REAL TIME COMPUTER DATA ACQUISITION AND CONTROL SYSTEMS: AN APPLICATION TO MODEL REFERENCE ADAPTIVE CONTROL OF A PACKED BED TUBULAR REACTOR

REAL TIME COMPUTER DATA ACQUISITION AND CONTROL SYSTEMS: AN APPLICATION TO MODEL REFERENCE ADAPTIVE CONTROL OF A PACKED BED TUBULAR REACTOR

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JEAN-PIERRE TREMBLAY, M. Eng.

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AUTHOR: Jean-Pierre Tremblay, M. Eng. (McMaster University)

SUPERVISORY COMMITTEE: DR. J.D. Wright, DR. T.W. Hoffman, DR. Della Torre.

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ABSTRACT

A pilot scale non-adiabatic packed bed reactor has been designed and constructed to carry out the hydrogenolysis of n-butane over a nickel on silica gel catalyst. The complex reaction scheme is highly exothermic and results in steep radial gradients within the reactor. The apparatus was interfaced to a minicomputer. A sophisticated executive program was developed to assist with on-line studies of the apparatus. It provided measurements of axial and radial reactor temperatures and composition data for the reactor effluent. A third order, discrete time state space model of the reactor was postulated from mechanistic arguments and the parameters fitted to dynamic data. The model served as the basis of a derivation of a model reference adaptive controller designed to satisfy Lyapunov's second theorem of stability. The control algorithm included terms for proportional, integral and setpoint actions. The objective of the controller was to regulate the reactor's production rate of intermediate reaction species. The control algorithm was implemented experimentally and its performance discussed. Problems with the controller are examined and recommendations made.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

1.1 Objectives of This Study

In his critique of chemical process control theory, Foss [1973] has suggested that improvements in the methodology for the design of multivariable control systems would result from developments in three areas: modelling, system configuration and adaptive systems.

Process models of low order form the basis of nearly all multivariable control strategies. The central role played by a dynamic model in the formulation of a control system accounts for the efforts spent in their development. Mechanistic forms are difficult to formulate properly because of poor understanding of a process' underlying mechanisms. As dynamic models become more sophisticated and consequently of greater order, it becomes increasingly difficult to achieve a reduction to a lower order form without the loss of essential dynamic characteristics. In contrast, statistical methods such as time series analysis assist in the identification of process transfer functions from process input/output data. The derivation of an empirical dynamic model is relatively simple and far less tedious when compared to the mechanistic approach. Model order reduction is not usually required since models produced in this manner must be parsimonious.

Economic considerations usually dictate the objectives of a

plant's control system. The configuration of the control system which is implemented to achieve these objectives is not easily determined. For instance, it is difficult to precisely know the effects of coupling between process inputs and outputs. Ideally, the strongest interactions should be used for control. Because it is usually not possible to manipulate the best inputs in the preferred way and often difficult to measure the best outputs accurately or frequently enough, compromise control system configurations must be examined. Since there exists no general criteria for determining the best combination of inputs and outputs which should be used, individual configurations must be studied. Discrimination is then by trial and error technique.

Finally, adaptation of model and controller parameters during load and setpoint changes can expand a system's operating region to cover a much wider range of operating conditions not possible otherwise. However, stable operation in an adaptive environment is difficult to ensure, particularly where a process exhibits time variant and non-linear behaviour.

This work is an attempt to encourage development in those areas singled out by Foss [1973], with particular attention given to their development in one branch of chemical engineering.

Chemical reaction systems of commercial interest are usually very complex and extremely difficult to model whether from fundamental mass and energy balances or by empirical methods. It is, therefore,

not surprising to discover that only a few investigations into the performance of modern multivariable control techniques have been reported for chemical reaction systems. Besides the usual modelling difficulties which accompany complex non-linear mass, energy and reaction processes, the model must be cast into a form which permits the application of modern multivariable control methods. Because such models always include numerous approximations, self-adjusting or adaptive methods which automatically compensate for these inherent model inaccuracies are worthy of experimental evaluation.

In a sampled data environment, problems arising from process data taken at non-uniform sampling rates have been difficult to handle. A specific example of this difficulty occurs when it is attempted to combine chromatographic data with the temperature and pressure data of a process. Typically, the refresh rate of the temperature and pressure data is one to two orders of magnitude greater than that of the chromatographic data. The discovery of a general method to effectively combine non-uniformly sampled data would make the application of modern multivariable control theories much more attractive.

The primary objectives of this study were threefold. Firstly, to arrive at a low order state space model of a heterogeneous packed bed pilot plant catalytic reactor which would be suitable for control purposes by using a combination of mechanistic and empirical arguments. The parameters of this model are to be fitted to actual pilot plant

dynamic data. Secondly, to resolve in a simple manner the problems related to the combination of non-uniformly sampled plant data for use by a multivariable controller. And thirdly, to evaluate experimentally the properties of a multivariable adaptive controller formulated according to a design technique based on Lyapunov's Second Theorem of stability. The reactor to be controlled would be complex enough to properly test the design method under reasonably adverse conditions.

Before any work related to the primary objectives could begin, it was first necessary to satisfy a few secondary objectives. A pilot plant reactor of adequate complexity had to be designed and constructed in order to conduct worthwhile experimental investigations. To this apparatus had to be interfaced a minicomputer system configured for data acquisition and control. Finally, an executive program for data acquisition and control had to be developed because none suitable for research applications was available for use on the Department's Data General Corp. minicomputers.

The scope of this project is considerable and is meant to explore the potential application of model reference adaptive control to chemical reactors. Several avenues for future studies potentially leading to significant improvements in adaptive control theory are major benefits resulting from this study.

1.2 Modelling Chemical Reactors for Process Control

During the last two decades and particularly with the more recent

development of minicomputer and microprocessor technology, it has become feasible to use digital computers for the simulation and control of chemical reactors. Despite the very powerful computational tools available at this time, most reactors are still modelled for control purposes by single variable transfer functions or steady state equations. The transfer functions derived from theoretical models or plant tests are used in the design of multiloop control systems. The sensitivity of a particular control system to parameter variations may be determined from Bode plots and Nyquist diagrams. Analysis of the control system results in a set of estimates of the controller gains. Of course, after a control system has been selected for use in a plant, in-plant tuning of the controller gains is generally required to account for initial model inaccuracies and the endless series of plant upsets. The steady state equations when fitted to plant data have largely been used to evaluate a reactor's day by day performance and to indicate the significant interactions among its inputs and outputs at a given operating level. Depending on prevailing market conditions for the products being produced, the reactor's operation would be altered to maximize profits or at least minimize losses. Transitions from one set of operating conditions to another would be based largely upon previous operating experience. Depending on the frequency of changes in operating conditions, dynamic models capable of assisting in the identification of optimal trajectories may also be developed to gain further economic advantage.

By their very nature, multiloop control systems cannot be designed to compensate for all interactions between reactor inputs and outputs. Compensation is normally provided for the major interactions but the quality of the control system relies heavily on the proper choice of controller gains. Multivariable models on the other hand do account to some degree for most input/output interactions. Therein lies the principle justification for the development of multivariable dynamic models and the application of multivariable control theory for packed bed chemical reactors (Foss [1973]). If the controller is equipped with an adaptive mechanism, greater advantages arise from the control system's ability to self compensate for known and unknown load changes or upsets (Unbehauen et al [1975]). Several approaches to the design of a multivariable control system are presently available and all may be readily implemented on digital computer systems equipped for data acquisition and control.

Jutan [1976] has determined that only a few investigators have reported attempts to apply modern multivariable control theory to packed bed chemical reactors. To date, results have been promising but much more research effort is needed before commercial applications can be considered. Work to date has typically involved only simple reaction systems: homogeneous and liquid phase reactions, isothermal or adiabatic configurations and linear reaction kinetics. Whatever the control design technique employed, no serious attemots have been made to incorporate analytical data into the final control schemes.

This deficiency is a direct result of the non-uniform sampling rates experienced when monitoring temperature, flowrate and composition data.

The primary objectives of this study have been explained in Section 1 and their justification is based on the above discussion. In order to fulfill these objectives, a multivariable dynamic model of a packed bed chemical reactor is required and two approaches at arriving at a suitable model will now be discussed. Adaptive control theory will be discussed in the following section.

As a design tool, the digital computer may be used to develop quite sophisticated multivariable models which simulate the dynamic behaviour of chemical reactors. The numerical methods which are inherent in the simulations lend themselves very well to real time sampled data systems. The complexity or sophistication of a model is then limited to one's ability to identify and describe quantitatively the underlying forces and processes of a chemical reactor. As most heterogeneous packed bed reactors are distributed parameter systems (Beck [1962]), a proper mechanistic model must comprise a set of non-linear highly coupled partial differential equations. Since these equations are often not useful for control in this form, simplifying assumptions must be made to render them tractable. Some approximations which result are quite reasonable in view of the physical properties of the system while others may result in partial loss of the dominant dynamic properties of the model. Another consequence of these simplifications is the loss of theoretical significance for the model parameters.

At some point, a decision must be made as to which approach to modelling -- empirical or mechanistic -- is most reasonable given that ultimately the model constitutes the basis of a multivariable controller. The essential question that must be answered has to do with the effort that must be expended to produce a model which serves the objectives of control. If one considers the mechanistic approach, a significant effort is required to formulate a comprehensive model of a reactor. Further efforts are often required to restructure it into a useful form for the application of modern control theory. Model parameters must then be estimated. Depending upon the situation, parameter estimation may become extremely complicated, so much so that the efforts of the estimation step exceed those of the modelling step. If further reduction of the fitted model is then contemplated, this effectively voids the validity of the original model formulation. On the other hand, an empirical model of appropriate dimensionality could produce the same result but with much less effort. The identification of meaningful models through the analysis of reactor input/output data is comparatively more efficient. In some cases, theoretical considerations may yield a model form which satisfies the control objectives and whose parameters may be estimated from process data. Since both empirical and mechanistic model parameters must be fitted to dynamic data, neither can be claimed to be better than the other in view of the end use.

Related to the problem of which modelling approach to use are the practical constraints on model dimensionality. Aside from the obvious

logistics problems which arise when dealing with complex models, one must consider the hardware limitations of digital computing systems.

In this study, an approach which involved a marriage of mechanistic and empirical modelling methods was employed to develop a multivariable dynamic model of a pilot scale n-butane hydrogenolysis reactor. Available detailed kinetic studies (Shaw [1974]) of the hydrogenolysis of n-butane provided significant a priori knowledge of the process. Using this information and a limited amount of pilot plant dynamic data, a reasonable form of a discrete time state space model of a pilot plant reactor could be postulated and the parameters estimated. The model states could be chosen to facilitate the formulation of a multivariable feedback controller.

The exercise of formulating a reactor model usually focuses much attention on simulating the reactor's dynamic behaviour correctly. This is obviously essential but some consideration must also be given to the manner by which measured process data is combined for use by a control algorithm. Because it is not uncommon to find that measured reactor outputs which are useful for control are not always measured at the same rate, some means of combining all useful information must be employed. The definition of dummy state variables in the reactor model could be used to account for missing information but this solution rapidly increases the order of the system under investigation. On the other hand, a state observer could be defined but the observer design

would have to account for the time-varying dimension of the measurement vector. Either of these approaches could be considered for on-line use but several practical aspects of the overall control problem preclude their use. The model order must be kept as small as possible to promote the stability of the model reference adaptive controller to be derived in Chapter 2. Dynamic adjustment of the measurement vector would be difficult to program and the momentary expansion and contraction of the measurement vector could introduce bumps into the state estimates.

Proper definition of the control objective can in some instances lead to another approach which is readily implemented provided that there is some insight into the properties of the reactor.

It is reasonable to assume that a usual objective of reactor control is the regulation of the production rate of one or more products in the reactor effluent. Given this premise, the states of a reactor dynamic model could then consist of an independent subset of these production rates. Because it is usually not possible to obtain reactor effluent composition data at a suitable rate, some means of estimating the states must be found. If the mass and energy equations for the reaction system are very complex, it still is often possible to find a simple correlation between the reactor model states and the reactant feed rates and reactor internal temperatures. The parameters of this state estimator may then be updated as new reactor effluent composition data becomes available. This approach was considered for the development

of a multivariable dynamic model of the n-butane hydrogenolysis reactor. The result was a model form well suited to the derivation of a model reference adaptive controller.

A detailed derivation of a discrete time state space model and state estimator for an n-butane hydrogenolysis packed bed reactor is discussed in Chapter 2. Details of the fitting of model parameters will be provided in Chapter 5.

1.3 Adaptive Algorithms for Process Control

Since it first appeared over a quarter century ago, adaptive control theory has been used extensively in the design of flight autopilots. It has also found use in the control of electrical drives and hydraulic servo-mechanisms and in a limited number of chemical engineering applications.

The general objective of adaptive control systems has essentially remained unchanged. In brief, the purpose of an adaptive system is to modify, subject to an index of performance the adjustable parameters of a process (for example, the gains of feedback controller) using information derived from the process itself.

Articles by Landau [1974] and Unbehauen and Schmid [1975] provide comprehensive reviews of the literature concerned with adaptive systems. Landau [1974] has attempted to define and classify the many facets of

model reference adaptive control systems according to their dominant characteristics. Design methods are also discussed with consideration given to the design particularities of the various system types. Unbehauen and Schmid [1975] have concerned themselves with presenting an overview of adaptive control techniques which have found use in the control of processes. Both review articles conclude with suggestions for future development. It is believed that present conditions will not foster wide use of the adaptive methods. Before significant industrial applications can be considered, new and very rapid algorithms are required and experimental confirmation of current and future design techniques must be provided. Because adaptive control schemes are relatively complex, digital computers must be used to implement them. Design methods must then be developed with some consideration given to the physical limitations imposed by the computer hardware.

Some experimental work dealing with adaptive control of chemical reaction systems has been reported. Typically, the systems being controlled have low order reaction kinetics and mathematical development of the control system has been with time as an independent and continuous variable. For instances where digital computers are used to implement the adaptive control algorithm, discretization occurs only after the pertinent continuous time equations have been derived. Often, the plant parameters being adjusted by the adaptive control algorithm are the gains of standard three term proportional-integral-derivative controllers.

For example, Schooley et al [1969] have successfully used a univariate adaptive controller on a batch rubber polymerization reactor. In this case, the controller was implemented on an analog computer. On-line optimization of a two variable control system has been used to control a water-gas shift reactor (Price et al [1967]). Ryan et al, [1971] have used a model reference adaptive controller to adjust the gains of a PI temperature controller for a first order reaction. An adaptive controller developed by the Lyapunov design technique has been used to control a rotary cement kiln. To the author's knowledge, no experimental investigations dealing with high order, non-linear chemical processes have been reported which test any of the adaptive control system design methods.

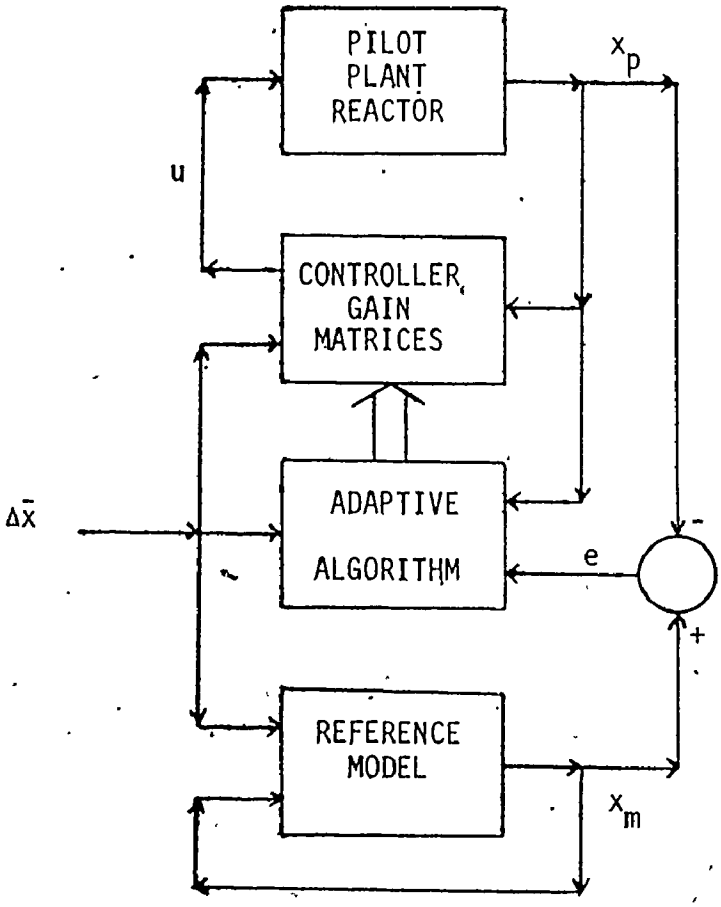
According to Landau [1974], adaptive control algorithms derived on the basis of a reference model enjoy an important advantage over other strategies because of their high speed of adaptation. The structure of a typical model reference adaptive control scheme is given in Figure 1-1. This type of system has a dual nature in that it may be used for control or parameter estimation. Since it is non-linear in nature, a model reference adaptive control system may be used on time variant, non-linear multivariable processes. Its structure has also promoted the development of "proportional-integral" adaptation, thereby providing the control law with a memory component.

In the past, model reference adaptive control systems have been

FIGURE 1-1

STRUCTURE OF A MODEL REFERENCE

ADAPTIVE CONTROLLER



designed on the basis of local parameter optimization. The objective of all local parameter optimization methods is to search for a set of parameter values which minimizes an index of performance used to measure the distance between a reference model and the process being controlled. Typical methods that have been used are the gradient and steepest descent optimization techniques.

Model reference adaptive control systems are by nature non-linear and for this reason, stability problems can arise. It is for this reason that current studies employ stability arguments for system design. Quite frequently, either one of two methods are employed. One method based on Lyapunov's second theorem of stability is used to assure the asymptotic stability of the difference between the states of the reference model and the process. A second method employs Popov's hyperstability criteria to provide asymptotic stability as well as bounded input/output properties (hyperstability) of the difference between the reference model and process states.

To the author's knowledge, only the Lyapunov design approach has been employed to derive a model reference adaptive controller for chemical engineering type systems. It has been mentioned that the method has been used successfully on a rotary cement kiln. The literature also contains an example of an evaporator (Oliver et al [1973]) which was controlled successfully by model reference adaptive control. However, no known references deal with the control of a noisy, unstable, highly

exothermic and non-linear packed bed reactor. In view of the fact that the Lyapunov design method had not been used to synthesize and implement a model reference adaptive controller for a complex reaction system, it was clear that an experimental investigation was required. As outlined in Section 1, a primary objective of this study was to evaluate experimentally the properties of a multivariable adaptive controller formulated according to a design technique based on Lyapunov's Second Theorem of stability. The reaction scheme employed in this study was considered to be sufficiently complex to adequately test any design method.

A methodology for the design of a multivariable model reference adaptive controller based on Lyapunov's second method has been advanced by Porter et al [1969]. Oliver et al [1973] have extended the design method to include both integral and setpoint action. In both cases, the derivations are in continuous time and as indicated previously, this may lead to unstable operation. To avoid this difficulty, the derivation of a model reference adaptive controller for this study was to be formulated entirely on a discrete time basis.

Certain difficulties were expected. Model reference adaptive control systems may be difficult to stabilize if the process exhibits non-minimum phase characteristics. Also, the stability of the control system may be jeopardized by a pseudo-inverse approximation called for in the calculation of the adaptive controller gains. The quantitative effect of these factors upon the ultimate stability of a model reference

adaptive controller was unknown and could not be determined beforehand. Since an objective of the study was to examine the properties of the adaptive controller under fairly reasonable adverse conditions, investigations were undertaken. The results of the experimental program will be presented in Chapter 5.

1.4 Experimental Considerations

The three secondary objectives mentioned earlier in Section 1 had to be satisfied before any of the primary objectives of this study could be undertaken. To begin, a pilot plant reactor had to be designed and constructed. It was desirable to have a reaction system which was complex and highly exothermic to contrast with the relatively simple systems on which the few reported works of applied reactor control have been done. The extensive kinetic studies by Shaw [1974] on the hydrogenolysis of n-butane over nickel catalyst made it reasonable to assume that the kinetics of this reaction were well known. Since this reaction exhibited the desired characteristics of complexity and high exothermicity, it was decided that a packed bed pilot scale reactor would be designed on the basis of the hydrogenolysis of n-butane reaction.

The experiments to be performed on the pilot scale reactor were sufficiently complex to warrant the use of an on-line minicomputer. This machine was interfaced to the reactor and could support both data acquisition and direct digital control applications. The pilot scale

reactor and the minicomputer system to which it is interfaced will be described in Chapter 3.

Finally, an executive program designed to support computer based research studies was developed for use on Data General Corp. minicomputers. Of the executive programs that were available at the time this work started, none was found to be compatible with Data General machines nor suited for use in an experimental environment. The executive program developed for this work is known by the acronym "GOSEX" and details of its structure will be provided in Chapter 4. However, the design basis of the program will be discussed at this time.

