SELF-TUNING AND ADAPTIVE CONTROL
OF A PILOT PLANT FLUIDIZED BED REACTOR

By

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ABSTRACT

A pilot plant fluidized bed reactor in which complex and highly exothermic catalytic hydrogenolysis reactions are taking place, is being used to investigate the computer control of temperature, conversion and selectivities in such reactors. The process is highly nonlinear, characterized by asymmetric dynamics and considerable change in catalyst activity. Moreover, a deadtime of 360 s is introduced by an on-line process gas chromatograph employed to obtain the composition measurements. As a result, the cascade control system comprising a proportional-integral controller for reaction temperature in the inner loop and a Dahlin controller for propane selectivity in the outer loop was reported in previous works to have performed well in certain regions of operation at a given time but revealed very oscillatory and nearly unstable performance in other regions or at different times.

This nonlinear behaviour of the reactor is further investigated. It is found that by better matching the process response characteristics and by detuning the Dahlin controller, this unstable oscillatory behaviour of the cascade control system can be overcome and acceptable performance can be achieved over a wider range of operating conditions. Later, self-tuning adaptive controllers are tried in an attempt to better account for the changing gains and time constants of the nonlinear process, as well as for the time-varying catalyst activity. The cascade control scheme with Dahlin and Self-tuning regulator (STR) demonstrated excellent performance. Finally a double STR configuration for both the inner and outer loops is carried out. Problems associated with this implementation are discussed and possible improvements suggested.
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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>2. THE FLUIDIZED BED REACTOR SYSTEM</td>
<td></td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>4</td>
</tr>
<tr>
<td>2.1.1 Background</td>
<td>4</td>
</tr>
<tr>
<td>2.1.2 The Chemical Reaction System</td>
<td>4</td>
</tr>
<tr>
<td>2.2 Process Description</td>
<td>5</td>
</tr>
<tr>
<td>2.2.1 The Reactor</td>
<td>5</td>
</tr>
<tr>
<td>2.2.2 Heating-Cooling System</td>
<td>9</td>
</tr>
<tr>
<td>2.3 Minicomputer System</td>
<td>10</td>
</tr>
<tr>
<td>2.4 Instrumentation and Process/Computer Interface</td>
<td>13</td>
</tr>
<tr>
<td>2.4.1 Instrumentation</td>
<td>13</td>
</tr>
<tr>
<td>2.4.1.1 Feed Flow System</td>
<td>13</td>
</tr>
<tr>
<td>2.4.1.2 Cooling Oil Temperature Control</td>
<td>15</td>
</tr>
<tr>
<td>2.4.1.3 Temperature Sensors</td>
<td>15</td>
</tr>
<tr>
<td>2.4.1.4 Gas Chromatograph System</td>
<td>18</td>
</tr>
<tr>
<td>2.4.2 Process-Computer Interface</td>
<td>19</td>
</tr>
<tr>
<td>3. THE DYNAMIC SIMULATION MODEL OF THE REACTOR SYSTEM</td>
<td></td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>21</td>
</tr>
<tr>
<td>3.2 Reaction Kinetics</td>
<td>21</td>
</tr>
<tr>
<td>3.3 Fluidized Bed Reactor Model</td>
<td>22</td>
</tr>
<tr>
<td>3.3.1 Material Balances</td>
<td>23</td>
</tr>
<tr>
<td>3.3.2 Enthalpy Balances</td>
<td>26</td>
</tr>
<tr>
<td>3.3.3 Reaction Rates and Heats of Reaction</td>
<td>28</td>
</tr>
<tr>
<td>3.4 The DYNYSYS Simulation</td>
<td>29</td>
</tr>
</tbody>
</table>
3.4.1 Introduction

3.4.2 Application of DYNSYS on Fluidized Bed Reactor System

3.4.3 Parameter Estimation

4. CONTROL METHOD USED ON THE PILOT PLANT FLUIDIZED BED REACTOR

4.1 Introduction

4.2 Temperature and Selectivity Control, Base Case: Dahlin + PI

4.3 Self-Tuning and Adaptive Control

4.3.1 Introduction

4.3.2 Review on Theory of STR

4.3.2.1 Minimum Variance (M.V.) Control with Recursive Least Squares Estimation

4.3.2.2 Constrained STR

4.3.3 Application to the Fluidized Bed Reactor

4.3.3.1 Control of the Reaction Temperature

4.3.3.2 Control of the Propene Selectivity

5. SIMULATION STUDIES ON THE REACTOR SYSTEM

5.1 Introduction

5.2 Computer Software for the Simulation

5.3 Results of the Simulation Runs

5.3.1 Introduction

5.3.2 Dahlin + PI

5.3.3 Dahlin + STR

5.3.4 STR + STR

6. EXPERIMENTAL STUDIES ON THE REACTOR SYSTEM

6.1 Introduction
6.2 Experimental Procedure
6.3 Minicomputer Program Setup for the Experimental Study
6.4 Results of the Experiments on the Reactor
   6.4.1 Dahlin + PI
   6.4.2 STR in Inner Loop for Reaction Temperature Control
   6.4.3 Dahlin + STR
   6.4.4 STR + STR

7. SUMMARY AND CONCLUSION
   7.1 Future Work

REFERENCES

NOMENCLATURE

APPENDICES

A. Calibration Procedures
   A.2.1 Calibration Procedure for Flow System
      A.2.1.1 n-Butane Flowrate
      A.2.1.2 Hydrogen Flowrate
   A.2.2 The Beckman Model 6700 Gas Chromatograph
      A.2.2.1 Setting of Component Boards in the Programmer
      A.2.2.2 Procedure for Preparation of a Calibration Sample
      A.2.2.3 Calibration Curves for Different Components

B. Illustration
   B.4.1 To Compute the Structure of Constrained STR for Temperature Control in Inner Loop
C. Computer Program Listings

<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>C.3.1</td>
<td>Program Listing of Module HOLD01: TYPE 8</td>
<td>135</td>
</tr>
<tr>
<td>C.3.2</td>
<td>Program Listing of KACT1</td>
<td>137</td>
</tr>
<tr>
<td>C.5.1</td>
<td>Program Listing of DASTFF2</td>
<td>141</td>
</tr>
<tr>
<td>C.5.2</td>
<td>Program Listing of STPLT2</td>
<td>151</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Fig. No.</th>
<th>Title</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Schematic diagram of fluidized bed reactor system.</td>
<td>6</td>
</tr>
<tr>
<td>2.2</td>
<td>Layout of the minicomputer system.</td>
<td>11</td>
</tr>
<tr>
<td>3.1</td>
<td>Structure of the DYNSYS simulation program in its application to the fluidized bed reactor.</td>
<td>32</td>
</tr>
<tr>
<td>3.2</td>
<td>Information flow diagram for DYNSYS simulation.</td>
<td>33</td>
</tr>
<tr>
<td>3.3</td>
<td>Main storage units for DYNSYS and information flow between them.</td>
<td>34</td>
</tr>
<tr>
<td>5.1</td>
<td>Flow chart for computer calling program DASTFF2.</td>
<td>55</td>
</tr>
<tr>
<td>5.2</td>
<td>Dahlin ($\tau = 250$, $\lambda = 350$) + PI cascade controller performance responding to a series of selectivity setpoint changes (simulation).</td>
<td>59</td>
</tr>
<tr>
<td>5.3</td>
<td>Dahlin ($\tau = 250$, $\lambda = 500$) + PI cascade controller performance responding to a series of selectivity setpoint changes (simulation).</td>
<td>60</td>
</tr>
<tr>
<td>5.4</td>
<td>Dahlin ($\tau = 450$, $\lambda = 500$) + PI cascade controller performance responding to a series of selectivity setpoint changes (simulation).</td>
<td>61</td>
</tr>
<tr>
<td>5.5</td>
<td>Dahlin ($\tau = 250$, $\lambda = 500$) + PI cascade controller performance responding to a selectivity setpoint and a load disturbance in $T_{oil,in}$ (simulation).</td>
<td>63</td>
</tr>
<tr>
<td>5.6</td>
<td>Parameter estimates and pole of the inner STR when FLAM = 1.0 (simulation).</td>
<td>66</td>
</tr>
<tr>
<td>5.7a</td>
<td>Dahlin + STR (FLAM = 0.98, $\xi = 0.5$) cascade controller performance (simulation).</td>
<td>67</td>
</tr>
<tr>
<td>5.7b</td>
<td>Parameter estimates and pole of the inner STR when FLAM = 0.98, $\xi = 0.5$ (simulation).</td>
<td>68</td>
</tr>
<tr>
<td>5.8</td>
<td>Parameter estimates and pole of the inner STR when FLAM = 0.95, $\xi = 0.5$ (simulation).</td>
<td>69</td>
</tr>
<tr>
<td>5.9a</td>
<td>Dahlin + STR (FLAM = 0.98, $\xi = 0.2$) cascade controller performance (simulation).</td>
<td>71</td>
</tr>
<tr>
<td>5.9b</td>
<td>Parameter estimates and pole of the inner STR when $\xi = 0.2$ (simulation).</td>
<td>72</td>
</tr>
<tr>
<td>Fig. No.</td>
<td>Title</td>
<td>Page No.</td>
</tr>
<tr>
<td>----------</td>
<td>-----------------------------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>5.10a</td>
<td>Dahlin + STR' (FLAM = 0.98, ( \xi = 2.0 )) cascade controller performance (simulation)</td>
<td>73</td>
</tr>
<tr>
<td>5.10b</td>
<td>Parameter estimate and pole of the inner STR when ( \xi = 2.0 ) (simulation)</td>
<td>74</td>
</tr>
<tr>
<td>5.11a</td>
<td>Dahlin + STR (FLAM = 0.98, ( \xi = 0.5 )) cascade controller performance responding to a selectivity setpoint change and a load disturbance in ( T_{oil,in} ) (simulation).</td>
<td>77</td>
</tr>
<tr>
<td>5.11b</td>
<td>Parameter estimation and pole of the inner STR (simulation).</td>
<td>78</td>
</tr>
<tr>
<td>5.12a</td>
<td>Double STR cascade controller performance responding to a selectivity setpoint change and a load disturbance in ( T_{oil,in} ) (simulation).</td>
<td>79</td>
</tr>
<tr>
<td>5.12b</td>
<td>Parameter estimates and pole of the inner STR (simulation).</td>
<td>80</td>
</tr>
<tr>
<td>5.12c</td>
<td>Parameter estimates and pole of the outer STR (simulation).</td>
<td>81</td>
</tr>
<tr>
<td>6.1</td>
<td>Structure of minicomputer software for the fluidized bed reactor system.</td>
<td>87</td>
</tr>
<tr>
<td>6.2</td>
<td>Dahlin + PI (experimental).</td>
<td>90</td>
</tr>
<tr>
<td>6.3a</td>
<td>STR in inner loop (experimental).</td>
<td>93</td>
</tr>
<tr>
<td>6.3b</td>
<td>Controller parameter estimates, controller pole and trace of ( P )_\text{matrix} for inner STR.</td>
<td>94</td>
</tr>
<tr>
<td>6.4a</td>
<td>Dahlin + STR (experimental).</td>
<td>98</td>
</tr>
<tr>
<td>6.4b</td>
<td>Controller parameter estimates, controller pole and trace of ( P )_\text{matrix} for inner STR.</td>
<td>99</td>
</tr>
<tr>
<td>6.5a</td>
<td>STR + STR (experimental).</td>
<td>103</td>
</tr>
<tr>
<td>6.5b</td>
<td>Controller parameter estimates, controller pole and trace of ( P )_\text{matrix} for inner STR.</td>
<td>104</td>
</tr>
<tr>
<td>6.5c</td>
<td>Controller parameter estimates, controller roots and trace of ( P )_\text{matrix} for outer STR.</td>
<td>105</td>
</tr>
<tr>
<td>A.2.1</td>
<td>Rotameter calibration for n-butane flow.</td>
<td>122</td>
</tr>
<tr>
<td>A.2.2</td>
<td>Computer calibration plot for n-butane flow.</td>
<td>122</td>
</tr>
<tr>
<td>Fig. No.</td>
<td>Title</td>
<td>Page No.</td>
</tr>
<tr>
<td>---------</td>
<td>------------------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>A.2.3</td>
<td>Rotameter calibration for hydrogen flow.</td>
<td>124</td>
</tr>
<tr>
<td>A.2.4</td>
<td>Computer calibration plot for hydrogen flow.</td>
<td>124</td>
</tr>
<tr>
<td>A.2.5</td>
<td>Computer calibration plot for methane composition.</td>
<td>128</td>
</tr>
<tr>
<td>A.2.6</td>
<td>Computer calibration plot for ethane composition.</td>
<td>129</td>
</tr>
<tr>
<td>A.2.7</td>
<td>Computer calibration plot for propane composition.</td>
<td>130</td>
</tr>
<tr>
<td>A.2.8</td>
<td>Computer calibration plot for butane composition.</td>
<td>131</td>
</tr>
</tbody>
</table>
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table No.</th>
<th>Title</th>
<th>Page No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Thermocouple Locations.</td>
<td>17</td>
</tr>
<tr>
<td>4.1</td>
<td>PI Parameter Estimates</td>
<td>42</td>
</tr>
</tbody>
</table>
1. INTRODUCTION

With the breakthrough in mini and microcomputer technology, computer control applications have been widely adopted in many industries over the past ten to fifteen years. Reactor control represents one of the most important control problems in chemical processes. But it is most difficult to generalize reaction kinetics since almost every reaction is unique, characterized by a specific chemical model, involving one or more phases and taking place in one of a great variety of reactor configurations. It was pointed out by Shinskey [1] that "In processes where transfer of mass or energy takes place, gain is a function of many factors, making generalization impossible. These processes are not only difficult to control because of dynamic behaviour, but are also difficult to understand. They are usually nonlinear in more than one respect, and compensation improperly applied can aggravate the situation."

No doubt, the control of the pilot scale fluidized bed reactor in which highly exothermic hydrogenolysis reactions are carried out represents one of the most challenging control problems.

The pilot plant exhibits a number of very important characteristics:

(1) The highly exothermic nature of the reactions coupled with the large activation energies necessitates direct control of reaction temperature for stable and safe operation of the reactor.

(2) The process is highly nonlinear and exhibits asymmetric dynamics with the time constants and gains dependent very
much upon the operating levels of reactor temperature, the temperature of the oil entering the reactor heating/cooling coils and the hydrogen-to-butane feedrate ratio.

(3) The reactor is a "changing plant". The catalyst activity changes with time. It can be different from one reaction run to another.

(4) The compositions of the product gas are measured by an on-line gas chromatograph. It takes 360 s to analyze a sample and this constitutes a long measurement delay in the system. As a result, previous works on control [4] using conventional cascade proportional-integral (PI) controllers with dead-time compensation that performed well in certain regions of operation at a given time were seen to perform very poorly at slightly different conditions or at different times.

In this work this nonlinear behaviour of the reactor is further investigated and it is shown that by better matching the process response characteristics and by detuning the controller algorithm, acceptable performance can be achieved.

In order to overcome some of the inherent problems associated with controllers employing fixed parameters on a process which has variable dynamic characteristics, self-tuning adaptive controllers are considered in an attempt to better account for the changing gains and time constants of the nonlinear process, as well as for the time varying catalyst activity.

The structure of the thesis is outlined as follows:

Chapter 2: provides the background, the process description and the instrumentation of the pilot plant fluidized bed reactor system.
Chapter 3: reviews the fluidized bed reactor model and the application of the DYNSYS simulation executive for dynamic simulation on the reactor system.

Chapter 4: discusses the different control methods to be used on the cascade control system for temperature and selectivity control.

Chapter 5: presents the simulation results for the reactor system including the effects of different choices of design parameters.

Chapter 6: describes the experimental application of both conventional multiloop and adaptive multiloop control on the real system.

Chapter 7: summarizes the general conclusions drawn from this work and provides recommendations for future work.
2. THE FLUIDIZED BED REACTOR SYSTEM

2.1 Introduction

2.1.1 Background

This process control study was conducted on a pilot-scale fluidized bed reactor (0.20 m diameter by 1.83 m high) in which butane hydrogenolysis reactions occur. The fluidized bed reactor was originally designed and constructed by Orlickas [2] and Shaw [3] and was used to study the phenomena occurring in fluidized bed reactors. Later McFarlane [4] carried out some preliminary control studies on this system; for this work, he upgraded the instrumentation, installed new control valves and interfaced a Nova 1200 minicomputer (Data General Corporation) with the control and instrumentation systems. The details of the reactor and the current control system are described in this chapter (Sections 2.2 and 2.4 respectively).

It is important to point out that the fluidized bed reactor was designed to be large enough to reduce wall effects and slugging but not so large as to entail excessive cost of chemicals over the long operating periods involved. At the same time, during operation, it exhibits many of the operating characteristics observed in industrial scale plants.

2.1.2 The Chemical Reaction System

The chemical reaction occurring in the fluidized bed is the hydrogenolysis of n-butane on a nickel-impregnated (10% by weight) silica-gel catalyst.

This reaction was extensively studied by Orlickas [2] and Shaw [3]. They showed that the following series-parallel reactions
occurred:

\[ \text{C}_4\text{H}_{10} + \text{H}_2 \rightarrow \text{C}_3\text{H}_8 + \text{CH}_4 \]  
\[ \text{C}_4\text{H}_{10} + \text{H}_2 \rightarrow 2\text{C}_2\text{H}_6 \]  
\[ \text{C}_3\text{H}_8 + \text{H}_2 \rightarrow \text{C}_2\text{H}_6 + \text{CH}_4 \]  
\[ \text{C}_2\text{H}_6 + \text{H}_2 \rightarrow 2\text{CH}_4 \]  

Although four hydrogenolysis reactions occur, only three are stoichiometrically independent. Not only are these reactions highly exothermic but also the kinetic studies of Orlikas and Shaw demonstrated that each of these reactions exhibit very high activation energies (ca. 210 kJ/mole). Their estimates of kinetic parameters and one of their fluidized bed reactor models are used in a simulation relating to this research program as described in Chapter 3.

2.2 Process Description

A simplified schematic diagram of the fluidized bed reactor system with its process control system along with the computer interfacing is shown in Figure 2.1. The cascade control scheme which is discussed in Chapter 4 is indicated on this diagram.

2.2.1 The Reactor

The reactor which is constructed from 16 gauge stainless steel consists of three sections: the bottom cone, the reactor barrel and the disengaging section. The reactor is 0.20 m diameter by 1.83 m high and the disengaging section, which is mounted on top, is 0.46 m diameter by 0.61 m high.
Figure 2.1 Schematic Diagram of the Fluidized Bed Reactor System

\[ X_{C_4} \]

\[ S_{C_3}, S_{C_2}, S_{C_1} \]

360 seconds

Dahlin or STR

Setpoint

Toil, in Setpoint

PI

E/P

Air Supply

to atm

15
cold water

16

to atm

10

11

14

13

12

100 psig steam supply

6

P

4

5

N\textsubscript{2} Supply

3

PDT

1 sec

\[ n-C_4 \]

Supply

PI

3

2

1

E/P

1 sec

H\textsubscript{2} supply

PI

1

E/P

2

PDT
Legend for Figure 2.1:

- \( X \): control valve
- \( \text{IT} \): multiplexed thermocouple
- \( \text{PDT} \): differential pressure transmitter
- \( \text{P} \): pressure gauge
- \( \times \): back-pressure regulator
- \( E/P \): electro-pneumatic transducer

- GC: Gas Chromatograph (Beckman Model 6700)

- Controller: PI: proportional-integral controller
- STR: self-tuning regulator
- Dahlin: controller using Dahlin algorithm

- \( T_R \): temperature of catalyst bed in reaction chamber
- \( T_{R}^{\text{set}} \): setpoint of \( T_R \)
- \( S \): selectivity

Subscripts for S:

- \( C_1 \): methane
- \( C_2 \): ethane
- \( C_3 \): propane
- \( X_{C_4} \): butane conversion

1. hydrogen and n-butane control valves
2. hydrogen and n-butane orifice plates
3. hydrogen and n-butane rotameters
4. nitrogen solenoid valve
Legend for Figure 2.1 (cont'd)

5. nitrogen flow indicator
6. feed preheater (steam)
7. backpressure regulator for feed system
8. feed preheater (circulating oil)
9. fluidized bed reactor, reaction chamber
10. fluidized bed reactor, disengaging section
11. air cooler (circulating oil system for heating/cooling coil)
12. heating tank, feed preheat circulating oil system
13. heating tank, heating/cooling coil circulating oil system
14. expansion chamber
15. reactor pressure relief valve
16. exit gas cyclone
17. heating/cooling coil
Feed gas enters the bottom cone of the reactor which is packed with 1.9 cm stainless steel Rasching rings to disperse the gas across the reactor cross-section. The gas then flows through a distribution/catalyst support plate, 0.0127 m thick drilled with 230, 1.4 mm-diameter holes. The 10% by weight nickel impregnated silica gel catalyst particles with diameters ranging from about 70 to 300 μm form a catalyst bed, the height of which is approximately 0.47 m under static conditions. A sheet of 200 mesh stainless steel screening placed over the distributor plate prevents the particles from falling through. The exit gas passes through a cyclone which returns any entrained catalyst particles to the catalyst bed. The reactor is maintained at constant positive pressure (ca. 115.1 kPa) by a back pressure valve (Brooks, model 66122BP) located after the cyclone and the exit gas sampling line. A 0.15 m flanged port on top of the disengaging section is used for charging catalyst and visual observation of bubbles when using nitrogen gas.

2.2.2 Heating-Cooling System

Two circulating oil systems are present; one in the feed-gas preheater system and the other in the heating-cooling coil system on the reactor. The circulating fluid is Sun 21 Heat Transfer Oil and electrical immersion heaters (4.5 kW for gas preheater system and 8.5 kW for reactor heating system) are used to heat the oil. The oil is circulated by Sihi centrifugal pumps.

1) Gas Preheater: Feed gas is preheated to reaction temperature (\( \geq 225^\circ C \)) by first heating it with 790.6 kPa steam in a brass shell-and-tube heat exchanger (single pass, 0.111 m\(^2\)) and then in two carbon steel heat exchangers (single pass, 0.185 m\(^2\) each) by the circulating oil.
3.4(i) Heating-Cooling System for the Reactor: At start-up, the fluidized bed is heated to reaction temperature by circulating hot oil through 1.27 cm diameter stainless steel tubing which is spiralled on 5.1 cm centres around the reactor barrel and approximately one half the disengaging section. This heating coil is imbedded in heat transfer cement (Thermon Company) to improve the heat transfer to the reactor wall.

Once the reaction starts, heat must be removed by the circulating oil. This is accomplished by passing the oil through an air-cooled heat-exchanger (single pass, shell-and-tube exchanger, 0.111 m² area), referred to hereafter as the air cooler.

2.3 Minicomputer System

The pilot plant fluidized bed reactor is interfaced to the minicomputer system (NOVA 1200) in the department's computer control laboratory. The computer system was used for all data logging programs and control algorithms that were implemented on the reactor. A layout of the computer facilities at the time of this study is given in Fig. 2.2.

The minicomputer system is a dual processor consisting of two Data General NOVA 1200, 16 bit minicomputers (A and B). They share an interprocessor bus (IPB), a 0.5 Mbyte fixed head disk and a Data Acquisition and Control Interface (DGDAC). The minicomputers can access to 48 analog to digital (A/D) and 12 digital to analog (D/A) channels, 32 TTL inputs, 32 TTL outputs, 16 relay outputs and 32 contact sense lines in the DGDAC through FORTRAN callable software driver routines in the library file AIO.LB which was first developed by Harris [5]. During a computer run, either system A or system B can access to the DGDAC, but not both.
Figure 2.2 Layout of the Minicomputer System
The peripheral devices on Minicomputer A include a cathode ray tube (CRT), a paper tape punch and reader, hardware floating point processor, hardware multiply and divide and a real time clock. System A is used for the production runs and communicates with a video console and keyboard (CRT). Because of the reduced computation time, the hardware floating point and multiply/divide System A allows the accommodation of the big production program which has three major sampling and control tasks on the flow, temperature and gas chromatograph systems; while the parameter interrupts as well as detalogging and control results are passed from and to System B via the IPB.

