \pm 11.95y_1 )</td>
<td>( u = 143y_1 )</td>
</tr>
</tbody>
</table>

### Table 2

System B, \( \frac{d^2y}{dt^2} = u - \frac{dy}{dt} \), \(|u| \leq 1\)

Along the singular trajectory \( u = \frac{S_1}{S_2}, y_2 = \pm \sqrt[3]{\frac{S_1}{S_2}} \cdot y_1 \)

\( S_1 = 1 \)

<table>
<thead>
<tr>
<th>( S_2 )</th>
<th>Singular Trajectory</th>
<th>Intermediate Trajectory</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Trajectory equation</td>
<td>Control Input (</td>
</tr>
<tr>
<td>0.1</td>
<td>( y_2 = \pm 3.16y_1 )</td>
<td>( u = 10y_1 + y_2 )</td>
</tr>
<tr>
<td>0.02</td>
<td>( y_2 = \pm 7.1y_1 )</td>
<td>( u = 50y_1 + y_2 )</td>
</tr>
<tr>
<td>0.007</td>
<td>( y_2 = \pm 12y_1 )</td>
<td>( u = 143y_1 + y_2 )</td>
</tr>
<tr>
<td>0.005</td>
<td>( y_2 = \pm 14.1y_1 )</td>
<td>( u = 200y_1 + y_2 )</td>
</tr>
</tbody>
</table>
FIG. 1. SKETCH OF SINGULAR AND BANG BANG TRAJECTORIES FOR A SYSTEM

WITH EQUATION \[ \frac{d^2y}{dt^2} = u, |u| \leq 1 \]

ERROR CRITERION = \[ \int_0^\infty (y_1^2 + y_2^2) \, dt \]

DESIRED COORDINATES \( y_1 = 0, y_2 = 0 \)

"Bang-bang" switching boundary

Along the singular trajectory

\( u = y_1, |u| \leq 1 \)

\( y_2 = -y_1 \)
FIG. 2. PHASE PLANE DIAGRAM FOR SYSTEM "A" WITH VARIOUS $g_2$ VALUES

<table>
<thead>
<tr>
<th>Value of $g_2$</th>
<th>Time to settle secs</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2.0</td>
</tr>
<tr>
<td>0.01</td>
<td>3</td>
</tr>
<tr>
<td>0.007</td>
<td>2.4</td>
</tr>
<tr>
<td>0.005</td>
<td>1.9</td>
</tr>
<tr>
<td>0.003</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>Oscillatory</td>
</tr>
</tbody>
</table>

$\frac{d^2 y}{dt^2} = u$

Velocity $y_2$

Position $y_1$

Minimum time

Intermediate mode

Limit control
FIG. 3 PHASE PLANE DIAGRAM FOR SYSTEM "B" WITH VARIOUS $q_2$ VALUES

\[ \frac{d^2y}{dt^2} = u - \frac{dy}{dt} \]

<table>
<thead>
<tr>
<th>Time to settle secs</th>
<th>Value of $q_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.1</td>
</tr>
<tr>
<td>5</td>
<td>0.02</td>
</tr>
<tr>
<td>2.45</td>
<td>0.005</td>
</tr>
<tr>
<td>2.1</td>
<td>0.003</td>
</tr>
<tr>
<td>3.6</td>
<td>0.001</td>
</tr>
<tr>
<td>7.0</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Minimum time

--- Intermediate mode

Limit control
FIG. 4. TIME FOR BOTH SYSTEMS TO SETTLE AGAINST $g_2$

In each case initial position error of $-1.0$
\[ g_2 = 0.003 \text{, "the optimal value"} \]

 Desired coordinates 
\[ y_1 = 0, y_2 = 0. \]

 Trajectory for initial error of \(-0.5\)

 Positive input +1 

 Negative input -1 

 Portion of trajectory with initial error of \(-1.0\)

 Intermediate mode

 Position \( y_1 \)

 Error velocity \( y_2 \)
APPENDIX 2

Physical Data

a) Physical Data

All physical data was obtained from "The Chemical Engineers Handbook" by Perry and the relationships used in the computer programmes are as follows:-

i) Vapour-liquid equilibrium relationship.

See Fig. 5(10) approximated by 50 values with linear interpolation.

ii) Enthalpy - composition data

This was approximated by two straight lines, for saturated vapour,

\[
\text{enthalpy} = 200x + 11580 \text{ cals/gm-mole}
\]

and for saturated liquid,

\[
\text{enthalpy} = 520x + 1750 \text{ cals/gm-mole}
\]

\(x\) is the molar fraction of ethyl alcohol.

iii) Boiling point data

This was approximated by three straight lines depending on the molar composition.

\[
\begin{align*}
0 \leq x < 0.1 & : T = 100 - 156x \degree C \\
0.1 \leq x < 0.54 & : T = 73.5 - 12.5x \degree C \\
0.54 \leq x < 1.0 & : T = 81.0 - 3.0x \degree C
\end{align*}
\]

\(T\degree C\) is the boiling point temperature.

iv) Specific heat

This was approximated by two straight lines depending on the
molar composition.

\[ 0 \leq x \leq 0.4 \quad \text{s.h.} = 19.7 + 40 x \text{ cals/gm/°C}, \]
\[ 0.4 < x \leq 1.0 \quad \text{s.h.} = 33.2 + 1.4 x \text{ cals/gm/°C}, \]

where s.h. is the specific heat.

v) Density

At boiling point,

\[ \rho = \frac{(0.967 - 0.214 x)}{(28 x + 18)}, \text{ gm-moles/cc} \]

where \( \rho \) is the density.

b) Column Data

i) Reflux relationship

Reflux ratio \( R = \frac{256}{B + 7.83} - 1, \)

where \( B \) is the binary keyboard number.

ii) Heat relationship

Heat input = 730 + 36 B watts

where \( B \) is the binary keyboard number.

iii) Keyboard voltage

Output voltage to Hermes = 0.05 B volts

iv) Thermistor relationship

Plate 6 temperature = \(-3.8V_6 + 4.29V_R + 82.93 ^\circ C\)
5 \quad = \(-3.8V_5 + 4.29V_R + 76.25 ^\circ C\)
4 \quad = \(-3.8V_4 + 4.29V_R + 68.7 ^\circ C\)
3 \quad = \(-3.8V_3 + 4.29V_R + 63.4 ^\circ C\)