The design of a digital computer executive program is based on many philosophical decisions which are meant to satisfy the varied needs of the end user. For this reason, an executive program designed for batch operations cannot support real time applications such as data acquisition and process control. Similarly, a real time executive program designed for use in industrial applications will not lend itself very easily for use in a research environment.

All real time executive programs have several things in common. Time is the most precious resource and tasks related to it must be executed without delay. The executive program must be interactive and respond promptly to user requests. In an industrial environment, the system structure is fixed and consequently the executive program is designed according to fairly rigid guidelines. In a research environment

however, needs change frequently and in this case great flexibility must be designed into the executive program. The rigidity or flexibility of an executive program is directly related to the mechanisms that must be used to make changes when on and off line. Changes include the alteration of calculation parameters and algorithm reprogramming.

A number of systems houses are currently marketing computer based data acquisition and control systems which are tailored to industrial applications. The FOX 1 and FOX 2 by Foxboro, the DC^2 by Fisher, the MOD III by Taylor and the TDC by Honeywell are systems which incorporate a wide variety of features essential for real time control applications. None of the systems can be considered perfect by any means but typically, they provide the capability to alter control structures and software while on-line.

The applications software language is structured to permit pre-compilation prior to program execution. This reduces the amount of storage needed for application software and significantly reduces the amount of system overhead that would be required otherwise (Shave [1975]). The sophistication incorporated into these industrially oriented data acquisition and control systems is essential in a processing environment but is clearly not essential in a research environment. For this reason, the purchase of such a system for research applications cannot usually be justified economically.

Executive programs for data acquisition and control are generally designed around real time operating systems which have been developed and are maintained by computer manufacturers. The general design considerations that must be incorporated into a real time operating system have been discussed by Purser et al [1975] and Sorenson et al [1975]. With this basis, software houses are now offering data acquisition and control systems which are assembled with proven hardware components sold by major equipment vendors such as Digital Equipment Corp., Data General Corp., RTP Inc., EMC Inc. and others.

The executive programs in this instance are usually much simpler and can be tailored to satisfy many small industrial and long term research applications. In these cases, changes to any of the applications programs often must be made by the vendor, thereby forcing the end user to rely heavily on the competence of the vendor's field service staff.

In a research environment where requirements change frequently, it is essential that the end user have the capability of making source changes to the applications software without recourse to a vendor. In order that this can be possible, the executive program must support a high level language such as BASIC, FORTRAN IV or ALGOL. Normally, the end user edits, compiles, links and loads the executive and applications programs before on-line use. No provisions are made to permit on-line modification of the user software. Recently however, a small number of software houses have marketed executive programs that provide the capa-

bility to write BASIC type programs while on-line. For example, BCS by Metromation Inc. includes an on-line editor which accepts and stores instructions for interpretation by the system at run-time. This technique is inefficient since there is no pre-interpretation of the user coding (Shave [1975]).

At the time this project was begun, no reasonably priced or technically acceptable executive programs for data acquisition and control were available that were designed for use on Data General Corp. NOVA minicomputers. Since an executive program was required for experiments investigating the properties of a model reference adaptive controller, one which satisfied the projects requirements was developed. The executive program was written in assembler language and was based on Data General Corp.'s Real Time Disk Operating System (RDOS). It was designed to support applications program written in FORTRAN IV. An overlay facility was employed to minimize the effective size of the executive core requirements. Several executive functions were developed which gave the user on-line control over data output record formats and application programs. A facility to change program parameters while on-line was also provided. Complete details describing the on-line capabilities of the program will be provided in Chapter 4.

In Chapter 2 which follows, a low-order, discrete time, state space model is developed for an n-butane hydrogenolysis packed bed reactor. The model is used in the derivation of a model reference adaptive

controller designed according to a methodology based on Lyapunov's second theorem of stability.

A description of the pilot scale packed bed reactor apparatus and the process minicomputer to which it was interfaced will be given in Chapter 3. This apparatus was used to investigate the properties of the model reference adaptive controller derived in Chapter 2.

The capabilities and on-line operation of an executive program developed during this work to support experiments on the reactor apparatus will be provided in Chapter 4. The application of the model reference adaptive controller was greatly simplified because of its development.

Details of the experimental program which was conducted to fit model parameters and evaluate the properties of the model reference adaptive controller will be given in Chapter 5.

Finally, conclusions and recommendations regarding this and other work will be summarized in Chapter 6.

CHAPTER 2

MODELLING AND MODEL REFERENCE ADAPTIVE CONTROL OF THE BUTANE HYDROGENOLYSIS REACTOR

2.1 Introduction

It is impractical and perhaps even impossible to formulate a dynamic model of a packed bed catalytic reactor which accounts for all types of disturbances or time varying parameters which may affect the reactor's operation. Nevertheless, an unsteady state model which simulates the reactor's principal dynamic characteristics must be developed if modern model based multivariable control theories are to be applied. The continuous and discrete time linear state space models

$$\dot{x} = Ax + Bu \qquad (2\text{-}1)$$

$$x(k+1) = Ax(k) + Bu(k) \qquad (2\text{-}2)$$

x: state vector, n x 1
u: input vector; r x 1
A: transition matrix, n x n
B: control matrix, n x r

are used to represent the dynamics of a process about a steady state or operating level. The order of the system is specified by the dimension of the transition matrix A. When the model is to be used in a sampled data control environment, the form of Equation 2-2 must be used.

In on-line applications using digital computers, it is desirable that the model be of low order for two main reasons. Firstly, computational difficulties may be encountered when attempting model based control

with a high order model. These may include numerical instability, lack of central processor memory or simply extremely long calculation times. Any one of these can preclude the use of a model for on-line control calculations. Secondly, most workers find it conceptually very difficult to deal with models of very high dimensionality: model development, parameter estimation and even relating model parameters to physical variables become formidable tasks. For practical purposes, it would appear reasonable to consider a tenth order model as a feasible upper bound on model dimensionality.

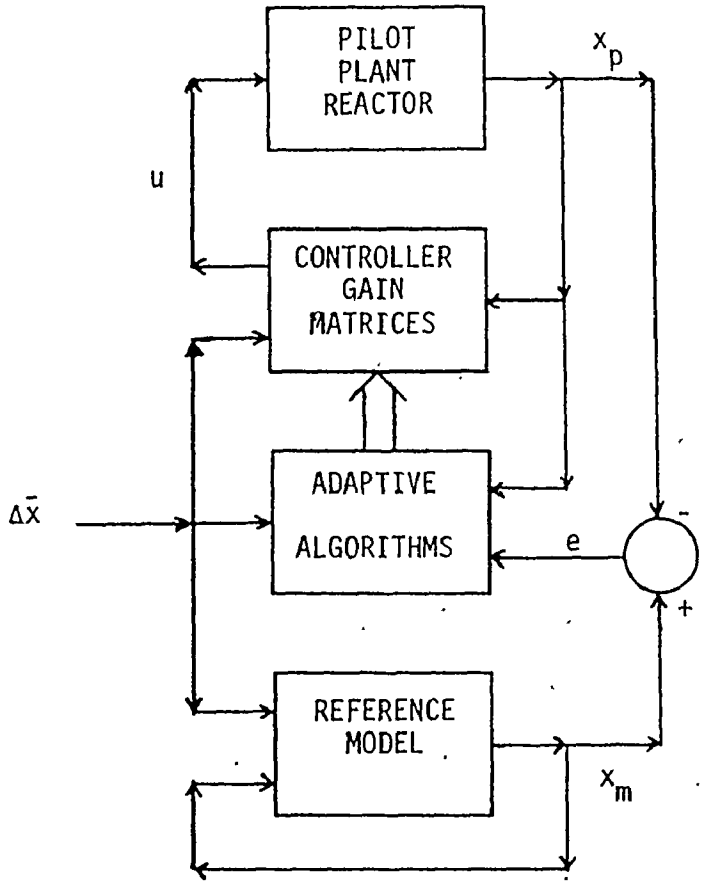
Because the dynamic behaviour of a complex plant cannot be precisely simulated by a low order model, it is advantageous to employ a control algorithm which is insensitive to the inherent modelling errors. A robust algorithm capable of self-tuning or adaptation of parameters is desirable, particularly if large excursions in plant operations occur. Large load or setpoint changes usually generate perturbations that can drive a plant into other regimes of operation. Model reference adaptive control systems may be used to adjust the inputs and parameters of a plant and it is usually based on the lowest order model that adequately represents the open loop plant dynamics.

As illustrated in Figure 2-1, the plant and reference model states and measured plant upsets are passed to an adaptive algorithm. The gain matrices of the controller are adjusted to force the plant states to follow those of the reference model. Above all, the resulting manipulation

FIGURE 2-1

STRUCTURE OF A MODEL REFERENCE

ADAPTIVE CONTROLLER



of the plant inputs must not cause instability.

In Section 2 of this chapter, a brief exposé summarizes the formulation of a low order model of the butane hydrogenolysis reactor. This model, structured in consideration of the control objectives forms the basis of a reference model which is central to the derivation in Section 3 of a model reference adaptive control algorithm. The stability of the control system is based on Lyapunov's direct method.

2.2 Unsteady-State Model of the n-Butane Hydrogenolysis Pilot Plant Reactor

The kinetics of the hydrogenolysis of n-butane (Shaw [1974]) are based on the following set of four equations of which only three represent independent reactions:

$$n\text{-}C_4H_{10} + H_2 \xrightarrow{F} C_3H_8 + CH_4 \qquad (2\text{-}3)$$

$$n\text{-}C_4H_{10} + H_2 \xrightarrow{1-F} 2C_2H_6 \qquad (2\text{-}4)$$

$$C_3H_8 + H_2 \longrightarrow C_2H_6 + CH_4 \qquad (2\text{-}5)$$

$$C_2H_6 + H_2 \longrightarrow 2CH_4 \qquad (2\text{-}6)$$

The hydrogenolysis of n-butane is an equimolar reaction and F is the fraction of the reacted n-butane which is converted to propane. An independent set of equations was formed by combining Equations 2-3, 2-4 and 2-6. For this study, it was advantageous to define for these independent reaction equations extents of reactions in terms of the amount of product formed per unit time. Symbols e_1, e_2 and e_3 were used to define the extents of reaction for the chemical reactions of Equations

2-3, 2-4 and 2-6 respectively. Overall steady state material balances for the five reaction species were then expressed as linear combinations of these. The appropriate algebraic equations derived in Appendix C, Section 3 are given by Equations 2-7 to 2-11:

$$Gc_{n\text{-}C_4H_{10}} = Gc^{I}_{n\text{-}C_4H_{10}} - f_{n\text{-}C_4H_{10}} \qquad (2\text{-}7)$$

$$Gc_{C_3H_8} = +f_{C_3H_8} \qquad (2\text{-}8)$$

$$Gc_{C_2H_6} = +3f_{n\text{-}C_4H_{10}} - 2f_{C_3H_8} - f_{H_2} \qquad (2\text{-}9)$$

$$Gc_{CH_4} = -2f_{n\text{-}C_4H_{10}} + f_{C_3H_8} + 2f_{H_2} \qquad (2\text{-}10)$$

$$Gc_{H_2} = Gc^{I}_{H_2} - f_{H_2} \qquad (2\text{-}11)$$

where G: total volumetric flowrate, cm^3/sec

c_i, c_i^I: concentration of component i at exit and inlet respectively, $gm\text{-}moles/cm^3$

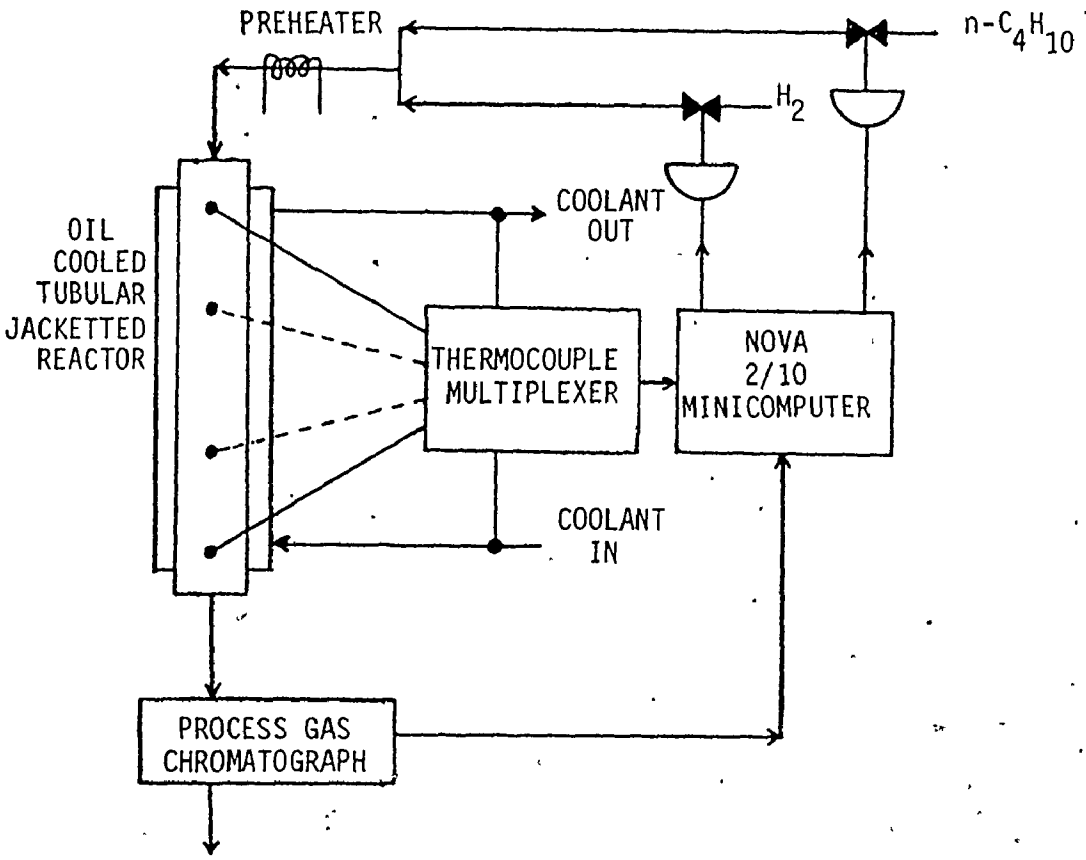
f_i: extent of reaction for component i, gm-moles/sec

In the development of these equations, it was assumed that the reactor feed was n-butane and hydrogen only and that inlet and outlet temperatures and pressures were identical. These assumed conditions were reasonable since the pilot plant reactor to be described was designed to approximate them as closely as possible. It is worthwhile noting here that the molar production rates of propane and ethane are simply linear combinations of the extents of reaction for n-butane, propane and hydrogen.

FIGURE 2-2

SCHEMATIC OF THE BUTANE

HYDROGENOLYSIS REACTOR



In his PhD thesis, Jutan [1976] has developed a mechanistic model which simulates the dynamic behaviour of the n-butane hydrogenolysis packed bed reactor about a steady state or operating point. The reactor itself was open loop unstable. Although a complete description of the pilot plant reactor (designed and constructed for this work) is provided in Chapter 3, a simplified description based on the schematic in Figure 2-2 is presented here. Independently manipulated hydrogen and n-butane feed streams were mixed and preheated before being fed to the top of the packed bed reactor. Inside the reactor, these were reacted to form propane, ethane and methane. The hydrogenolysis of n-butane was promoted by a nickel catalyst described in Appendix A. The cylindrical bed was 4.1 cm in diameter and 25.6 cm long. Partial removal of the heat of reaction was achieved by jacket cooling of the reactor. This precluded isothermal or adiabatic operation. Due to the reactor design, it was possible to assume that the reactor wall temperature equalled the average of the coolant inlet and outlet temperatures. Within the reactor, feed gases were heated to the reactor wall temperature before entering the catalyst bed. The reactor was subjected to various small disturbances. The only known large disturbance affecting the pilot plant reactor had to be synthesized by forcing step changes in the coolant temperature. All major pilot plant variables were monitored by a minicomputer. These included two coolant temperatures, nine axial and three radial reactor temperatures, reactant flowrates and the composition of the product stream. The acquisition of temperature and flow data was controlled by

computer program whereas a programmable process gas chromatograph provided the concentration data. Temperature measurements were taken once every twelve seconds and flow measurements once every second. Analytical information on concentrations was only available at six minute intervals.

A great deal of thought went into the derivation of the differential equations describing the dynamics of the butane hydrogenolysis reactor. Justification and a detailed discussion of the key assumptions for the following set of four coupled highly non-linear partial differential equations (PDE's) are available in Jutan's [1976] thesis.

$$V_C \frac{\partial c_i}{\partial z} + \frac{D_{er}}{R^2 r} \frac{\partial}{\partial r}\left(r \frac{\partial c_i}{\partial r}\right) - \frac{\rho_B \bar{R}_i}{\varepsilon} = \frac{\partial c_i}{\partial t} \qquad (2\text{-}12)$$

$$i = 1,2,3$$

$$V_T \frac{\partial T}{\partial z} + \frac{\lambda_{er}}{R^2 \bar{C} r} \frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) + \frac{\sum_{j=1}^{3} \Delta h_j R_j \rho_B}{\bar{C}} = \frac{\partial T}{\partial t} \qquad (2\text{-}13)$$

$$\left.\begin{aligned} V_C &= \frac{-G_S}{\varepsilon L} \\ V_T &= \frac{-G_S \rho_G C_{PG}}{L \bar{C}} \\ \bar{C} &= C_{PS}\rho_B + C_{PG}\rho_G \varepsilon \end{aligned}\right\} \qquad (2\text{-}14)$$

Boundary Conditions

$$\left.\begin{aligned} r=0,\ & \frac{\partial c_i}{\partial r} = \frac{\partial T}{\partial r} = 0 \\ r=1,\ & \frac{\partial c_i}{\partial r} = 0,\ \frac{\partial T}{\partial r} = B_i(T_w - T) \end{aligned}\right\} \qquad (2\text{-}15)$$

$$\left.\begin{array}{l} z=0,\ T = T_w \text{ for all } r \\ \qquad c_i = c_i^I,\ i = 1,2,3 \text{ for all } r \\ t=0,\ T(r,z) = T \text{ initial} \\ \qquad c_i(r,z) = c_i \text{ initial},\ i = 1,2,3 \end{array}\right\} \qquad (2\text{-}16)$$

where z: axial distance (normalized)
r: radial distance (normalized)
t: time (sec)
L: reactor length (cm)
R: radius of reactor (cm)
c_i: concentration of species i (gm-moles/cm^3)
T: temperature of gas or solid catalyst in reactor bed (^oK)
T_w: reactor wall temperature (^oK)
V_T: thermal wave velocity (cm/sec)
V_C: concentration wave velocity (cm/sec)
$\bar{C}$: inhomogeneous heat capacity (kcal/gm/^oK)
B_i: Biot number
G_S: superficial gas velocity (cm/sec)
ε: catalyst bed void fraction
D_{er}: effective radial diffusivity (cm^2/sec)
λ_{er}: effective radial conductivity (kcal/cm/^oK/sec)
ρ_B: bulk density of catalyst (gm/cm^3)
ρ_G: gas density (gm/cm^3)
C_{PG}: specific heat of gas (kcal/gm/^oK)
C_{PS}: specific heat of solid (kcal/gm/^oK)
$\bar{R}_i$: net reaction rate for species i (gm-moles/gm catalyst/sec)
R_j: heat of reaction for reaction j (gm-moles/gm catalyst/sec)
Δh_j: heat of reaction for reaction j (kcal/gm-moles)

Equations 2-12 and 2-13 express the time variation of the radial and axial gradients of temperature and concentration. These equations include the following simplifying assumptions:

-The free gas and the catalyst particle temperatures were essentially the same at a given location in the reactor;

-The reactor was assumed to be an homogeneous system with negligible pressure drop;

-Free gas movement along the reactor axis was assumed to be in plug flow with a constant average velocity in spite of the existence of thermal gradients in both the axial and radial directions;

-Axial diffusion terms were considered negligible when compared to the bulk flow terms;

-Physical property data were evaluated at an average operating condition and were assumed constant over the range of operation.

The system of equations did not exhibit special forms or characteristics. Without an indication of the nature of these differential equations, it was not obvious which theoretical and numerical techniques could be employed. Since it was apparent that numerical solutions of the PDE's were altogether impractical in this instance, it was felt that simplifications should rely on a priori knowledge of the nature of the reactor's concentration and temperature profiles in the axial and radial directions. The next few paragraphs summarize the steps Jutan [1976] followed in arriving at a low order approximation of the PDE's.

The first simplification of the PDE's resulted from the use of orthogonal collocation numerical techniques (Finlayson [1972]).

Low order orthogonal polynomials were chosen to approximate the expected radial temperature and concentration profiles and to satisfy available radial boundary conditions. When the polynomials were differentiated with respect to "r", formulae for the various radial

derivatives resulted. Application of these formulae to Equations 2-12 and 2-13 yielded a reduced system of seven, two dimensional PDE's: one temperature and six concentration equations. An algebraic equation for the temperature at the reactor wall also arose.