System B is interfaced to two 5 Mbyte disks, one of which is removable and is used to store all the data. Any on-line parameter changes may also be communicated to System B via a teletype with a QTY port (QTY:1, is a CRT). The measurements and the setpoints introduced can be read from a hardcopy when the information has transferred from System A to System B and dumped out through another QTY port (QTY:0, a Centronics line pointer). After each experimental run, it is advisable to store all the data onto a magnetic tape using the magnetic tape drive. In addition, Minicomputer B is able to transfer data directly to the University’s main Control Data Corporation (CDC) Cyber computer.

The computers use Data General’s Real-Time Disk Operating System (RDOS) revision 6.62. All user software for this study was written using Real-Time FORTRAN in a multitasking environment.
2.4 Instrumentation and Process/Computer Interface

2.4.1 Instrumentation

2.4.1.1 Feed Flow System. The hydrogen and n-butane gases are fed to the reactor from cylinders. Six hydrogen cylinders (each containing 6.5 m$^3$ at S.T.P.) are connected to a common manifold; usual operation entails using one at a time and each can last for about one hour under normal reactor operating conditions (ca. 0.1 m$^3$/min). The butane originates from one large cylinder. Hot water is run over the cylinder as a film to maintain a reasonable operating pressure.

Two flowrate measuring systems are employed. Rotameters are used as a visual indication; that for hydrogen is a Fisher-Porter FP-1/2-21-G-10/80 and that for butane is Brooks ER-1/2-25G10. Originally there were two floats in the butane rotameter, but since only low flowrates were required only the light float was used. Orifice plates (2.50 mm diameter for n-butane and 2.00 mm diameter for hydrogen) along with pressure differential (ΔP) transmitters (Rosemount Alphaline: n-butane, model C1151DP4E22MBCE, hydrogen, model C115DP4C22MBCE, 4-20 ma output) were used to monitor (datalog) the flowrates by the computer. These were installed upstream of the rotameters. To ensure a constant calibration of these flow measuring devices, a constant pressure of 128.9 kPa was maintained on them by a back-pressure regulator (Fisher, type 38L) installed downstream of the rotameters.

The hydrogen and butane flowrates are controlled by pneumatically-activated valves (Badger Meter Inc. Research and Control Valves, air to open, type TY7SS; n-butane, Trim J; hydrogen, Trim G).
Interfacing the pressure transducers with the computer and the computer with the pneumatically controlled valves requires analog-to-digital (A/D) conversion and electro-pneumatic (E/P) converters respectively. The A/D converters are able to digitize input signals of 0 to 10 volts* and produce output voltages over a similar range. Thus, the milliamp signal from the pressure transducers was converted to a suitable voltage by installing dropping resistors across the outputs of the ΔP transmitters. The reverse procedure, that is producing the required pneumatic signal from the output voltage from the computer (D/A converters) requires conversion from voltage to current (1-9 V to 2-50 ma) and then an E/P converter (Fisher Controls Co., Type 546) to linearly convert this current to pneumatic signals for actuation of the control valves. The calibration procedures and results for butane and hydrogen are given in Appendix A.2.1.

It is important to maintain the feed flowrate ratio \( \frac{u_{H_2}}{u_{C_4}} \) of the incoming gases above some critical ratio depending upon the reactor operating temperature, since it was observed on one occasion that severe coking of the catalyst occurred when the \( \frac{u_{H_2}}{u_{C_4}} \) ratio fell to around 3 for about 5 to 10 minutes. This coking led to severe catalyst deactivation. Since the catalyst could not be easily reactivated, complete replacement of catalyst was required. This experience led to the design and construction of an automatic device which caused the butane to be immediately shut off if the feed flowrate ratio was reduced to less than some specified value (usually 4.0). This safety device com-

* This is done in terms of computer units; 0-4095 computer units correspond to 0-10 V at the D/A output.
compares the ratio of the voltages which are transmitted to each flowrate control valve. In addition to this device, which was activated essentially all the time during reaction operation, computer software also ensured that the required ratio, as calculated by the control algorithms, was always above a specified ratio. The physical device was used as back-up; however, it was essential during manual operation or in case of computer malfunctioning.

2.4.1.2 Cooling Oil Temperature Control. The air cooler is used to maintain a constant, preset oil temperature to the reactor cooling coils. In this way an attempt is made to maintain a constant heat load on the reactor. Cooling air from the 790 kPa lab system is used to control the outlet oil temperature. The air flowrate is controlled by a pneumatically operated valve (Badger Meter Inc., Research Control valve, air to open, Type TY7SS, Trim E) using similar auxiliary equipment as for the feed gas. A manually operated by-pass valve around the control valve can be used if a high rate of cooling is required.

During operation of the reactor, it was found advisable to have the electrical power on to the heaters in the oil hold tank (ca. 70% of maximum depending upon the conversion level and butane flowrate to the reactor).

2.4.1.3 Temperature Sensors. The temperatures throughout the reactor system (as indicated in Figure 2.1) are measured by Chromel-Alumel thermocouples (Thermo Electric (Canada) Ltd). These sensors are located at various vertical positions in the fluidized bed, on the outer wall of the reactor and in the oil and gas lines; exact locations are
given in Table 2.1. Radial traverses within the bed at various locations indicated essentially isothermal conditions, except in the immediate vicinity of the wall, as long as the gas velocity was in excess of about ten times that required for minimum fluidization.

Sixteen separate temperature measurements may be made at any instant. A multiplexing system (internal design) transmits any two signals at any given time. These relatively low level signals require amplification and transmission to the A/D input channels.

The particular amplifier (ACROMAG, Model 314-WM-U) which was used did create a problem in that it was somewhat incompatible with the multiplexer chip since the existing combination gives rise to a relatively long settling-out-time of 3 to 5 seconds, depending on the difference in voltages between consecutive readings. Thus, this system should require about 24 to 40 seconds to step through the eight channels connected to each of the two amplifiers. This means that a "snapshot" of all the temperatures cannot be taken at one time under a given operating condition. The problem was alleviated to some extent by judicious choice of the consecutive temperatures which were multiplexed to the amplifier. For example, the representative temperature of the bed was assumed to be the average of these measured 0.15 m and 0.30 m from the distributor plate. Thus these temperatures were measured consecutively. The oil temperature to the cooling coils is also controlled. Since it
<table>
<thead>
<tr>
<th>THERMOCOUPLE #</th>
<th>LOCATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Out of order</td>
</tr>
<tr>
<td>2</td>
<td>Not in use</td>
</tr>
<tr>
<td>3</td>
<td>Out of order</td>
</tr>
<tr>
<td>4</td>
<td>$T_{W,9^\circ}$: Reactor wall, 0.23 m from distributor plate</td>
</tr>
<tr>
<td>5</td>
<td>$T_{tank}$: Oil line exiting circulating oil heating tank</td>
</tr>
<tr>
<td>6</td>
<td>$T_{R,2'}$: Reactor chamber, 0.61 m from distributor chamber</td>
</tr>
<tr>
<td>7</td>
<td>$T_{W,36^\circ}$: Reactor wall, 0.91 m from distributor plate</td>
</tr>
<tr>
<td>8</td>
<td>$T_{oil,preheater}$: Oil line entering feed preheater</td>
</tr>
<tr>
<td>9</td>
<td>$T_{W,18^\circ}$: Reactor wall, 0.46 m from distributor plate</td>
</tr>
<tr>
<td>10</td>
<td>$T_{oil,out}$: Oil line exiting heating/cooling coil</td>
</tr>
<tr>
<td>11</td>
<td>$T_{feed}$: Reactor feed line</td>
</tr>
<tr>
<td>12</td>
<td>$T_{R,3}$: Reactor chamber, 0.91 m from distributor plate</td>
</tr>
<tr>
<td>13</td>
<td>$T_{R,4'}$: Reactor chamber, 0.22 m from distributor plate</td>
</tr>
<tr>
<td>14</td>
<td>$T_{oil,in}$: Oil line entering heating/cooling coil</td>
</tr>
<tr>
<td>15</td>
<td>$T_{R,1'}$: Reactor chamber, 0.30 m from distributor plate</td>
</tr>
<tr>
<td>16</td>
<td>$T_{R,2'}$: Reactor chamber, 0.15 m from distributor plate</td>
</tr>
</tbody>
</table>

Table 2.1: Thermocouple Locations
is only slightly lower than the reactor temperature it, too, was measured immediately before the reactor temperatures. This measurement sequence also ensured that control procedures were executed under the same conditions.

Another problem which was encountered with the ACROMAG transmitter-amplifier was the continual slow drifting of the calibration of the amplified signals from the thermocouples. Moreover the calibration was non-linear so frequent recalibration (ca. every one or two hours) was necessary. Although a new multiplexing-amplifier system was designed, construction was not completed in time for the experimental program reported here.

2.4.1.4 Gas Chromatograph System. As Figure 2.1 indicates, a process gas chromatograph (Beckman Model 6700) was used to analyze the exit gas stream from the reactor. The chromatograph consists of an analyzer and programmer. The latter schedules the injection of samples to the columns and the transmission of data and pulses to and from the computer. Details of the gas chromatograph, its interface to the reactor and computer systems as well as its operation are not presented here. Both Tremblay [6] and McFarlane [4] have included comprehensive summaries of its operation in their theses. However some of the new settings of the component boards in the programmer, the procedure for preparing a calibration sample and the calibration curves for the different components are described in Appendix A.2.2.

For this chemical system, the time required by the chromatograph to process the complete analysis is 360 s. This introduces a considerable
dead-time between sampling and measurement which is very important in designing the control system for the reactor.

2.4.2 Procesa-Computer Interface

The reactor is started up under manual control. Thus variable voltage sources (0 to 10 volts D.C.) are required to allow manipulation of the control valves through the E/P converters. Four separate variable sources are available: one to manipulate hydrogen flow, one for butane and one for the air supply to the air cooler; the fourth is a spare.

A "Manual/Computer" switch at the reactor control station adjacent to the reactor allows the operator to select the manual or computer control mode. In the manual mode, manipulation of each of the valves is effected by a potentiometer on the voltage supplies. The start-up procedure recommended by Shaw [3] was easily carried out using this equipment.

In the computer mode, the voltage sources are manipulated by the computer via the D/A converter output channels. The voltages to be transmitted to the E/P converters are set or calculated within the user-generated software in terms of computer units (4095 units = 10 volts at the output of D/A unit).

Detailed schematics and information about some of the devices described above can be found in the technician's file in the Department. They are as follows:

- The circuit diagram and the details of the ratio comparator device in Section 2.4.1.1.
- The block diagrams, input-output connection diagram of the multiplexing system and the multiplexer-cable connections in Section 2.4.1.3.
The wiring of the Manual-Computer control box, a schematic of the process-computer interface and the pin connections for the interface cable in Section 2.4.2.
3. DYNAMIC SIMULATION MODEL OF THE REACTOR SYSTEM

3.1 Introduction

The simulation model used in this study for the fluidized bed reactor system was based on the previous work done by Ørlikas [7] and Shaw [3]. Shaw tested a number of steady-state models which had been proposed for heterogeneous catalytic chemical reactions in fluidized beds and indicated that most models provided reasonable predictions (from a control point of view) as long as one parameter which related to the fluid-mechanical behaviour and also another parameter relating to catalyst activity were evaluated from reactor response data. It is the extension of these steady-state models to include the main dynamic effects which is described in this chapter. The essence of the chemical reaction kinetic model and the steady-state model is briefly reviewed prior to presentation of the dynamic model of the system.

3.2 Reaction Kinetics

The hydrogenolysis reactions which took place in the reactor were described in Section 2.1.2. The mechanistic kinetic model for the reaction system which was developed by Ørlikas [2, 7] and further investigated by Shaw [3, 8] has been shown to describe the chemical kinetics for this reaction quite well. It was shown that this mechanistic model gave good predictions of conversion and selectivities over a wide range of conditions in the small packed bed integral reactor used for the study. A catalyst activity parameter \( \frac{k}{k_0} \) was included in the model since even the same catalyst exhibited differences in activity depending on the initial 'conditioning' treatment to which it was subjected. This parameter as included in the model was shown to account
for differences in catalyst activity during this experimental program.

The main characteristics of the reactions are that they are all highly exothermic \((\Delta H_R = -167.4 \text{ kJ/mol})\), leading to a doubling of the reaction rates for about every 3°C increase in reaction temperature.

3.3 Fluidized Bed Reactor Model

Prior experimental and steady-state modelling studies conducted on this reactor by Shaw et al. \([3, 8]\) found that the simple, two-phase model of Orcutt, Davidson and Pigford \([9]\) described the conversion and product distribution (selectivity) with acceptable accuracy even though other models provided a better representation of the reactor under certain conditions. Therefore our dynamic model was based upon the Orcutt model because of its simplicity. The model assumes

1. The reactor consists of two separate phases: a bubble phase in plug flow and a perfectly mixed emulsion phase.

2. Spherical bubbles of constant size within which the gas is perfectly mixed but which contain no solid catalyst (hence no reaction occurs in bubble phase).

3. Gas is perfectly mixed in emulsion phase; the gas flowrate into and out of the emulsion phase is that required to keep the solids in a fluidized rate (minimum superficial fluidization velocity, \(u_{mf}\)).

4. The mass transfer coefficient for the transfer of gas between the bubble and emulsion phases is constant over the bed height.

5. The system is isothermal throughout.
The mathematical model based on these assumptions is described below.

### 3.3.1 Material Balances

(i) **Bubble Phase**: At any instant, for any component \( i \) in the bubble phase, its concentration as a function of the height \( h \) through the bed is given by

\[
\frac{dC_b^i}{dt} = Q(C_e^i - C_b^i) \quad i = 1, 2, 3
\]

(3.3.1)

with initial conditions \( C_b^i = C_o^i \) at \( h = 0 \). \( Q \) is the transfer or interchange rate for any component between a bubble of volume \( V_b \) and the emulsion. Since \( V_b, u_b, C_e \) and \( Q \) are assumed to be independent of height in the bed, the bubble material balance equations in (3.3.1) can be integrated from \( h = 0 \) to \( h = H \) to give the exit bubble concentrations as

\[
C_{b,H}^i = C_e^i + (C_o^i - C_e^i) \exp(-QH/u_bV_b) \quad i = 1, 2, 3
\]

(3.3.2)

(ii) **Emulsion Phase**: For any component \( i \), a material balance over the entire perfectly mixed emulsion phase yields (with the use of Equation (3.3.2))

\[
\frac{dC_e^i}{dt} = S(C_o^i - C_e^i)(u_mf + Nu_bV_b[1 - \exp(-QH/u_bV_b)]) - r_iV_e
\]

(3.3.3)

for \( i = 1, 2, 3 \).

Simultaneous solution of this set of differential equations gives the emulsion phase concentrations through the reactor.

Using \( V_e = V(1 - NV_b) \) and \( H = V/S \), Equation (3.3.3) becomes

\[
H(1 - NV_b) \frac{dC_e^i}{dt} = (C_o^i - C_e^i)(u_mf + Nu_bV_b[1 - \exp(-QH/u_bV_b)]) - H(1 - NV_b)r_i
\]

(3.3.4)
Since it has been found for this system that the time constant of Equation (3.3.4) is small compared to the time constant of the Equation describing the enthalpy or temperature change of the reactor contents (Equation (3.3.12)) the concentration of the various reacting species was assumed to be at their pseudo steady-state values throughout. Therefore change of concentration with respect to time is assumed to be zero; thus, there results:

\[
(C_o - C_e) \left\{ \frac{u_m}{u_b} + Nu_b V_b \left[ 1 - \exp(-\frac{QH}{u_b V_b}) \right] \right\} = H(1-NV_b) \frac{r}{r_i} \tag{3.3.5}
\]

Knowing the division of flow into each phase, the bed exit concentration can then be solved simultaneously from the set of Equations (3.3.2) and (3.3.5). Note that the calculation of concentration involves only algebraic equations.

(iii) **Disengaging Section**: Since the concentrations are measured by a process chromatograph at the exit of the reactor, the dynamics of the disengaging section may also be important under some operating conditions at least. Here, this section is modelled as a perfectly mixed vessel. Thus, the transient mass balance for each component \(i\) may be written:

\[
\frac{dM_i}{dt} = F_{i,\text{in}} - F_{i,\text{out}} \tag{3.3.6a}
\]

\[
= F_{i,\text{in}} - \frac{M_i}{Q_{\text{out}} V} \tag{3.3.6b}
\]

where \(M_i\) = mass of component \(i\) in the vessel (Kg)

\(F_{i,\text{in}}\) = inlet mass flowrate of component \(i\) (Kg/s)

\(F_{i,\text{out}}\) = outlet mass flowrate of component \(i\) (Kg/s)
\[ Q = \text{volumetric flowrate of the stream (L/S)} \]
\[ V = \text{volume of the vessel (L)} \]

Since
\[ Q_{\text{out}} = Q_{\text{in}} \frac{T_{\text{out}}}{P_{\text{out}}} \frac{P_{\text{in}}}{T_{\text{in}}} \]

(3.3.7)

where \( T \) = absolute temperature of the stream (K)
\( P \) = total pressure in the stream (kPa)

Note that both \( F_{\text{in}} \) and \( Q_{\text{in}} \) are required and these may be obtained from the calculation of the product exit stream from the reactor. Thus Equation (3.3.6) can be integrated to give the mass hold up of the component \( i \), \( M_{i} \), in the vessel.

The mass flowrate of each component \( i \) in the outlet stream may be obtained from:
\[ F_{i,\text{out}} = \frac{M_{i}}{V} \]

(3.3.8)

**Empirical Correlations:** Several empirical correlations available from literature were used for predicting certain physical phenomena in the bed:

1. **Bubble diameter, \( d_{b} \),** as a function of bed height was given by Kato and Wen [10]:

\[ d_{b} = 0.14 \rho_{p} \frac{d_{h}}{\mu_{mf}} \left( \frac{u_{b}}{u_{mf}} \right) + \left[ 6 \left( \frac{u_{b} - u_{mf}}{u_{mf}} \right) \right]^{0.4} g^{-0.2} \]

(3.3.9)

Since the Orcutt model assumes a constant bubble diameter with respect to height, an integrated average value of \( d_{b} \) was calculated by Shaw et al. [8].
(2) The interchange rate $Q$ between the bubble and the emulsion phases was calculated from the correlation [11):

$$ Q = 0.11 \frac{V_b}{d_b} \quad (3.3.10) $$

It was assumed that the form of the correlation applied but an additional multiplying factor (interchange parameter) was required to compensate for difference in the reactor system employed here. A sensitivity analysis [3] demonstrated that this was by far the most important parameter in the fluid mechanical part of the model.

(3) The bubble rise velocity $u_b$ was predicted by Shaw et al. [8]

$$ u_b = 0.711 (g \cdot d_b)^{1/2} + (u - u_{mf}) \quad (3.3.11) $$

3.3.2 Enthalpy Balances

1. Reactor Contents: Assuming that the gas and the catalyst particles are at the same uniform temperature in the bed, then an enthalpy balance on the chemical gas/solid phases yields:

$$ (W_{PB} + \varepsilon V \rho_g C_{pg}) \frac{dT_R}{dt} = V \frac{C_{og} \rho_g (T_o - T_R)}{\rho} + h_w A_w (T_w - T_R) + \sum_{j=1}^{F} R_j \Delta H_j W \quad (3.3.12) $$

Since the second term on the left hand side of this equation is small compared to the first term, it can be neglected. Thus, the final form of the enthalpy balance on the reactor contents is

$$ W_{PB} \frac{dT_R}{dt} = V \frac{C_{og} \rho_g (T_o - T_R)}{\rho} + h_w A_w (T_w - T_R) + \sum_{j=1}^{F} R_j \Delta H_j W \quad (3.3.13) $$
where \( r \) = number of reactions where heat is generated (equal to 3 as explained in Section 3.3.3.)

(ii) Reactor Wall: The reactor wall, cooling coils, and supporting structure in contact with the wall was judged to have a mass sufficient to make their dynamic effect an important consideration in the temperature dynamics of the overall system. If these elements are lumped into a single mass \( (M_w) \) at a uniform temperature \( (T_w) \), an enthalpy balance yields

\[
M_w C_w \frac{dT_w}{dt} = h_w A_w (T_R - T_w) + h A (T_{oil} - T_w) - Q_{loss} \tag{3.3.14}
\]

(iii) Reactor Heating/Cooling Coils: The temperature response of both heat exchanger units was assumed to be rapid in relation to the rest of the system; therefore the instantaneous outlet temperature from the cooling coils was calculated from the steady-state relationship for a heat exchanger with a constant source temperature using the effectiveness factor relationship as follows:

\[
\varepsilon = \frac{1 - \exp[-(NTU)(1-R)]}{1 - R \exp[-NTU(1-R)]} \tag{3.3.15}
\]

where \( R = \frac{(WC_p)_{oil}}{M_w C_w} = 0 \)

\[
NTU = \frac{h c c}{(WC_p)_{oil}}
\]

Also,

\[
\varepsilon = \frac{T_{oil, out} - T_{oil, in}}{T_w - T_{oil, in}} \tag{3.3.16}
\]

Knowing \( T_w \) and \( T_{oil, in} \), Equation (3.3.15) and (3.3.16) are combined to eliminate \( \varepsilon \) and to calculate \( T_{oil, out} \).
The mean bulk temperature of oil in the heating/cooling coils is taken as the arithmetic average of the oil inlet and outlet temperature:

\[ T_{\text{oil}} = T_{\text{oil,in}} + \frac{(T_{\text{oil,out}} - T_{\text{oil,in}})}{2} \]  \hspace{1cm} (3.3.17)

3.3.3 Reaction Rates and Heats of Reaction

If \( F \) is the fraction of n-butane that reacts to form propane and methane, Equations (2.1.1) and (2.1.2) are rewritten respectively, as

\[ FC_4H_{10} + FH_2 \rightarrow FC_3H_8 + FCH_4 \]  \hspace{1cm} (3.3.18)

\[ (1-F)C_4H_{10} + (1-F)H_2 \rightarrow 2(1-F)C_2H_6 \]  \hspace{1cm} (3.3.19)

These are added to give:

\[ C_4H_{10} + H_2 \rightarrow FC_3H_8 + 2(1-F)C_2H_6 + FCH_4 \]  \hspace{1cm} (3.3.20)

Equations (2.1.3), (2.1.4) and (3.3.20) are three heat-producing reactions for which heats of reaction may be calculated; thus \( \tau \) is equal to three in Equation (3.3.13). Their rates of reaction are given by \( R_P \), \( R_E \) and \( R_B \) respectively as follows:

Let

- \( R_B \) = net rate of reaction of n-butane
- \( R_P \) = net rate of reaction of propane
- \( R_E \) = net rate of reaction of ethane

with units = mol/(unit volume emulsion phase-sec).

It is easy to show that the rates of reactions can be expressed in terms of the rate of hydrocarbon reacting as exemplified by the rate of reaction of propane in the following illustration:

\[ C_4H_{10} \rightarrow \text{rate} = R_B \cdot F \]

\[ C_3H_8 \text{ [net rate of production of } C_3H_8 = R_P \text{]} \rightarrow \text{rate of reaction, Equation (2.1.3)} \]

\[ C_2H_6 \]
Define the rate of reaction of Equation (2.1.3), RP (g moles propane reacted/unit volume emulsion phase-sec)

\[ RP = (RB \cdot F) - RP_2 \] (3.3.21)

Similarly, for ethane, the rate of reaction of Equation (2.1.4), RE is given by

\[ RE = RP + 2(1 - F)RB - RE_2 \] (3.3.22)

Heats of reaction for Equations (2.1.3), (2.1.4) and (3.3.20) are calculated using heats of formation of the product and reactant species, evaluated from polynomial expressions in temperature as given by Kjaer [12].

3.4 The DYNSYS Simulation

3.4.1 Introduction

A computer simulation program called DASTFF2 was modified from an existing program written by McFarlane [4], for use on the CDC Cyber Computer System in the University's Computer Centre. The program was written using a modular dynamic simulation approach utilizing the DYNSYS simulation executive which was developed by Bobrow [13, 14] to allow convenient dynamic simulation of chemical processes. A DYNSYS module consists of a steady state or a dynamic model to be written in terms of first ordinary differential equations, which are solved simultaneously in all modules by an Adams-Morton-Shell formulated third order predictor corrector routine.

The original DYNSYS executive main program was restructured by McFarlane [4] into a Subroutine Model 1 and a program external to
DYNSYS was created to define all inputs, setpoint changes, load disturbances, etc. in performing the control function. Through this modification, Model 1 can conveniently integrate the appropriate modules over one time interval when provided with updated inputs and returns the prediction of the system outputs at one time step ahead to the calling program.

3.4.2 Application of DYNSYS on Fluidized Bed Reactor System

Since the temperature response of the air cooler was assumed to be rapid in relation to the rest of the system, the instantaneous outlet oil temperature from the air cooler, which is the temperature of the oil entering the reactor heating/cooling coils, \( T_{oil, in} \), was taken to be freely adjustable as an input to the reactor. Therefore the DYNSYS simulation does not include the air cooler. The fluidized bed reactor has been simulated by two processing units: REACO1, the reactor, including the wall and heating/cooling coil and HOLDO1, the disengaging section, modelled as a well mixed vessel with a mass hold up.

With the modification of the DYNSYS executive main program into a subroutine, Model 1 and a calling program to be created, the computer program has the following structure:

Program DASTFF2 - the calling program provided by the user to fulfill the desired (control) function

Subroutines: MODEL 1, TYPE 1 (REACO1), TYPE 8 (HOLDO1), ORCMIX, HREACT.
The DYNYSYS subprograms:

Subroutines:  DYN1, DYN2, GET, FETCH, FETCHR, OUTPUT

Functions:  Y1, PROPS.

The relationship between the calling program, the subroutines and
function subprograms are illustrated by Figure 3.1. For the detailed
functions and descriptions of the DYNYSYS subprograms, the reader is
referred to the DYNYSYS manual by Bobrow et al. [13].

An information flow diagram for the system is shown in Figure 3.2
and each unit is described separately in the sections REAC01 and HOLD01.

The main features of the DYNYSYS program are outlined here so that
the reader obtains some impression of what is involved. All the details
of the DYNYSYS executive program are available in the manual.

There are four main storage arrays for DYNYSYS and the general
flow of information between them is indicated in Figure 3.3. The numbers
shown in the figure are representative of the fluidized bed reactor and
are the initial values read into the computer program.

The process matrix MP(I,J), dimensioned as 20 x 8, contains the
ordered list of unit numbers, module type and the associated streams
(input streams shown positive, followed by output streams shown negative).
There are two processing units involved: REAC01 and HOLD01 with their
corresponding type numbers 1 and 8. Their related streams are shown in
Figure 3.2. It should be noted that the last element in each row is used
for the storage of a pointer for locating extra parameter in the EX(100)
vector to be described below. All the unfilled locations in the storage
arrays are initialized to be zero.

The equipment parameter storage array EP(20,5) contains up to five
equipment parameters for each unit. If more than five parameters are
Legend:

- Main Program
- Subroutines
- Function Subprogram

* DYN2 executed twice with IC=1 and IC=2

Figure 3.1 Structure of the DYNSYS Simulation Program in Its Application to the Fluidized Bed Reactor
Stream 1 oil inlet to reactor heating/cooling coil
2 reactor feed
3 oil exiting reactor heating/cooling coil
4 product gas exiting from reactor to disengaging section
5 reactor information stream
6 exit gas from disengaging section
7 disengaging section information stream

Figure 3.2 Information Flow Diagram for DYNSYS Simulation
### MP(20,8)

<table>
<thead>
<tr>
<th>Unit No.</th>
<th>Type</th>
<th>Streams</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>3 4 5 6 7 8</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1. 2. -3. -4. -5. 1</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>4. -6. -7. - - 6</td>
</tr>
</tbody>
</table>

### EP(20,5)

<table>
<thead>
<tr>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2 3 4 5</td>
</tr>
<tr>
<td>7000.0    1.87 21.4 17.36 0.0165</td>
</tr>
<tr>
<td>124.6      10. - - -</td>
</tr>
</tbody>
</table>

### EX(100)

<table>
<thead>
<tr>
<th>Additional Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>3000. 0.64 0.25 0.1</td>
</tr>
<tr>
<td>0. 0. 0. 0. 0.</td>
</tr>
<tr>
<td>26.22 4. 5.3 39.35 8.65</td>
</tr>
</tbody>
</table>

### S(2,50,20)

<table>
<thead>
<tr>
<th>No. Flag</th>
<th>Flow Temp Pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 2 3 4 5 6 7 8 9 10 11 12 ...</td>
<td></td>
</tr>
<tr>
<td>1 5. 565.7 247. 1.1 0. 0. 0. 0. 0. 565.7 0.</td>
<td></td>
</tr>
<tr>
<td>2 5. 0. 260. 1.1 0. 0. 0. 0. 0. 0. 0.</td>
<td></td>
</tr>
<tr>
<td>3 5. 565.7 0. 0. 0. 0. 0. 0. 0. 565.7 0.</td>
<td></td>
</tr>
<tr>
<td>4 5. 0. 0. 1.1 0. 0. 0. 0. 0. 0. 0.</td>
<td></td>
</tr>
<tr>
<td>5 11. 247.4 253. 260. 0. 0. 0. 0. 0. 0. 0.</td>
<td></td>
</tr>
<tr>
<td>6 5. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.</td>
<td></td>
</tr>
<tr>
<td>7 11. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.</td>
<td></td>
</tr>
</tbody>
</table>

---

Figure 3.3 - Main Storage Units for DYNSYS and Information Flow Between Them
required for a unit computation, these parameters are stored in the extra-
equipment parameter vector EX(100). The executive sets up the last column
in the process matrix MP( ) as a pointer to this table. This feature
allows storage of an indefinite amount of information for the EX vector
in the data set. The physical significance of these parameters are to be
described in the modules.

The stream information array S(I,J,K), dimensioned as 2 x 50 x
20, is used to store the stream information for the present time step, I =
1 and for the previous time step, I = 2. Each row (J) is allocated for
each stream number (J) as defined in the process matrix MP( ). The
stream number is stored in K = 1 location.

For K = 2, the stream flag serves the dual purpose of identifying
the stream type and, if negative, suppresses printing of the stream
variables in the output. In general, there are two types of streams:

1. material information stream (flags with absolute value $\lt 10$); these
   are indicated by solid connecting lines on the information flow
diagram in Figure 3.2 and may include total flow, temperature,
pressure and the flows or concentrations of the components. For
this simulation, the stream list has been defined as:

\[ K = 1 \] stream number, \( (1,2,3,4,6) \)

2 - stream flag, \( = 5 \)
3 - total mass flow \( (\text{g/sec}) \)
4 - temperature \( (^\circ\text{C}) \)
5 - pressure \( \text{(atm)} \)
6 - \( \text{CH}_4 \) flowrate
7 - \( \text{C}_2\text{H}_6 \) flowrate
8 - C₃H₈ flowrate
9 - C₄H₁₀ flowrate
10 - H₂ flowrate
11 - circulating oil flowrate
12 - air flowrate

flowrates in g/sec

(2) control information streams (flags with absolute value >10) represented by dashed lines indicate that the information flow is concerned with control variables (such as the pressure used to activate a valve) or sensed variables (such as temperature in a tank). The stream list for stream 7, which is a control information stream is the same as that for material information stream because the sampled stream coming out from the disengaging section requires the same information whereas the control information stream 5 has the following stream list:

K = 1 - stream number, = 5
2 - stream flag, = 11
3 - T_{oil}, mean bulk temperature of oil in cooling coil (°C)
4 - T_w, average wall temperature over bed height (°C)
5 - T_R, reaction temperature (°C)
6 - S₁, selectivity of methane (moles methane produced/moles butane reacted)
7 - S₂, selectivity of ethane
8 - S₃, selectivity of propane
9 - CONV, conversion of butane
REAC01: Type 1

The reactor module REAC01 (TYPE 1) consists of the following equations which were described in Section 3.3:

1. algebraic equation describing the pseudo-steady state reactor mass balances: Equation (3.3.5).
2. differential equation describing temperature dynamics of reactor contents: Equation (3.3.13).
3. differential equation describing temperature dynamics of reactor wall: Equation (3.3.14).
4. algebraic equation describing enthalpy balance on oil in heating/cooling coil: Equations (3.3.15) to (3.3.17).

A solution to the steady state mass balance was provided by Shaw [3] as the Subroutine ORCMIX. It incorporates the reaction rate expressions Equations (3.3.1) to (3.3.3) and solves the (pseudo) steady state mass balance Equation (3.3.5) for each component. While the heats of reaction Equations (2.1.3), (2.1.4) and (3.3.20) are calculated in subroutine HREACT.

The calculation flowcharts and listings, together with the argument list, for subroutines ORCMIX, and HREACT may be found in Section 3.3.1 and Appendix A3.1 of McFarlane's thesis [4].

HOLD01: TYPE 8

The dynamic effects of the open volume above the fluidized bed and constituting the disengaging section are also important. The mixing patterns within this free space are unknown. In fact, a mixing model (for example, part of the volume could be considered perfectly mixed, another part in plug flow) should be formulated perhaps on the basis of pulse testing experiments, which would account for the mixing process which occurs there. In the absence of this experiment, the volume above the fluidized
bed was considered to be perfectly mixed. Thus, module HOLD01 is based on
the differential equation describing the unsteady state mass balance for
each component in the incoming stream, i.e. Equation (3.3.6).

The information flow diagram showing the associated streams with
this module is given in Figure 3.2. A program listing of TYPE 8 is
included in Appendix C.3.1. The equipment and extra parameter list
defined for this unit on Figure 3.3 are given below:

**Equipment List:**

<table>
<thead>
<tr>
<th>EP(2,1)</th>
<th>V'</th>
</tr>
</thead>
<tbody>
<tr>
<td>EP(2,2)</td>
<td>T\textsubscript{in} - T\textsubscript{out}</td>
</tr>
</tbody>
</table>

**Extra List:**

<table>
<thead>
<tr>
<th>EX(1)</th>
<th>M\textsubscript{C1} (corrector step)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EX(2)</td>
<td>M\textsubscript{C2} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(3)</td>
<td>M\textsubscript{C3} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(4)</td>
<td>M\textsubscript{C4} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(5)</td>
<td>M\textsubscript{H2} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(6)</td>
<td>M\textsubscript{C1} (predictor step)</td>
</tr>
<tr>
<td>EX(7)</td>
<td>M\textsubscript{C2} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(8)</td>
<td>M\textsubscript{C3} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(9)</td>
<td>M\textsubscript{C4} (&quot;&quot;&quot;)</td>
</tr>
<tr>
<td>EX(10)</td>
<td>M\textsubscript{H2} (&quot;&quot;&quot;)</td>
</tr>
</tbody>
</table>

3.4.3 **Parameter Estimation**

Many of the parameter values in the foregoing model were readily
available in the literature, or had been previously well estimated from
statistically designed kinetic experiments \([2, 8]\). There still remained,
however, a number of unknown parameters, which related to the dynamics of
the reactor system, that had to be estimated by least-squares methods from
data collected on the fluidized bed reactor itself by McFarlane \([4]\).

* initial values, to be replaced by values calculated in corrector step
  using the computer program.

\# initial values, estimated from the mass flowrate of each component
  exiting the reactor bed.
At the time of data collection for this parameter estimation program, the Beckman Gas Chromatograph was not in service and so exit stream selectivities were not available. In this work, the catalyst activity was re-estimated by non-linear least squares optimization algorithm for multiresponse parameter using the exit stream selectivities from reaction run data. The subroutine UWHAUS, based on Marquardt algorithm [16], is used to estimate the parameter in a model (Subroutine ORCMIX) given experimental data. A listing of the calling program KACT1 with the modified subroutines is given in Appendix C.3.2.
4. CONTROL METHODS USED ON THE PILOT PLANT FLUIDIZED BED REACTOR

4.1 Introduction

The highly exothermic nature of the reactions coupled with the large activation energies meant that direct control of the reaction temperature was a necessity for safe and stable operation. This was accomplished by manipulating the ratio of hydrogen to n-butane feedrates. The other manipulable variables, oil temperature and inlet feed temperature, could not be used for this purpose since their effect on $T_R$ was slow due to heat transfer limitations. However, maintaining stable reaction temperature is not the ultimate goal of control for this system. The primary control objective is propane selectivity control.

Propane selectivity is defined as the number of moles of propane produced per mole of n-butane reacted. Propane is one of the intermediate products of the reactions described by Equations (2.1.1) to (2.1.4), and it was chosen for two reasons: the control scheme reported here is univariate and so independent control of only one product is possible; and of all the products, propane is the most sensitive to changes in the operating conditions.

A cascade control configuration resulted and Figure 2.1 shows how the cascade control system interfaced to the process equipment. At the lowest level, the individual feedrates of hydrogen and n-butane were controlled at one second intervals; at the next level the feedrate ratio was controlled by the reaction temperature controller every 30 seconds; and at the highest level the reaction temperature setpoint was controlled by the selectivity controller when the product selectivities became available from the chromatograph every 360 seconds. An independent
controller, manipulating the air flowrate through an air-cooled heat exchanger, was used to maintain the oil temperature at any preselected value.

The dominant feature in the selectivity control loop is that the effluent gas is sampled every 360 s and analyzed with an on-line Beckman process gas chromatograph. The complete chromatographic analysis cycle requires 360 s for completion thereby introducing a considerable deadtime in obtaining the concentration measurements. This was known to cause problems for proportional-integral (PI) controllers [1] and so a controller with inherent dead time compensation was required. This was an important consideration in the control studies.

4.2 Temperature and Selectivity Control, Base Case: Dahlin + PI

The cascade control configuration using PI algorithm to control the reaction temperature in the inner loop and Dahlin algorithm [17] to control the propane selectivity in the outer loop was used as a base case for comparison to the other control schemes tested in this thesis.

A dynamic simulation model was developed for the system and control of the reactor temperature was simulated using a discrete PI controller in the velocity form

\[
\frac{u_{H_2}}{u_{C_4}} = \frac{u_{H_2}}{u_{C_4}}_{t-1} + K_P [\varepsilon_{T_R,t} - \varepsilon_{T_R,t-1} + K_I \varepsilon_{T_R,t}] \tag{4.2.1}
\]

where \( \varepsilon_{T_R,t} = \frac{T_{R,t}^{\text{measured}} - T_{R,t}^{\text{set}}}{T_{R,t}} \)

\( K_P = \) proportional gain

\( K_I = \) integral gain
The tuning of this PI controller [4] was accomplished by minimizing a weighted sum of squares criterion with respect to the controller parameters, $K_p$ and $K_I$. Four consecutive setpoint changes were made while the following criterion was evaluated:

$$
\min_{K_p, K_I} \left\{ \sum_{i=1}^{N} \left( \frac{T_{R,i} - T_{R,i}^{\text{set}}}{T_{R,i}^{\text{set}}} \right)^2 + \sum_{j=1}^{N} \left( \frac{S_{3,j} - S_{3,j}^{\text{set}}}{S_{3,j}^{\text{set}}} \right)^2 \right\}
$$

(4.2.2)

where $N = 200$ control intervals

$$w = \text{relative weighting of } S_3 \text{ deviations with respect to } T_R \text{ deviations}$$

A measurement error $\mathcal{N}(0, 0.35^2)$ was added to the predicted response of $T_R$, and to the response $S_3$ was added an error $\mathcal{N}(0, 0.008^2)$. The PI parameter estimates under different weightings are summarized in Table 4.1.

The open loop behaviour of the reactor was examined by step-testing using the simulation model [4]. It was found that the heating and cooling responses vary widely depending upon the reactor operating temperature, the catalyst activity, the hydrogen-to-butane feed ratio, and the cooling-oil temperature. This means that there are significant differences in the system gains and time constants for the heating and cooling responses.

Table 4.1

<table>
<thead>
<tr>
<th>$w$</th>
<th>$K_p$</th>
<th>$K_I$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.</td>
<td>1.508</td>
<td>0.268</td>
</tr>
<tr>
<td>(minimize squared variation in $T_R$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.000125</td>
<td>1.030</td>
<td>0.340</td>
</tr>
<tr>
<td>(equal weighting of $S_3$ and $T_R$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.</td>
<td>0.573</td>
<td>0.073</td>
</tr>
<tr>
<td>(minimize squared variation in $S_3$)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Because a 360 s dead-time was introduced by the chromatograph analysis time in the selectivity control loop, the Dahlin algorithm [17] was used for selectivity control. This controller algorithm has been shown to be most useful when it is desired that the closed-loop response (here the selectivity loop) resembles a first-order plus dead-time process. Here the dead-time was specified as 360 s and the desired closed-loop time constant, \( \lambda \), could be adjusted on-line. The response of the propane selectivity to a set-point change in reactor temperatures may be further approximated as a first order plus dead-time response (time constant \( \tau \) and gain \( K \)). The resulting Dahlin controller was simply a discrete-time PI controller with one period of dead-time compensation, that is

\[
V_{R,t}^{\text{set}} = a_1 V_{R,t-1}^{\text{set}} + \frac{a_1}{a_3} [\varepsilon_{S_3,t} - a_2 \varepsilon_{S_3,t-1}]
\]

(4.2.3)

where

\[
a_1 = 1 - e^{-360/\lambda}
\]

\[
a_2 = e^{-360/\tau}
\]

\[
a_3 = K(1 - a_2)
\]

\[
\varepsilon_{S_3} = S_3^{\text{set}} - S_3^{\text{measured}}
\]

At one set of nominal operating conditions, step tests on the simulation model were used to estimate an approximate inner loop gain \( K = -0.0173 \) and time constant \( \tau = 180 \) s. Since the up and down responses of the system were substantially different, these average values were a compromise. Upon implementing this control system on the pilot plant reactor at conditions close to that used in the simulation model, the controller performance for small set-point changes was quite
acceptable and in accordance with what was expected \( [4] \). However, after a few days when the catalyst activity had increased (from 1.87 to 2.50 estimated by the procedure described in Section 3.4.3) and a substantial set-point change (about \( .10 \) change) in selectivity was called for, the controllers led to the oscillatory and unstable behaviour. This very poor controller performance was attributed to the fact that the Dahlin algorithm was tuned very tightly (a desired closed-loop time constant of \( \lambda = 150 \text{ s} \) was called for). Then when the process response (represented by \( K \) and \( \tau \)) changed substantially due to the time varying catalyst activity and due to the very nonlinear behaviour of the process over the selectivity change requested, the Dahlin controller exhibited this nearly unstable behaviour.

This nonlinear behaviour of the reactor system was investigated further and the results are reported in this work. It will be shown in Section 5.3.2 that by better matching the process response characteristics and by detuning the Dahlin algorithm, this unstable oscillatory behaviour of the cascade control system can be overcome and acceptable performance can be achieved over a wider range of operating conditions.

In order to overcome some of the inherent problems associated with controllers employing fixed parameters on a process which has variable dynamic characteristics, it is logical to consider the use of self-tuning and adaptive controllers. These control schemes should be able to retune the controller as the catalyst activity changes with time, or as the process gain and time constants change when moving into a different region of operation. Self-tuning and adaptive control is discussed in the following section.
4.3 Self-Tuning and Adaptive Control

4.3.1 Introduction

The design of automatic control systems normally requires an accurate model of the system to be controlled before a suitable controller can be designed. However, for many industrial processes, it is very difficult to get an accurate model because of changing process conditions and disturbances in the system. Furthermore, even though identification schemes can be used to determine models for stationary processes, they may involve excessive plant experimentation and off-line analysis. It also demands a level of expertise sometimes not available in the industry. Thus an adaptive control system in which the parameters of a simple model are estimated on-line and subsequently used in the controller is very attractive for practical applications.

In developing a self-tuning regulator (STR), the parameters of a single-input, single-output stochastic model are estimated on-line using a linear least square recursive technique. The updated parameter estimates are then used in a minimum variance controller to calculate the control signal at each sampling instant. Very little a priori information about the process is required and the regulator can be easily implemented. This approach takes into account system time delays and can be used to control processes with slowly time varying parameters.

This section presents the basic equations for the self-tuning regulators (STR) as well as constrained STR. Their application to the fluidized bed reactor is also discussed.
4.3.2 Review on Theory of STR

The principal theoretical developments of self-tuning regulators, as discussed in Astrom et al. [18] and Clarke et al. [20], presumes that the process may be described by a model of the form

\[ Y_{t+b} = \frac{\tilde{R}(z^{-1})}{A(z^{-1})} U_t + \frac{C(z^{-1})}{A(z^{-1})} a_{t+b} \]  

(4.3.1)

whereas Box and Jenkins [21] use the notation

\[ Y_{t+b} = \frac{\omega(z^{-1})}{\delta(z^{-1})} U_t + \frac{\theta(z^{-1})}{\nu_d \phi(z^{-1})} a_{t+b} \]  

(4.3.2)

Both forms are capable of providing an adequate representation of a dynamic-stochastic system. However it is felt that the Box and Jenkins notation provides more insight into the nature of the process dynamics and stochastic disturbances by separating them into two terms. The common denominator in Astrom's representation mixes up the dynamic and stochastic models and it is no more than a mathematical representation of the output. The Box-Jenkins notation is to be adopted in this thesis because it clearly indicates the form of the estimation model in an adaptive environment.

The definitions of the symbols are given in the Nomenclature. It should be noted that in the Auto-regressive-integrated-moving-average (ARIMA) model for the white noise, all the roots in the numerator and denominator polynomials should lie inside the unit circle in the z-plane for stable operation. Furthermore, the allowance for d roots equal to unity (usually d = 0 or 1) enables integral action in the controller.

The next two sections summarize all the important equations to be used in the self-tuning and adaptive control on the reactor. For details of the derivation, the reader is referred to Harris [22,23].
4.3.2.1 Minimum Variance (M.V.) Control with Recursive Least Squares Estimation

Assume that the single-input, single-output plant can be represented by Equation (4.3.2) or

\[ Y_{t+b} = \frac{\delta(z^{-1})}{\phi(z^{-1})} U_t + N_{t+b} \]  \hspace{1cm} (4.3.3)

where \[ N_{t+b} = \frac{\phi(z^{-1})}{\phi(z^{-1})} a_{t+b} \]

The disturbance model can be reexpressed as

\[ N_{t+b} = \frac{\psi_1(z^{-1})}{\phi(z^{-1})} a_{t+b} + \frac{T(z^{-1})}{\phi(z^{-1}) \psi_1(z^{-1})} a_t \] \hspace{1cm} (4.3.4)

where \[ \psi_1(z^{-1}) a_{t+b} \] is the forecast error; and \[ \psi_1(z^{-1}) \] is a polynomial of order \( b-1 \)

\[ \frac{T(z^{-1})}{\phi(z^{-1}) \psi_1(z^{-1})} a_t \] is the \( b \) step ahead forecast.