A continuous state space model was obtained by discretizing a linearized version of the reduced system along the axial dimension "z". Since 20 steps were taken, the order of the state space model became 140. It was clear that a reduction to a significantly lower order was required. Reduction by modal analysis was not feasible. The concept of aggregation due to Aoki [1968] was used to transform the high order system to an 80th order system. Although the transformation was not exact, the result was, in the least squares sense, the best that one could achieve.

The state space model of order 80 was still too large for the purpose of on-line control. An approach other than discretization in the "z" direction had to be considered. As for most solid catalysed gas reactions, the ratio of the concentration wave velocity to the thermal wave velocity for this reactor was very large (about 1400). This implied that perturbations would cause the reactor concentration profile to quickly reach a quasi-steady state level. Concentrations would nevertheless respond to the slower dynamics of the temperature wave, thereby attaining their ultimate steady state level as temperature reached its own. The quasi-steady state assumption removed the explicit dependence

of concentration on time. The dependence still existed by virtue of the coupling between concentration and temperature. As a result of the quasi-steady state assumption, the set of seven, two dimensional PDE's was reduced to a single two dimensional PDE for temperature and a set of six ordinary differential equations for concentration. Only the temperature PDE included time as a dimension.

Further model simplification was necessary for control purposes. Under the assumption that the axial temperature and concentration profiles could be approximated by high order orthogonal polynomials, once again it was possible to further reduce the newly simplified system. The linearized seventh order continuous state space model which resulted expressed the time variation of the axial collocation point temperatures about their steady-state or operating levels. Algebraic equations expressing the component concentrations throughout the reactor as a function of the system states and inputs were derived. The fact that the effluent concentrations could be expressed as a linear combination of the axial collocation point temperatures and the manipulated inputs was a key result and is extremely relevant to later discussions in this thesis.

Because the reactor model was to be used for on-line control, the continuous seventh order state space model had to be discretized. A simple numerical technique which accomplishes the conversion is described by Noton [1965]. Briefly, the integration of the linearized continuous

state space model over the discrete time control interval generates the necessary discrete state space model matrices. By this method, Jutan [1976] arrived at the following time-invariant linearized discrete state space model of the reactor. Real matrices A, B and H were estimated from temperature and concentration data.

$$x(k+1) = A\,x(k) + B\,u(k) \qquad (2\text{-}17)$$

$$y(k) = H\,x(k) \qquad (2\text{-}18)$$

where x: state vector of collocation point temperatures, nx1
u: vector of inputs, rx1
y: vector of measured temperatures, mx1
A: transition matrix, nxn
B: control matrix, nxr
H: measurement matrix, mxn
n = 7
r = 2
m = 9

The collocation point at z = 0.0 is not included since no dynamics exist at this axial position.

The essential dynamics of the reactor were well modelled by Equation 2-17. The incorporation of product stream analysis data into measurement Equation 2-18 would lead to serious difficulties since this information was not usually available when control action had to be computed. For this reason, the derivation of a stochastic multivariable control law was based on estimates (by Kalman filtering) of the collocation point temperatures from pilot plant temperature data. The

objective of this law was to minimize the variance of the vector of estimated reactor effluent concentrations about their steady state or operating point values.

Despite the fact that Jutan's controller worked reasonably well, the real control problem is related to the production rate and composition of the reactor effluent. In this study, we were specifically interested in the control of the rate of production of reaction intermediates, propane and ethane. In order to derive a multivariable control law which will satisfy these objectives, a state space model expressing the time variation of the reactor effluent extents was required. Instead of achieving state variable feedback control, output feedback control was desired, where the outputs were extents of reaction as opposed to temperatures.

It has already been pointed out that the quasi-steady state approximation made it possible to express the concentration in the reactor effluent as an algebraic function of the manipulated reactor inputs and axial collocation point temperatures. This same assumption suggested that it may be possible to describe the behaviour of the reactor by a lower order dynamic model with the reactor effluent stream extents as the states. This postulate is based on the following arguments. Assume an experiment was to be conducted in a plant to obtain a multivariable relationship between input flow rates and effluent stream extents. It is assumed that the reactor has been operating at a steady state condition.

Subject to a step change of the reactor inputs, the effluent compositions will also change rapidly and appear to level off within a few seconds. Since the thermal wave "time constant" of the reactor is known to be of the order of 5 minutes (Tremblay [1973]), the temperature profile will not vary significantly for several seconds after the disturbance. However, as the thermal wave responds to the new input levels, the effluent composition will vary in response to the changing temperature profile. Variations in the effluent stream composition will persist until the thermal wave transients disappear. From these observations, it could be postulated that the dynamics of the effluent stream reaction extents defined by Equations 2-7 to 2-11 may be suitably represented by a system of the form of Equation 2-19. A state space model in terms of reaction extents could be used to satisfy the objectives of control.

$$x(k+1) = A\,x(k) + B\,u(k) \qquad (2\text{-}19)$$

$$y(k) = I\,x(k) \qquad (2\text{-}20)$$

where x: state vector of effluent stream reaction extents, nx1 : $\begin{bmatrix}\text{extent of n-butane}\\ \text{extent of propane}\\ \text{extent of hydrogen}\end{bmatrix}$

u: vector of inputs, rx1 : $\begin{bmatrix}\text{n-butane flow}\\ \text{hydrogen flow}\end{bmatrix}$

y: vector of measured reaction extents, nx1
A: transition matrix, nxn
B: control matrix, nxr
I: identity matrix, mxm
n = 3
m = 3
r = 2

As indicated by Equations 2-8 and 2-9, the molar flowrates of propane and ethane in the effluent are simply linear combinations of the extents of n-butane, propane and hydrogen.

Heterogeneous catalytic packed bed reactors are distributed parameter systems and typically exhibit non-minimum phase behaviour. The n-butane hydrogenolysis pilot plant reactor has been observed to exhibit this property and to account for it in a model of the reactor would require the existence of right half plane zeroes. As described in Chapter 5, all parameters of the reactor model Equations 2-19 and 2-20 were to be fitted to experimental data. Since no prior information about the process zeroes was available, no attempt was made to force the fitted model parameters to assume any right half plane zeroes. The state space reactor model would therefore only possess those characteristics imparted by the experimental data itself.

Experience with this pilot plant reactor indicates that action must be taken several times during the six minute analysis cycle of the process gas chromatograph if control of the effluent composition is to be achieved. In order that Equation 2-19 be applicable to the control of this reactor, some means of predicting the reaction extents of the reactor effluent stream is required. It was previously mentioned that Jutan [1976] was able to express the effluent stream concentration in terms of the reactor inputs and temperatures along the reactor axis. For this study however, a low order empirical correlation of the form of

Equation 2-21 was found to satisfactorily predict effluent extents.

$$y(k) = E\ t(k) + G\ u(k-1) \qquad (2\text{-}21)$$

where y: vector of estimated reaction extents in the reactor effluent, nx1
t: vector of functions of temperature data, mx1
u: vector of inputs, rx1
E: correlation matrix, nxm
G: correlation matrix, nxr
n = 3
r = 2
m = 3

The extents were linearly related to the two reactor inputs and three independent functionals of the reactor axial collocation point temperatures. A discussion of this equation will be presented in Chapter 5.

Equation 2-21 may be used to predict the reactor effluent stream extents from input and axial temperature data. If the elements of matrices E and G are not updated on-line, these predictions will be unreliable, particulary during plant upsets. These may result from load or setpoint changes or from time variations of key plant parameters such as catalyst activity. To reduce prediction errors, matrices E and G may be updated recursively from actual concentration data while on-line if it is assumed that Equation 2-21 represents a set of independent multivariable, single response, linear equations. Since our prime interest was on-line prediction of concentration data, the fact that these equations were not truly independent was ignored. Any of the popular recursive estimation algorithms could have been used in the updating of matrices E and G. However, a study (Soderstrom et al [1974]) has demon-

strated that all would yield equally good estimates of the matrices if the errors were assumed to be white noise only. In this light, it was decided that the method of least squares would be employed. The selection was based on computation speed alone. Row elements of matrices E and G may be updated on-line by the following recursive algorithm (Soderstrom et al [1974]) for a real-time environment:

$$\hat{\Theta}(k+1) = \hat{\Theta}(k) + c(k+1)\varepsilon(k+1) \qquad (2\text{-}22)$$

$$c(k+1) = \frac{P(k)\,\Psi(k+1)}{\lambda + \Psi(k+1)^T P(k) \Psi(k+1)} \qquad (2\text{-}23)$$

$$P(k+1) = P(k) - \left[\frac{P(k)\Psi(k+1)\Psi(k+1)^T P(k)}{\lambda + \Psi(k+1)^T P(k)\Psi(k+1)^T}\right] \Big/ \lambda \qquad (2\text{-}24)$$

$$\varepsilon(k+1) = y(k+1) - \hat{\Theta}(k)^T \Psi(k+1) \qquad (2\text{-}25)$$

where $\hat{\Theta}$: vector of parameter estimates, row elements of matrices E and G, $(m+r) \times 1$
Ψ: vector of independent variables, $(m+r) \times 1$
y: measured response, scalar
ε: residual of measured and predicted response, scalar
c: weighting vector, $(m+r) \times 1$
P: matrix proportional to the covariance matrix $(m+r) \times (m+r)$
λ: forgetting factor, scalar $0 < \lambda \leq 1$

The P matrix is proportional to the covariance matrix and will converge in a stable manner to the null matrix if the forgetting factor is unity. The undesirable consequence of this is that the updating algorithm will be insensitive to disturbances once P becomes too small. By setting the forgetting factor slightly less than unity, P cannot converge exactly to the null matrix. In this case, only $(1/(1-\lambda))$ past residuals will

actually influence the current parameter estimates. Typical values of λ are 0.95 to 1.

Together, Equations 2-19 to 2-21 define the form of the reactor model that was used for this control study. From reactor temperature and input data, the states of Equation 2-19 were estimated by Equations 2-21 and 2-20. Control action based on these estimates was then computed by the algorithm described in Section 3. As new analytical data about the reactor effluent were obtained, the elements of the matrices E and G of Equation 2-21 were updated by a recursive algorithm which is defined by Equations 2-22 to 2-25.

Initial estimates of real matrices A, B, E and G of Equations 2-19 and 2-21 were determined from data obtained while the reactor operated under single variable feedback control. The estimation is discussed in Chapter 5.

2.3 Model Reference Adaptive Control Based on Lyapunov's Direct Method

Because multivariable control laws are generally designed to exploit process interactions, they should perform better than multiloop control systems. This has not been the case since most multivariable control structures are not robust enough to compensate for unmeasured disturbances and drift. Multivariable control laws also cannot function effectively should key measurements or manipulated inputs become unavail-

able through failure. Since all plants are subjected to these phenomena, adjustments must be made to the multivariable controller in order to maintain operating objectives. There are two ways of arriving at the necessary adjustments. The first approach is to analyze recent operating data and either re-estimate new controller parameters or restructure the control system. With the recent development of adaptive algorithms, on-line estimation of controller parameters using a process control digital computer has become an attractive alternative. There is every indication (Unbehauen et al [1975]) that model based adaptive control systems will find wide acceptance in several chemical engineering applications. Experimental studies like this one with complex pilot plants are intended to test the power of existing adaptive control theory and point out the inherent weaknesses.

The design of a model reference adaptive controller based on Lyapunov's direct method is developed for application to the control of the butane hydrogenolysis pilot plant. Early work (Luders et al [1974]) with continuous adaptive control systems encountered serious numerical instabilities when solutions were attempted with a digital computer. It has since been recognized (Sebakhy [1976]) that the difficulties arose from the direct discretization of the pertinent continuous equations. These problems can be avoided if the system is derived in discrete form. The discrete time derivation is also required for application of the theory in a sampled data environment.

The usual objectives of a commercial plant are basically to produce a certain material at a given rate and quality. To ensure relevance, the controller developed herein is designed with these objectives in mind. In order to maintain the production rates of reaction intermediates propane and ethane at specified setpoints without offset, integral action is incorporated in the derivation.

In Section 2, it was postulated that the dynamic behaviour of the butane hydrogenolysis pilot plant in terms of reactor effluent extents could be represented by the linear state space model:

$$x(k+1) = A\,x(k) + B\,u(k) \qquad (2\text{-}19)$$

The implementation of integral and setpoint action in the control of the production rates of propane and ethane requires the definition of two new states, such as those defined by Equations 2-26 and 2-27:

$$\bar{x}(k) = F\,x(k) \qquad (2\text{-}26)$$

$$z(k+1) = z(k) + \bar{x}(k) + \Delta\bar{x} \qquad (2\text{-}27)$$

where $\bar{x}$: deviation of the production rates of propane and ethane about the fitted mean, sx1

F: real constant matrix, $\begin{bmatrix} 0 & 1 & 0 \\ 3 & -2 & -1 \end{bmatrix}$, sxn (Refer to Equations 2-8 and 2-9)

$\underline{z}$: integral sum vector, sx1

$\Delta\bar{x}$: deviation of the production rate setpoints from the fitted mean values for propane and ethane (fitted mean value of the production rates − desired values of the production rates), sx1

An augmented time-invarient discrete linear dynamic model of the reactor is obtained by combining Equations 2-19, 2-26 and 2-27. The result given

by Equation 2-28 is an open loop model of the reactor system:

$$x_m(k+1) = A_m x_m(k) + B_m u(k) + D_m \Delta\bar{x} \qquad (2\text{-}28)$$

where x_m: $\begin{bmatrix} x \\ z \end{bmatrix}$, augmented state vector, $(n+s)x1$

A_m: $\begin{bmatrix} A & 0 \\ F & I \end{bmatrix}$, transition matrix, $(n+s)x(nxs)$

B_m: $\begin{bmatrix} B \\ 0 \end{bmatrix}$, control matrix, $(n+s)xr$

D_m: $\begin{bmatrix} 0 \\ I \end{bmatrix}$, $(n+s)xs$

If load change information was available, it could be included as an input to the model by augmenting the last term of Equation 2-28. In this way, feedforward action could be produced. The adaptive algorithm developed in this section associates all differences between model and plant states with improper process regulation. Although not treated here, it is possible to include a suitably identified noise model to account for a portion of these differences.

The auxiliary form of Equation 2-28 can serve as the basis for the design of an optimal controller for the pilot plant. If a quadratic performance index with a penalty for control is defined and minimized (see Appendix C, Section 2) a time-invariant, asymptotically stable closed loop model would result. In order that this model included the possibility of setpoint changes, it is altered to yield Equation 2-29:

$$x_m(k+1) = A_m^* x_m(k) + D_m \Delta\bar{x} \qquad (2\text{-}29)$$

where A_m^*: inherently stable transition matrix, $(n+s)x(n+s)$

Despite the fact that the form of Equation 2-28 was obtained using reasonable arguments and that elements of the A_m and B_m matrices were fitted to real plant data, this linear model can only represent an approximation of the real plant. Consequently, Equation 2-29 cannot be optimal for the real plant.

The real plant is assumed to be governed by the following time-invariant linear state space system:

$$x_p(k+1) = A_p\, x_p(k) + B_p\, u(k) + D_p\, \Delta\bar{x} \qquad (2\text{-}30)$$

where x_p: process state vector, (n+s)x1
u: vector of inputs, rx1
A_p: transition matrix, (n+s)x(n+s)
B_p: control matrix, (n+s)xr
D_p: (n+s)xs

Because Equation 2-30 does not figure directly in the development of the adaptive algorithm, the fact that the underlying process may be non-linear and time variant is unimportant (Lindorff et al [1973]). Although there is no requirement that the governing system and the process model have the same order (Nguyen Thuc Loan [1971]), the development which follows demands it.

Oliver et al. [1973] have reported the use of a linear multivariable control law in the derivation of a continuous time adaptive algorithm. Following their example, it was postulated that the control law

$$u(k) = \left[K_{FB}(k) \;\vdots\; K_I(k)\right] x_p(k) + \left[K_{SP}(k)\right] \Delta\bar{x} \qquad (2\text{-}31)$$

where K_{FB}: proportional feedback gain matrix, rxn
K_I : integral feedback gain matrix, rxs
K_{SP}: setpoint gain matrix, rxs

was valid for this discrete time formulation. The gain matrices have been partitioned to emphasize the proportional, integral and setpoint blocks. A closed loop representation of the reactor system, Equation 2-32, is obtained by substitution of Equation 2-31 into Equation 2-30. The gain matrices defined by Equation 2-31 become the plant parameters to be manipulated by the adaptive algorithm.

$$x_p(k+1) = A_p^*(k)\, x_p(k) + D_p^*(k)\Delta\bar{x} \qquad (2\text{-}32)$$

where $A_p^*(k)$: $A_p + \Gamma(k)$, $(n+s)x(n+s)$
$\Gamma(k)$: $B_p \cdot \left[K_{FB}(k) \;\vdots\; K_I(k)\right]$, $(n+s)x(n+s)$
$D_p^*(k)$: $D_p + \Omega(k)$, $(n+s)xs$
$\Omega(k)$: $B_p \cdot \left[K_{SP}(k)\right]$, $(n+s)xs$

To ensure the stability of this closed loop plant, the values of the gain matrices will be determined from a stability analysis. Lyapunov's second theorem or direct method has been used in this study.

The derivation of a discrete time model reference adaptive control system synthesized using Lyapunov's direct method parallels the continuous time case reported by Oliver et al [1973]. Quite like the continuous time formulations, this discrete time equivalent is essentially an attempt to force a plant -- such as our closed loop reactor -- to track the dynamic

behaviour of an inherently stable reference system. The reference system or model is meant to exhibit the desired dynamic behaviour of the system represented by Equation 2-32. Although any stable model would do (Porter et al [1969]), one which was formulated from an analysis of the process would seem appropriate.

The reference model selected for this work was in fact Equation 2-29. As illustrated in Figure 2-1, the reference model will assist in the adjustment of the gain matrices $K_{FB}(k)$, $K_I(k)$ and $K_{SP}(k)$ to ensure stability.

The formulation of a model reference adaptive control system begins by the definition of an error vector

$$e(k) = x_m(k) - x_p(k) \qquad (2\text{-}33)$$

which is a measure of the approach of the manipulated system to the reference system. An objective of the synthesis is to drive the error defined by Equation 2-33 to zero. This is done by manipulating the elements of the plant parameters $K_{FB}(k)$, $K_I(k)$ and $K_{SP}(k)$. Equation 2-34 is the result of subtracting Equation 2-32 from Equation 2-29:

$$e(k+1) = A_m^* e(k) + \Phi(k)x_p(k) + \Psi(k)\Delta\tilde{x} \qquad (2\text{-}34)$$

where $\Phi(k)$: $A_m^* - A_p^*(k)$

$\Psi(k)$: $D_m - D_p^*(k)$

By definition, the auxiliary system

$$e(k+1) = A_m^* e(k) \qquad (2\text{-}35)$$

is inherently stable. A Lyapunov function for it is

$$V(k) = e^T(k)Pe(k) \qquad (2\text{-}36)$$

where P is a symmetric positive definite matrix defined by the matrix equation

$$A^*_m{}^T P A^*_m - P = -Q \qquad (2\text{-}37)$$

Q is an arbitrary symmetric positive definite matrix. The Q matrix may be selected to reflect the relative importance of the error vector elements when obtaining the P matrix. However, since it is not usually possible to determine the weighting precisely, the unit matrix is most often selected. Details of the solution of Equation 2-37 for the P matrix are found in Appendix C, Section 1. A Lyapunov function (Porter et al [1969]) for the system described by Equation 2-33 is given by

$$V(k) = e^T(k)Pe(k) + \sum_{i=1}^{n+s}\sum_{j=1}^{n+s}\frac{\phi^2_{ij}(k)}{\xi_{ij}} + \sum_{i=1}^{n+s}\sum_{j=1}^{s}\frac{\psi^2_{ij}(k)}{\gamma_{ij}} \qquad (2\text{-}38)$$

where ξ_{ij}, $\gamma_{ij} > 0$ are adaptive loop gains. These may be set to reflect the relative importance of the states in the adaptation. In practice, the absolute value of these gains has a marked effect upon the performance of the adaptive control algorithm. By way of analogy, these could be compared to the gain of a univariate proportional feedback controller. Typically, a small gain does not permit the controller to respond effectively until a large difference between process state and controller setpoint exists. Oscillatory behaviour is characteristic of a controller with large gain. It is therefore important to obtain suitable values of the adaptive

loop gains. Although some workers have offered systematic techniques for estimating the values of the adaptive loop gains (Gromeyko et al [1969]), on-line adjustment of these is usually required. Because the manipulated inputs are constrained due to physical considerations, the proper choice of gains becomes more difficult.

In order that the system described by Equation 2-34 be asymptotically stable, the change between two successive Lyapunov function values must be negative. The backward difference at time k

$$\Delta V(k) = V(k) - V(k-1) \qquad (2\text{-}39)$$

may be evaluated by substituting Equations 2-34 and 2-38 into Equation 2-39. Equation 2-40 is the result:

$$\begin{aligned}
\Delta V(k) = {} & e^T(k-1)\left[A^*_m{}^T P A^*_m - P\right] e(k-1) \\
& + 2e^T(k-1)A^*_m{}^T P\Phi(k-1)x_p(t-1) \\
& + 2e^T(k-1)A^*_m{}^T P\Psi(k-1)\Delta\bar{x} \\
& + x_p{}^T(k-1)\Phi^T(k-1)P\Phi(k-1)x_p(k) \\
& + \Delta\bar{x}^T\Psi^T(k-1)P\Psi(k-1)\Delta\bar{x} \\
& + 2x_p{}^T(k-1)\Phi^T(k-1)P\Psi(k-1)\Delta\bar{x} \\
& + \sum_{i=1}^{n+s}\sum_{j=1}^{n+s}\left[\frac{\Phi_{ij}{}^2(k) - \Phi_{ij}{}^2(k-1)}{\xi_{ij}}\right] \\
& + \sum_{i=1}^{n+s}\sum_{j=1}^{s}\left[\frac{\Psi_{ij}{}^2(k) - \Psi_{ij}{}^2(k-1)}{\gamma_{ij}}\right] \qquad (2\text{-}40)
\end{aligned}$$

The second to sixth terms of Equation 2-40 can be decomposed into a sum of products as shown in Equations 2-41 to 2-45.

$$E(1) = e^T(k-1)A_m^T P\Phi(k-1)x_p(k-1)$$
$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{n+s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{n+s} e_l(k-1)\, A^*_{m_{kl}}\right]\cdot P_{ki}\right]\cdot\Phi_{ij}(k-1)\, x_{p_j}(k-1)\right] \quad (2\text{-}41)$$

$$E(2) = e^T(k-1)A_m^T P\Psi(k-1)w$$
$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{n+s} e_l(k-1)\, A^*_{m_{kl}}\right]\cdot P_{ki}\right]\cdot\Psi_{ij}(k-1)\,\Delta\bar{x}_j\right] \quad (2\text{-}42)$$

$$E(3) = x_p^T(k-1)\Phi^T(k-1)P\Phi(k-1)x_p(k-1)$$
$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{n+s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{n+s} x_{p_l}(k-1)\,\Phi_{jl}(k-1)\right]\cdot x_{p_k}(k-1)\,\Phi_{ik}(k-1)\right]\cdot P_{ji}\right] \quad (2\text{-}43)$$

$$E(4) = w^T\Psi^T(k-1)P\Psi(k-1)w$$
$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{s}\Delta\bar{x}_l\,\Psi_{kl}(k-1)\right]\cdot P_{ki}\right]\cdot\Delta\bar{x}_j\,\Psi_{ij}(k-1)\right] \quad (2\text{-}44)$$

$$E(5) = E(6) = x_p^T(k-1)\Phi^T(k-1)P\Psi(k-1)w$$
$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{n+s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{s}\Delta\bar{x}_l\,\Psi_{il}(k-1)\right]\cdot x_{p_k}(k-1)\,\Phi_{jk}(k-1)\right]\cdot P_{ji}\right] \quad (2\text{-}45a)$$

$$= \sum_{i=1}^{n+s}\left[\sum_{j=1}^{s}\left[\sum_{k=1}^{n+s}\left[\sum_{l=1}^{n+s} x_{p_l}(k-1)\Phi_{kl}(k-1)\right]\cdot P_{ki}\right]\cdot\Delta\bar{x}_j\,\Psi_{ij}(k-1)\right] \quad (2\text{-}45b)$$

The organization of the summation nests resulted from programming considerations.

To ensure the stability of the system of Equation 2-34 -- hence, to

ensure the stability of the system of Equation 2-32 -- it is necessary that Equation 2-38 be positive definite and Equation 2-40 negative definite for all time. The Lyapunov function given by Equation 2-38 is positive definite by virtue of its form. Equation 2-40 can at best be negative semidefinite if all terms except the first of Equation 2-40 are summed to zero. When this is done, an algorithm for computing $\Gamma(k)$ and $\Omega(k)$ and hence the gain matrices of Equation 2-31 is obtained. Equation 2-40 simplifies to Equation 2-46. The recursive equations for generating $\Phi(k)$ and $\Psi(k)$ are given by Equations 2-47 and 2-48:

$$\Delta V(k) = -e^T(k-1)Qe(k-1) \qquad (2\text{-}46)$$

$$\phi_{ij}^2(k) = \phi_{ij}^2(k-1) - \xi_{ij}\left[2\cdot E(1) + E(3) + E(5)\right]_{ij} \qquad (2\text{-}47)$$

$$\psi_{ij}^2(k) = \psi_{ij}^2(k-1) - \gamma_{ij}\left[2\cdot E(2) + E(4) + E(6)\right]_{ij} \qquad (2\text{-}48)$$

If the right hand side of Equations 2-47 and 2-48 approach zero for all elements of $\Phi(k)$ and $\Psi(k)$, the plant is tracking the reference model exactly. When this occurs, the adaptive algorithm will fail to respond to process disturbances. This occurrence is unlikely in noisy and highly non-linear systems. Without a noise term perturbing the reference model, the algorithm will naturally adapt to zero deviations because the reference model states decay asymptotically to zero. To prevent the occurrence of complex values when solving for $\Phi_{ij}(k)$ and $\Psi_{ij}(k)$ by Equations 2-47 and 2-48, the approximations

$$\phi_{ij}^2(k) = \Phi_{ij}(k)\,\Phi_{ij}(k-1) \qquad (2\text{-}49)$$

$$\psi_{ij}^2(k) = \Psi_{ij}(k)\,\Psi_{ij}(k-1) \qquad (2\text{-}50)$$

are used. In turn, matrices $\Gamma(k)$ and $\Omega(k)$ are updated by the recursive relationships 2-51 and 2-52 derived from the definitions of $\Phi(k)$ and $\Psi(k)$:

$$\Gamma(k) = \Gamma(k-1) - \left[\Phi(k) - \Phi(k-1)\right] \qquad (2\text{-}51)$$

$$\Omega(k) = \Omega(k-1) - \left[\Psi(k) - \Omega(k-1)\right] \qquad (2\text{-}52)$$

Finally, the gain matrices for Equation 2-31 are extracted from Equations 2-51 and 2-52 by application of a pseudo-inverse of the process control matrix:

$$\left[K_{FB}(k) \vdots K_I(k)\right] = V \cdot \Gamma(k) \qquad (2\text{-}53)$$

$$\left[K_{SP}(k)\right] = V \cdot \Omega(k) \qquad (2\text{-}54)$$

where $V = \left[B_p^T B_p\right]^{-1} B_p^T$

The above system of equations forms the basis of an algorithm for the adjustment of the $\Gamma(k)$ and $\Omega(k)$ matrices (hence the $A_p^*(k)$ and $D_p^*(k)$ that would force the process states to follow those of the model. The stability of the closed loop system would be assured if it were possible to directly manipulate each element of these matrices. However, because there are fewer inputs than states and the process control matrix is invariant, it is not always possible to calculate a set of controller gain matrices that will result in stable operation. The gain matrices are nevertheless the best that can be obtained given the form of the pseudo-inverse being used. Because the gain matrices of this adaptive control

algorithm are approximating the information provided by the $\Gamma(k)$ and $\Omega(k)$ matrices, one thing is clear. As the difference in the number of states and inputs increases, the approximation becomes worse and stability less likely. For a given system, it may be possible to discover a pseudo-inverse which would yield a better approximation, thereby imporving the likelihood of stable operation. Recalling from Chapter 1, the stability of the control system is jeopardized under the pseudo-inverse.

Since integral action has also been included in this derivation, the stability problem is aggravated due to the introduction of a lag not characteristic of the true process.

Matrices $\Phi(k)$ and $\Psi(k)$ are updated by Equations 2-47 and 2-48 using information at time (k-1). However, new data at time k are available and may be incorporated in the update. An indirect way of doing this is to arrange Equations 2-32 and 2-34 to yield expressions in terms of recent data. If matrices $A_p(k-1)$, $D_p(k-1)$, $\Phi(k-1)$ and $\Psi(k-1)$ have not converged to their ultimate values, numerical instabilities could result. A more direct approach would be to consider the new data as just an approximation of the old. This latter technique was employed in the control studies detailed in Chapter 5.

The sensitivity of the adaptive scheme to the value of the control matrix B_p, its pseudo-inverse, the approximations and data substitutions when solving Equations 2-47 and 2-48 had to be determined. Although a

non-linear dynamic model of the reactor was available (Jutan [1976]), a simulation to evaluate these aspects of the adaptive control algorithm was not attempted. It was simpler and much more appropriate to test the algorithm on the pilot plant itself.

For future reference, the algorithm for adaptive control can be summarized by the following steps:

- Sample the reactor axial temperature data and compute the axial collocation point temperatures. Calculate $x_p(k)$ from Equations 2-19 to 2-21;
- Equation 2-28 is used to calculate $x_m(k)$. The error vector $e(k)$ is then available;
- Using the new data at time (k), evaluate matrices $\Phi(k)$ and $\Psi(k)$ by Equations 2-47 and 2-48;
- The controller gain matrices are obtained from Equations 2-51 and 2-52;
- Equation 2-31 is used to implement control.

The model reference adaptive control algorithm developed in this chapter has been cast into a form suited to on-line studies. Before delving into the details of these studies presented in Chapter 5, a description of the experimental system is first given. Chapter 3 provides the reader with an extensive description of the n-butane hydrogenolysis pilot plant reactor. The design and run-time operation of a real time executive program developed for this work is provided in Chapter 4.

CHAPTER 3

EXPERIMENTAL APPARATUS

3.1 Introduction

The butane hydrogenolysis pilot plant described in this chapter was designed and built by the author. Its design was based on a similar apparatus designed for use during the author's Masters Degree program (Tremblay [1973]). Industrial instrumentation was used to interface the pilot plant and a minicomputer. Within the computer, a program processed transmitted plant data and the result was used for the manipulation of the plant's inputs. In an attempt to give the reader an appreciation of the extent of the apparatus used for this work, descriptions centre around its major components. In Section 2, a brief description of the process computer and its peripherals is provided. An extensive description of the butane hydrogenolysis pilot plant is given in Section 3. Details on most of the instrumentation interfacing the computer and the pilot plant are found in Section 4. Finally, in Section 5, the scheme for product stream analysis by gas chromatography is discussed along with details of the hardware required to interface the process chromatograph to the process computer. Calibration data for the process chromatograph and the various other transducers found within the pilot plant are provided in Appendix B. Complete pilot plant operating

instructions are available (Wright et al [1977]).

3.2 Process Control Computer

A schematic of McMaster University's Chemical Engineering Control Laboratory computer facility is given in Figure 3-1. For this work, the NOVA 1200 and the NOVA 2/10 operated under Data General Corporations' Real Time Disk Operating System (RDOS). They shared a 0.5 megabyte ALPHADATA fixed head disk without the use of an interprocessor bus (IPB). Neither machine was equipped with memory mapping, hardware multiply-divide or floating point processor. However, each contained 32K words of 16 bit central processor memory, real time clock and power-fail monitor. The cycle time of these machines was approximately one microsecond.

Due to the nature of this installation, the NOVA 1200 could only be used for program development. Consequently, all data acquisition and control applications relied upon the NOVA 2/10. The interface between the NOVA 2/10 and the laboratory apparatus was established through the following peripheral devices:

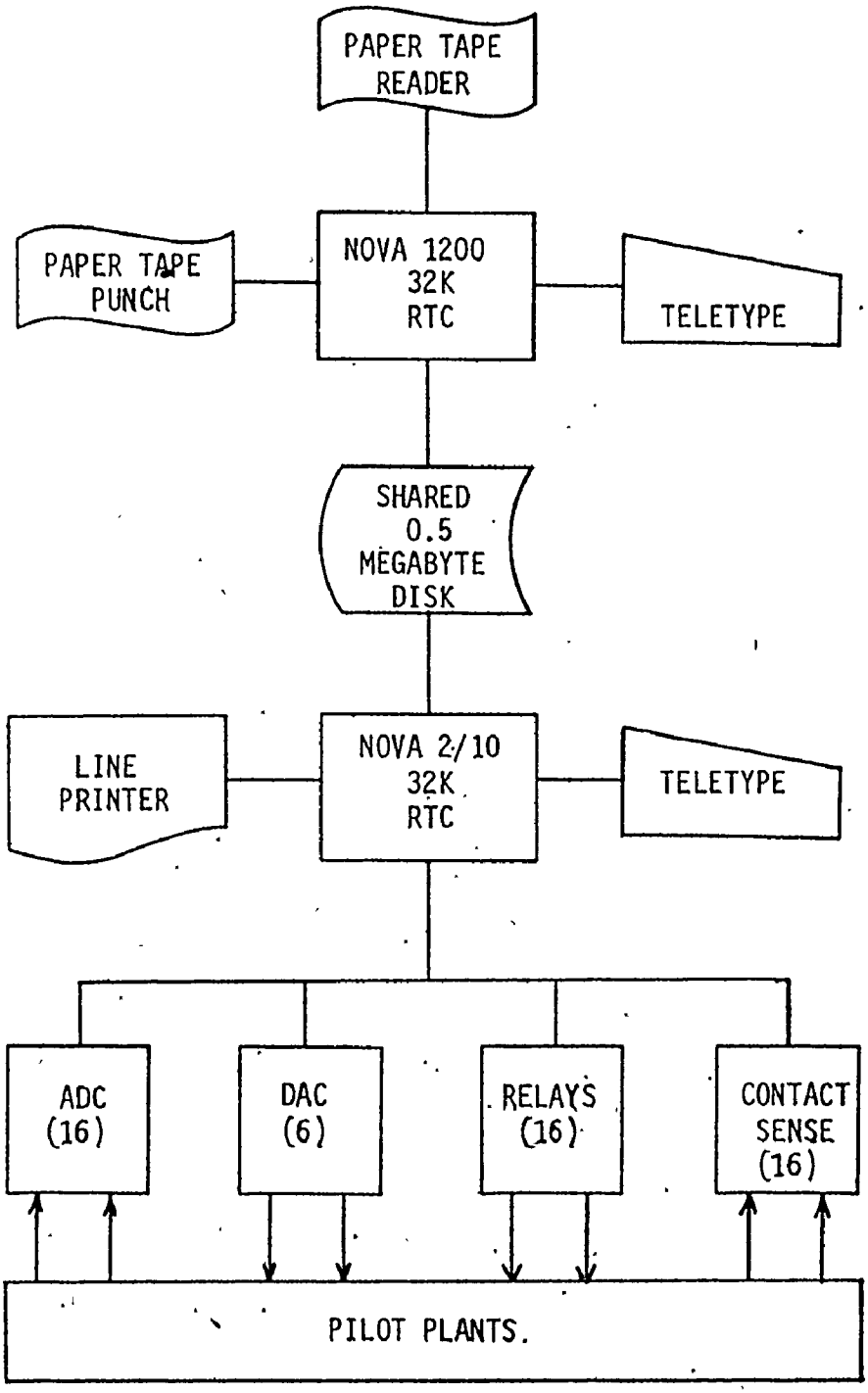
- -16 channels of analog input (-10 to +10 VDC) multiplexed into a single 10 bit analog to digital converter (ADC)
- -16 contact sense inputs
- -16 relay outputs
- -6 channels of analog output (-10 to +10 VDC) from 10 bit digital to analog converters (DAC)

Details of the computer facility are available (Wright [1975]).

FIGURE 3-1

CONTROL LABORATORY

COMPUTER FACILITY



Both assembler and FORTRAN IV languages were used to program the NOVA 2/10 for real-time control operation. The reader is referred to Chapter 4 for a description of the executive program developed to support data acquisition and control studies.

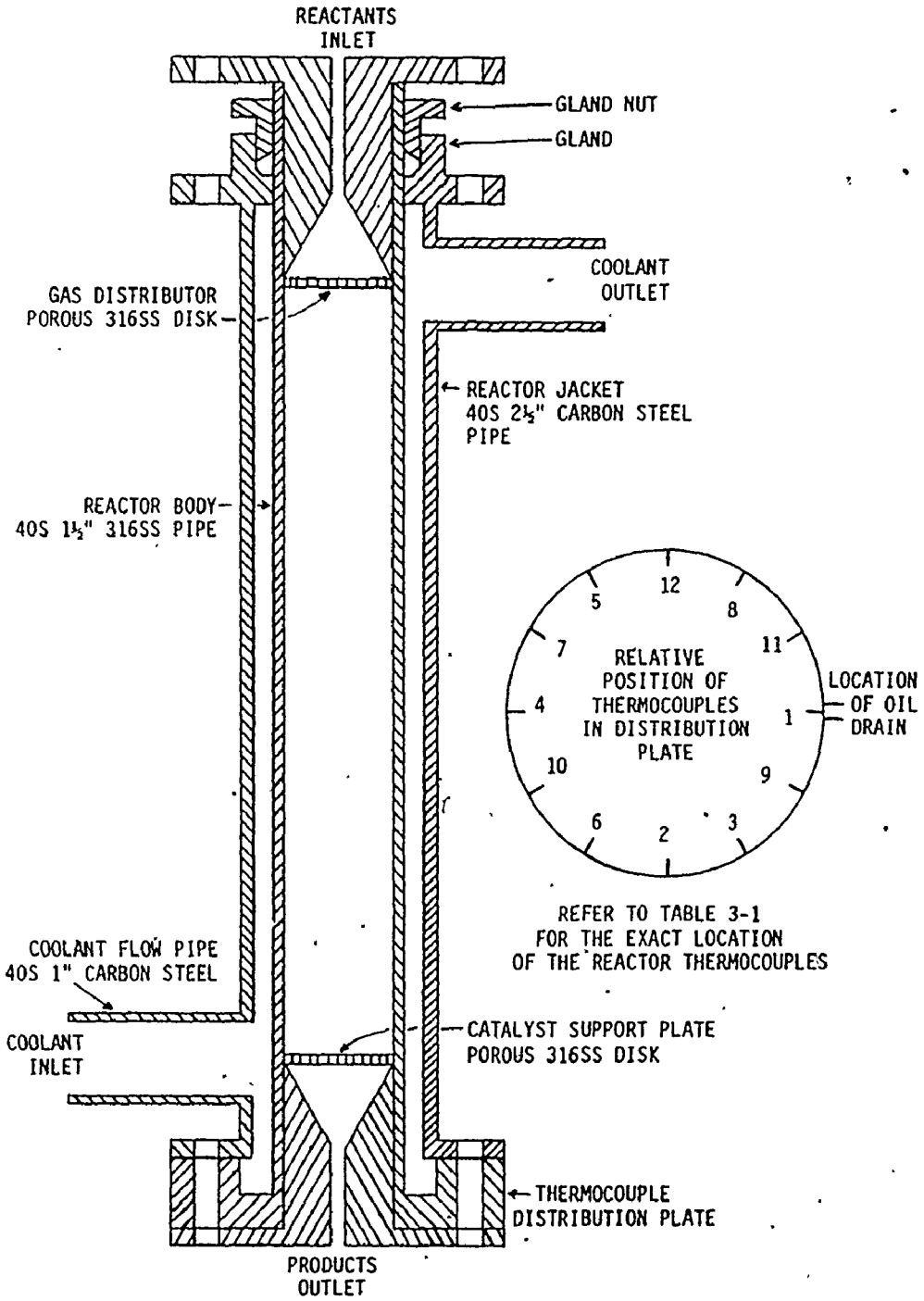
3.3 Butane Hydrogenolysis Pilot Plant

The description of the butane hydrogenolysis pilot plant will first centre on the reactor used for this work. Following this, the various networks needed to operate this reactor are described. The entire pilot plant apart from gas cylinders, gas chromatograph and the electrical heater's power supplies was mounted within a tubular steel frame 2.5 m long by 2.0 m high by 0.75 m wide.

The objectives of this work were dominant factors affecting the design of the reactor illustrated in Figure 3-2. A prime consideration was that the reactor exhibit dynamics characteristic of those of industrial gas phase catalytic packed bed chemical reactors. This implied that operation could be neither adiabatic nor isothermal. In addition, a short residence time and a distribution of reaction produots were desirable. These factors led to the design of a jacketted tubular reactor for the hydrogenolysis of butane. However, to simplify the analysis of the reaction process, the design ensured that the wall temperature was essentially equal to the temperature of the fluid flowing through the jacket. From the experimental point of view, simplicity of reactor servicing had to be considered.

FIGURE 3-2

n-BUTANE HYDROGENOLYSIS REACTOR



The butane hydrogenolysis reaction was selected for this work principally because it was similar to many industrial reactions: complex reaction mechanism coupled with high exothermicity. The main advantage of this reaction over many others was that the kinetic equations and rate constants were well known (Shaw [1974]). In addition, analysis of reaction mixtures was relatively simple and none of the components was toxic although all were highly flammable. Hydrogen and n-butane of suitable purity were easily obtained at modest cost.