The minimum variance controller \( U_t \) in terms of \( Y_t \) is given by

\[ U_t = -\frac{\delta(z^{-1})}{\omega(z^{-1})} \frac{1}{\psi_1(z^{-1})} \frac{T(z^{-1})}{\phi(z^{-1}) \psi_1(z^{-1})} Y_t \] \hspace{1cm} (4.3.5)

Expressing the process output \( Y_{t+b} \) explicitly in terms of the M.V. controller parameters \( \alpha_i, \beta_i \)

\[ Y_{t+b} = \alpha(z^{-1}) Y_t + \beta(z^{-1}) \psi d U_t + \epsilon_{t+b} \] \hspace{1cm} (4.3.6)

where \[ \alpha(z^{-1}) = \alpha_0 + \alpha_1 z^{-1} + \ldots + \alpha_m z^{-m} \]

\[ \beta(z^{-1}) = \beta_0 + \beta_1 z^{-1} + \ldots + \beta_l z^{-l} \]

and \( \epsilon_{t+b} \) is the \( b \) step ahead forecast error \( \psi_1(z^{-1}) a_{t+b} \).
The orders of \( m \) and \( l \) are

\[
m = \tilde{r} + \max(q - b, p + d - 1) \quad (4.3.7)
\]

\[
l = s + p + b - 1 \quad (4.3.8)
\]

Define

\[
\hat{\phi}_t = [-Y_t, -Y_{t-1}, \ldots, -Y_{t-m+1}, WU_{t-1}, \ldots, WU_{t-l}]^T
\]

\[
\hat{\theta} = [\alpha_0, \ldots, \alpha_m, \beta_0, \beta_1, \ldots, \beta_l]^T
\]

Equation (4.3.6) can be rewritten as

\[
Y_{t+b} = \hat{\phi}_t \hat{\theta} + e_{t+b} \quad (4.3.9)
\]

Equation (4.3.9) admits linear least squares estimation which may be expressed recursively

\[
\hat{\theta}_t = \hat{\theta}_{t-1} + K_t (Y_t - \hat{\phi}_{t-b} \hat{\theta}_{t-1}) \quad (4.3.10)
\]

where

\[
K_t = \frac{P_t \hat{\phi}_{t-b}^T}{1 + \hat{\phi}_{t-b} P_t \hat{\phi}_{t-b}^T}
\]

The parameters after being updated at every sampling interval can be used in the control law

\[
\gamma^d U_t = -\frac{\gamma(z^{-1}) Y_t}{\beta(z^{-1})} \quad (4.3.11)
\]

4.3.2.2 Constrained STR

M.V. controller sometimes calls for excessively large variation in the manipulated variable. In situations where this manipulation is too severe, it is common practice to calculate control laws which minimize the variance of \( Y \) subject to a constraint on the variance of \( WU_t \), that is to minimize
\[ I_1 = E[Y_t^2 + \xi' (v_t^d)^2] \quad (4.3.12) \]

However, the solution required to solve this linear quadratic control problem needs spectral factorization [24], or the steady-state solution of a matrix Riccati equation [25].

An alternative and much simpler approach to constraining the variations in the manipulated variable has been proposed by Clarke and Hastrys-James [26] and Clarke and Gawthrop [26]. Rather than minimizing Equation (4.3.12), they treat the simpler problem of minimizing an instantaneous performance index

\[ I_2 = \{ \hat{Y}_{t+b/t}^2 + \xi' (v_t^d)^2 \} \quad (4.3.13) \]

where \( \hat{Y}_{t+b/t}^2 \) is the minimum variance forecast of \( Y_{t+b} \) made at time \( t \).

Clarke and Gawthrop [20] proved that minimizing (4.3.13) is equivalent to minimizing

\[ I_3 = E[Y_{t+b} + \xi v_t^d]^2 = E[\phi_{t+b}]^2 \quad (4.3.14) \]

where \( \xi = \xi' / \omega_0 \)

The resulting controller can be shown [22] to be

\[ v_t^d = \frac{-a(z^{-1})}{\beta(z^{-1}) + \xi \delta(z^{-1}) \phi(z^{-1})} Y_t \]

\[ = \frac{\delta(z^{-1}) T(z^{-1})}{\omega(z^{-1}) \psi(z^{-1}) \phi(z^{-1}) + \xi \delta(z^{-1}) \phi(z^{-1})} Y_t \quad (4.3.15) \]

\( \xi \) is a tuning parameter. If \( \xi = 0 \), a M.V. controller without constraint is obtained. Note that \( \xi = \xi' / \omega_0 \) and since \( \xi' \) is positive, the sign of \( \xi \) must be that of \( \omega_0 \).
4.3.3 Application to the Fluidized Bed Reactor

4.3.3.1 Control of the Reaction Temperature

In the fluidized bed reactor a self-tuning regulator was first implemented on the inner temperature loop since the performance of this loop was observed to change with time and with process conditions, and it also strongly affects the selectivity controller. The performance index upon which the controller was based was the constrained one-step ahead criterion [20].

\[
\min_{U_t} \sum_{j=t}^T \left[ (T_R - T_{R_{set}})^2 + \xi \Delta U_t^2 \right] \tag{4.3.16}
\]

where \(U_t\) is the hydrogen-to-butane feedrate ratio and \(\Delta U_t\) is the change in the ratio.

In developing a control model for the reaction temperature, the following reasonable assumptions may be made:

(i) a first-order transfer function with no delay is a reasonable approximation for the reactor temperature dynamics,

(ii) the major disturbances to the inner (temperature-control) loop were white measurement noise, and

(iii) step disturbances in the temperature setpoint were called for every 6 minutes by the outer loop selectivity controller.

Using these assumptions, the process described by Equation (4.3.2) can be represented by:

\[
Y_{t+1} = \frac{\omega_0}{1 - \delta z^{-1}} U_t + \frac{1 - \theta z^{-1}}{1 - \delta z^{-1}} a_{t+1} \tag{4.3.17}
\]

As illustrated in Appendix B.4.1, the orders \(i, m, b\) and \(d\) were determined to be \(i = m = 1, b = d = 1\). This means that the optimal (in
the sense that the output variance is minimized) constrained controller
structure would be of the form:

$$\beta_0 V_t = \beta_1 V_{t-1} + \alpha_0 (T_R - T_{R \text{set}})_t + \alpha_1 (T_R - T_{R \text{set}})_{t-1} \quad (4.3.18)$$

where $u_t$ is the hydrogen-to-butane feedrate ratio and $V_t$ is the change in
this ratio from the previous control time to the present one.

Furthermore, the reactor temperature can be expressed in terms of
the input as in Equation (4.3.9)

$$(T_R - T_{R \text{set}})_t = -\alpha_0 (T_R - T_{R \text{set}})_{t-1} - \alpha_1 (T_R - T_{R \text{set}})_{t-2} + \beta_0 W_{t-1}$$

$$- \beta V_{t-2} + e_t \quad (4.3.19)$$

The controller parameter vector $\theta$ was estimated using the
exponentially discounted recursive least squares algorithm [18]

$$\hat{\theta}_t = \hat{\theta}_{t-1} + \frac{K_t (Y_t - \hat{\phi}_{t-1} \hat{\theta}_{t-1})}{\phi_{t-1}^T \phi_{t-1}} \quad (4.3.20)$$

where

$$K_t = \frac{P_t \hat{\phi}_{t-1}^T}{\phi_{t-1} P_{t-1} \phi_{t-1}} \quad (4.3.21)$$

and

$$P_t = \frac{1}{\phi_{t-1}^T \phi_{t-1}} \left( P_{t-1} - \frac{P_{t-1} \hat{\phi}_{t-1} \phi_{t-1} \phi_{t-1}^T}{\phi_{t-1} P_{t-1} \phi_{t-1}} \right) \quad (4.3.22)$$

$\phi_{t-1} \leq 1.0$, is the exponential discounting factor in the recursive least
square algorithm to allow the controller to track changing parameters.

4.3.3.2 Control of the Propane Selectivity

As mentioned earlier in Section 4.1, the primary control objective
is propane selectivity control. Again the Clarke and Gathrop[20] method
is used to minimize the instantaneous performance index:
\[
\text{Min } E \sum_{T^\text{set}_R} \left( (S_3 - S_3^\text{set})^2_{j+1} + \xi V(T^\text{set}_R)_{j}^2 \right) \tag{4.3.23}
\]

As explained previously in Section 4.2, the closed-loop response of the selectivity loop can be specified to resemble a first-order plus dead-time process, where the dead-time was 360 s. By a similar derivation, as in that presented in Section 4.3.3.1, the optimal controller structure of the outer STR would be of the form

\[
\beta_0 V(T^\text{set}_R)_{t} - \beta_1 V(T^\text{set}_R)_{t-1} + \alpha_0 (S_3 - S_3^\text{set})_{t} \\
+ \alpha_1 (S_3 - S_3^\text{set})_{t-1} \tag{4.3.24}
\]

The selectivity expressed in terms of the reactor temperature setpoint is

\[
(S_3 - S_3^\text{set})_{t} = -\alpha_0 (S_3 - S_3^\text{set})_{t-1} - \alpha_1 (S_3 - S_3^\text{set})_{t-2} \\
+ \beta_0 V(T^\text{set}_R)_{t-1} - \beta_1 (T^\text{set}_R)_{t-2} + e_{t} \tag{4.3.25}
\]

Again, the estimates of the parameters \(\alpha_0, \alpha_1, \beta_0\) and \(\beta_1\) can be updated at each time instant by a recursive least squares algorithm using equation (4.3.25) and then used in equation (4.3.24) to calculate the current control action. An exponential discounting factor used in the recursive least squares algorithm will further allow the controller to track changing parameters.
5. SIMULATION STUDIES ON THE REACTOR SYSTEM

5.1 Introduction

In this pilot scale fluidized bed reactor system, complex and highly exothermic hydrogenolysis reactions are taking place. For this reason, the dynamic simulation model for the reactor system, as described in Chapter 3, was used to study the system before the experimental studies were performed.

The objective of this simulation study was to investigate:

1. the sensitivity of the system response to the parameter values in the Dahlin controller on propane selectivity, given a proportional-integral (PI) controller on the reactor temperature in the inner loop of the cascade control system,

2. the behaviour of the system when a self-tuning regulator (STR) is substituted for the PI controller in the inner loop, and

3. the behaviour of the system when a STR was substituted for the Dahlin controller in the outer loop.

5.2 Computer Software for the Simulation

In order to accommodate the simulations indicated above, a calling program (DASTFF2) was written to call those subroutines (as discussed in Section 3.4.2) which are appropriate for the study of a given control scheme. The characteristic feature is that the program could be run interactively to allow the following options:
(a) Measurement noise could be included if desired.

(b) The inner and/or outer loop could be opened or closed.

(c) Any desired controller could be implemented in the inner and outer loop. This option provided flexibility in the choice of a PI or STR controller on the inner loop and a Dahlin or STR controller on the outer loop.

As shown in the flow chart in Figure 5.1, the program begins with the initialization of constants/parameters and definition of the input variables to subroutine MODEL1 which, in turn, integrates the reactor variable equations from \( t_n \) to \( t_{n+1} \). It then enters into the various control option specifications. Process measurement noise can be added. Inner control loop options include no control, using PI controller or the STR for the temperature control while the outer loop can have the option of no control, implementing Dahlin algorithm or STR to control propane selectivity. For all closed loop runs, the control signals are constrained to conform to the physical limitations of the reactor system.

After each integration step, the reactor and controller (if any) variables of interest are stored in a data file to be used in a plotting routine. At the end of the desired number of integration steps, the variables of interest for each run are printed. A plotting program STPLT2 is used to plot the variables. Listings of the calling program DASTFF2 and the plotting program STPLT2 are included in Appendices C.5.1 and C.5.2 respectively.

5.3 Results of the Simulation Runs

5.3.1 Introduction

The cascade control configuration used in this study is shown in
Figure 5.1 Flow Chart for Computer Calling Program DASTFF2
Figure 5.1 (cont'd)

B

CONTROL CONSTRAINTS

STORE REACTOR AND CONTROLLER VARIABLES IN DATAFILE

FINISHED?

NO

A

YES

PRINT REACTOR AND CONTROLLER VARIABLES

STOP
Figure 2.1 and different control methods have been discussed in Chapter 4. This section presents the results of the dynamic simulation described in Chapter 3 using the various controllers. In all the simulation runs, a measurement error $\sim N(0, 0.1^2)$ was added to the predicted response of reactor temperature, and to the response of propane selectivity was added an error $\sim N(0, 0.002^2)$.

5.3.2 Dahlin + PI

Throughout all the reported simulations, total volumetric feed-rate of hydrogen and butane combined and oil inlet temperature were constant at 0.1 m$^3$/min (S.T.P.) and 247°C respectively. The tuning parameters of the PI algorithm, $K_p = 1.03$ and $K_i = 0.34$ were used for the inner temperature loop. As for the Dahlin controller implemented in the outer selectivity loop, the gain $K = -0.022$ was used and $\tau$ and $\lambda$ were allowed to vary to determine the sensitivity of the system to these parameter values.

Three sets of $\tau$ and $\lambda$ values were chosen to further investigate the performance of the cascaded Dahlin and PI controllers. They were $\tau_1 = 250$, $\lambda_1 = 350$; $\tau_2 = 250$, $\lambda_2 = 500$ and $\tau_3 = 450$, $\lambda_3 = 500$ as shown in Figures 5.2, 5.3 and 5.4 respectively. The choice of these three sets of values originated from the fact that $\tau$ and $\lambda$ were thought to be under-specified in previous work [4]. It should be noted that all the graphs which are to be presented in this thesis will have the same format with the different variables of interest plotted versus the number of control intervals. This control interval refers to the time interval between control action on the reactor temperature (inner loop) which, for the experimental system, was 30 s. Thus, 240 control intervals represent a
time elapse of two hours. In the temperature plot, the top solid curve
gives the reactor temperature response $T_R$; the dotted lines represent
the setpoints $T_{R \text{ set}}$ which are the outputs from the outer loop controller
(Dahlin or STR); and the bottom curve is the inlet temperature ($T_{\text{oil, in}}$)
of the cooling oil for the reactor. The second and third plot responses
of the butane conversion and propane selectivity ($S_3$), respectively.
Propane selectivity was the controlled variable; its desired value
($S_{3 \text{ set}}$) is indicated by dotted lines on the third plot and was preset at
any desired value by the operator. The last plot shows the response of
the manipulated variable, the ratio of hydrogen-to-butane feedrates
$u_{H_2}/u_{C_4}$.

In the set of graphs shown in Figure 5.2, the selectivity setpoint
was changed in a series of steps in the order: 0.32, 0.25, 0.32, 0.36
and 0.40. This was the range of selectivities expected during the
actual experimental runs.

It should be noted that only during simulation studies can the
$S_3$ response be predicted using the model in between the sampling interval
(6 minutes) of the selectivity loop. And the heavy dots on the graphs
of $T_R$, $S_3$ and $u_{H_2}/u_{C_4}$ indicate the time when a chromatographic sample is
taken.

Figures 5.2, 5.3 and 5.4 indicate the responses of the system for
the same $S_3$ setpoint changes but with different values of the Dahlin
parameters $\tau$ and $\lambda$. Looking at these results, it is obvious that the
results in Figure 5.3 ($\tau = 250$, $\lambda = 500$) give the best response to
changes in $S_3$ setpoint. Using $\lambda = 350$ as in Figure 5.2 gave a similar
$S_3$ response but required greater variations in $u_{H_2}/u_{H_4}$. These responses
for $\lambda \geq 350$ appear to represent a considerable improvement over that.
Figure 5.3  Dahlia($\tau=250, \lambda=500$) + PI cascade controller performance responding to a series of selectivity setpoint changes (Simulation)
Figure 5.4  Dahlin (τ=450, λ=500) + PI cascade controller performance responding to a series of selectivity setpoint changes (Simulation)
obtained in previous work [4] with smaller \( \lambda \)'s. This implies that the model mismatch was probably too great to demand reasonable responses from the system. This is further illustrated in Figure 5.4 when \( \tau \) was increased to 450 (\( \tau = 250 \) being more realistic). There even with \( \lambda = 500 \) the model mismatch had become severe enough that oscillations had set in.

The simulation results in Figure 5.5 show the performance of the detuned Dahlin (\( \tau = 250 \) and \( \lambda = 500 \)) plus PI cascade controller responding to a change in \( S_3^{\text{set}} \) from .32 to .27 and a load disturbance on the reactor wall by lowering the \( T_{\text{oil, in}} \) from 247 to 242°C. The control system was well behaved.

As a setpoint change in \( S_3 \) was introduced, the Dahlin controller computed a new \( T_R^{\text{set}} \) for the reactor temperature controller which in turn calculated a new setpoint by the PI algorithm for the hydrogen-to-butane feed ratio. The \( u_{H_2} / u_{C_4} \) decreased instantaneously in order to raise the \( T_R \). The \( S_3 \) stepped down smoothly to the new desired level.

Later on when the load disturbance occurred at \( A \), the reactor temperature decreased in response to the decreased oil inlet temperature because the rate of heat transfer to the wall from the catalyst bed increased. A greater heat generation by the reaction was required to maintain reaction temperature; the temperature controller called for decreasing \( u_{H_2} / u_{C_4} \) which in turn, fell very quickly. This action caused the selectivity to drift off the target. On the other hand, a decrease in \( T_R^{\text{set}} \) was called for when the Dahlin controller realized the deviation of \( S_3 \) from its target and brought the \( S_3 \) back to the desired level after two sampling intervals. Note that the decrease in \( T_R^{\text{set}} \) was requested by
Figure 5.5  Dahlin($\tau=250, \lambda=500$) + PI cascade controller performance responding to a selectivity setpoint change and a load disturbance in $T_{oil,in}$ (Simulation)
the Dahlin algorithm at point C, two sampling intervals after the load
disturbance had taken place. The reason for this becomes apparent when
one realizes that the selectivity data on the graphs is plotted against
the time at which the sample was taken; those data are not really avail-
able to the computer until six minutes later. Thus at the subsequent
sampling point B, the Dahlin controller was comparing \( S_{3}^{\text{set}} \) with \( S_{3} \) at
point A and, finding no error, the controller did not take any action.
It was not until the next sampling interval at C, that the Dahlin con-
troller did detect an error and act accordingly.

In summary, this simulation suggests that the performance of the
cascade control system with the tuning parameters \( \tau = 250 \), \( \lambda = 500 \), \( K_p = 1.03 \) and \( K_I = 0.34 \) is satisfactory.

5.3.3 Dahlin + STR

A self-tuning algorithm has been developed for the fluidized bed
reactor as described in Section 4.3. Basically the algorithm can be
divided into two parts at every sampling instant: (1) estimation of the
new parameters in the control model, and (2) implementation of appro-
priate control action. Before the self-tuning algorithm can be used,
the constants and initial values listed below must be specified:

- Model order: \( m, \lambda \)
- Discounting factor: \( FLAM \)
- Constraining factor: \( \xi \)
- Initial parameter estimates: \( \Theta_0 \)
- Initial covariance matrix: \( \Sigma_0 \)
- Scaling factor: \( \beta_0 \)
The model structure of the controller was taken to be \( m = 2 = 1 \) as explained in Section 4.3.3.1. When the discounting factor, FLAM, in the recursive least squares (RLS) algorithm is less than 1.0, passed data is discounted exponentially as

\[
\sum_{s=1}^{t} \text{FLAM}^{t-s} e_s
\]

The effective time span (window length) over which data plays a role in the evaluation of the least squares is given by \( 1/(1 - \text{FLAM}) \). Thus, decreasing FLAM from .99 to .95 decreases the effective number of observations used in estimating the parameters from 100 to 20. The adaptation of the parameters although faster will then also be less smooth. There is no discounting of past data when FLAM = 1. Figures 5.6 (FLAM = 1.), 5.7b (FLAM = .98) and 5.8 (FLAM = .95) demonstrate the effects of varying FLAM on the controller parameters. The first two plots give the variations in the STR parameter estimates and the last plot shows the behaviour of the pole of the controller when the system was subject to the same sequence of setpoint changes in \( S_3 \) as in Figure 5.2. Despite the significant differences in the three sets of parameters, the system responses in each case are nearly identical as shown in Figure 5.7a.

After initialization of the parameter estimating procedure (first four sampling periods), the controller parameters started adapting. The first setpoint change in \( S_3 \) at the 31st sampling instant led to the most severe changes in the parameters for FLAM = .95 (Figure 5.8). The parameters for FLAM = 1. (Figure 5.6) seemed to change hardly despite the fact that a series of setpoint changes in \( S_3 \) were later introduced. On the other hand, changes in parameter values were observed in the case
Figure 5.6 Parameter estimates and pole of the inner STR when FLAM=1.0 (Simulation)
Figure 5.7a Dahlin + STR(FLAM = 0.9α, ξ = 0.5) cascade controller performance (Simulation)
Number of control intervals, temperature loop (30 s)

Figure 5.7b Parameter estimates and pole of the inner STR when FLAM=.9R, ε=.5
(Simulation)
Figure 5.8 Parameter estimates and pole of the inner STR when FLAM=95 (Simulation)
of FLAM = .95. At some particular instants, the pole of the controller lay outside the unit circle but stability was achieved as these values moved quickly back into the unit circle (see lower plot of Figure 5.8). The behaviour of the parameters for FLAM = .98 gave intermediate responses between the two extreme cases. Since the performance of the system was basically insensitive to the values of FLAM in the simulation study, FLAM = .98 was used for the rest of the simulation runs.

The $\xi$ in Equation (4.3.14) is a constraining factor used to weigh the past control actions. For $\xi = 0$, a minimum variance controller without constraint is obtained. The constraining factor is generally very effective in reducing the variance of the manipulated variable without significantly increasing the variance of the controller variable.

Figures 5.9 and 5.10 show the two cases of $\xi = .2$ and $\xi = 2$, respectively. These results are to be compared to Figure 5.7 with $\xi = .5$. The relatively unconstrained controller with $\xi = .2$ gave rise to large step changes in the manipulated variable $u_{H2}/u_{C4}$ (Figure 5.9a). In effect tighter control was implemented on the reactor temperature. These excessive variations in the feedrate ratio upset the production rate of the desired products of reaction giving the oscillating behaviour of $S_3$. This response can be improved by increasing the $\xi$ value to .5 as shown in Figure 5.7a. The consecutive changes in the feedrate ratio decreased in magnitude and the behaviour of the $S_3$ is more acceptable. However, further increasing the constraining factor to 2.0, the results as shown in Figure 5.10a indicate that the manipulated variable was so heavily constrained that it could not bring $T_R$ to the appropriate setpoint in a reasonable time. In this case, the dynamics of the reactor temperature
Figure 5.9a  Dahlin + STR(FLAM=0.98, ξ=0.2) cascade controller performance (Simulation)
Figure 5.9b parameter estimates and pole of the inner STR when $\varepsilon = 0.2$ (Simulation)
Number of control intervals, temperature loop (30 s)

Figure 5.10b Parameter estimates and pole of the inner STR when \( \xi = 2 \). (Simulation)
were slowed to a great extent; consequently, oscillatory behaviour in $S_3$
was observed.

Initial choices of the parameters $\Theta_0$ and $P_0$:

The initial parameter estimates $\Theta_0$ (except $\beta_0$), were chosen to be
zero based on the assumption that prior information about the reactor
system was unknown. However better initial guesses are possible by using
the tuning parameters from the PI algorithm. The behaviour of the system
and the responses of the controller parameters were found to be the same
whether the initial value for the parameters were assumed to be zero
(except $\beta_0 = 1$) or were taken as the PI tuning parameters.

At the same time initial estimates for $P_0$ are needed to start the
recursive estimation scheme. Since $\Theta_0$ represents the prior expectation
of $\Theta$ and $P_0$ represents a matrix proportional to the covariance matrix of
the prior distribution of $\Theta$, one can either achieve very rapid updating
under the situation of little prior knowledge using large values for $P_0$
or very slow but smooth updating under the situation of substantial prior
knowledge ($P_0$ small). The choice of $100I$ for $P_0$ seems to be appropriate
in this case (with no prior information).

For the scaling factor $\beta_0$, there is some controversy as to
whether it should be constant. Poor guesses of a fixed $\beta_0$ can cause
problems of system stability and poor convergence. However if $\beta_0$ is
being estimated, poor behaviour can occur when the parameter converges to
a wrong value or a singular estimation situation can arise when all the
parameters converge. Here in the simulation runs $\beta_0$ was allowed to adapt
in order to observe possible changes which might occur over the range of
operation. Later, during the actual reaction runs as discussed in
Chapter 6, $\beta_0$ is fixed because the initial parameter estimates are calcu-
lated from the operating PI tuning parameters and $\beta_0$ in that case can be considered as a good estimate. This procedure should avoid any problems of stability or convergence.

The results in Figure 5.11a show an identical simulation run as in Figure 5.5. In this case the difference is that the PI controller on the inner temperature loop was replaced by a self-tuning regulator (STR) while the previously described detuned Dahlin algorithm ($\lambda = 500$, $\tau = 250$) was used on the outer loop for selectivity control. For the STR, the constraining factor, $\xi$, and the least squares discounting factor FLAM were set equal to 0.5 and 0.98 respectively.

On a setpoint change in $S_3$, the controller gave an initial overshoot in $T_R$ but kept close to the target until a load disturbance on the reactor occurred. The STR had tuned itself in to provide comparable control as in the PI case in Figure 5.5a. Starting off with initial parameter estimates of zero for all parameters except for $\beta_0$ which was taken as unity, the variations in the controller parameter estimates are shown in Figure 5.11b.

5.3.4 STR + STR

Figure 5.12a shows the same simulation run using a double STR configuration for both the inner and outer loops. The inner STR had the same tuning parameters as the one referred to in Figure 5.11 under Section 5.3.3. The structure of the outer STR was taken to be $m = 1$ as described in Section 4.3.3.2. The constraining factor $\xi = 0.5$ and least square discounting factor FLAM = .98 were the same as those used in inner STR. The initial parameters were based on the values calculated from the Dahlin algorithm ($\alpha_0 = 6$, $\alpha_1 = 1.4$, $\beta_0 = .2$, $\beta_1 = .1$). Since these
Figure 5.11a  Dahlin + STR(FLAM=.98, ε=.5) cascade controller performance responding to a selectivity setpoint change and a load disturbance in $T_{oil,in}$ (Simulation)
Figure 5.11b: Parameter estimates and pole of the inner STR (Simulation)
Figure 5.12c. Parameter estimates and pole of the outer STR (Simulation)
could be regarded as good estimates, the initial $P_0$ was chosen to be 10 times the

On the setpoint change in $S_3$, the outer STR called for a big adjustment in $T_{R}^{\text{set}}$ and this was followed by a smaller second adjustment in $T_{R}^{\text{set}}$ to bring the $S_3$ right onto the target. When the load disturbance on the reactor occurred, the adjustments in $T_{R}^{\text{set}}$ were so gradual that the $S_3$ could not recover until after four sampling intervals, one sampling period later than the Dahlin case. The variations in the inner STR parameter estimates are shown in Figure 5.12b and those for outer STR are shown in Figure 5.12c. There are little variations in the tuning parameters $\alpha_0$ and $\alpha_1$ of the outer STR. As for $\beta_0$ and $\beta_1$, the only change occurred at the setpoint change of $S_3$. It was recognized later (after the reactor control runs to be described in Section 6.4.4) that these little variations in $\alpha_0$ and $\alpha_1$ were due to the fact that the starting covariance values in $P_0$ for $\alpha_0$ and $\alpha_1$ were not properly scaled according to their magnitudes as compared to the magnitudes of $\beta_0$ and $\beta_1$. Later on, load disturbance occurring in the reactor wall caused the deviation of $S_3$ from its target. However, the magnitude of this deviation value was small and the outer STR regarded $S_3$ essentially as nearly always on target and therefore did not carry out any adjustment in the controller parameters.
6. EXPERIMENTAL STUDIES ON THE REACTOR SYSTEM

6.1 Introduction

This chapter reports the experimental observations associated with the cascade control strategies which were applied to the pilot plant fluidized bed reactor. The details associated with these strategies were developed through the dynamic simulation program which was presented in Chapters 4 and 5.

6.2 Experimental Procedure

Because the chemical system is potentially quite dangerous and considerable quantities of highly flammable gases are involved in the reactor at a relatively high temperature level, it is important to implement safe operating procedures from start-up to shut-down. This procedure also entails a thorough check of the reactor system prior to starting it up. Detailed instructions for experimental check-out, catalyst conditioning and reactor operation were described in previous work [3]. These procedures were followed throughout but an improvement was made here by upgrading the flow control system to enable much closer control of the operation than was previously achieved.

The entire reactor system can be operated either manually at the site or remotely under computer control using the Nova 1200 minicomputer. It was found to be more convenient to allow computer-controlled operation at the reactor site rather than in the computer room. This not only reduced the operator travel from computer to reactor, but also meant that fewer operating personnel were required. This was important since, the experimental runs extended over long operating periods (16-18 hours).
The computer program can be initiated at the start up of the reactor for datalogging only. The reactor data is collected and stored on disk files at each sampling interval of the three major loops:

1. the flow loop sampled at every second
2. the temperature loop sampled at every 30 s
3. the gas chromatograph loop sampled at every 360 s.

Prior to the initiation of any of the controllers, satisfactory operating conditions must be obtained under manual operation. As soon as the flow control loop has been activated, the whole system can be switched over to computer control. The different control loops are then initiated one at a time:

1. the air cooler controller to control the inlet oil temperature to the reactor heating/cooling coil
2. the temperature controller to control the average temperature as measured in the reaction chamber at 0.15 and 0.30 m from the distributor plate
3. the selectivity controller to maintain the propane selectivity at a desired operating level.

Control action for each loop is taken at every sampling interval. The control signals calculated from the control algorithms were set as setpoints to the individual DDC control loops, that is, at every 360 s the controller for propane selectivity computes according to the control algorithm a setpoint to the reaction temperature whose controller in turn calculates a setpoint for the $\frac{U_{H_2}}{U_{C_4}}$ ratio to the two flow controllers giving rise to different setpoints for hydrogen and n-butane flows based on a constant total flowrate of the mixture.
At the end of each run, all the collected data were printed and also stored on magnetic tapes. They were then transferred to the computer system (Control Data Corporation) in the University's computer centre to have the results plotted.

6.3 Minicomputer Program Setup for the Experimental Study

The real-time multitasking computer programs that were used in the experimental study of the fluidized bed reactor system were modified and extended so that they could take care of the following aspects:

(1) All values were echoed to the CRT screen and checked before final entry into the computer. This is very important in on-line implementation because a mistakenly entered number may result in disastrous consequences for the reacting system.

(2) Many different control strategies can be used. This means that:
   a. step changes in the $\frac{u_{H_2}}{u_{C_3}}$ ratio may be introduced with open reaction temperature and propane selectivity loops.
   b. either a PI or STR controller may be used in inner loop for temperature control.
   c. either a Dahlin or STR controller may be implemented in the outer loop for propane selectivity control.

(3) Transition from manual manipulation to computer control must be smooth.

Since the computer programs have been extended to the extent that the entire program is more than double its original size, the previous
The arrangement of the computer system did not provide enough memory to allow the programs to be executed. The configuration of the existing facilities had to be modified as described in Section 2.3. However, with this configuration the computer is more susceptible to I/O runtime errors; as a result these errors occurred more frequently.

A list of the various tasks and subroutines of the user software developed for these data acquisition and control studies is included in Figure 6.1. The arrows indicate their interactions. The main task, MSBA, in system A receives any parameter changes from system B. It activates the other three tasks:

1. FSBA: flow sampling and control task
2. TSBA: temperature sampling and control task
3. GCSBA: gas chromatograph sampling and control task

and coordinates their sampling and controlling as indicated by the user through parameter interrupts. The flow task which is sampled at the fastest rate of 1 s is responsible for the transfer of all the update measurements of the different loops to system B through the inter-processor bus (IPB). In system B, the main task XPBP receives any interrupt from the console and facilitates the parameter changes as requested by the user. It then passes the parameters to system A to effect the changes via IPB. It also activates a printing task PRBA which prints out the different measurements and setpoints when appropriate flags are set.

This computer program has the option of filtering the flow and temperature measurements if they are found to be too noisy but it was not used in the reaction runs to be presented.
Figure 6.1 Structure of Minicomputer Software for the Fluidized Bed Reactor System.
6.4 Results of the Experiments on the Reactor

To verify the main results of the simulation study, a similar set of experimental runs were performed except under somewhat different operating conditions as described in the next paragraph. The cascade control using PI and Dahlin for the inner temperature and outer propane selectivity control respectively was applied first. Then the STR was used for temperature control only. It was allowed to tune itself before the propane selectivity control by the Dahlin algorithm was turned on. Finally a double STR cascade control strategy was implemented. Under most conditions the parameter values obtained from the simulation were used. When the outer STR was used, the actual system demonstrated quite large deviations from simulation results. The effects of various design decisions and parameter values were investigated.

There were some differences in the operating conditions between the actual reaction and simulation runs. The actual reaction depends very much on the activity of the catalyst and the initial starting conditions such as inlet oil temperature to attain steady state operation. These differences in operating conditions should be kept in mind when the simulation results are compared with the experimental results.

The ratio of the hydrogen-to-butane flowrates was constrained between 4 and 20 throughout all the runs; similarly a constant total volumetric flow rate of .081 m$^3$/min (S.T.P.) was used. The oil inlet temperature was held constant around 264°C by the air cooler controller.

The testing sequence of the proposed control strategies is as follows. The cascade scheme with PI and Dahlin for temperature and propane selectivity control respectively was evaluated first (Figure 6.2)
by first turning on the PI controller for temperature control and a set-
point change for $T_R$ was introduced to test whether the PI tuning para-
meters were appropriate or not. The $S_3$ loop was then activated and the
control system was evaluated for step changes in $S_3$.

6.4.1 Dip + PI

As a basis of comparison for the different control schemes on the
fluidized bed reactor, the cascade control system was chosen with a PI
controller on the inner loop for reactor temperature and the Dahlin
algorithm for control of propane selectivity on the outer loop. The con-
trol intervals on temperature and propane selectivity were 30 s and 360 s,
respectively. The response under the control scheme is shown in Figure
6.2. Testing of the temperature loop was first performed using a step
increase of $T_R^{\text{set}}$ from 265 to 267°C with the PI tuning parameters $K_p = 1.03$
and $K_i = 0.34$ (which were used in the simulation runs and found to be
adequate). Note that the PI controller for the feed ratio responds
instantaneously to the change resulting in large initial decrease in
$u_{H_2}/u_{C_4}$. The reactor temperature achieves its setpoint temperature
within five sampling periods (1 sampling period = 30 s); note initially
there is an overshoot of about 1°C but this is quickly damped. The set-
points for the $T_{\text{oil,in}}$ were introduced according to the reactor tempera-
ture so as to maintain a temperature difference of about 3 to 5°C between
oil inlet temperature and $T_R$. It was found that this difference serves as
a reasonable driving force for heat transfer from the reactor.

The Dahlin controller for propane selectivity was then activated
and tested for setpoint changes in $S_3$: a step up from .3 to .33 and a
step down from .33 to .28. Since a dead time of 360 s is introduced by
the gas composition chromatograph analysis cycle, this controller was designed (in Section 4.2) to incorporate dead time compensation by specifying that the desired closed-loop response of the selectivity loop resemble a first-order plus dead time process. The parameters, time constant $\tau$, gain $K$ and the desired closed-loop time constant $\lambda$ were chosen to be 250 s; -0.22 and 500 s respectively based on the simulation results.

Figure 6.2 demonstrates that the performance of the control system with the above controller parameters was satisfactory; $S_3$ moved smoothly with some overshoot to the new setpoint .33. The reader is reminded that the plotted $S_3$ responses in all the subsequent graphs correspond to the time at which the chromatograph samples were taken; the analysis information was known 360 s later. Thus when the change to $S_3^c$ was made from .3 to .33, the setpoint change would not be effective until after the chromatograph sample had been analyzed. After the 360 s analysis time, control action would then be taken based on the error computed from the difference between the new setpoint and the previous measured $S_3$. The Dahlin controller calculated that the reactor temperature should change by -0.82°C to meet the desired propane selectivity.

Figure 6.2 indicates that after about 120 control intervals, the controller calls for a continual increase in reactor temperature to meet the desired $S_3$ level. At the same time, the reactor feed ratio increased continuously. The selectivity and conversion remain nearly constant. The reason for this behaviour can be traced to a gradual change in catalyst activity. The catalyst had been stored in the reactor for a long period prior to this run. The reactivation period had probably been
too short and the catalyst was gaining activity during this reaction run. Furthermore, it must be remembered that the reactor together with the support structure has a relatively large thermal capacity which requires considerable time to be heated to operating temperature. As it reaches operating temperature, it represents less of a heat sink and thus the reactor operating conditions change gradually with time during this initial time. Note that the Dahlin controller was able to handle this nonstationary condition reasonably well. And when a stepdown in $S_3^{\text{set}}$ was introduced, the propane selectivity moved smoothly right to the target resembling a first-order system as predicted by the Dahlin algorithm.

6.4.2 STR in Inner Loop for Reaction Temperature Control

The experimental runs for the STR in inner loop to control the reaction temperature without closing the outer selectivity loop are presented in this section. The highly exothermic nature of the reactions coupled with the large activation energies means that direct control of the reaction temperature, $T_R$, is necessary for safe and stable operation even though the propane selectivity is the ultimate economic control variable. Moreover, it is wise to tune for $\xi$, the constraining parameter, first, without the complication of the additional outer loop.

Model orders of $m = l = 1$ were used, based on an assumed or previously identified transfer function model for the process and the noise model. The choice of model orders was previously verified by simulation (Section 5.3.3).

Section 1: Minimum variance STR

For the run shown in Figure 6.3(a) and (b), the performance of
the STR to control the reactor temperature in the inner loop was evaluated. The initial parameters of the STR, $Q_0: (1.840, -1.373, -0.320)$ were calculated from the tuning parameters of the PI controller, to ensure a very smooth transition from PI control to STR control. As soon as the STR started at point A, the first four sampling intervals were devoted to filling the $VU$ and $Y$ vectors, but with the PI controller still operative. Since we were confident that the initial guesses for the values of the STR parameters were reasonably good, the initial conditions for the estimation algorithm were $E_0 = 1I$, $FLAM = 0.95$ and $\xi = 0.0$. Here $\beta_0$ was allowed to adapt.

It was found that when a setpoint change in $T_R$ was introduced, this minimum variance control called for excessively large variations in the manipulated variable resulting in a bang-bang type of control action on the feedratio controller. These excessive variations in the butane flowrate would upset the level of propane selectivity and were therefore unacceptable. Thus the inner STR was deactivated at point B and the PI controller was allowed to take over.

**Section 2: $\xi = 0.4$**

In order to reduce the variations in the manipulated variable, Clarke's [20] constrained minimum variance algorithm which minimizes the performance index in Equation (4.3.16) was used. The inner STR was initiated at point C for a second time with the initial conditions for the estimation algorithm as $E_0 = 1I$, $FLAM = 0.95$ as previously in Section 1 and with some basis from the simulation $\xi$ was chosen to be 0.4. The parameter, $\beta_0$, was fixed at a value of 1.33 (found from the simulation)
since it was felt that this value was a good guess and hence it was not necessary for it to adapt.

Four sampling periods were required to fill the \( VU \) and \( Y \) vectors. After this initial period, the controller parameter estimates (Figure 6.3b) started adapting (except \( \beta_0 \) which was fixed purposely). As soon as the first setpoint change to \( T_R \) from 266 to 268°C was introduced, the controller parameter estimates made immediate changes. As a piece of new information had come in, the sum of the diagonal elements of the \( P \) matrix (trace) which is proportional to the average variance of the controller parameter estimates was found to decrease instantaneously. Since no major new disturbances were entering the system between setpoint changes, the variances of the parameter estimates were seen to grow by a factor of \( 1/FLAM \) (FLAM being the discounting factor). We could observe this kind of trend for the rest of the STR runs.

After a few setpoint changes from 268 to 270 and then to 267°C, the controller had tuned itself to give steady control on the reaction temperature holding it to 267°C. However it was thought that the variations in the controlled variable, \( T_R \), caused by the variations in the manipulated variable, \( u_{H_2}/u_{C_4} \), were still too large in the initial transient. Other values for the parameter, \( \xi \), were investigated.

At point D, it was found that the supply of hydrogen gas ran out and the butane gas supply was cut off by the safety device mentioned in Section 2.4.11. The system was momentarily under manual control. The reactor temperature was observed to decrease severely.
Sections 3 and 4 of Figure 6.3: $\xi = 0.8$ and $\xi = 1.6$

The inner STR was re-initiated again at point E with $P_0 = 0.5$ for a slower and smoother adapting of the controller parameters. The other initial conditions were the same except for $\xi = 0.8$ and later $\xi = 1.6$ (at point F). This change is readily accomplished on-line by simply changing the value of the constraining parameter $\xi$.

The controller parameters were found to converge to progressively smaller values than before. The increase in $\xi$ value effectively caused the pole of the controller to move further inside the unit circle (Figure 6.3b) and reduces the variability in the $u_H/u_C$ gradually but at the expense of increased variation in the reaction temperature. The controller parameter also slowed down the response of the reaction temperature.

Since the variations found in propane selectivity for different $\xi$ values were roughly the same, it was decided to take the $\xi = 0.4$ setting with the hope that the reaction temperature could be stabilized within the 360 s analysis cycle time of the outer propane selectivity loop.

6.4.3 Dahlin + STR

The value of parameter, $\xi$, was then changed on-line to 0.4 and two successive step down changes in $T_R^{\text{set}}$ were introduced from 270 to 269 and then to 267°C (Figure 6.4a) in order for the STR to obtain new information to tune its parameters. However, sustained oscillations were observed this time. The $T_R$ response to a decrease in setpoint change of $T_R$ was different from the last time under similar conditions. When the reactor temperature reached 267°C, the $S_3$ was still at a low level of 0.2. Another decrease of 2°C in $T_R^{\text{set}}$ was intended in the subsequent setpoint change to increase the propane selectivity level. In order to maintain a driving force of 3°C difference for heat transfer across the wall, $T_{\text{oil,in}}$ was
Figure 6.4a  Dahlin + STR (Experimental)
lowered from 264 to 262°C. The air cooler responded instantaneously by opening wide the air valve and brought the T_{oil,in} down to 262°C almost immediately. However this load change on the reactor wall forced the ratio controller for the feedrates to react in order to maintain the T_R at the desired setpoint. Unfortunately the temperature oscillations persisted.

At this point, the Dahlin controller on the propane selectivity was ready to be turned on. With this kind of sustained oscillations on T_R, it was expected to upset the level of S_3. Hence the constraining parameter ξ was backed off to a value of 0.8 at point A. Two more setpoint changes of T_R were made in order to allow the STR to adapt. The Dahlin controller was activated at point B. There were some initial oscillations in S_3 due to the unsteady behaviour of T_R. After the controller parameters in Figure 6.4b had some abrupt adjustments at each setpoint change of T_R as requested by the Dahlin algorithm, they tuned themselves in by the STR and converge nicely bringing the T_R to target by the end of 360 s.

At point A, as soon as the first setpoint change for T_R from 267 to 265°C was introduced, the controller parameter estimates made an immediate adjustment, and the trace of the P matrix was found to decrease instantaneously again. At point C, the discounting factor FLAM was changed to 0.98 in order to have a relatively slow updating in the estimation algorithm.

The performance of the control system was evaluated for a few setpoint changes in S_3: 0.23 to 0.19 and then to 0.21. The propane selectivity was brought to the desired setpoint gradually each time according to an overdamped first-order behaviour as designed in the Dahlin
algorithm. This was facilitated by the inner STR which brought the $T_R$ right onto the $T_{R \text{set}}$ as requested by the Dahlin controller at the end of 360 s.

In general, this control scheme performed satisfactorily. Given that the parameters used in the Dahlin algorithm gave rise to a very detuned controller, it is not surprising to see that it took a very long time (approximately 45 minutes to 1 hour) for $S_3$ to reach the desired value. This is because the $S_3$ is very close to the setpoint, the error computed from the difference between $S_3^{\text{set}}$ and $S_3^{\text{measured}}$ has a magnitude such as 0.01 that could only introduce a tiny fraction of a degree Centigrade change in $T_{R \text{set}}$.

6.4.4 STR + STR

The last control scheme to be tested is the double STR configuration for both the temperature and selectivity control. There were difficulties in running the outer STR for the selectivity control and some potential problems are disclosed and discussed in turn below.

(1) Initial estimates for $\Theta_0$ and $P_0$

As mentioned in Section 5.3.4, if $\Theta_0$ represents the best guess for $\Theta$ and $P_0$ represents the uncertainty in $\Theta_0$, one can achieve very rapid updating when little prior knowledge is available (large values of $P_0$ are used). On the other hand, very slow but smooth updating occurs when substantial prior knowledge on the parameters is available. However, the usual choice of $P_0 = \sigma I$ where $\sigma$ is a constant giving rise to homogeneous values for the diagonal elements in the $P_0$ matrix cannot be applied in this case because of the difference in the magnitude of the parameters in $\Theta_0$: (6.119, -1.444, 0.2, 0.103). Since the diagonal
elements of $P_{\xi}$ represents $\text{var}(\Theta_{1,2}, \epsilon)$, if the variances for 0.2 and 0.103 are of equal magnitude, the variance for $-1.444$ should be about 10 times as large and that for $6.119$ about 30 times the magnitude.

(2) The constraining factor $\xi$

Figure 6.5 shows the experimental results for the evaluation of the double STR configuration. As usual there was an initial transient for the fluidized bed reactor to reach a thermal equilibrium. The inner STR was turned on first at point A with FLAM = 0.95, $\xi = 0.8$, $P_0 = 0.5$, $\Theta_0 = (1.840, -1.373, 1.333, -0.320)$ as determined from the PI tuning parameters and $\beta_0$ was fixed. After the first few setpoint changes in $T_R$ from 265 to 266°C, the controller parameter estimates started to tune themselves in. The STR led to an initial overshoot on $T_R$. On subsequent adjustments in the tuning parameters, $T_R$ was brought to the setpoint value quickly.

At point B, the outer STR was activated with FLAM = 0.95 and $\xi = 1$. These parameters were chosen on the basis from the simulation and the plant experience with implementing the inner STR. The initial parameters for the outer STR, $\Theta_0$: $(6.119, -1.444, 0.2, 0.103)$, were calculated from the parameters of the Dahlin controller and the diagonal elements of $P_0$: $(7500, 2500, 250, 250)$ were scaled to the appropriate ratio as discussed in previous section. The initial four sampling intervals of the outer STR were used to fill $VU$ and $Y$ vectors; therefore, the Dahlin controller was operating during this stage.

The propane selectivity was controlled at 0.285 by the Dahlin controller. On the next setpoint change in $S_3$ to 0.23 the outer STR was effective and called for a large adjustment of $T_R^{\text{set}}$ from 265.3 to 268.3°C.
Figure 6.5b Controller Parameter Estimates, Controller Pole and Trace of P Matrix for Inner STR
The inner STR brought the $T_R$ right to the target by decreasing the set-point to the feedratio controller which responded accordingly. Hence the $S_3$ dropped to the desired level in the following sampling interval and remained around there for a few subsequent sampling intervals. So far the inner STR was performing extremely well and the controller parameters had converged, thus the discounting factor was changed to 0.98 on line for a relatively slow updating in the estimation algorithm at point C.

Later on at point D, it was detected that the zero of the outer STR moved outside the unit circle and remained there for two sampling periods. It was mistakenly thought that this might result in an unstable controller. The outer STR was immediately de-activated and the Dahlin controller took over for selectivity control. In fact there is no problem with zero's of controller being outside unit circle. It is the pole, if being outside the unit circle, that will give stability problems.

After two sampling intervals, the $S_3$ was still maintained at a steady desired level and the $T_R$ and $u_{H2}/u_{C4}$ were reasonably constant, the outer STR was re-activated again at point E. The values of FLAM and $\xi$ were the same as the previous values of 0.95 and 1.0 respectively. $\sigma_0$ was re-initialized to $(6.19, -1.444, 0.2, 0.103)$ again. However there was a bug in the computer software so $\sigma_0$ could not be re-initialized and took the values of those left behind from the outer STR that was last used: $(88.3, 76.3, .078, .080)$. The ratios between these values were adequate.