As indicated in Figure 3-2, the reactor tube was made from Schedule 40 1½ inch (4.09 cm ID) Type 316 stainless steel pipe. Thermocouples destined for location in the reactor interior were introduced through a flange welded to the bottom end of the reactor tube. Grooves machined into the exterior wall of the reactor tube led the thermocouple wires to the points at which they were to penetrate the reactor wall. These points were one half inch below the desired axial positions. Inside the reactor tube, the thermocouple wires were bent so that the thermocouple beads were located at the desired positions. Twelve thermocouples in all were located inside the reactor, nine along the reactor axis and three at radial positions at various points along the reactor. The precise layout is given in Table 3-1. A jacket fabricated from Schedule 40 2½ inch carbon steel pipe was bolted to the thermocouple distribution flange. The cylindrical annulus formed by the coaxial reactor tube and jacket was approximately 0.75 cm wide. A gland at the top end permitted the removal of the reactor tube from the assembly. Plugs at either end of

TABLE 3-1

Location of Reactor Thermocouples[+]

Thermocouple Number (*)	Distance From Top of Bed (**)	Radial Position (***)
1	0.034	0.0
2	0.158	0.0
3	0.282	0.6
4	0.282	0.0
5	0.407	0.0
6	0.531	0.0
7	0.531	0.6
8	0.655	0.0
9	0.779	0.0
10	0.904	0.0
11	0.904	0.6
12	1.000	0.0

\+ All thermocouples were type K (chromel-alumel).

* Refer to Figure 3-2.

** Normalized distance. Bed length was 25.6 cm.

*** Normalized position. Reactor inside diameter was 4.09 cm.

the reactor tube were made from Type 316 stainless steel rod and porous Type 316 stainless steel disks (Pall Trinity Micro Corporation, Type H, 5 micron pore, 1/8 inch thick) were mounted within them. Both plugs were bolted into place, the bottom one providing support for catalyst and the top one distributing feed gases over the reactor bed. Thermocouples were mounted inside the plugs to measure the gas temperatures near the porous disks. The reactor tube was 28 cm long and consisted of the volume between the reactor plugs. It was packed with a nickel catalyst supported on silica gel. Catalyst particles were roughly spherical with an average diameter of about 1 mm. The preparation of this catalyst is outlined in Appendix A. In Section 2 of Chapter 2, the use of a high order orthogonal polynomial to approximate the axial temperature profile was mentioned. A requirement of this approximation was that the temperature at the top and bottom of the catalyst bed be measured. Because end effects had to be eliminated, the catalyst bed could not rest directly on the support disk and the feed gas distributor could not contact the top of the bed. In order that reactor thermocouple #12 be located at the end of the catalyst bed, the bottom 1.3 cm of the reactor were filled with inert silica gel and the volume above reactor thermocouple #1 was left unpacked. The effective bed length and volume were estimated to be 25.6 cm and 336 cm^3 respectively. Bed voidage was estimated to be 0.4.

The oil circulation network outlined in Figure 3.3 served a dual purpose. During pilot plant startup, it provided the threshold

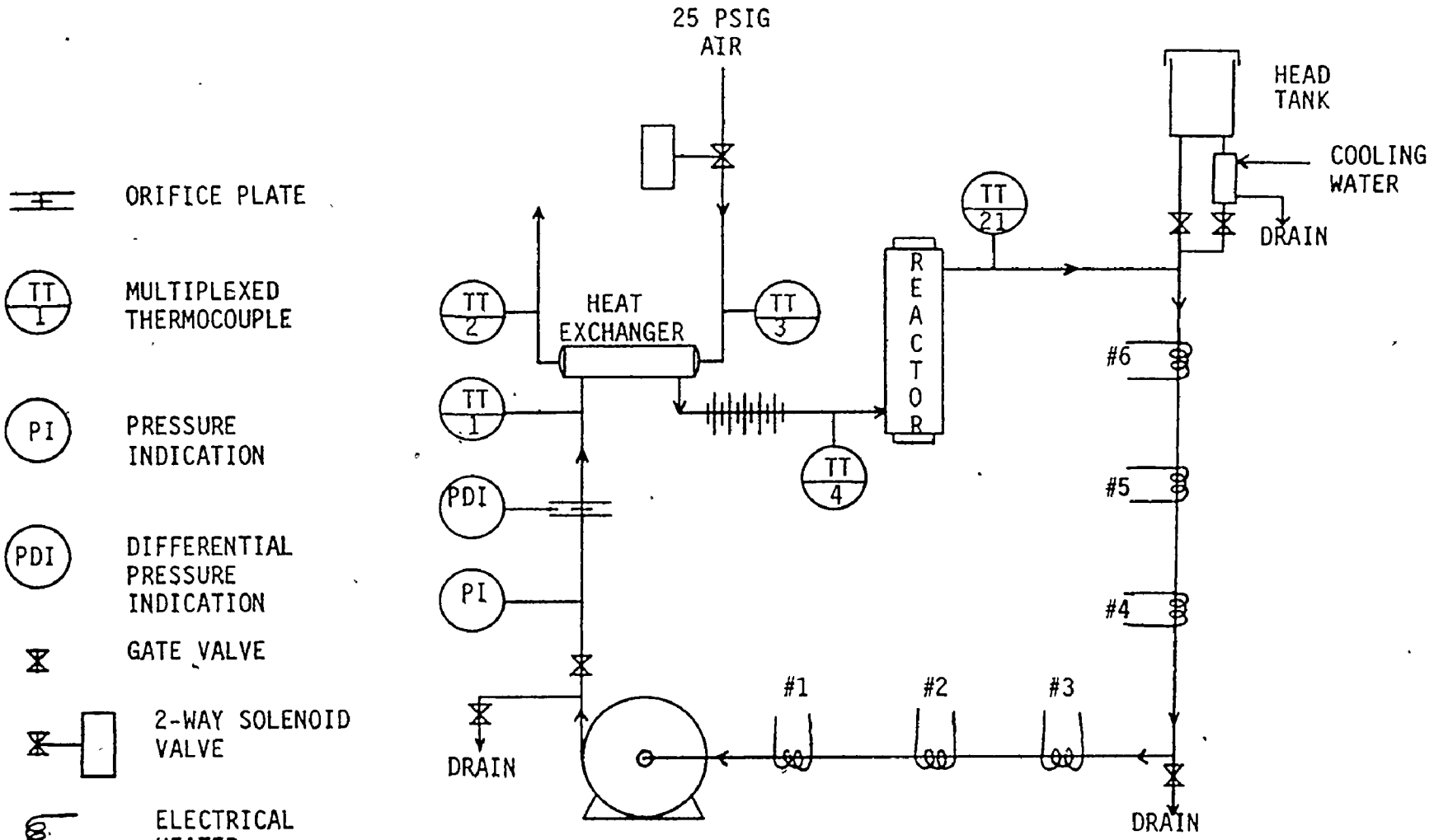


FIGURE 3-3

OIL CIRCULATION NETWORK

temperature needed to initiate the hydrogenolysis of butane. During normal operation, it kept the reactor wall temperature constant. Heat transfer oil (Sun Oil #21) was continuously circulated by a centrifugal pump (SIHI Pumps Co., Model ZLLE 4017/155Q). The pump seals were designed for high temperature operation. The oil circulation rate was estimated from the pressure drop across a 5/8 inch diameter orifice plate located downstream of the pump. The oil then flowed through the shell side of a single pass heat exchanger (American Standard Model 200-8) and was cooled by compressed air at 25 PSIG which was supplied to the tube side. To reduce thermal stresses in the network, a 30 cm section of flexible pipe was installed between the heat exchanger and the pilot plant reactor. The reactor, shown in Figure 3-2 is a jacketted tubular reactor. Oil leaving the reactor jacket was heated by a series of six electrical heaters. Total capacity of these heaters was about 6 kilowatts. A head tank was located just above the heating section of the network. Because normal reactor operation was at high temperature, the head tank acted as an expansion chamber for the heat transfer oil during reactor startup. A small water cooler was installed to ensure that the expansion tank remained cool during high temperature operation.

Piping from the pump outlet to the section just before the electrical heaters was constructed from 1 inch carbon steel pipe. The remaining portion which consisted of the heating section only was made from 1½ inch carbon steel pipe. The electrical heaters (Kanthal resistance strips) were imbedded in a layer of refractory cement applied

to the exterior surface of the 1½ inch carbon steel pipe. Each heater was supplied by a one kilowatt, 24 Volt (MAX), high current AC source. Power cables were #6 gauge Type TWH stranded. Power was controlled by powerstats on a 240 VAC, 3-phase source with 10:1 step down voltage transformers.

Thermocouples were installed in the oil circulation network at the locations indicated in Table 3-2.

The schematic of the reactor gas network is found in Figure 3-4. Effectively, four separate flow paths may be identified within it. The primary path is the one which supplied the reactor with reactants. However, two others were provided to facilitate the calibration of the various transducers in the network. A fourth was used only during pilot plant operation to flush the reactor with pure hydrogen. It bypassed the three curcuits to be described. Both hydrogen and n-butane were throttled by pneumatically actuated control valves (Badger Meter Inc., Research Control Valves, Type 78S, Trim N, Linear, CV=0.006, air to open). The total combined flow under normal operating conditions was about 100 cm^3/sec (1 ATM and 25^oC). The flowrate of each gas -- to a maximum of 160 and 30 cm^3/sec (1 ATM and 25^oC) for hydrogen and n-butane respectively -- was determined from the pressure drop across a length of stainless steel needle tubing (details on the calibration of these flow meters are given in Appendix B). Each pressure drop was measured by a differential pressure transmitter and optionally by the manometer located at the transmitter calibration station (see Figure 3-5). The metered

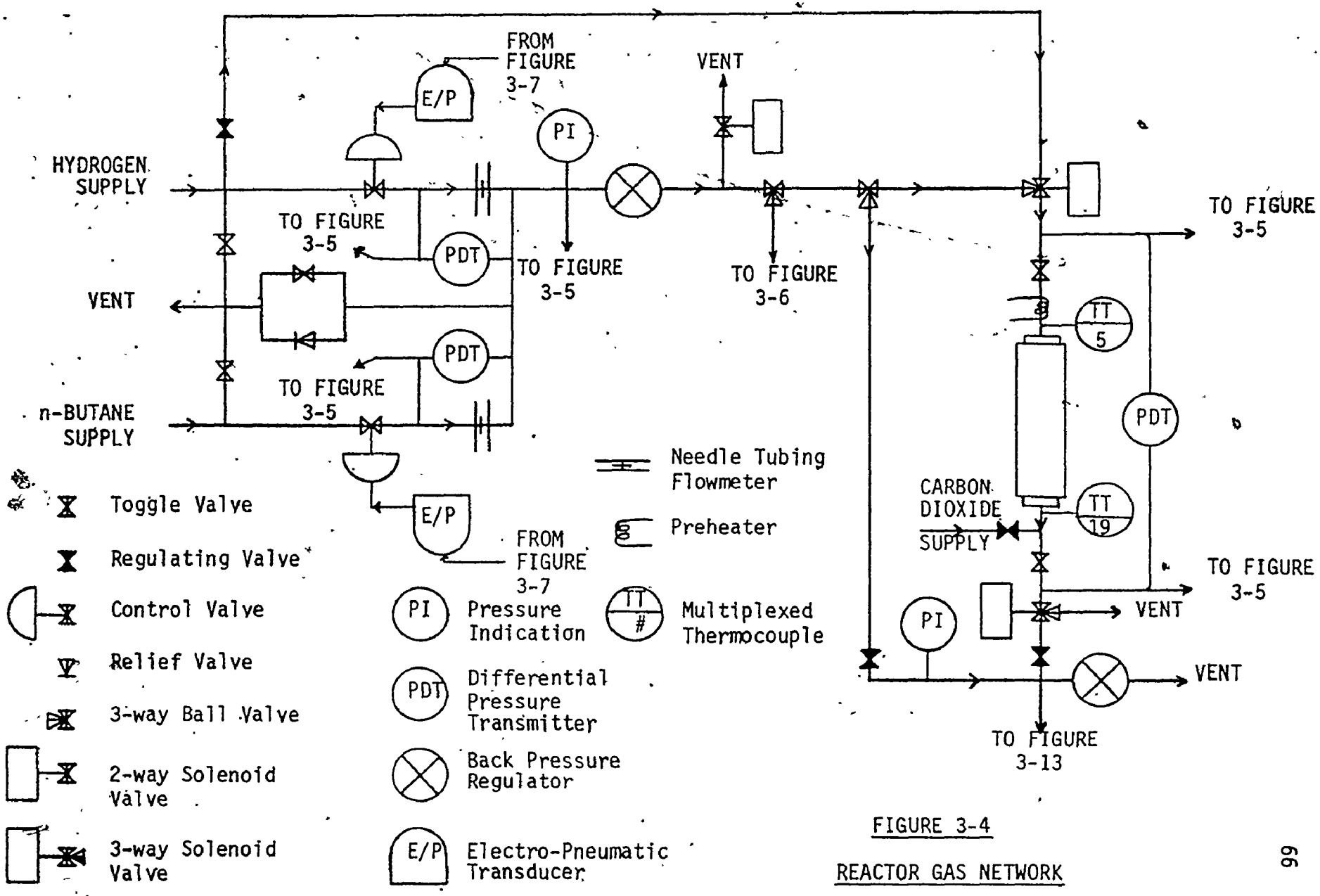


FIGURE 3-4

REACTOR GAS NETWORK

TABLE 3-2

Location of Oil Circulation Network Thermocouples[+]

TT/1	Oil inlet of heat exchanger
TT/3	Air inlet of heat exchanger
TT/2	Air outlet of heat exchanger
TT/4	Oil inlet of reactor jacket
TT/21	Oil outlet of reactor jacket

+ All thermocouples were type K (chromel-alumel). Refer to Figure 3-3.

gases were mixed and the mixture flowed through a back pressure regulator (Fairchild Inc., Model 10BP) which maintained the downstream pressure of the flowmeters at 10 PSIG. A pressure gauge provided an indication of this pressure. At this point, the mixture could be directed to three different sections of the network. During calibration of the hydrogen and butane flowmeters, gas was directed to the flowmeter calibration station (see Figure 3-6). Prior to pilot plant startup, the reactor bypass was selected. Of course, during pilot plant startup and operation, gases were directed to the reactor itself. Preheating of the reactor feed was provided by passing it through an electrically heated packed bed of coarse silica gel. The feed temperature was controlled manually. The downstream pressure of the reactor was maintained at 8 PSIG by another back pressure regulator. It provided the necessary pressure to push a portion of the reactor effluent through the gas chromatograph flow network (see Section 5 for a description of this part of the pilot plant). The rest of the reactor effluent was simply vented through a high volume explosion proof building exhaust fan. A pressure gauge provided an indication of the reactor exit pressure. The pressure drop across the reactor was measured by a differential pressure transmitter or optionally by the manometer located at the transmitter calibration station. The two-way solenoid valve located just downstream of the first back pressure regulator provided venting of the reactor feed. The three-way solenoid valves about the reactor were used to flush the reactor with pure hydrogen gas.

The schematic of the differential pressure transmitter calibration station is given in Figure 3-5. Quite simply, both sides of a single manometer (80 cm max differential height, Meriam Fluid, SG-2.95) were manifolded to the appropriate sides of the differential pressure transmitters of this apparatus. By selecting the high and low pressure sources, one could directly measure the pressure drop across a particular element of the reactor gas network.

During calibration of the hydrogen and butane flowmeters, gas was directed to the flowmeter calibration station represented schematically in Figure 3-6. Depending on the flowrate being measured, either a bubble or wet test flowmeter was used. The bubble flowmeter was used when flowrates were less than 12 cm^3/sec.

The schematic of the gas supplies is given in Figure 3-7. Two sources of hydrogen were required. The major supply required for the reactor, calibration mixture preparation station (see Section 5) and catalyst conditioning unit (see Appendix A) consisted of two cylinders manifolded into a single pressure regulator. The other supplied the carrier gas required for the process gas chromatograph (see Section 5). N-butane was supplied to the reactor and calibrated mixture preparation station. The propane, ethane and methane gases were only used at the calibrated mixture preparation station. Carbon dioxide was required during the preparation and storage of active nickel catalyst. The air supply for this pilot plant was fairly extensive. It supplied the heat exchanger located in the oil circulation network, the process gas