Again for the first four sampling intervals the $S_3$ was still controlled by the Dahlin algorithm. When the outer STR became effective,
the controller parameters started to tune themselves and at the third sampling interval $a_0$ was observed to decrease drastically as in the previous case. Nevertheless, the gain of the controller remained at low values for the rest of the experimental run. Despite the fact that two consecutive setpoint changes in $S_3$ from 0.23 to 0.28 and then to 0.33 were made, the $S_3$ stayed at the same level and never moved closer to the new setpoints except for the first two sampling periods after each setpoint changes was made. In fact after the change in $S_3^{set}$ was introduced from 0.23 to 0.28, the outer STR had only called for the first two significant adjustments in $T_R^{set}$. The inner STR responded accordingly to lower the $T_R$ by calling for a change in $u_{H_2}/u_{C_4}$. Later on no appreciable setpoint changes in $T_R$ were requested by the outer STR and the reactor temperature remained on the setpoint value, thus requiring little adjustment in the feedratio.

Detailed analysis of the phenomenon has disclosed the following reason for this observed behaviour. A value of 1.0 was assigned to $\xi$ in this experimental run. We can see that $a_0$ decreases significantly from 6.0 to 1.0 at that point where the trouble seems to arise. This means that the gain was effectively reduced by six times as compared to the Dahlin algorithm. Since the controller was designed to minimize the performance index given by Equation (4.3.23)

$$\min_{T_R^{set}} \sum_{j+1}^{t} \left[ (S_3 - S_3^{set})^2 + \xi \lambda (T_R^{set})^2 \right]$$

that is minimizing a weighted sum of the variances of the output and input of the controller. For a step change in $S_3$ from 0.23 to 0.28 and then to 0.33, the variance of the output is of the magnitude of $(0.02)^2$
while the change in $T_{R}^{\text{set}}$ can be of two to three degrees Centigrade having a variance of about $(0.5)^{2}$. If we put $\xi$ as 1.0, the second term in the bracket of Equation (4.3.23) is about 600 times the first term. This implies that the controller was designed to minimize the variance in $T_{R}^{\text{set}}$ rather than in the propane selectivity. It explains why this controller ignored the variance in $S_{3}$ but tuned the outer STR in such a way so as to maintain the $T_{R}^{\text{set}}$ at a steady level. Obviously $\xi$ would have to be of the order of $10^{-3}$ to obtain a reasonable STR.

Later on at point F, the estimation portion of the regulator was turned off for the inner STR because the trace of $P$ matrix was observed to grow by a factor of $1/FLAM$ due to lack of information. Furthermore, the controller parameters were believed to be well-tuned and converged at this stage. The trace of $P$ matrix was then leveled off.
7. **SUMMARY AND CONCLUSION**

The main purpose of this research program was to determine the adequacy of conventional and adaptive multiloop cascade control on a pilot-plant fluidized bed involving an extremely non-linear complex chemical reaction. Three cascade control schemes were examined for temperature and selectivity control:

Control Scheme 1: a fixed proportional integral (PI) controller on the inner temperature loop and a Dahlin algorithm for the outer loop selectivity controller.

Control Scheme 2: an adaptive self-tuning regulator (STR) on the inner loop and a Dahlin controller for the outer loop.

Control Scheme 3: a double STR scheme for both the inner temperature and outer selectivity loops.

The use of self-tuning and adaptive controllers were considered in order to overcome the following challenging problems associated with the control of the fluidized bed reactor:

1. **Asymmetric dynamics**: the time constants and gains depend upon the operating levels of $T_R - T_{oil}$ and the feedrate ratio.

2. **Time varying parameter**: the catalyst activity changes with time and the history of operation.

3. **Long measurement delay**: the chromatograph takes 360 s to analyze a sample.

Based upon the mechanistic model equations describing the mass and energy balances of the system, an existing simulation [4] was modified to include the dynamic effects of the disengaging section above the
fluidized bed which was modelled as a perfectly mixed vessel and to enable the investigation of the different control schemes of interest. Extensive simulation studies were carried out. The conventional cascade control system, consisting of a PI controller for the reaction temperature in the inner loop and Dahlin controller for the propane selectivity in the outer loop was improved by increasing the desired closed-loop time constant parameter, \( \lambda \), in the controller. The performance of the Dahlin algorithm with \( \lambda = 500 \text{ s} \) \( (\tau = 250 \text{ s}) \) was satisfactory in the simulation results over a wide range of propane selectivity changes and even when the reactor system was subject to a load disturbance. The acceptable range of operation of the controller has thus been greatly extended, by effectively detuning the Dahlin controller. The well-behaved detuned Dahlin was further verified in the experimental run. The tuning parameters for the PI controller, \( K_p = 1.03 \) and \( K_i = 0.34 \) were used at all times.

For control scheme 2 (with \( \lambda = 500, \tau = 250 \)) for the Dahlin algorithm, the inner STR was first implemented with the following design parameters in the simulation:

1. model structure \( m = l = 1 \)

2. discounting factor \( \text{FLAM} = 0.98 \)

3. constraining factor \( \xi = 0.5 \)

4. initial parameter estimates \( \theta = 0 \) for all parameters except for \( \theta_0 \) which was taken to be unity.

5. initial covariance matrix \( P_0 = 100 I \)

This cascade control scheme in the simulation runs provided
Adequate control when the system was subjected to the same range of propane selectivity changes and load disturbance.

Later, an actual reactor run was conducted using the same Dahlin controller while the STR has the following characteristics:

1. model structure \( m = 2 = 1 \)
2. discounting factor \( \text{FLAM} = 0.95 \) initially and 0.98 later afterwards
3. constraining factor \( \xi = 0.8 \)
4. initial parameter estimates \( \Theta = (1.840, -1.373, 1.333, -0.320) \) calculated from the PI tuning parameters
5. initial covariance matrix \( P_0 = 0.5 I \).

The control scheme 2 was found to provide effective control and was able to better handle the control problems (1) and (2) mentioned earlier.

The double STR control configuration for both the temperature and selectivity control, i.e. the control scheme 3, was used to better account for all the control problems mentioned above. It should be noted that this control scheme was only tentatively tested by the simulation.

The inner STR had the same simulation tuning parameters as described above. The outer STR had the model structure of \( m = 2 = 1 \) and the same initial parameters for the estimation algorithm except for the \( \Theta_0 \) parameters which were \( (6, 1.4, .2, .1) \). These values were calculated from the Dahlin algorithm and \( P_0 = 10 I \). The performance of the control scheme was found to be quite acceptable. Several unsuccessful attempts were made in the reaction runs. However, it is felt that the reasons for the failure were not a fault of the basic algorithm but of poor choice of parameters used in this implementation.
Based on the experience of implementing the STR on the temperature loop with the Dahlin controller on the outer selectivity loop in one case and a double STR on both loops in the other case, the conclusions concerning the practical considerations in using self-tuning regulators in this particular application can be summarized as follows:

1) **RLS Discounting Factor, FLAM**

The discounting factor, FLAM, in the exponentially discounted least squares algorithm was found to be very useful in the tracking of the parameters in time-varying processes. In this case, FLAM is set less than 1.0.

Starting off with a value of 0.95, FLAM was changed periodically on-line as follows: it should be increased when the parameters have nearly converged and decreased when known changes (for instance, in set point or in constraining factor \( \xi \)) are being made.

2) **Constraining Factor \( \xi \)**

The numerical value of \( \xi \) was found to be different in the experimental runs than in the simulation work. The appropriate value for \( \xi \) has to be tuned on-line. A judicious choice for the value of \( \xi \) in the outer STR requires further investigation and is recommended to be of the order of \( 10^{-3} \).

3) **Initial Choices of the Parameters \( \vartheta_0 \) and \( E_0 \)**

The initial estimates \( \vartheta_0 \) were based on the tuning parameters of the PI controller in the case of inner STR and those of Dahlin controller in the case of outer STR. With this prior knowledge, small values for \( E_0 \) were adequate for slow but smooth updating of the controller para-
meters. Bearing in mind the difference in the magnitude of the parameters \( \theta : (6.19, -1.444, 0.2, 0.103) \) in the outer STR, the initial estimates \( P_0 \) should be scaled accordingly. If not, poor control performance results.

(4) Deterministic Disturbances

The major disturbances to the inner (temperature) loop and the outer (selectivity) loop were the measurement white noise and deterministic step disturbances in the form of setpoint changes. The disturbances must be frequent enough to excite the system so that the \( P \) matrix does not become excessively large due to lack of information. The sum of the diagonal elements of the \( P \) matrix (trace) which is proportional to the average variance of the controller parameter estimates was found to grow by a factor of \( 1/\sigma^2 \) between setpoint changes. It decreased instantaneously as a piece of new information had come in. In this application, it is advisable to implement the STR to allow tuning of the controller over the periods when setpoint changes are introduced. As soon as the controller parameters have converged, the estimation portion of the regulator can be turned off when no major new disturbances are entering the system.

7.1 Future Work

The simulation and experimental studies in this thesis gave not only satisfactory results but also offered some insight into the control of the fluidized bed reactor. However there are a number of areas that require further investigation and these will be discussed as follows:

1. The double STR control configuration should provide a fruitful area of investigation by decreasing the value of \( \xi \) and supplying appropriate \( P_0 \) values.
2. An obvious extension of the univariate STR is to multivariate STR to account for process interactions. A rather straightforward extension of the STR concept was proposed by Borisson [27]. However for the multivariable STR, a large number of parameters has to be identified. Unless some model reduction techniques are applied, this extension appears too cumbersome to use.

3. The on-line measurement of the product gas compositions via the gas chromatograph with an analysis cycle of 360 s is in fact too slow for a direct feedback control scheme. Some predictions of the exit conversion and product selections in between the sampling intervals are necessary. Some form of inferential control based on complex multivariable models of the reactor (see, for example, references [28], [15] and [29]) should provide better and more effective control of the fluidized bed reactor system.
REFERENCES


### NOMENCLATURE

#### Section 3.3

- **$A_c$**  
  area for heat transfer between oil in heating/cooling coil and wall, $m^2$

- **$A_w$**  
  area for heat transfer between catalyst bed and wall, $m^2$

- **$C$**  
  concentration, $mg \, mol/m^3$

- **$C_{PB}$**  
  heat capacity of catalyst particles, $J/(kg \, K)$

- **$C_{pg}$**  
  average molal heat capacity of gas, $J/(kg \, mol \, K)$

- **$C_{p oil}$**  
  heat capacity of oil, $J/(kg \, K)$

- **$C_{pw}$**  
  effective heat capacity of wall, $J/(kg \, K)$

- **$d_b$**  
  bubble diameter, $m$

- **$d_p$**  
  average particle diameter, $m$

- **$F$**  
  = 0.9, fraction of n-butane that reacts to form propane

- **$g$**  
  acceleration due to gravity, $m/s^2$

- **$H$**  
  height of bed at fluidization conditions, $m$

- **$\Delta H_j$**  
  heat of reaction of the jth reaction, $kJ/Kg \, mol$

- **$h_c$**  
  effective heat transfer coefficient between oil and wall, $J/(s \cdot m^2 \cdot K)$

- **$h_w$**  
  effective heat transfer coefficient between catalyst bed and wall, $J/(s \cdot m^2 \cdot K)$

- **$M_w$**  
  mass of reactor wall, $kg$

- **$n_o$**  
  number of holes in perforated plate per unit area, $m^{-2}$

- **$N$**  
  number of bubbles per unit volume of bed, $m^{-3}$

- **$Q$**  
  transfer rate, $m^3/(s \cdot bubble)$

- **$Q_{loss}$**  
  heat loss from the wall, $J/s$

- **$R$**  
  gas law constant, $m^3 \cdot Pa/(kg \, mol \cdot K)$

- **$r_i$**  
  rate of reaction of a component, $kg \, mol/s$

- **$R_j$**  
  rate of reaction of a component, $kg \, mol/s$
S  cross sectional area of bed, m²
S  surface area of bubble, m²
 t  time, s
T  temperature, K

Subscripts for T:
oil,in  oil entering heating/cooling coil
oil,out oil exiting heating/cooling coil
R  reactor catalyst bed
oil  average bulk temperature of oil in heating/cooling coil
w  reactor wall
ub  bubble rise velocity, m/s²
umf  superficial velocity at minimum fluidization, m/s
V  = SH, bed volume under fluidizing conditions, m³
Vb  average bubble volume, m³
ve  volume of emulsion phase, m³
Vo  total volumetric flowrate of inlet gas, m³/s
W  weight of catalyst, kg
w_oil  mass flowrate of oil in heating/cooling circulating system, kg/s

Greek Letters:
ε  bed void fraction, dimensionless
ρ_g  average molal density of gas, kg mol/m³
ρ_p  average particle density, kg/m³
Subscripts:

b       bubble phase

\( e \)       emulsion phase

\( o \)       feed

Section 4.3

\( A(z^{-1}) \) denominator of process dynamic transfer function (4.3.1)

\( a_t \)       random shock

\( \beta(z^{-1}) \) numerator of process dynamic transfer function (4.3.1)

\( b \)       number of whole periods of delay

\( C(z^{-1}) \) polynomial \( \beta \) in \( z^{-1} \)

\( d \)       order of the pole lying on unit circle of disturbance model (4.3.2)

\( E() \)       mathematical expectation operator

\( FLAM \) forgetting factor for discounted least squares (4.3.21)

\( K_t \)       weighting vector for recursive least squares (4.3.10)

\( \zeta \)       order of \( \beta(z^{-1}) \)

\( m \)       order of \( \alpha(z^{-1}) \)

\( N_t \)       disturbance affecting process output (4.3.3)

\( (p, d, q) \) orders of polynomials in disturbance model

\( P \)       weighting matrix for recursive least squares

\( t \)       time

\( U \)       manipulated variable or process inputs (mean corrected)

\( Y \)       controlled variable or process output (setpoint corrected)

\( z \)       feedforward variable

\( z^{-1} \)       backward shift operator

\( \alpha(z^{-1}) \) numerator of controller transfer function

\( \beta(z^{-1}) \) denominator of controller transfer function
$\varepsilon_{t+b}$  b step ahead forecast error (4.3.6)

$\Theta_t$  vector of controller parameters to be estimated

$\Theta(z^{-1})$  moving average term in disturbance model (4.3.2)

$\phi(z^{-1})$  autoregressive term in disturbance model (4.3.2)

$\phi_t$  objective function for constrained control

$\delta(z^{-1})$  denominator of process dynamic transfer function (4.3.2)

$\xi, \xi', \xi''$  constraining weights

$\omega(z^{-1})$  numerator in process transfer function (4.3.2)

$\mathcal{V}$  difference operator ($1 - z^{-1}$)

Superscripts:

- estimate of the particular value
APPENDICES

A. Calibration Procedures
B. Illustration
C. Computer Program Listings
A.2.1 Calibration Procedure for the Flow System

A.2.1.1 n-butane flowrate

A wet-test meter was used to calibrate the flowrates of n-butane which ranged from .0045 m³/min (.15 s.c.f.m.) to .02 m³/min (.70 s.c.f.m.) for a total volumetric feedrate of .1 m³/min at S.T.P. when the ratio was constrained between 4 and 20. The zero and span on the butane ΔP transmitter was adjusted so that approximately 2 to 9.5 volts were produced respectively, across the dropping resistor on the output of the transmitter. At a supplying pressure of 239.2 kPa (20 p.s.i.g.) and a backpressure of 128.9 kPa (4 p.s.i.g.) on the rotameter, the calibration curve for the rotameter is shown in Figure A.2.1. A straight line fit to the calibration data in Figure A.2.2 gave the n-butane calibration equation for minicomputer software:

\[( u_{C_4} )^2 = -0.6233 + 0.15876 \times ( \text{ADC units}) \]

where \( u_{C_4} \) was in s.c.f.m.

and ADC units are 0-4095 computer units corresponding to 0-10 volts at the A/D input.

A.2.1.2 hydrogen flowrate

The flowrates of hydrogen ranged from .08 m³/min (2.8 s.c.f.m.) to .095 m³/min (3.34 s.c.f.m.) for the same total volumetric feedrate of .1 m³/min at S.T.P. and the ratio being constrained between 4 and 20. Since these are high flowrates, nitrogen and a precision nozzle (Cox Instruments) was used and the results were corrected for hydrogen. The
Figure A.2.1 Rotameter Calibration for n-butane Flow

Figure A.2.2 Computer Calibration Plot for n-butane Flow
zero and span on the ΔP transmitter was again adjusted to produce approximately 2 to 9.5 volts respectively across the dropping resistor.

At a supplying pressure of 211.6 kPa (16 p.s.i.g.) and a back-pressure of 128.9 kPa (4 p.s.i.g.) on the rotameter, the rotameter calibration curve is shown in Figure A.2.3. The straight line fit to the calibration data in Figure A.2.4 gave the hydrogen calibration equation:

\[(u_{H_2})^2 = -6.1101489 + 3.1037964 \times \text{(ADC units)}\]

where \(u_{H_2}\) was in s.c.f.m.
Figure A.2.3 Rotameter Calibration for Hydrogen Flow

Figure A.2.4 Computer Calibration Plot for Hydrogen Flow
A.2.2 The Beckman Model 6700 Gas Chromatograph

A.2.2.1 Settings of component boards in the programmer

The settings of the component boards used for the experimental study reported in Chapter 6 were as follows:

<table>
<thead>
<tr>
<th>Component</th>
<th>C₁</th>
<th>C₂</th>
<th>C₃</th>
<th>C₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time On</td>
<td>212</td>
<td>300</td>
<td>39</td>
<td>90</td>
</tr>
<tr>
<td>Time Off</td>
<td>279</td>
<td>348</td>
<td>74</td>
<td>195</td>
</tr>
<tr>
<td>X₁ range</td>
<td>OFF</td>
<td>ON</td>
<td>OFF</td>
<td>OFF</td>
</tr>
<tr>
<td>X₁₀ range</td>
<td>OFF</td>
<td>OFF</td>
<td>ON</td>
<td>ON</td>
</tr>
<tr>
<td>Auto zero</td>
<td>OFF</td>
<td>OFF</td>
<td>OFF</td>
<td>OFF</td>
</tr>
<tr>
<td>Function polarity</td>
<td>OFF</td>
<td>OFF</td>
<td>OFF</td>
<td>OFF</td>
</tr>
<tr>
<td>Switches reverse</td>
<td>ON</td>
<td>ON</td>
<td>ON</td>
<td>ON</td>
</tr>
<tr>
<td>hi/lo</td>
<td>LO</td>
<td>LO</td>
<td>LO</td>
<td>LO</td>
</tr>
<tr>
<td>Memory</td>
<td>6</td>
<td>5</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>Select</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
A.2.2.2 Procedure for preparation of a calibration sample

The procedures for preparing a calibration mixture is as follows:

1. Vent bottle with 'BOTTLE VENT'
2. Close all 'A' valves (i.e. hydrogen, butane etc)
3. Ensure 'VACUUM TO ATMOSPHERE' and 'VACUUM SOURCE' are closed
4. Turn on vacuum pump and slowly open 'VACUUM SOURCE' until the vacuum is \(131\text{ mm Hg}\) on left leg of Hg manometer.
5. Start adding gases
   a) butane
      - crack cylinder, pressure = 20 p.s.i.g.
      - open main butane valve on packed bed front panel
      - quickly vent butane supply line by opening 'SUPPLY VENT'
      - add butane by opening 'A' valve for butane
      - close butane valve on front panel
   b) propane
      - crack cylinder, pressure = 30 p.s.i.g.
      - vent line with 'SUPPLY VENT' toggle
      - add desired amount by opening 'A' valve for propane
   c) ethane
      - same procedure as (b), but pressure = 48 p.s.i.g.
   d) methane
      - same procedure as (b), but pressure = 30 p.s.i.g.
   e) hydrogen
      - same procedure as (a)
6. Shut off all cylinders. Vent supply lines with 'VENT'
A.2.3 Calibration curves for different components

The calibration procedure for the gas chromatograph can be found

4. The calibration data used to fit the calibration equation for
methane, ethane, propane and butane are shown in Figures A.2.5, A.2.6,
A.2.7 and A.2.8 respectively. The straight line fit to the data gave
the calibration equation for each of the components:

\[
X_{C_1} = -1.2230 + 0.1633e^{-3} \times \text{ (ADC units) }
\]

\[
X_{C_2} = -7.1312e^{-2} + 0.89712e^{-5} \times \text{ (ADC units) }
\]

\[
X_{C_3} = -4.5635e^{-2} + 0.70969e^{-5} \times \text{ (ADC units) }
\]

\[
X_{C_4} = -4.4743e^{-1} + 0.55301e^{-4} \times \text{ (ADC units) }
\]

where \( X \) is the absolute mole fraction of the component in the sample.
Figure A.2.7 Computer Calibration Plot for Propane Composition
Figure A.2.8 Computer Calibration Plot for Butane Composition
B.4.1 To Compute the Structure of Constrained STR for Reaction Temperature Control in Inner Loop

From Equation (4.3.17), the term

\[ N_{t+1} = \frac{1 - \theta z^{-1}}{1 - z^{-1}} a_{t+1} \]  

(B.4.1)

can be represented by the one step ahead forecast and the forecast error as in Equation (4.3.4)

\[ \frac{1 - \theta z^{-1}}{1 - z^{-1}} a_{t+1} = \psi(z^{-1}) a_{t+1} + \frac{T(z^{-1})}{1 - z^{-1}} a_t \]  

(B.4.2)

\[ \psi(z^{-1}) \text{ and } T(z^{-1}) \] can be found by equating the coefficients on left-hand-side and right-hand-side of Equation (B.4.2)

\[ 1 - \theta z^{-1} = 1(1 - z^{-1}) + T(z^{-1}) z^{-1} \]

\[ 1 - \theta z^{-1} = 1 - z^{-1} + (1 - \theta) z^{-1} \]

\[ \psi(z^{-1}) = 1 \]

\[ T(z^{-1}) = 1 - \theta \]  

(B.4.3)

(B.4.4)

The Equation (B.4.2) becomes

\[ \frac{1 - \theta z^{-1}}{1 - z^{-1}} a_{t+1} = a_{t+1} + \frac{1 - \theta}{1 - z^{-1}} a_t \]  

(B.4.5)

Substituting Equation (B.4.5) into Equation (4.3.17) yields

\[ Y_{t+1} = \frac{\omega_0}{1 - \delta z^{-1}} u_t + a_{t+1} + \frac{1 - \theta}{1 - z^{-1}} a_t \]  

(B.4.6)

The minimum variance controller can be derived by minimizing \( E(Y_{t+1}^2) \).
Taking expectation of the square of Equation (B.4.6) gives
\[
E(Y_{t+1}^2) = E\left\{ \frac{\omega_0 U_t + \frac{1 - \theta}{1 - z^{-1}} a_t}{1 - \delta z^{-1}} \right\} + E(a_{t+1})^2 +
2 E\left\{ \frac{\omega_0 U_t + \frac{a_t}{1 - z^{-1}}(a_{t+1})}{1 - \delta z^{-1}} \right\} \tag{B.4.7}
\]

The third term on the right-hand-side of Equation (B.4.7) is equal to zero, thus Equation (B.4.7) becomes
\[
E(Y_{t+1}^2) = E\left\{ \frac{\omega_0 U_t + \frac{1 - \theta}{1 - z^{-1}} a_t}{1 - \delta z^{-1}} \right\} + E(a_{t+1})^2 \tag{B.4.8}
\]

\[E(Y_{t+1}^2)\] can be minimized by setting
\[
\frac{\omega_0}{1 - \delta z^{-1}} U_t = \frac{1 - \theta}{1 - z^{-1}} a_t \tag{B.4.9}
\]

Thus
\[
\nu U_t = \frac{(1 - \delta z^{-1})(1 - \theta)}{\omega_0} a_t \tag{B.4.10}
\]

where \(\nu U_t = U_t - U_{t-1}\)

Under this controller, \(Y_{t+1} = a_{t+1}\) or \(Y_t = a_t\). Substitute \(a_t\) into Equation (B.4.10) gives
\[
\nu U_t = \frac{(1 - \delta z^{-1})(1 - \theta)}{\omega_0} a_t \tag{B.4.11}
\]

By Equation (4.3.15) Clarke and Gawthrop [20] constrained STR will be of
the form

$$\mathcal{V}U_t = \frac{(1 - \delta z^{-1})(1 - \theta)}{\omega_0 + \frac{\xi}{\omega_0}(1 - \delta z^{-1})} \mathcal{V}_t$$

(B.4.12)

The controller thus has the structure

$$B_0 \mathcal{V}U_t = B_1 VU_{t-1} + \alpha_0 y_t + \alpha_1 y_{t-1}$$

(B.4.13)
C.3.1 Program Listing of Module HOLD01 : TYPE 8

SUBROUTINE TYPE 8
COMMON/CON/IG, KLOOP, NCOMP, NC5, DELT, ME, TIME(30), NS, NPR, TOLL, TOLU,
+ EMAX, NPOL, TMAX, NCOUNT, JM, KJ, MPR, NGIM
COMMON/MAT/MP(20,6), EP(20,5), S(2,500,20), EX(100)
COMMON/UNIT/IM, NMP
COMMON/PRED/S1, S2, S3, CON
REAL MW(5)
DIMENSION Y(10), X(5), DY(10)
DATA MW/58., 44., 30., 16., 2.7/

REACTOR DISENGAGING SECTION MODULE
WRITTEN DEC 07, 80; SH YANG
PERFECTLY MIXED TANK

INITIAL CONCENTRATIONS IN THE DISENGAGING SECTION TAKE THE VALUE OF THE CONC OF THE GAS LEAVING THE REACTION SECTION OBTAINED AFTER THE FIRST PREDICTOR STEP

INFORMATION STREAM LIST
1 STREAM NO
2 FLAG
3 TOTAL FLOW
4 TEMP DES C
5 NAME THE STREAMS AND INFORMATION

IN=MPI(MP, 3)
IOUT=MTABS(MP(MP, 4))
T=S(SIG, IN, 4)-EP(IM, 2)

DETERMINE VOLUMETRIC FLOW RATE IN
AMOLE = TOTAL # MOLES IN
QIN = VOLUMETRIC FLOW RATE IN

AMOLE=0.
DO 10 I=1, 5
II=I+5
AMOLE=AMOLE+S(SIG, IN, II)/MW(I)
QIN=AMOLE*22.4

DETERMINE VOLUMETRIC FLOW RATE OUT
QO=QIN*(TO+273.2)/273/S(SIG, IN, 5)

DETERMINE MASS HOLD-UP OF EACH COMPONENT IN THE VOLUME ON CORRECTOR STEP
INDEX=MPI(MP, NMP+1)
IF(SIG.EQ.1) GO TO 21
DO 20 I=1, 5
II=I+5
INDEX+II-1=S(SIG, IN, II)*EP(IM, 1)/QIN
20 EX=INDEX+II-1=S(SIG, IN, II)*EP(IM, 1)/QIN

DO 30 I=1, 5
Y(I)=EX(INDEX+(SIG-1)*S+I-1)
DO 40 I=1, 5
II=I+5
40 DY(I)=S(SIG, IN, II)-QO*Y(I)/EP(IM, 1)

CARRY OUT INTEGRATION VIA FUNCTION Y1
DO 50 I=1, 5
II=I+5
FILLING IN OUTLET STREAMS

50 CONTINUE

CHECK IF SAMPLING STREAM IS NECESSARY

IF(MP(I,i)GE 0) GO TO 500

SET UP SAMPLING STREAM

OUT =ABS(HP(I,i))

CALCULATE SELECTIVITY

S(I,i) = S(I,i-1) + I(i,i-1)/HM(I)

DO 70 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

70 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

DO 90 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

90 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

DO 100 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

100 S(I,i) = S(I,i)*OUT(I,i)*0.25*XI(I,i)

END
C.3.2 Program Listing of KACT1

PROGRAM KACT1(INPUT,OUTPUT,KXIOU,KXOOU,TAPE5=KXIOU,TAPE6=OUTPUT,TAPE3=KXOOU)

DIMENSION Y(75),TH(1),DIFF(1),SIGNS(1),SCRAT(250)

DIMENSION XY(25,40)

EXTERNAL MODEL

COMMON/NFLOW(25),T(25),FEED(5,9),NR

DATA NPROB,MTA/1,1/

DATA NR,IOBS/3,9/

DATA TH/5.3/

DATA EPSI,EPS2/0.1,1.E-3/

DATA MTI,FLAM,FNU/15.,1.10.1/

DATA DIFF,SIGNS/01,1.1/

REWR 3

REWR 5

I=1,1.IOBS

READ(5,107)I1,I2,I3

WRITE(3,107)I1,I2,I3

READ(5,106)XI(J),J=1,8

WRITE(3,108)XI(J),J=1,8

READ(5,106)TI(J),J=9,16

WRITE(3,108)TI(J),J=9,16

READ(5,108)HI(J),J=17,23

WRITE(3,108)HI(J),J=17,23

READ(5,108)YI(J),J=24,30

WRITE(3,108)YI(J),J=24,30

TF=XY(I,16)+273.1

CS=SCM=XY(I,18)

SCF=XY(I,19)

FL=SCF*TF/273.1

TR=XY(I,20)

F=TR*9.8532

FEED(1,1)=0.

FEED(2,1)=0.

FEED(3,1)=0.

FEED(4,1)=0.

FEED(5,1)=P-FEED(4,1)

CONTINUE

FORMAT(1X,3I4)

FORMAT(1X,3F9.2)

FORMAT(1X,3F6.0,16F7.2)

READ S3 AND CONVERSION DATA

DO 501 I=1,1.IOBS

READ(5,510)IM1,IM2,IM3

WRITE(3,510)IM1,IM2,IM3

READ(5,510)S1,S2,S3,CONV

WRITE(3,511)S1,S2,S3,CONV

XY(I,31)=S2

XY(I,32)=S3

XY(I,33)=CONV

READ(5,511)X1,X2,X3,X4

WRITE(3,511)X1,X2,X3,X4

Y(I-1)=S2

Y(I-1)=S3
Y(3*I) = CONV
501 CONTINUE
510 FORMAT(1X,3I5)
511 FORMAT(1X,4F10.5)
502 CONTINUE

WRITE XY MATRIX
WRITE(6,220)
WRITE(3,220)
220 FORMAT(3X,'T',5X,'H2SCFM',4X,'C4SCFM',4X,'FLOW',6X,'TR',8X,
+ 'PC4',6X,'PH2',6X,'S2',6X,'S3',6X,'CONV'/)
DO 505 I=1,I0BS
505 WRITE(6,515) I, (XY(I,J), J=17,18), FLOW(I), T(I), FEED(4,I), FEED(5,I),
+ (XY(I,J), J=31,33)
WRITE(6,515) I, (XY(I,J), J=17,18), FLOW(I), T(I), (FEED(J,I), J=4,5),
+ (XY(I,J), J=31,33)
515 FORMAT(1X,4F10.5)
I0BS=I0BS+NR
CALL UWHAUS(NPROB,MODEL,NOB,TH,DIF,SIGNS,EPS1,EPS2,MIT,FLAM
+ FNU,SCRAT)
STOP
END

SUBROUTINE MODEL(NPROB,TH,YPRED,NOB,NP)
INTEGER P
DIMENSION A(13), OUT(5)
DIMENSION TH(NP), YPRED(NOB)
COMMON/AFLOW(25), T(25), FEED(5, 9), NR
A(1)=5.1E04
A(2)=4.0E04
A(3)=3.0E04
A(4)=1.6E04
A(5)=1.5E04
A(6)=1.0E04
A(7)=1.2E02
A(8)=6.0E1
A(9)=-2.5E05
A(10)=-2.0753
A(11)=-2.0E04
A(12)=4.5200
A(13)=-2.2115
A(14)=1.0E0
A(15)=1.0E0
A(16)=1.0E0
A(17)=1.0E0
A(18)=1.0E0
A(19)=1.0E0
H0=47.6
XFA=0.426
GRAV=9.800
DBMAX=1.0
UMF=0.77
HN=20.0
RHCH=0.957
DP=0.015
I0BS=N0B/NR
DO 500 I=1,I0BS
U = FLOW(I)*1.46042
TEMP = (T(I)-32.)*(5./9.) + 273.1
UEMUL = UMF
HMF = H0*1.043
DO = 0.3261*(UUEMUL)*HN**0.4
G1 = 1.0
UX = U/G1
HDBMAX = (DBMAX-DD)*UMF/(1.4*RHOS*DP*U)
DBMEAN = DBMAX - 0.9

HT = HMF*1.1*0 + (U-UEMUL)/(0.711*SQRT(980.*DBMEAN))
DBSAVE = DBMEAN
DBMEAN = ((DBMAX-DD)*0.5*HDBMAX + DBMAX*(HT-HDBMAX))/HT

IF(ABS(DBSAVE=DBMEAN).GT.0.0001)GO TO 2
Q = XFACT*11.0/DBMEAN
X = Q*HT/10.711*SQRT(GRAV*DBMEAN)
N=2 = 0
MSW = 1
TOL = 0.000001
RTT = 1.99*TEMP
FAC = (1.0-0.557)/(1.0-0.449)
RK=TH(1)*FAC*A(5)*EXP(-A(1)/RTT)
RK2=TH(1)*FAC*A(6)*EXP(-A(2)/RTT)
RKE=A(7)*EXP(-A(3)/RTT)
RKE=A(8)*EXP(-A(4)/RTT)
EXPX = EXP(X)
GAM = (U*(1.0-INDEXUMUL/U)/EXPX))/0.06*TEMP*HMF
P5 = FEED(5,I)

REACTION KINETICS FOR EMULSION WHERE THE ONLY REACTION OCCURS

Y2 = P5**A(9)
P2 = (FEED(4,I)*GAM)/(GAM + RK*Y2)
RB = RKBP42*Y2
Z1 = 0.9*R8
Z3 = RKP1*P5**A(10)
P3 = (Z1+FEED(3,I)*GAM*(1.0+RKP2))/(Z3+GAM*(1.0+RKP2))
RP2 = (Z1+3*P32)/(1.0+RKP2)
Z4 = RKE2*P5**A(13)
P22 = (1.1*RB-RP2+1.0+RKE)*GAM*FEED(2,I)/(Z4*(1.0+RKE)*GAM)
RE2 = (1.1*RB-RP2-Z4*P22)/(1.0+RKE)
P12 = (4.0*RB-3.0*RKP-2.0*RE2)/GAM
P5 = (FEED(5,I)*GAM - 3.0*R8 + 2.0*RKP2 + RE2)/GAM
SEARCH SO THAT GUESSED H2 WILL BE THE SAME AS THE CALCULATED H2
PDIF = P5

IF(NH2.EQ.2) GO TO 703
IF(PDIFF.LE.0.0) GO TO 700
MSW = 2
PRT = P5
P5 = P5 - 0.10
DIFF = PDIFF
IF(P5.GE.0.0) GO TO 800
P5 = 0.0001
IF(NH2.EQ.0) GO TO 701
P5 = 0.0001
PRINT = -999
GO TO 704

701 NH2 = 1
GOTO 800
700 IF(NSH.EQ.1) WRITE(6,996) IPRINT,P5,P5,P2,PDIF,PLT=P5
DIFF=PDIF
NSH=2
GO TO 750

703 IF(ABS(PDIFF).LT.TOL) GO TO 704
IF(ABS(PDIFF).LT.(ABS(DIFF)+0.1*ABS(PDIFF))/LT. ABS(DIFF)) GO TO 710
WRITE(6,996) IPRINT,P5,P5,P2,PLT,PRT,PDIF,DIFF

710 IF(PLT.GT.P5) GO TO 730
IF(PRT = P5
DIFF = PDIF
GO TO 750
PRT = PLT
DIFR = DIFL
PLT = P5
DIFL = PDIF
GO TO 750
730 IF(PRT.LT.P5) GO TO 735
PLT = P5
DIF = PDIF
GO TO 750
735 PLT = PRT
DIFL = DIFR
PRT = P5
DIFR = PDIF
750 PLT = DIFL*(PRT-PLT)/(DIFR-DIFL)
GOTO 800

C

704 PB1 = P12 + (FEED(1,I)-P12)/EXPX
PB2 = P22 + (FEED(2,I)-P22)/EXPX
PB3 = P32 + (FEED(3,I)-P32)/EXPX
PB4 = P42 + (FEED(4,I)-P42)/EXPX
PB5 = P52 + (FEED(5,I)-P52)/EXPX
F1 = UEMUL/U
F2 = (U-UEMUL)/U
OUT(1)=F1*PB2+PB1*F2
OUT(2)=F1*PB2+PB2*F2
OUT(3)=F1*PB3+PB3*F2
OUT(4)=F1*PB4+PB4*F2
OUT(5)=F1*PB5+PB5*F2.

380 IF(FEED(4,I).EQ.0) GO TO 390
F=FEED(4,I)
DD=FEED(4,I)-OUT(4)
S1=OUT(3)/DD
S2=OUT(2)/DD
GOTO 410
390 IF(FEED(3,I).EQ.0) GO TO 400
F=FEED(3,I)
DD=FEED(3,I)-OUT(3)
S3=0.
S2=OUT(2)/DD
GOTO 410
400 F=FEED(2,I)
DD=FEED(2,I)-OUT(2)
S3=0.
S2=0.
410 CONV=100.*DD/F
S1=OUT(1)/DD
EMULH2=P52
YPRED(3*I-2)=S2
YPRED(3*I-1)=S3
YPRED(3*I)=CONV

500 CONTINUE

996 FORMAT(1X, 40HNEGATIVE ON FIRST STEP OF SEARCH FOR P52, 5X,I3,3F14.4)
999 FORMAT(1X, 45H THE ORCUTT SEARCH MAY BLOW UP FOR IPRINT = ,I4, RETURN)
END
C.5.1 Program Listing of DASTFF?

PROGRAM DASTFF2 (INPUT, OUTPUT, DATA, 0235, TAPE5=DATA, TAPE6=OUTPUT
1, TAPE3=0235) *
***
DIMENSION G(6, 6), G2(6, 6)
DIMENSION VS10(10), VS10(10), ZS10(10), P(6, 6), THETA(10), PHI(10)
DIMENSION VS12(10), VS12(10), ZS12(10), PHI2(10)
DIMENSION YTP(100), YUTP(100), Y2TP(100), YU2TP(100)
DIMENSION AC(12), CC(12)
DIMENSION VS3(1200)
COMMON/PRED/S1, S2, S3, CON
COMMON/HAT/HI(20, 8), EP(20, 5), S(2, 50, 20), EX(100)
COMMON/AREA4/IFLAG
***
REAL NT, NT
DATA THETA, THETA2/10*0.9, 6, 1.4, 2, 1.6*0.9 /
DATA NP, NP2/2*6 /
DATA IC, IP/0, 0 /
DATA NT1/0 /
DATA K1, K2, KL, K2L/2*100, 2*10 /
DATA KNT/0 /
DATA B0, RAD, RA1, RA2, RB1, BA1, BA2, BB/1*0.5 /
DATA B20, R2A1, R2A2, R2B1, B2A1, B2A2, B2B/6*0.5 /
C
MAIN PROGRAM TO SIMULATE RESPONSE FROM REACTION TEMP
TO RATIO OF HYDROGEN TO N-BUTANE FEEDRATES
NSTEP IS THE NUMBER OF INTEGRATION STEPS REQUIRED
REWIND 5
PRINT *, "ENTER NSTEP"
READ, NSTEP
PRINT *, "NOISE TO BE ADDED?"
READ, NOIZ
PRINT *, "INNER TEMP CONTROLLER TO BE ACTIVATED?"
READ, I1
PRINT *, "INNER STR TO BE ACTIVATED?"
READ, I1
IF (I1 .NE. 1) GO TO 5
PRINT *, "ENTER NA, NB & NC"
READ, NA, NB, NC
PRINT *, "ENTER FLAM, ZETA, AETA"
READ, FLAM, ZETA, AETA
I1 = 1
NP = NA + NB + NC
INITIALIZING COVARIANCE MATRIX TO ZERO
DO 19 IR = 1, NP
DO 19 IJ = 1, NP
P(IJ) = 0
19 CONTINUE
INITIALIZING THETA, PHI VECTORS TO ZERO, P DIAGONAL ELEMENTS TO 100.
DO 29 IR = 1, NP
PHI(IR) = 0
P(IR, IR) = 100.
29 CONTINUE
THETA(NA + 1) = 1.
INITIALIZING VS10 & VS10 TO ZERO
DO 39 IR=1,10
US10(IR)=0.
YS10(IR)=0.
39 CONTINUE

5 PRINT*,'OUTER LOOP ACTIVATED? -- 1.DAHLIN 2.STR-
READ*,IOP
IF(IOP.GE.2)GO TO 10
PRINT*,'ENTER NA2, NB2 & NC2'
READ*,NA2,NB2,NC2
PRINT*,'ENTER FLAM2, ZETA2 & AETA2'
READ*,FLAM2,ZETA2,AETA2
PRINT*,'ENTER I82'
READ*,I82
NP2=NA2+NB2+NC2
DO 219 IR=1,NP2
DO 219 J=1,NP2
P2(IR,J)=0.
219 CONTINUE
DO 229 IR=1,NP2
PHI2(IR)=0.
P2(IR,IR)=1.
IF(IR.GT.NA2)P2(IR,IR)=1.
229 CONTINUE
THETA2(NA2+1)=.2
DO 239 IR=1,10
US102(IR)=0.
YS102(IR)=0.
239 CONTINUE

10 NOELT=30
C INFORM SUBROUTINE MODEL1 THAT A NEW INTEGRATION HAS BEEN INITI-
IFLAG=0
C DEFINE INITIAL TR TW AND TOIL
TR1=253.
TM1=249.1
TOIL1=247.1
C DEFINE DESIRED TOTAL VOL FLOWRATE TO REACTOR
SCFM=3.5
C DEFINE VECTOR OF INPUTS, TFEED AND TOILIN
TFEED1=253.
TFEED2=TFEED1
TOILIN1=247.
C DEFINE VECTOR OF DESIRED S3 SETPOINTS
S3SET=.1

****
CREATE VECTORS OF ERRORS FOR OBSERVED RESPONSES
AM=0.
SD1=.1
SD2=.1
SD3=.002
DEFINE THE FIRST 25 TR SETPOINTS WHICH WILL BE USED FOR THE INF LOOP UNTIL THE S3 CONTROLLER TAKES OVER

TRSET=253.

IF(IT1 .EQ. 0) GO TO 1100

INITIALIZE PAST ERROR FOR TR-RATIO CONTROLLER

E2=0.

SET TR - RATIO PI PARAMETERS

C1=1.03
C2=0.34

DEFINE INITIAL FEED FLOWS FOR INTEGRATION STEP, UNTIL TR RATIO CONTROLLER TAKES OVER

1100 RATIO1=10.29
C4SCFM1=SCFM/(RATIO1+1.)
C4SCFM2=C4SCFM1
H2SCFM1=SCFM-C4SCFM1
H2SCFM2=H2SCFM1

U=RATIO1
USSP=RATIO1

IF(ITOP .EQ. 0) GO TO 1900

SET DAHLIN'S PARAMETERS

EK=.022
T=66.0
TAU=2.65
ELAMBD=5.00
A1=1.-EXP(-T/ELAMBD)
A2=EXP(-T/TAU)
A3=EXP(1.-EXP(-T/TAU))

INITIALIZE PAST ERRORS FOR S3 CONTROLLER

ERR2=0.
TR2=253.
TR3=253.

PROCEED WITH NSTEP-1 INTEGRATIONS, APPLYING CONTROL ACTION AFTER EACH STEP

1900 NUMB=NSTEP-1
DO 2000 I=1,NUMB

DEFINE CURRENT AND ONE STEP AHEAD INPUTS
2 IS CURRENT TIME, 1 IS ONE STEP AHEAD

TOILIN2=TOILIN1
IF(I .GT. 252)TOILIN1=242.

INTEGRATE MODULES OVER ONE TIME INTERVAL

CALL MODEL1(TR1,TH1,TOIL1,TFEED1,TFEED2,TOILIN1,TOILIN2,
1H2SCFM1,H2SCFM2,C4SCFM1,C4SCFM2,TRP,TWP,TOILP)
ADD NORMALLY DISTRIBUTED ERROR TO RESPONSES

* * *
IF(NOIZ EQ 0) GO TO 2010

CALL GAUSS(13231, SD1, AM, ER1)
NT=NT+1+ER1
TRP=TRP+ER1
CT1=NT
CALL GAUSS(137, SD2, AM, ER2)
TWP=TWP+ER2
CALL GAUSS(1331, SD2, AM, ER3)
TOILP=TOILP+ER3
CALL GAUSS(1234567, SD3, AM, ER4)
S3=S3+ER4

C

STORE THE PREDICTIONS IN THE APPROPRIATE PREDICTION VECTORS

2010 VS3(I)=S3

* * *

C

TAKE CONTROL ACTION

* * *

C

DAHLMIN'S ALGORITHM ON OUTER S3 LOOP

TEST IF THE 12TH TR-RATIO CONTROL ACTION IS COMING UP. IF IT IS
NEW S3 DATA ARE AVAILABLE AND AN S3 CONTROL ACTION IS REQUIRED

IF(IOPO EQ 0) GO TO 120

IF(I) LT 25) GO TO 124
IF(I) LT 30) S3SET=32
IF(I) LT 11) GO TO 120
IC=IC+1
IP=1
IF(IP EQ 1) GO TO 1126
Y2=VS3(I-12)
U2=TRP
USPP2=TRP
YSP12=S3SET
YSP12=YSP12

1125 YSPM2=AETA2*YSPM12+(1-AETA2)YSP12

1126 CONTINUE
IF(I) GT 30) S3SET=25
IF(I) GT 50) S3SET=32
IF(I) GT 130) S3SET=36
IF(I) GT 190) S3SET=40
IF(IOPEQ 1) GO TO 2020

YSP2=S3SET
ZSP2=YSP2*YSP12
IF(NC2 EQ 0) YSPM2=YSP2

1129 IF(I) LT MP2) GO TO 1129
CALL UYINCR12, YSPM2, Z2, US102, VS102, ZS102
CALL FORMPHI12, YS102(I+102), US102(I+102), ZS102(I+102), MA2, N82, MP2

1129* OBFN2=YS102(I)+ZETA2*US102(I+1IB2)
DO 11 J=1,NP2
   P2(J,3)=0.
   P2(J,3)=0.
11 CONTINUE

   CALL RLS(OBFCN2,P2,PHI2,THETA2,FLAM2,NP2)
   IF(N2A.EQ.2) R2A1=-THETA2/(2)/THETA2(1)
   R2A0=THETA2(NA2+1)
   R2A1=THETA2(1)/R20
   R20=THETA2(NA2+2)/R20
   IF(NA2.NE.31) GO TO 92
   R2A2=THETA2(3)/R20
   DISC2=R2A1*R2A1-4*R2A0*R2A2
   IF(DISC2.LT.0.) GO TO 72
   TWO REAL ROOTS
   R21=-5*(-R2A1*SQRT(DIS C2))
   B2A1=SQRT(R21*R21)
   R22=-5*(-R2A1-SQRT(DIS C2))
   B2A2=SQRT(R22*R22)
   GO TO 92

72 DISC2=SQRT(DIS C2*DIS C2)
   B2A1=5*(SQRT(R2A1*R2A1+DISC2))
   B2A2=B2A1
   92 B29=THETA2(NA2+2)/R20

   CALL MD(P2,6,NP2,DET2,IDET2,G2)
   PRINT 1072,I,(P2(J,J),J=1,6),DET2,IDET2

82 CALL FORM(PHI2,YS102(1),US102(1),ZS102(1),NA2,NB2,NC2,NP2)

   PRINT*,"KNT",",KNT,DU2TP(KNT)
1127 USP2=U2
   YSP12=YSP2
   YSPM12=YSPM2
   TR1=U2
   IF(TR1.LT.250.) TR1=250.
   GO TO 128
1129 CALL UYINCR(Y2,YSPM2,Z2,US102,YS102,ZS102)
   YSP12=YSP2
   YSPM12=YSPM2
2020 ERR1=SSSET-YS3(I-12)
   TR1=(A1/A3)*ERR1-2*ERR2 + (1.-A1)*TR2 + A1*TR3
   IF(TR1.LT.250.) TR1=250.