FIGURE 3-5

DIFFERENTIAL PRESSURE TRANSMITTER

CALIBRATION STATION

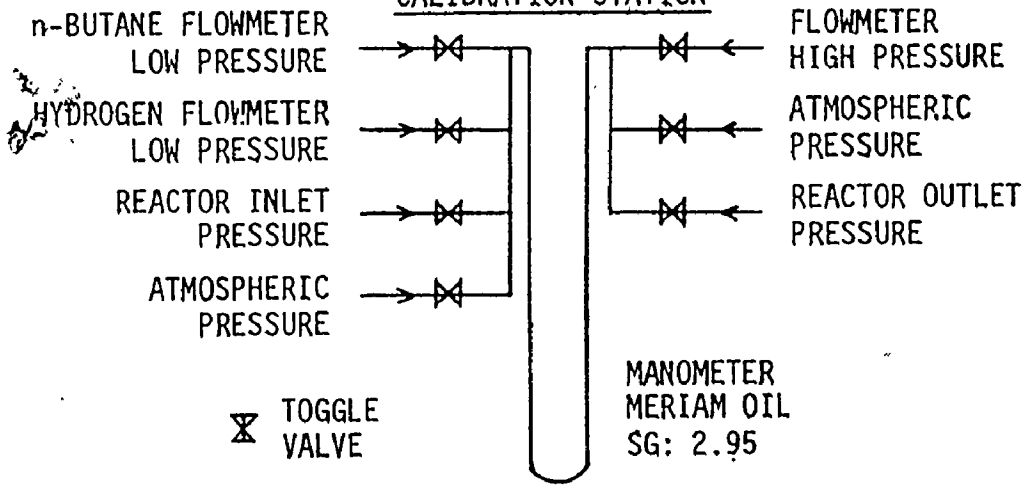


FIGURE 3-6

FLOWMETER CALIBRATION STATION

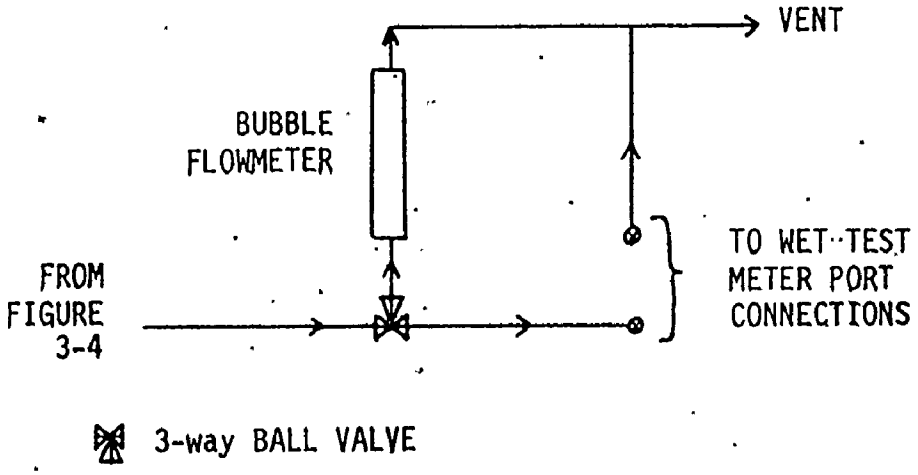


FIGURE 3-7
GAS SUPPLIES

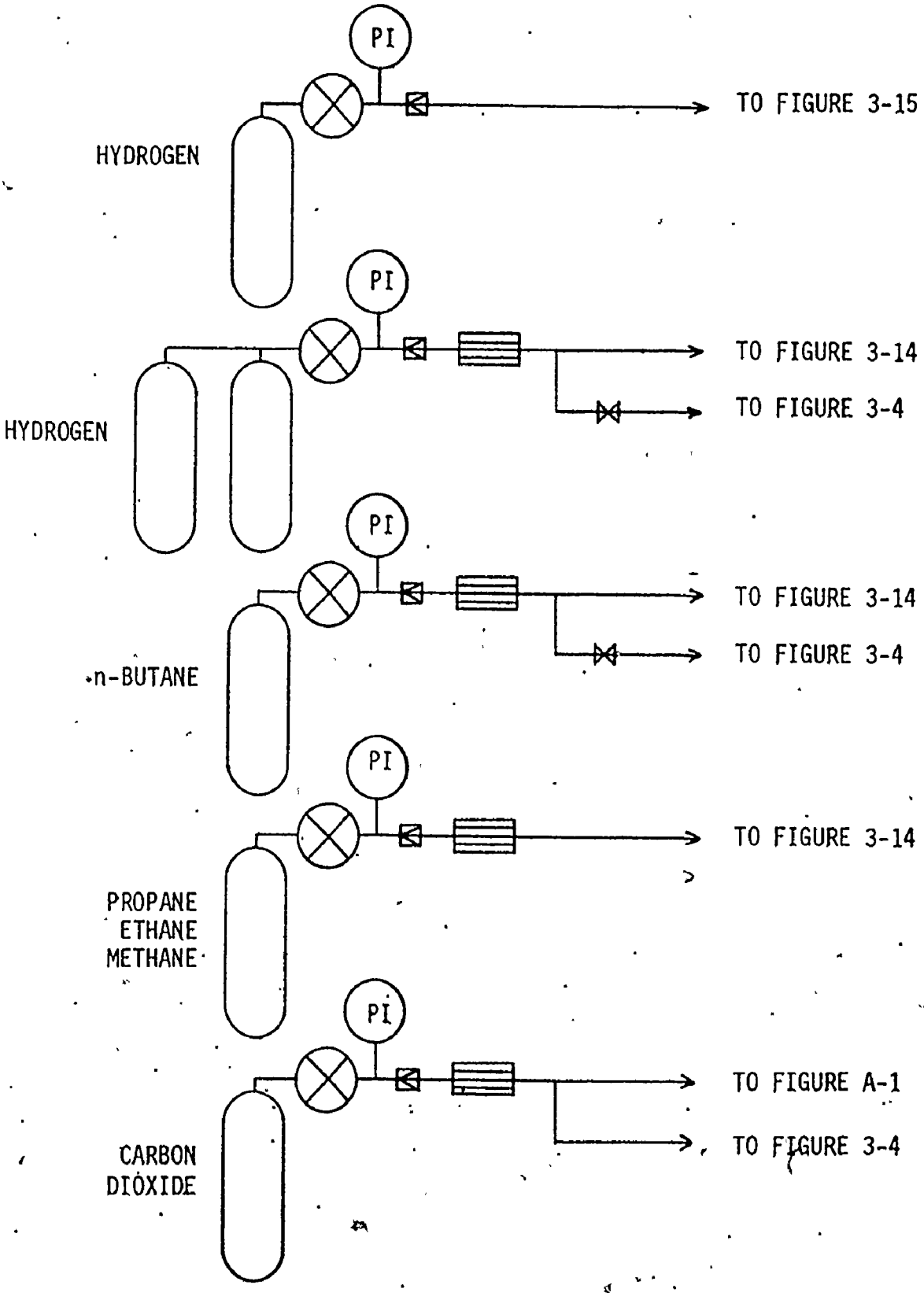
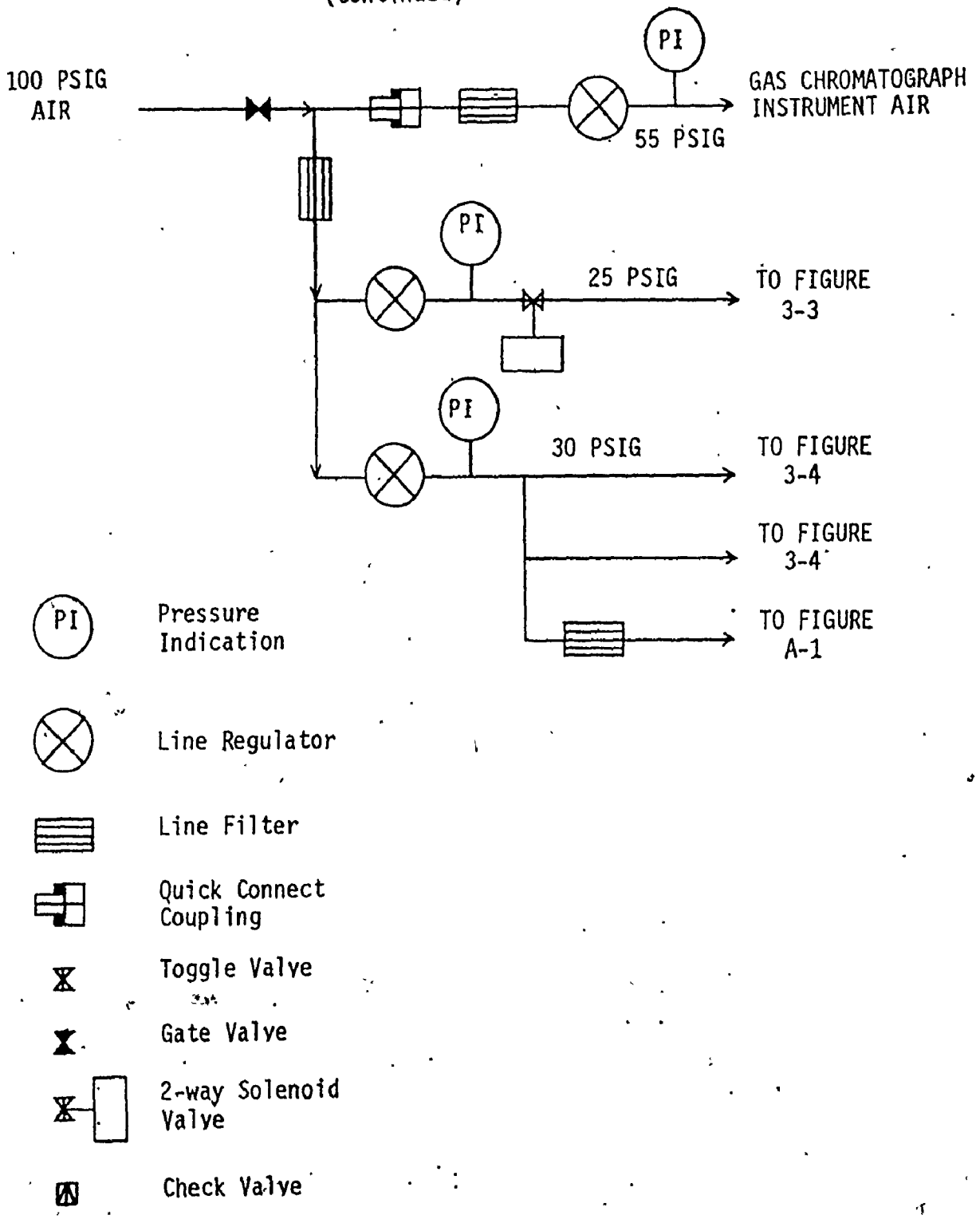


FIGURE 3-7
(continued)



chromatograph, the E/P transducers used to actuate the control valves and finally the catalyst conditioning unit.

SAFETY: The final remarks of this section are related to the venting of the various gases used in this pilot plant. Since all process gases are flammable and have wide explosion limits, all vented gases were collected into a header which ensured that these flammable gases were discharged outside the building. To guarantee this venting, the laboratory fans had to be operating at all times and all venting tubes had to be connected to the header. Further, no smoking or open flames were allowed in the laboratory at any time that gas flows existed.

3.4 Pilot Plant Instrumentation

The principal purpose of this section is to indicate to the reader the type of instruments used to establish the link between the pilot plant and the control computer. These will be classified into three groups:

- transducers to measure process variables for transmission to the process computer
- transducers to enable manipulation of the pilot plant's inputs
- switching networks to provide either manual or automatic manipulation of the pilot plant inputs.

The process variables of interest were temperature, differential pressure and product stream composition. Details on the process gas chromatograph used for analysis of the product stream are given in Section

5. The acquisition of temperature and differential pressure data was controlled by a computer program. Concentration data was acquired by a programmable process gas chromatograph. The chromatograph operated independently of the computer.

In all, 19 temperatures were measured and all were sensed using chromel-alumel thermocouples (1/8 inch OD Ceramo wire, Thermo Electric Co.). Due to the limited capacity of the computer's analog to digital converter (ADC) and to the cost of sufficient numbers of transmitters, a switch described later in this section was used to multiplex the thermocouple signals of the pilot plant into two identical thermocouple transmitters (Acromag Inc., Model 314-WM-U). Up to 22 inputs could be multiplexed into two computer ADCs. The multiplexer input assignment is given in Table 3-3. Note that unused inputs were not left opened or shorted. A thermocouple measuring room temperature was used to occupy unneeded inputs. Details on the calibration of the thermocouple transmitters are given in Appendix B. However, once calibrated, they would output a current in the range of 10 to 50 mA through a 200 ohm resistive load located at the input of the computer's ADC.

The flowrates of hydrogen and n-butane were determined by measuring the differential pressure across calibrated flow restrictors. The differential pressure transmitters (Foxboro Co., Model E13DM-SAM1) consisted of a transducer equipped with a separate power supply. Two transmitters were needed for the flow measurements and a third was used

TABLE 3-3

Thermocouple Multiplexer Input Assignment

Input #		Thermocouple Location
1	---	heat exchanger oil inlet (**)
2	---	heat exchanger air outlet (**)
3	---	heat exchanger air inlet (**)
4	---	reactor oil inlet (**)
5	---	reactor reactants inlet (***)
6	---	reactor thermocouple #10 (*)
7	---	reactor thermocouple #4 (*)
8	---	reactor thermocouple #7 (*)
9	---	reactor thermocouple #5 (*)
10	---	reactor thermocouple #12 (*)
11	---	room temperature
12	---	reactor thermocouple #6 (*)
13	---	reactor thermocouple #2 (*)
14	---	reactor thermocouple #3 (*)
15	---	reactor thermocouple #9 (*)
16	---	reactor thermocouple #1 (*)
17	---	reactor thermocouple #11 (*)
18	---	reactor thermocouple #8 (*)
19	---	reactor products outlet (***)
20	---	room temperature
21	---	reactor oil outlet (**)
22	---	room temperature

* Refer to Table 3-1 for the location of these thermocouples within the reactor

** Refer to Table 3-2 for the location of these thermocouples

*** Refer to Figure 3-4 for the location of these thermocouples

to monitor the pressure drop across the reactor during operation. For zero differential pressure, these transmitters were adjusted to output 10.5 mA into a 200 ohm resistive load located at an input of the computer's ADC. Refer to Appendix B for details of the calibration of the differential pressure transmitters.

As indicated in Figures 3-3 and 3-4, the following pilot plant inputs could be manipulated:

- -the flowrate of air through the oil circulation network's heat exchanger
- -the flowrates of hydrogen and n-butane through their respective flowmeters.

In addition, the reactor feed line could be vented and the reactor flushed with pure hydrogen.

Since the heating section of the oil circulation network was always operating at maximum capacity during operation, some cooling was provided in order to maintain the reactor wall at a constant temperature. For this work, cooling of the oil was accomplished by feeding compressed air at 25 PSIG to the oil circulation network's heat exchanger. Actuation of a two-way normally closed solenoid valve (Ascoelectric Ltd., Model 8210D2, 6 VDC coil) provided the mechanism for thermostat control of the oil temperature.

Voltage to pressure (E/P) transducers (Fisher Governor Co., Model 546) were used to convert a 1 to 9 VDC signal into a pneumatic signal varying linearly between 3 and 15 PSIG. This pneumatic signal was applied to the diaphragm of the control valves used to adjust the

flowrates of hydrogen and n-butane.

To provide rapid venting of the reactor feed section of the reactor gas network, a normally closed two-way solenoid valve (Ascoelectric Ltd., Model 8262B202, 6 VDC coil) could be actuated. Similarly, flushing of the reactor with pure hydrogen was achieved by two Universal Type three-way solenoid valves (Ascoelectric Ltd., Model 8320A11, 6 VDC coil).

During normal operation, manipulation of the pilot plant inputs was done through the computer. However, it was necessary to provide some means of overriding the computer to gain manual control of the pilot plant under abnormal circumstances. These would include startup and shutdown. To this end, two separate types of switching networks were assembled.

The line drawing of the one designed to operate a control valve is given in Figure 3-8. As illustrated, the rotary switch had four modes of operation. If it was in either of the automatic posisions (A&B), the computer digital to analog converter (DAC) signal was directed to an E/P transducer which in turn actuated a control valve. If this switch was in either of the two manual positions (C&D), the voltage to the E/P transducer was supplied by a 0 to 10 VDC manually operated variable voltage source (see Figure 3-12). The computer's contact sense facility was used to detect movement of the rotary switch between positions B and C. Futhermore, it was also possible to monitor the voltage from the

FIGURE 3-8

CONTROL VALVE SWITCHING

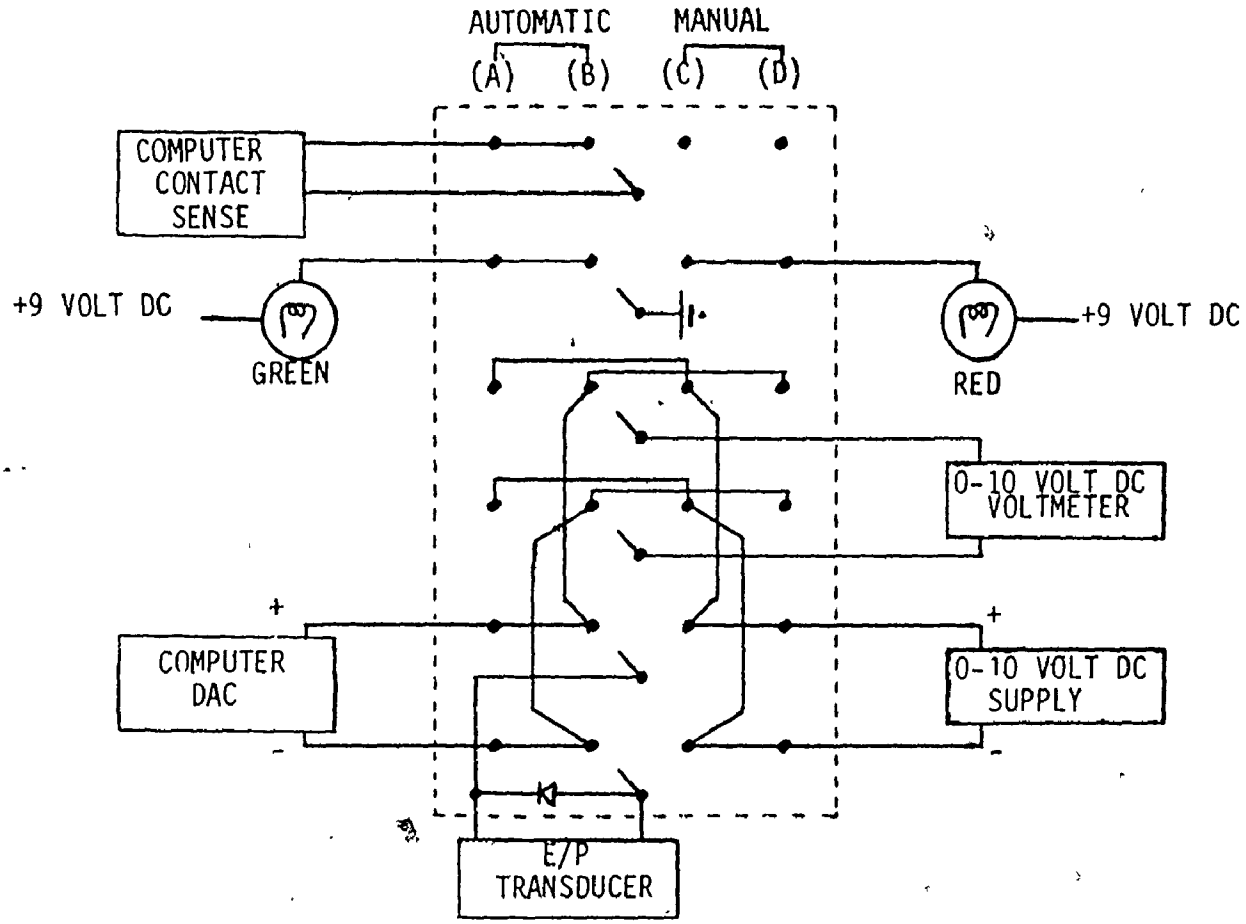
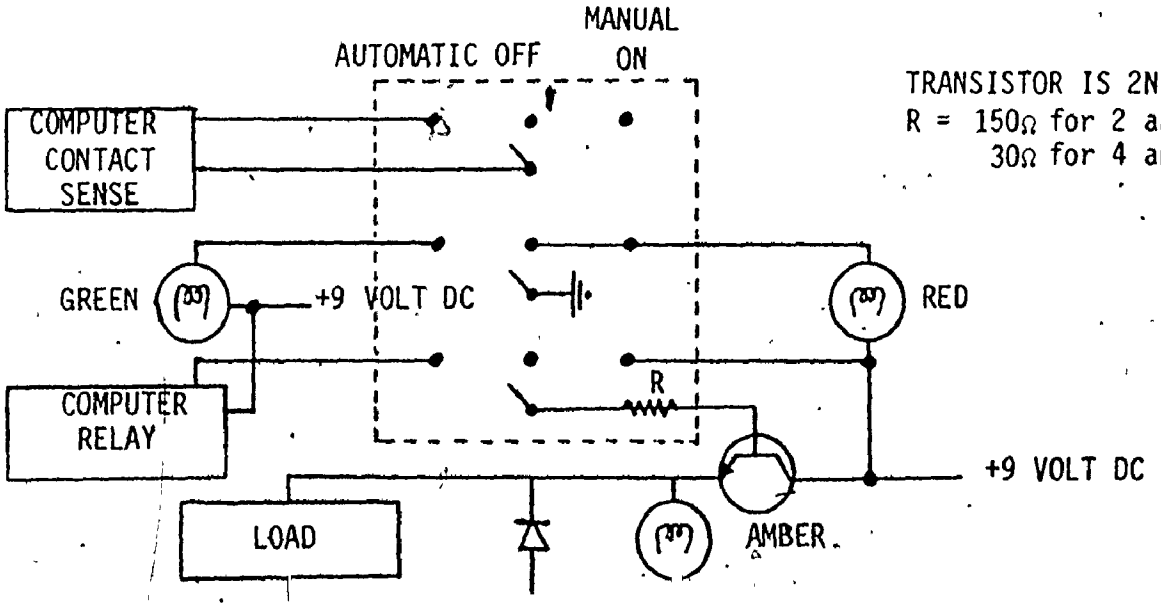


FIGURE 3-9

SOLENOID VALVE SWITCHING



computer DAC or the variable DC source.

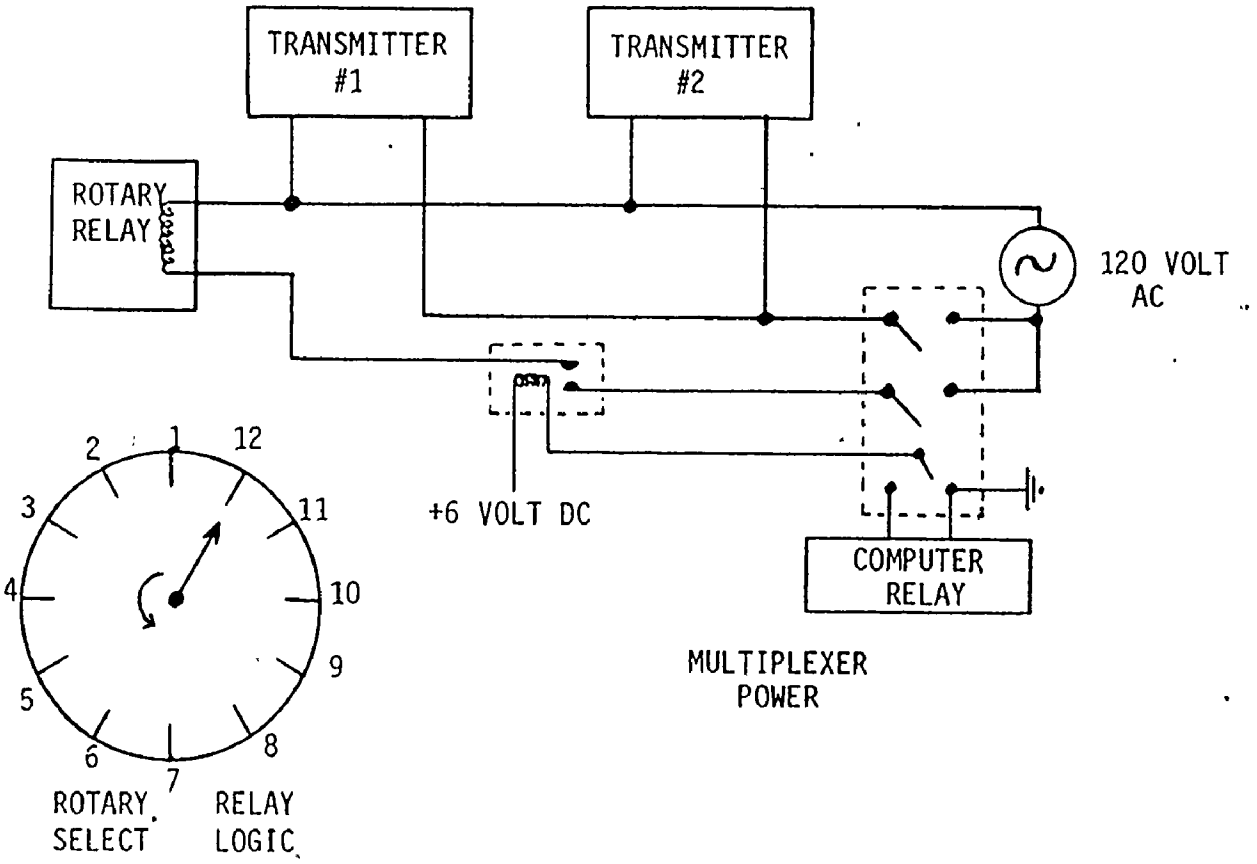
The second type of switching network was designed for actuation of a solenoid valve. The line drawing for this network is shown in Figure 3-9. When the rotary switch was in the automatic position (A), a computer relay was used to activate the transistor which powered a solenoid valve. Position B effectively deenergized the load. Manual actuation of the load occured when the rotary switch was in position C. The computer's contact sense facility was used to detect movement of the rotary switch between positions A and B.

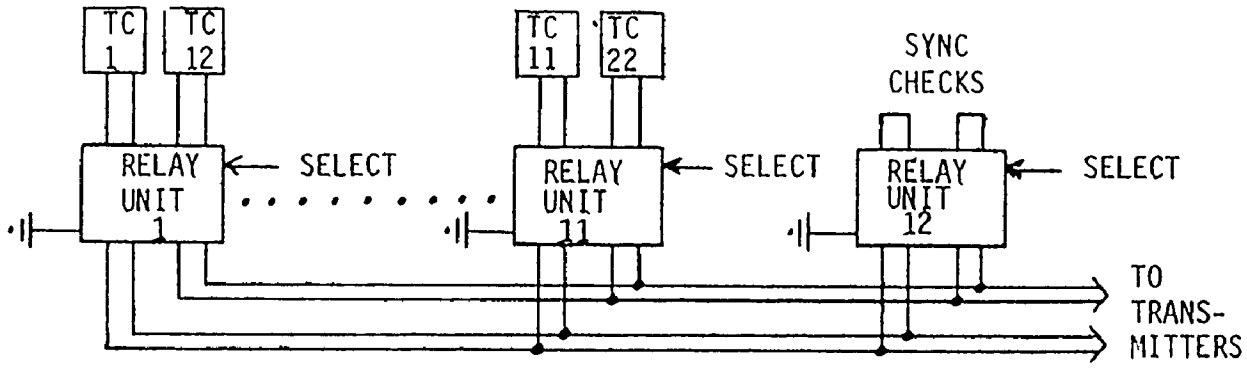
A schematic of the switch designed to multiplex the pilot plant thermocouples into two thermocouple transmitters is found in Figure 3-10. A twelve point rotary relay actuated by a computer relay (or manually if necessary) selected via 4-pole single throw dry reed relays the pair of thermocouples to be switched into the inputs to the thermocouple transmitters. To provide a check on the phasing of the rotary relay, the inputs to the thermocouple transmitters were shorted when the 12 o'clock position on the rotary relay was reached. The multiplexer could accept up to 22 thermocouple inputs. The response time of the transmitters and the nature of the rotary relay limited the multiplexer cycle time to 12 seconds.

Power to energize the pilot plant solenoid valves was provided by a pair of 9 VDC supplies rated at 15 amperes. The line drawing for these supplies is given in Figure 3-11. The line drawing for the 0 to

FIGURE 3-10

THERMOCOUPLE MULTIPLEXER





REED RELAY ASSIGNMENT

FIGURE 3-11

9 VOLT POWER SUPPLIES

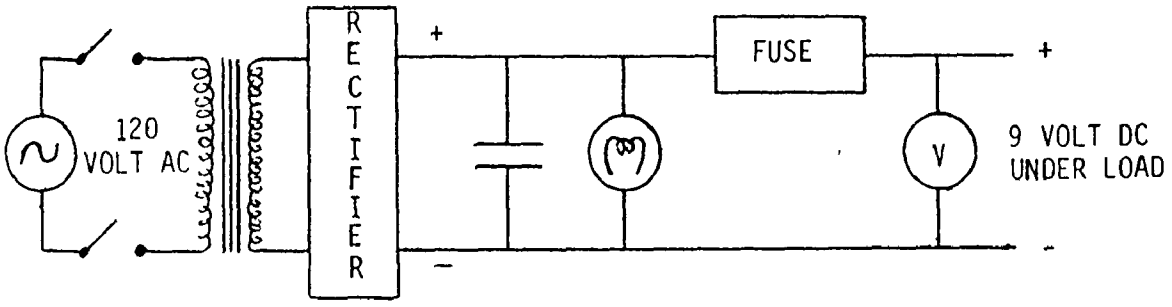
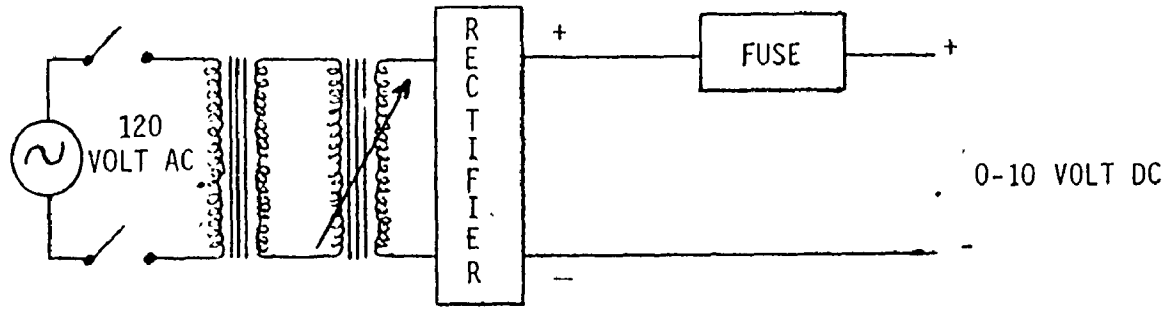


FIGURE 3-12

0-10 VOLT VARIABLE SUPPLIES



10 VDC variable sources used for manual operation of the control valves is shown in Figure 3-12.

3.5 Reactor Effluent Analysis

For any processing operation, some means of determining the nature and quality of the product is absolutely necessary. In the chemical and petroleum industries, the usual instrument used for analysis is the gas chromatograph. Although different instruments (spectrophotometers for example) could have been used for the particular analysis at hand, a basic requirement for this study was that the pilot plant resemble a typical process as closely as possible. For this reason, a process gas chromatograph was chosen to perform the stream analysis. The one selected was the Beckman Instruments Inc. Model 6700 Process Chromatograph equipped with thermal conductivity detector. The essential features of this instrument were that it was programmable and that it could be interfaced to the process computer. Typical programmable functions were:

- -analysis cycle time
- -multiple valve timing
- -component signal gain
- -component area gain.

The process gas chromatograph consisted of two physically distinct units: an analyzer and a programmer. The actual analysis occurred within the analyzer. The programmer provided the control signals to operate the analyzer and established an interface with the computer. The programmer

was equipped with mercury wetted reed relays which signaled the start and end of each analysis. Each signal was a pulse of 60 milliseconds duration detected by the computer's contact sense. The occurence of a start pulse would cause the activation of a program to record the operating conditions prevailing at the time of sample injection. Another program would process the analysis data upon an end of analysis pulse signal. All analysis data appeared as a programmer current output. The voltage drop across a 500 ohm (¼ watt, 1%) resistance connected across these outputs was sampled by the computer's ADC.

Before considering the analytical scheme in detail, information about the analyzer feed will first be presented. The stream being sampled by the analyzer may originate from one of two sources. Referring to Figures 3-4, 3-13 and 3-14, the reactor effluent or a calibrated gas mixture may be fed to the analyzer. If the normally closed three-way solenoid valve (Ascoelectric Model 8320A3, 120 VAC coil) shown in Figure 3-13 was energized (whenever instrument calibration was desired), the source was the calibrated gas mixture. Otherwise (which was the usual case during normal operation of the reactor), a portion of the reactor effluent constituted the feed. The pressure upstream of the flow controller (Figure 3-13) was maintained at 8 PSIG, either by the back pressure regulator at the reactor exit (Figure 3-4) or by the line regulator at the calibrated mixture preparation station (Figure 3-14). The flow controller (Emerson Electric Co., Model 8944) provided 100 cm^3/min of feed to the

FIGURE 3-13

GAS CHROMATOGRAPH FLOW NETWORK

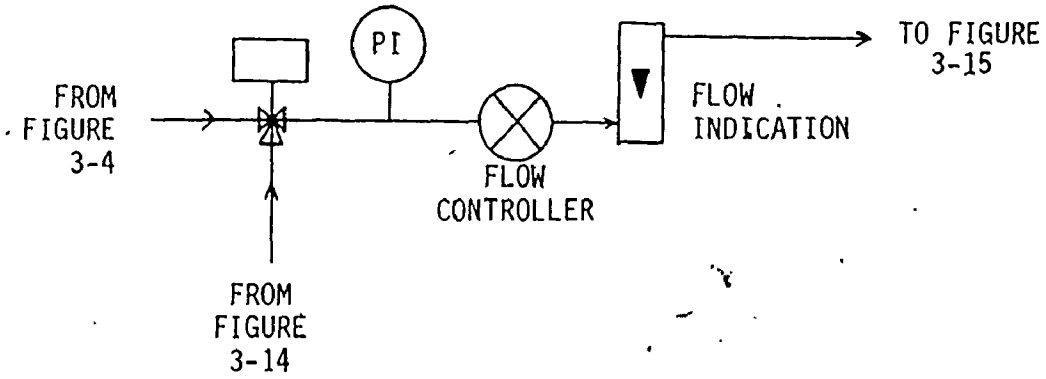
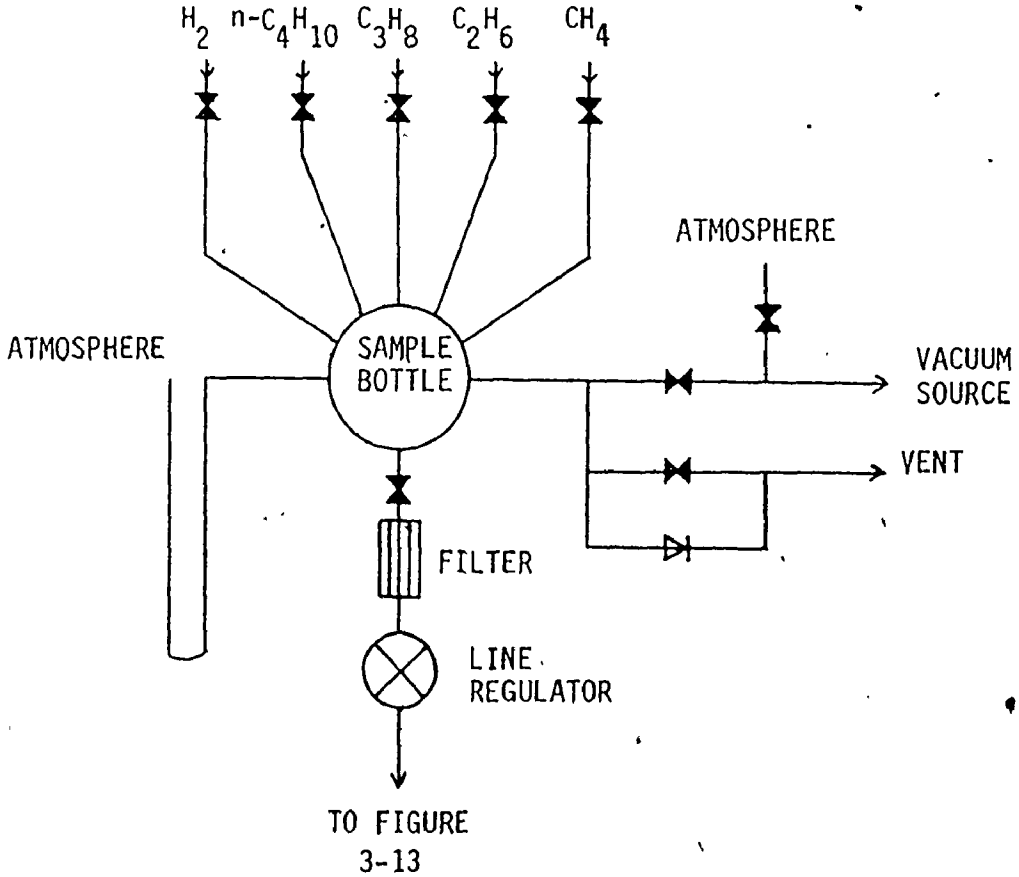


FIGURE 3-14

CALIBRATED MIXTURE PREPARATION STATION



analyzer. All analyzer wastes were vented through the pilot plant exhaust header.

The reactor effluent was known to contain only five species: hydrogen, butane, propane, ethane and methane. The hydrogen fraction was usually quite significant and previous work (Shaw [1974]) had indicated that analysis for all five components was simple but required abnormally long times. The design of the Beckman Model 6700 Programmer had the requirement that the minimum time between successive component peaks had to be at least 15 seconds. This complicating factor had to be considered when determining the operating conditions for the chromatographic columns. Fortunately, this time was short enough to allow a determination of all hydrocarbon species. Since it was possible -- as explained later -- to separately calculate the hydrogen component of a mixture from this determination, the analytical scheme remained comparatively simple. For this reason, hydrogen was selected as carrier gas, thereby masking out the hydrogen component of all samples.

Chromatographic analysis of a mixture for its hydrocarbon species only would usually result in biased estimates of all components in the mixture. In this case, the bias could be removed since independent information about a mixture was available. The carbon to hydrogen ratio in the feed and product streams of the reactor must be equal if the molar flowrates of the butane and hydrogen in the feed are fixed. This ratio is given by Equation 3-1.

$$R = \frac{2x^{I}_{C_4H_{10}}}{5x^{I}_{C_4H_{10}} + x^{I}_{H_2}} \qquad (3\text{-}1)$$

where x^{I}_{i}: mole fraction of component i in the reactor feed

R: carbon to hydrogen ratio

The available calibration data (given in Appendix B) provides estimates of the hydrocarbon mole fractions in a given mixture. The relative values of the mole fractions were assumed to be correct: their absolute levels were believed to be incorrect. It was postulated that the true and estimated levels differed only by a constant as indicated by Equation 3-2.

$$x_{C_4H_{10}} = f\bar{x}_{C_4H_{10}} \qquad x_{C_2H_6} = f\bar{x}_{C_2H_6}$$
$$x_{C_3H_8} = f\bar{x}_{C_3H_8} \qquad x_{CH_4} = f\bar{x}_{CH_4} \qquad (3\text{-}2)$$

x_i, $\bar{x}_i$: respectively, actual and estimated mole fractions of component i.

f: correction factor relating x_i to $\bar{x}_i$

The mole fraction of hydrogen in a mixture is then given by Equation 3-3.

$$x_{H_2} = 1 - f(\bar{x}_{C_4H_{10}} + \bar{x}_{C_3H_8} + \bar{x}_{C_2H_6} + \bar{x}_{CH_4}) \qquad (3\text{-}3)$$

The carbon to hydrogen ratio of the product stream is expressed by Equation 3-4.

$$R = \frac{fz}{2(fz + 1)} \qquad (3\text{-}4)$$

where

$$z = 4\bar{x}_{C_4H_{10}} + 3\bar{x}_{C_3H_8} + 2\bar{x}_{C_2H_6} + \bar{x}_{CH_4}$$

Rearrangement of Equation 3-4 yields an expression for the correction factor "f".

$$f = \frac{2R}{z(1 - 2R)} \qquad (3\text{-}5)$$

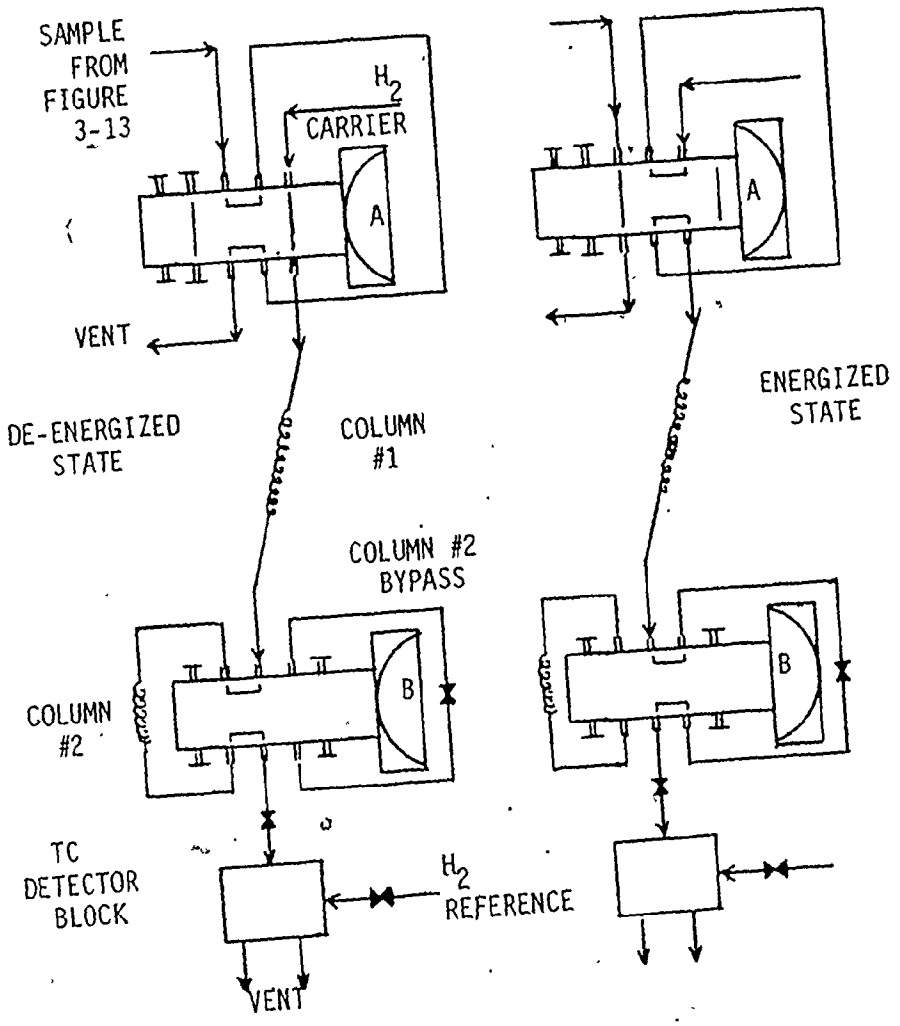
In Equation 3-5, "R" is determined from Equation 3-1 and "Z" from the definition of Equation 3-4. From Equations 3-2 and 3-3, the composition of a mixture may be determined.

The above algorithm for correcting analysis data is valid only if the reactor feed rates are fixed. In practice, control of the butane hydrogenolysis reactor will cause these inputs to vary in time. The transportation lag between the reactants' control valves and the gas chromatograph was estimated to be 1.5 seconds when the total reactants flow was 100 cm^3/sec (1 ATM and 25^oC). Provided that flow changes did not occur within 3 seconds before a sample was injected into the gas chromatograph, it was believed that the strategy was valid.

The problem was then reduced to finding a scheme which would quickly analyze the four hydrocarbon species. The one that was finally used is illustrated in Figure 3-15. Dual columns and 10-port valves were required. Both columns were made from ¼ inch OD copper tubing packed with 50-80 mesh PORAPAK S. All other tubing was 1/8 inch OD Type 316 stainless steel tubing. Column #1 was 0.25 meters long and column #2 3.0 meters. The first meter of column #2 was used for pure delay only. The analyzer (containing the 10-port valves, columns, detector and flow restrictors) was maintained at 110°C. Detector filament current was 150 ma. Under programmer control, valve A would inject a sample (about 0.8 cm^3) essentially at atmospheric pressure into chromatographic column #1. Injection occurred one second after the start of analysis. The start of analysis for this instrument occurs at time one second. With the carrier gas flowing at 60 cm^3/min., methane and ethane were completely eluted into column #2 at 39 seconds after the start of analysis, leaving propane and butane still in column #1. At this time, valve B was energized, trapping methane and ethane in column #2 and allowing propane and butane to elute from column #1 directly into the detector. At 199 seconds after the start of analysis, butane had completely eluted from column #1. Valve B was then de-energized and the components in column #2 resumed elution. Total analysis cycle time was 360 seconds. The programmer cycle time was then 361 seconds which included a one second delay for instrument reset at zero time. The precise programmer sequence and details of the calibration of

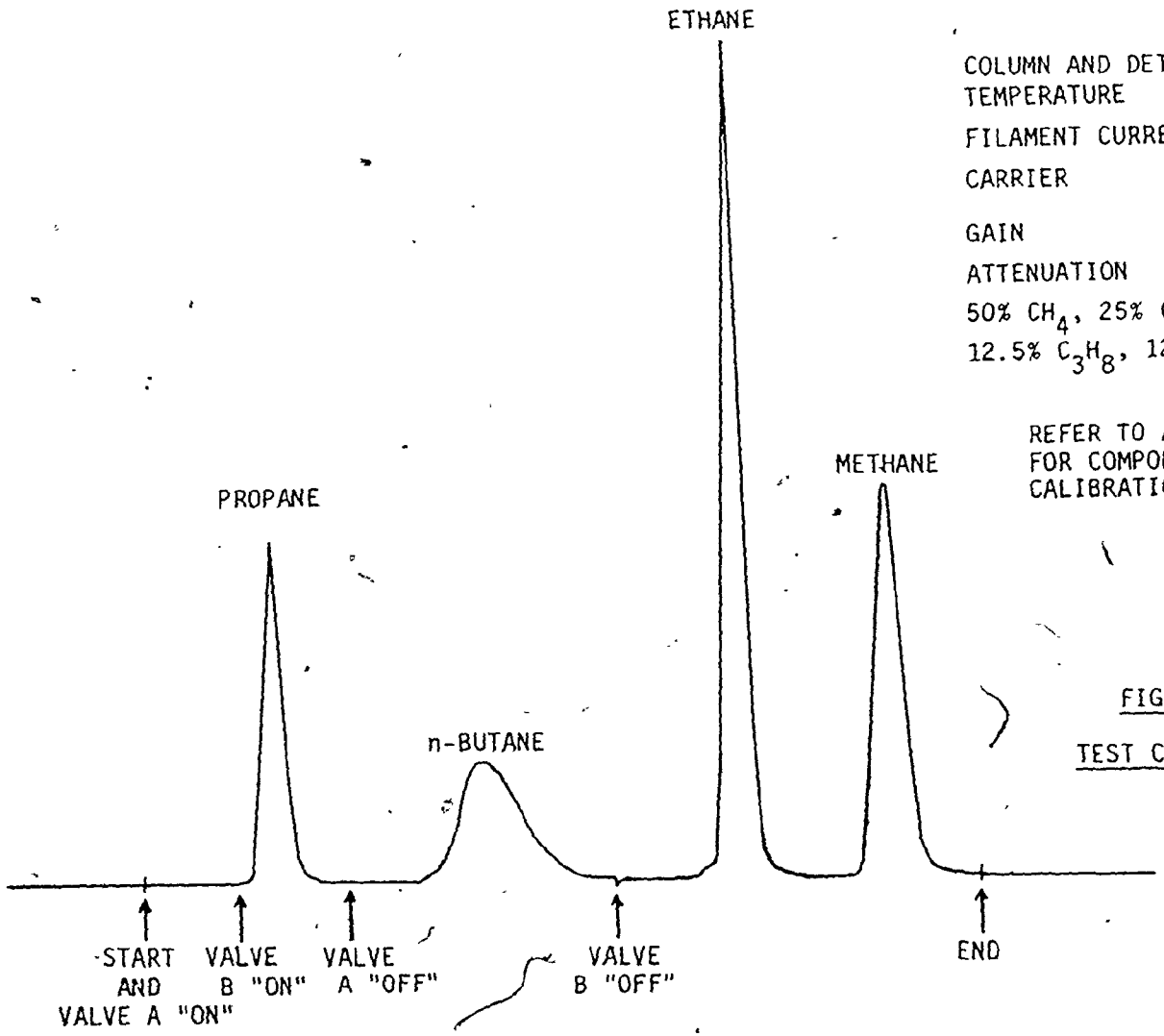
FIGURE 3-15

ANALYSIS SCHEME FOR LIGHT HYDROCARBONS CH_4, C_2H_6, C_3H_8 and n-C_4H_{10}



the process gas chromatograph are provided in Appendix B. A test chromatogram is found in Figure 3-16.