C: UPDATE FOR NEXT CONTROL ACTION
   ERR2=ERR1
   TR3=TR2
   TR2=TR1

128 CONTINUE

   IF IST=1, IMPLEMENT S.T.R.
   IF(IST.NE.1) GO TO 130
Y = Y2P
IF (I .GT. 1) GO TO 125
YSP1 = TRSET
YSPH1 = YSP1
125 YSPM = ETA * YSPH1 + (1 - ETA) * YSP1
IF (IP .EQ. 1) GO TO 126
YSP = TRSET
Z = YSP - YSP1
GO TO 127
126 CONTINUE
YSP = TR1
Z = YSP - YSP1
127 CONTINUE
**** IF (NC .EQ. 0) YSPM = YSP
****

IF (I .LT. NP) GO TO 129
CALL UYINCR (Y, YSPM, Z, US10, YS10, ZS10)
CALL FORM (PHI, YS10(1 + IB), US10(1 + IB), ZS10(1 + IB), NA, NB, NC, NP)
OBFCN = YS10(1 + IB) * ETA * US10(1 + IB)
CALL RLS (OBFCN, P, PHI, THETA, FLAM, NP)

IF (NA .EQ. 2) BAI = -THETA(2)/THETA(1)
BI = THETA(NA + 1)
RA1 = THETA(1)/BI
RA2 = THETA(2)/BI
RA1 = THETA(NA + 2)/BI
IF (NA .NE. 3) GO TO 9
RA2 = THETA(3)/BI
DISC = RA1 * RA1 - 4 * RA1 * RA2
IF (DISC .LT. 0.) GO TO 7
TWO REAL ROOTS
R1 = .5 * (-RA1 + SQRT(DISC))
BA1 = SQRT(R1) - R1
B1 = .5 * (-RA1 - SQRT(DISC))
BA2 = SQRT(R2) - R2
GO TO 9
IMAGINARY ROOT
COMPUTE MAGNITUDE
DISC = SQRT(DISC * DISC)
BA1 = .5 * (SQRT(RA1 + RA1 + DISC))
BA2 = BA1
9 BI = -THETA(NA + 2)/BI
IREM = MOD (I, 10)
IF (IREM .NE. 0) GO TO 8
CALL M0D (P, NP, DET, IDET, G)
PRINT 107, I, (P(J, J), J = 1, G), DET, IDET
8 CALL FORM (PHI, YS10(1), US10(1), ZS10(1), NA, NB, NC, NP)
CALL STRC1 (U, USSP, THE1A, PHI, NP, NA)
US10(1) = U - USSP
81 USSP = U
YSP1 = YSP
YSPH1 = YSPM
PRINT 109, I, Y, U, US10(1), (THETA(J), J = 1, NP), (PHI(J), J = 1, NP)
RATIO1 = U
GO TO 562
129 CALL UXINCR(Y, YSPM, Z, US10, HS10, ZS10)
YSP1=YS
YSPM1=YS
C TR-RATIO CONTROLLER
C IF IP=0, 3 CONTROL HAS NOT TAKEN ITS FIRST CONTROL ACTION
C SO USE PREVIOUSLY SUPPLIED STARTING TR SETPOINTS
130 IF(IT1 .EQ. 0) GO TO 562
***  IF(IP .EQ. 1) GO TO 540
E1=TRSET-TRP
***  IF(E1 .LT. 4.0) GO TO 542
E1=-E1
TRSET=TRP+4.
542 E1=-E1
GO TO 560
540 E1=TR1-TRP
***  IF(E1.LT.4.0) GO TO 546
E1=-E1
546 E1=-E1
560 CONTINUE
RATIO1=RATIO1 + C1*(E1-E2 + C2*E1)
C BASED ON THIS NEW RATIO, SET C4 AND H2 FEEDRATES, SCFM
562 IF(RATIO1 .LE. 4.) RATIO1=4.
IF(RATIO1 .GE. 20.) RATIO1=20.
C4SCFM1=SCFM/(RATIO1+1.)
C4SCFM2=C4SCFM1
H2SCFM1=SCFM-C4SCFM1
H2SCFM2=H2SCFM1
C UPDATE FOR NEXT CONTROL INTERVAL
IF(IT1 .EQ. 0) GO TO 590
E2=E1
C RECORD NEW RATIO, C4SCFM AND H2SCFM FOR LATER PLOTTING
C INCREMENT COUNTER FOR S3 LOOP
IC=IC+1
C IF S3 LOOP HAS TAKEN OVER SETTING TRSET, RECORD THESE FOR LATER OUTPUT
IF(IP .EQ. 0) GO TO 590
TRSET=TR1
590 CONTINUE
C
C ************************************************************
C END OF CONTROL ACTION
TO CHANGE CATALYST ACTIVITY

IF(I .GT. 50)EP(1,2)=-9997476*EP(1,2)
IF(I .GT. 1150)EP(1,2)=5.25

J=J+1
F=I
WRITE(3,108)I,TRP,TWP,TOILP,S3,
ICON,RATIO,TOILIN1,
+RSET,S3SET,EP(1,2)
WRITE(3,1088)(THETA(K),K=1,4),BB,BA1,
+(THETA2(K),K=1,4),B2B,B2A1

1234 CONTINUE
2000 CONTINUE

 THIS IS THE END OF NSTEP-1 INTEGRATIONS, OUTPUT TO LINE
PRINTER AND DISC

WRITE(6,110)
110 FORMAT(72X,'I',3X,'TR',4X,'TH',4X,'TOIL',3X,'S1',3X,'S2',
+3X,'COM',3X,'C4',3X,'H2',1X,'RATIO',1X,'TOILIN1',
+1X,'TRSET',1X,'S3SET',1X,'A0',2X,'A1',2X,'B0',2X,
+2X,'B1',7X)

TIME=0.

TIME=TIME+DEL
J=J+1
WRITE(6,108)I,TRP,TWP,TOILP,VS3(I),
ICON,RATIO,TOILIN1,
+RSET,S3SET,EP(1,2)
WRITE(6,1088)(THETA(K),K=1,4),BB,BA1,
+(THETA2(K),K=1,4),B2B,B2A1

107 FORMAT(1X,I4,7F10.3,'E',I4)
108 FORMAT(1X,I4,6E10.3,'E',I4)
109 FORMAT(1X,12F5.2)

999 STOP
END

SUBROUTINE UYINCR(Y,YSPP,Z,US10,YS10,ZS10)
DIMENSION US10(10),YS10(10),ZS10(10)
DO 9 J=1,9
I=11-J
US10(I)=US10(I-1)
YS10(I)=YS10(I-1)
ZS10(I)=ZS10(I-1)
9 CONTINUE
US10(1)=0.0
YS10(1)=(Y-YSPP)
ZS10(1)=Z
RETURN
END

SUBROUTINE FORM(X,YS10,US10,ZS10,NA,NB,NC,NP)
DIMENSION YS10(NA),US10(NB),ZS10(NC),X(NP)
X(NP)=1.0
DO 9 I=1,NA
   X(I)=YS10(I)
9 CONTINUE
DO 19 I=1,MB
   X(NA+I)=US10(I)
19 CONTINUE
DO 29 I=1,NC
   X(NA+NB+I)=ZS10(I)
29 CONTINUE
RETURN
END
SUBROUTINE STRCL(U,USSP,THETA,X,NP,NA)
   DIMENSION X(NP),THETA(NP)
   SUM=0.
   DO 19 I=1,NP
      SUM=SUM+X(I)*THETA(I)
19 CONTINUE
   U=USSP-SUM/THETA(NA+1)
   RETURN
END
SUBROUTINE RLS(YP,PHI,THETA,FL,NP)
   DIMENSION P(6,6),PHI(NP),THETA(NP),S(10)
   REAL K(10)
   SUM=0.
   DO 9 I=1,NP
      SUM=SUM+PHI(I)*PHI(J)*P(I,J)
9 CONTINUE
   DEN=SUM+FL
   ERRS=0.
   DO 19 I=1,NP
      SUM=0.
      DO 29 J=1,NP
         SUM=SUM+P(I,J)*PHI(J)
      29 CONTINUE
      S(I)=SUM
      K(I)=SUM/DEN
      ERRS=ERRS+PHI(I)*THETA(I)
19 CONTINUE
   ERRS=Y-ERRS
   DO 5 I=1,NP
      DO 4 J=1,NP
         P(I,J)=(P(I,J)-S(I)*S(J)/DEN)/FL.
4 CONTINUE
   THETA(I)=THETA(I)+K(I)*ERRS
5 CONTINUE
RETURN
END
SUBROUTINE CRCORR(X,Y,CC,SDX,SDY,N,NL)
   DIMENSION X(N),Y(N),CC(I)
   SX = 0.
   SY = 0.
   SXX = 0.
   SYY = 0.
   DO 2 I=1,N
      SX = SX+X(I)
      SY = SY+Y(I)
      SXX = SXX+X(I)*X(I)
      SYY = SYY+Y(I)*Y(I)
2 CONTINUE
   TN = N
   SDX = SQRT((SXX-SX**2/TN)/TN)
   SDY = SQRT((SYY-SY**2/TN)/TN)
   NL1 = NL+1
   DO 3 K=1,NL1
      SXY = 0.
3 CONTINUE
RETURN
END
NN = N-K+1
DO 4 I=1,NN
4  SXY = SXY+(X(I)-SX/TN)*(Y(KK)-SY/TN)
KK = I+K-1
3  CC(K) = (SXY/TN)/(SDX*SDY)
RETURN
END
SUBROUTINE ACORR(Z, AC, SDZ, N, NL)
DIMENSION Z(1), AC(I)
NL1 = NL+1
TN = N
SZ = 0
DO 13 I=1, N
SZ = SZ+Z(I)
ZBAR = SZ/TN
DO 10 JJ=1, NL1
J = JJ-1
SZZ = 0.
NN = N-J
DO 11 I=1, NN
11  SZZ = SZZ+Z(I)-ZBAR)*(Z(I+J)-ZBAR)
10  AC(JJ) = SZZ/TN
SDZ = SQRT(AC(I))
WZ = AC(I)
DO 12 J=1, NL
12  AC(J) = AC(J+1)/WZ
RETURN
END
C.5.2 Program Listing of STPLT2

PROGRAM STPLT2(INPUT, OUTPUT, 0236, TAPE3=0236, TAPE6=OUTPUT)

COMMON XY(400, 23)
COMMON XYOLIN, XDMIN, XMAX, YDMIN, YMAX
COMMON PLTSpec, IPEN, XLEN, YLEN, XOFF, YOFF

RESTART 3

ENTER PARTICULARS
PRINT*, "ENTER NSTEP"
READ*, NSTEP
NEQ=NSTEP-1
DELT=0

PRINT*, "INNER STR PARAMETERS?"
READ*, IST
IF(IST .NE. 1) GO TO 11
PRINT*, "ENTER NA, NB"
READ*, NA, NB

11 PRINT*, "OUTER STR PARAMETERS?"
READ*, IOST
IF(IOST .NE. 1) GO TO 21
PRINT*, "ENTER N2A, N2B"
READ*, N2A, N2B

READ AND VERIFY DATA

21 WRITE(6, 110)
+"B1", 3X)
DO 105 I=1, NOB
READ(3, 108)(XY(I, J), J=1, 11)
F=I
XY(I, 1)=F
105 READ(3, 108)(XY(I, J), J=12, 23)
WRITE(6, 109)(XY(I, J), J=1, 11)
WRITE(6, 108)(XY(I, J), J=12, 23)

109 FORMAT(1X, F4.0, 10F9.3)
108 FORMAT(1X, 12F5.2)

START PRINTING ROUTINES

PLOT 7. RATIO,

IPEN=3
XMIN=XY(1,1)
XMAX=241
YMIN=4
YMAX=20
XOFF=2.5
XLEN=7.5
YOFF=1.25
YLEN=1.5

CALL FRME
CALL XTIIC(20, 0)
CALL XTIIC(4, 0)
CALL XTIC(4.***08)
CALL YTIC(2.***05)
CALL SPLT(1,7,N0B)

PLOT 5.S3, 10.S3SET
YDMIN=0.1
YDMAX=0.5
YOFF=2.875
YLEN=1.

CALL FRME
CALL XTIC(20.***08)
CALL XTIC(4.***05)
CALL YTIC(.1,***05)

CALL CPLT(1,5,N0B)
CALL DPLT(1,10,N0B)

PLOT 6.CONV
YDMIN=.2
YDMAX=.6
YOFF=4.
YLEN=1.

CALL FRME
CALL XTIC(20.***08)
CALL XTIC(4.***05)
CALL YTIC(.1,***05)

CALL CPLT(1,6,N0B)

PLOT 2.TR, 4.TOIL, 9.TRSET, 11.TOILSP
YDMAX=260.
YDMIN=240.

YLEN=1.875
YOFF=5.125
CALL FRME
CALL XTIC(20.***08)
CALL XTIC(4.***05)
CALL YTIC(10.***08)
CALL YTIC(5.***05)
CALL CPLT(1,2,N0B)
CALL CPLT(1,4,N0B)
CALL DPLT(1,9,N0B)

CALL PLOT(12,0,**-3)

PLOT INNER STR PARAMETER ESTIMATES

IF(IST .LT. 1) GO TO 900
YDMIN=-4.
YDMAX=4.
YLEN=1.85
YOFF=5.2
CALL PARPLT(1,12,13,N0B)

YOFF=3.225
YDMIN=-4.0
YDMAX=4.0
CALL PARPLT(1,14,15,N0B)

YOFF=1.25
YDMIN=-2.0
YDMAX=2.0
CALL PARPLT(1,16,17,N0B)
CALL UNITTO(XY(1,1),1.,X1P,ZE)
CALL UNITTO(XY(NOB,1),1.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)
CALL UNITTO(XY(1,1),-1.,X1P,ZE)
CALL UNITTO(XY(NOB,1),-1.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)

CALL PLOT(12.,0.,-3)

PLOT OUTER STR PARAMETER ESTIMATES

900 IF(IOST .NE. 1) GO TO 999
YDMIN=-7.0
YDMAX=7.0
YLEN=1.85
YOFF=5.2
CALL PARPLT(1,18,19,N0B)
CALL UNITTO(XY(1,1),0.,X1P,ZE)
CALL UNITTO(XY(NOB,1),0.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)

YOFF=3.225
YDMIN=-2.0
YDMAX=2.0
CALL PARPLT(1,20,21,N0B)
CALL UNITTO(XY(1,1),0.,X1P,ZE)
CALL UNITTO(XY(NOB,1),0.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)

YOFF=1.25
YDMIN=-4.0
YDMAX=4.0
CALL PARPLT(1,22,23,N0B)
CALL UNITTO(XY(1,1),0.,X1P,ZE)
CALL UNITTO(XY(NOB,1),0.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)
CALL UNITTO(XY(1,1),1.,X1P,ZE)
CALL UNITTO(XY(NOB,1),1.,X2P,ZE)
CALL DASH(X1P,ZE,X2P,ZE,1)

CALL PLOT(12.,0.,-3)

END ALL PLOTTING

999 CALL PLOT(0.,0.,999)
STOP
END

SUBROUTINES
SUBROUTINE FRME
COMMON/XYDLM/XDMIN,XDMAX,YDMIN,YDMAX
COMMON/PLTSPEC/IPEN,XLEN,YLEN,XOFF,YOFF
CALL NEWPEN(4)
XSCALE=(XDMAX-XDMIN)/XLEN
YSCALE=(YDMAX-YDMIN)/YLEN
XORG=XDMIN-XOFF*XSCALE
YORG=YDMIN-YOFF*YSCALE
XMIN=XORG
YMIN=YORG
XMAX=XDMAX+3.
YMAX=YDMAX+3.
CALL PLTN(XSCALE,YSCALE,XORG,YORG,XMIN,XMAX,YMIN,YMAX)
CALL FRAME
CALL NEWPEN(2)
RETURN
END

SUBROUTINE CPLT(ITH,IJ,NOB)
CONTINUOUS CURVE
COMMON XY(400,23)
COMMON/XYDLM/XDMIN,XDMAX,YDMIN,YDMAX
COMMON/PLTSPEC/IPEN,XLEN,YLEN,XOFF,YOFF
MOVE PEN TO FIRST DATA POINT, PEN UP
CALL PLOTT(XY1,ITH),XY1(IJ),3)
CALL NEWPEN(IPEN)
J=25
DO 63 I=1,NOB
IF(I .NE. 2 .AND. IJ .NE. 5) GO TO 63
IF(I .NE. J) GO TO 63
J=J+12
CALL UNITTO(XY(I,ITH),XY(I,IJ),XC,YC)
CALL GRAF(XC,YC,.08,11)
63 CALL PLOTT(XY(I,ITH),XY(I,IJ),2)
RETURN
END

SUBROUTINE DPLOT(ITH,IJ,NOB)
DOTTED CURVE
COMMON XY(400,23)
COMMON/XYDLM/XDMIN,XDMAX,YDMIN,YDMAX
COMMON/PLTSPEC/IPEN,XLEN,YLEN,XOFF,YOFF
DO 64 I=1,NOB
IF(I .LT. 25) GO TO 63
CALL UNITTO(XY(I,ITH),XY(I,IJ),XC,YC)
CALL GRAF(XC,YC,.08,11)
63 CALL PLOTT(XY(I,ITH),XY(I,IJ),3)
64 CALL NEWPEN(4)
CALL PLOTT(XY(I,ITH),XY(I,IJ),2)
RETURN
END

SUBROUTINE GPlot(ITH,IJ,IS3,CODE)
CALL SUBROUTINE GRAF
COMMON XY(400,23)
COMMON/XYDLM/XDMIN,XDMAX,YDMIN,YDMAX
COMMON/PLTSPEC/IPEN,XLEN,YLEN,XOFF,YOFF
J=25
DO 67 I=1,IS3
IF(I .NE. J) GO TO 67
J=J+12
CALL UNITTO(XY(I,ITH),XY(I,IJ),XC,YC)
CALL GRAF(XC,YC,.08,CODE)
67
CONTINUE
RETURN
END
SUBROUTINE SPOINT(IHM, IJ, NOB)
ZERO HOLD CURVE
COMMON XY(400, 23)
COMMON/XYOLIM, KDMIN, KMAX, YDMIN, YMAX
COMMON/PLTSPEC/IPEN, XLEN, YLEN, XOFF, YOFF
CALL PLOTT(XY(1, IHM), XY(I, IJ), 3)
J=25
DO 72 I=2, NOB
IF(I .NE. J) GO TO 71
J=J+12
CALL UNITTO(XY(I, IHM), XY(I-1, IJ), XC, YC)
CALL GRAP(XC, YC, -08, 1)
CALL PLOTT(XY(I, IHM), XY(I-1, IJ), 2)
CALL PLOTT(XY(I, IHM), XY(I, IJ), 2)
RETURN
END
SUBROUTINE PARPLT(IHM, MA, NA, NOB)
COMMON XY(400, 23)
COMMON/XYOLIM, KDMIN, KMAX, YDMIN, YMAX
COMMON/PLTSPEC/IPEN, XLEN, YLEN, XOFF, YOFF
CALL FRME
CALL XTC(20, 0)
CALL XTC(4, 05)
CALL YTC(1, 05)
CALL UNITTO(XY(I, 1), 0, X1P, ZE)
CALL UNITTO(XY(NO, 1), 0, X2P, ZE)
DO 10 I=MA, NA
IF(I .LT. 19) GO TO 8
CALL GLOM(IHM, I, NOB, I-MA+1)
CALL CLOM(IHM, I, NOB)
CONTINUE
RETURN
END
SUBROUTINE XTC(XINTVL, TICLEN)
COMMON/XYOLIM, KDMIN, KMAX, YDMIN, YMAX
COMMON/PLTSPEC/IPEN, XLEN, YLEN, XOFF, YOFF
NTICS=1(/KMAX-KDMIN)/XINTVL+.5+1
XD=XDMIN
YD=YDMIN
DO 20 I=1, NTICS
XD=XDMIN+FLOAT(I-1)*XINTVL
CALL UNITTO(XD, YD, XP, YP)
CALL PLOTT(XP, YP, 3)
CALL PLOTT(XP, YP+TICLEN, 2)
CALL PLOTT(XP, YP+YLEN, 3)
CALL PLOTT(XP, YLEN+YP+TICLEN, 2)
CONTINUE
RETURN
END
SUBROUTINE YTC(YINTVL, TICLEN)
COMMON/XYOLIM, KDMIN, KMAX, YDMIN, YMAX
COMMON/PLTSPEC/IPEN, XLEN, YLEN, XOFF
NTICS=1(/YMAX-YDMIN)/YINTVL+.5+1
XD=XDMIN
YD=YDMIN
DO 20 I=1, NTICS
YD=YDMIN+FLOAT(I-1)*YINTVL
CALL UNITTO(XD, YD, XP, YP)
CALL PLOTT(XP, YP, 3)
CALL PLOTT(XP, YP+TICLEN, 2)
CALL PLOT(XP+XLEN,YP,3)
CALL PLOT(XP+XLEN-10LEN,YP,2)
CONTINUE
RETURN
END
SUBROUTINE XTLAB(XINTVL,HEIGHT)
COMMON/XYDLM/XDMIN,XMAX,YDMIN,YMAX
NLABS=((XMAX-XDMIN)/XINTVL+.5)+1
YP=YDMIN
XO=XDMIN
CALL UNITTO(XO,YP,XP,YP)
YPP=YP-1.5*HEIGHT
DO 100 I=1,NLABS
XO=XDMIN+FLOAT(I-1)*XINTVL
CALL UNITTO(XO,YP,XP,YP)
XP=XP+(-.5*HEIGHT)
ENCODF(2,20,ICH)XD
CALL LETTER(1,HEIGHT,0.,XP,YPP,ICH)
100 CONTINUE
20 FORMAT(F2.0)
RETURN
END
SUBROUTINE YTLAB(YINTVL,HEIGHT)
COMMON/XYDLM/XDMIN,XMAX,YDMIN,YMAX
NLABS=((YMAX-YDMIN)/YINTVL+.5)+1
XD=YDMIN
YD=YDMIN
CALL UNITTO(XD,YP,XP,YP)
XPP=XP-1.5*HEIGHT
DO 100 I=1,NLABS
YD=YDMIN+FLOAT(I-1)*YINTVL
CALL UNITTO(XD,YD,XP,YP)
YP=YP+(-.5*HEIGHT)
ENCODF(2,20,ICH)YD
CALL LETTER(1,HEIGHT,0.,XPP,YP,ICH)
CONTINUE
20 FORMAT(F2.0)
RETURN
END
SUBROUTINE FRAME
COMMON/XYDLM/XDMIN,XMAX,YDMIN,YMAX
CALL PLOT(XDMIN,YMIN,3)
CALL PLOT(XMAX,YMIN,3)
CALL PLOT(XMAX,YMAX,2)
CALL PLOT(XMIN,YMAX,2)
CALL PLOT(XMIN,YDMIN,2)
RETURN
END
SUBROUTINE PLOT(XD,YD,N)
CALL UNITTO(XD,YD,XP,YP)
CALL PLOT(YP,N)
RETURN
END