One aspect of the experimental system -- the pilot plant apparatus -- has been described in this chapter. In order that meaningful experimental studies be undertaken with this apparatus, a real time executive program was developed and is described in Chapter 4 which follows.



COLUMN AND DETECTOR TEMPERATURE : 110°C

FILAMENT CURRENT : 150 ma

CARRIER : 1 cm^3/sec H_2

GAIN : 100

ATTENUATION : 4

50% CH_4, 25% C_2H_6, 12.5% C_3H_8, 12.5% C_4H_{10}

REFER TO APPENDIX B, SECTION 5 FOR COMPONENT TIMING AND CALIBRATION

FIGURE 3-16

TEST CHROMATOGRAM

CHAPTER 4

GENERALIZED OPERATING SYSTEM EXECUTIVE

4.1 Introduction

The economics of a processing plant are based on its mode of operation. Plants may operate in one of three modes:

- market limited
- production limited
- resource limited.

The conditions which lead to the first two modes of operation do not change rapidly and profitable control strategies may be maintained for extended periods of time. Recently however, most process plant managers have been forced to operate in the resource limited mode. This means that changes in operating conditions can be expected at any time. In spite of these changes, product quality must be tightly controlled. Profitable operation of a plant in this type of environment requires a robust but highly flexible control system. Considering the type of hardware now available and anticipated for the future, a modern plant's control system must be based on process computers. These permit the implementation of alarm and control strategies which may be quickly altered to meet production constraints. The changing direction of process control has forced plant managers to consider the use of minicomputers for data acquisition and control.

Historically, the use of minicomputers for data acquisition and control entailed the development of an operating system. It and all application software had to be written in assembler language. This clearly precluded the implementation of complex data reduction algorithms while on-line. Frequently, the complete process had to be repeated each time a new application was considered. Presently, most minicomputer manufacturers are supplying sophisticated and reliable operating systems to their customers. Typically, an operating system provides the user with access to a multitask scheduler and device drivers for all standard peripherals. High level languages such as FORTRAN IV are also supported. The development of software for a given application has become less involved. Coupled with the proven reliability and low cost of minicomputer systems, plant managers have begun to acquire them for data acquisition and control. In view of this trend, academic institutions are beginning to introduce students to the various aspects of on-line computer technology.

Data acquisition and control is classified as an on-line system. In such systems, logically independent programs called tasks must normally execute at specific times of the day or at specific time intervals. These tasks appear to execute in parallel but in fact, at a given instant in time, only one task is executing. Computer resources are allocated by a task scheduler to the various tasks on a priority basis. For further details, the reader is referred to any text on multitask programming.

Most minicomputer manufacturers have provided customers with powerful off-line (BATCH) executives supported by their operating systems. Executives for on-line (REAL-TIME) operations are not, however, usually available from most vendors. Computer system vendors such as Foxboro, Honeywell and Fischer & Porter to name only a few have developed on-line executives for use in plant environments. The systems are indeed impressive but are not suited to a research environment where a variety of data acquisition and control applications exist. The dynamic nature of academic research coupled with the fact that academic institutions cannot normally afford packaged computer systems thereby eliminate these vendors from any consideration at all. Vendors like Digital Equipment or Data General offer several suitable models of minicomputers but do not market an on-line executive program. Some software houses have developed on-line software for these machines but then again, it is not designed for use in a research environment.

The Chemical Engineering Department at McMaster University has a number of Data General NOVA series minicomputers which had limited use until this research program was undertaken. Since applied research in control could not be attempted efficiently without a suitable on-line executive program, a highly flexible and powerful on-line executive program was developed. Its structure is not application dependent and is readily converted from one application to another with minimal effort. The executive program was based on Data General Corporation's Real Time Disk Operating System.

The development of an interactive on-line executive or man-machine interface must follow a careful study of the needs of all users and the structure of the operating system being used. For effective use, communications based on a symbolic language is desirable. The interpretation of commands must include extensive diagnostic checks and precise error reporting. Error-free commands must execute promptly.

Any on-line executive must provide a number of fundamental functions. These are summarized below:

- A facility to start, kill or report on the current status of any user task.
- Output of data in log or plot format is necessary. On-line formatting is desirable.
- The displaying and altering of user program parameters must execute in real time.
- User alarms must be reported promptly.
- The package must maintain the plant interface from control information provided in tabular form.
- Support for user tasks written in FORTRAN IV must be provided.

Many more additional functions are usually included to expand a package's flexibility.

Data General Corporation's Real Time Disk Operating System (RDOS) provides the facilities essential to the development of an executive. The major ones involved in the operation of the executive described in this chapter follow:

- disk based operating system
- scheduling of tasks based on software priorities
- multiple user overlays
- disk buffering of output to slow peripherals.

The Generalized Operating System Executive, known by its acronym "GOSEX" makes extensive use of the operating system's overlay facility. All text strings used for dialogue or alarming are kept in specially formatted disk files. Together, these provide for a very compact program. Because the entire program was written in assembler language following modular concepts, the executive is extremely efficient and flexible. All executive tasks compete with user tasks on a priority basis. User tasks may be written in either assembler or FORTRAN IV language.

The GOSEX structure is illustrated in Figure 4-1. Three classes of routines may be identified and are listed in Table 4-1. The utilities are reentrant core resident subroutines for use by the executive tasks, functions and user tasks. These are outlined in Section 2 of this chapter. The executive tasks described in Section 3 form the heart of the GOSEX package. Control over executive output and user tasks is provided by the functions. These are presented in Section 4. Finally, the link between GOSEX and the user tasks is summarized in Section 5.

Flexibility was the major objective behind the design of the GOSEX package. At setup time, the user provides a simple interface

FIGURE 4-1

THE STRUCTURE OF GOSEX

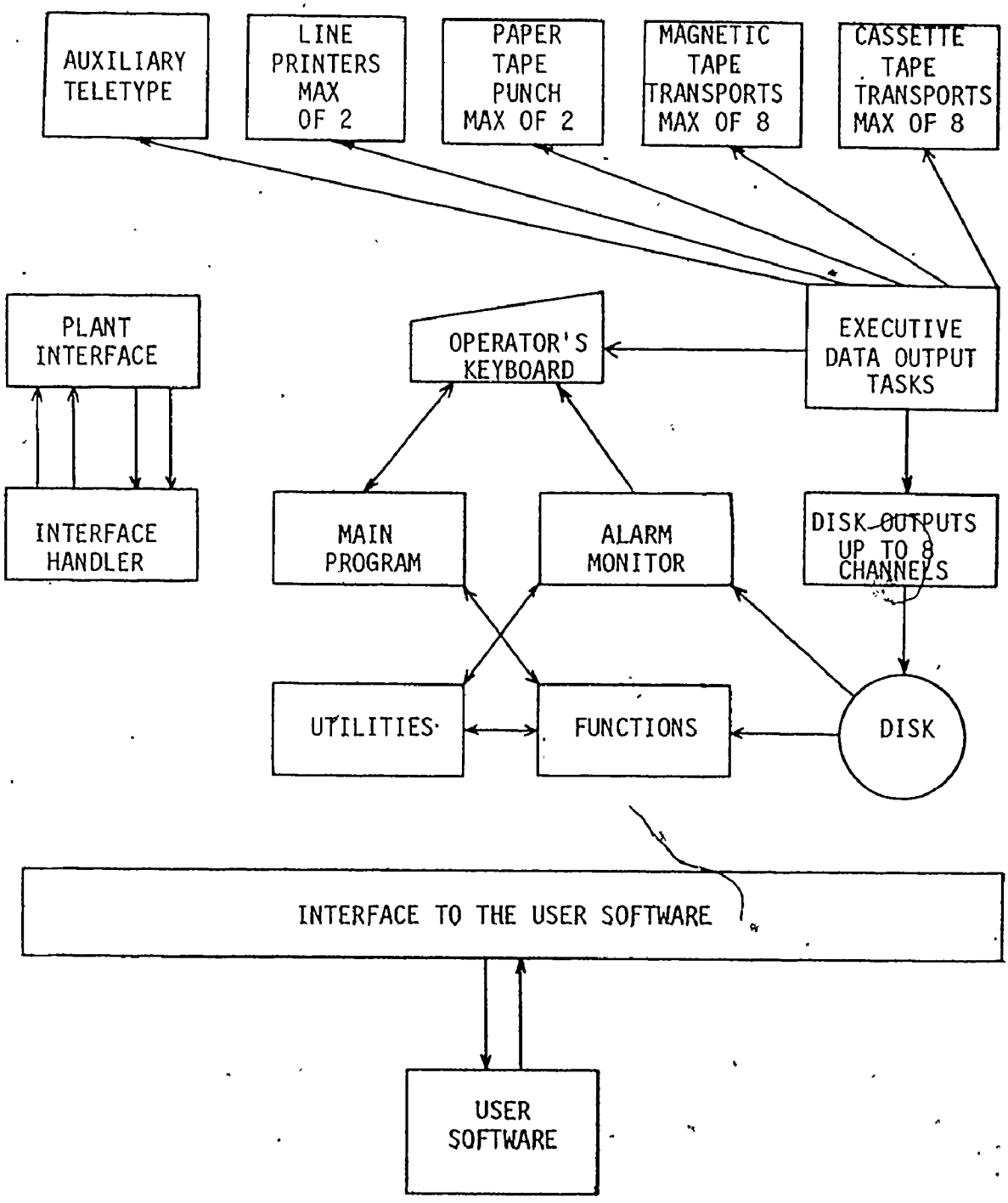


TABLE 4-1

GOSEX ROUTINES

UTILITIES

ERROR	-fatal error reporting
KEYED	-keyboard input buffering
ENCOD	-string encoding
DECOD	-string decoding
BDEC	-binary to decimal convert
BOCT	-binary to octal convert
BFLT	-binary to floating point convert
DBIN	-decimal to binary convert
OBIN	-octal to binary convert
FBIN	-floating point to binary convert
MTPLY, MTPLA	-single precision unsigned multiply
DIVID, ROUND	-single precision unsigned divide
LOCAT, RETRV	-buffered character storage and retrieval
LNEAR, LNVRS	-linear integer polynomial
QUAD, QNVRS	-quadratic integer polynomial
NUMBS	-single precision signed integer compare
RANGE	-absolute address testing
MFINT, MFENT, MFEXT	-access to the floating point interpreter in a multitask environment
DSKMG	-disk message file access
CONTL	-single variable three term controller
FLTER	-first order filter

EXECUTIVE TASKS

INTRP	-main program
MNITR	-user alarm monitor
MTPLX	-interface handler
LOGER	-logging routine
PLTER	-plotting routine
PFILE	-profiling routine
COPER	-copying routine
CHTER	-analog output routine

TABLE 4-1

(cont'd)

FUNCTIONS

USER TASK CONTROL	START	-start a user task
	CEASE	-kill a user task
	STATS	-obtain status of a user task
EXECUTIVE DATA OUTPUT TASK CONTROL	LOG	-data logging initiator
	MYLOG	-data logging initiator
	PLOT	-data plotting initiator
	PROFL	-data profilling initiator
	COPY	-data transfer initiator
	CHART	-analog output initiator
	ENDIO	-kill a selected output task
	ENDAL	-kill all output tasks
	CHNGE	-change display rate of a selected output task
ON-LINE PARAMETER DISPLAY AND CHANGE	PARAM	-general parameter display and change
	TUNER	-controller parameter display and change
MISCELLANEOUS		
	DIALG	-operator report generation
	CLEAR	-delete a disk log file
	READY	-initialize a magnetic tape device or disk subdirectory
	RELSE	-release a magnetic tape device or disk subdirectory
	CLOCK	-output time of day and day's date
	RETRN	-return to the RDOS CLI

between his programs and GOSEX. This interface characterizes his application. At run-time, the operator controls all operations of the GOSEX package and user tasks through an expandable set of functions. For complete information about the GOSEX package, the reader is directed to two references: Tremblay [1975] and Tremblay [1977a].

The GOSEX package occupies approximately 4K of central processor memory. The actual usage depends on the number of devices and the size of buffers configured for a particular application. A typical memory layout of a 32K computer at run-time is given in Figure 4-2. In a FORTRAN IV environment, available core for user programming exceeds 14K in a 32K machine.

Up to 30 standard output devices are supported by GOSEX. They are:

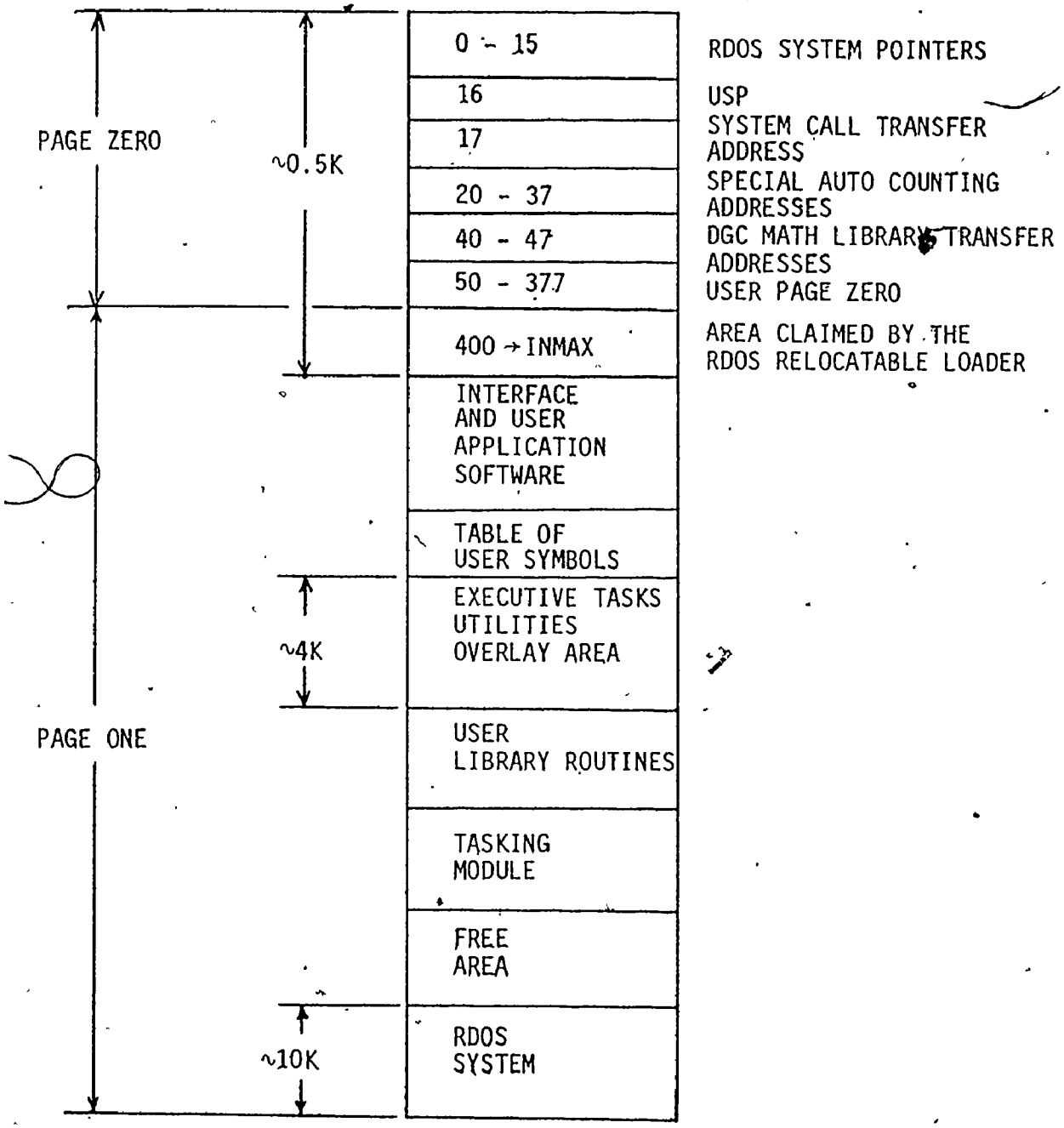
- 2 teletypers (or similar devices)
- 2 line printers
- 2 high speed paper tape punches
- 8 magnetic tape transports
- 8 cassette tape transports
- 8 parallel disk channels.

In addition, user tasks may output on other disk channels. Under GOSEX, the output devices are identified by the following names and unit numbers:

CONSL	- operator's console
TTYPE	- auxiliary teletyper
PRINT(O&1)	- line printer

FIGURE 4-2

GOSEX MEMORY LAYOUT AT RUN-TIME



The tasking module occupies about 1K when user tasks are in assembler only. When FORTRAN IV tasks exist, the tasking module occupies about 1.5K. The FORTRAN IV library routines must also be included. The free area is claimed for the run-time stack at run-time.

PUNCH(0&1) - high speed paper tape punch
CASET(0-7) - cassette tape transport
MAGTP(0-7) - magnetic tape transport
DISK - disk

The GOSEX package has been tested extensively and is now widely used in computer based control research at McMaster University. GOSEX is being used in process research at Ontario Hydro's Bruce Heavy Water Plant in Tiverton, Ontario.

4.2 GOSEX Utilities

Twenty-eight subroutines have been developed and form a library of core resident utility programs. These have been listed in Table 4-1. All subroutines are reentrant since they store data in an area indexed by the calling tasks's "USP". Under RDOS, each active task is assigned its own "USP": memory cell 16. The "USP" may be considered as a reentrant storage register.

Except for utilities DSKMG and CONTL, the minimum work area is 10 (decimal) words. This area provides temporary and return address storage for all utilities and is often used to exchange information between the utility and the calling task. Utility DSKMG requires a 17 (decimal) word work area and CONTL requires 49 (decimal). Some locations in the extensions to the basic 10 (decimal) word work area must contain special data required by the DSKMG and CONTL utilities.

Because most of the GOSEX utilities have been designed to assist

executive operations, only a few are useful in the development of application software. Those that may be called by the user are denoted by an asterisk. This section is devoted to the description of each utility. The descriptions follow.

ERROR - Fatal Error Reporting (*)

A special subroutine for the identification of unusual error conditions is available. A call to this routine causes the calling task to be raised to the highest software priority level and all parallel tasks of lower priority to be killed. A message is then output to the keyboard and has the form:

CRASH @ ADDR [TASK ID] RDOS TEXT MESSAGE

"ADDR" specifies the absolute core address from which the call to the error subroutine was made. The task identification code of the task which made the call is specified within the square brackets. Since a call to this utility causes an unconditional return to the CLI (RDOS' off-line executive), the operating system is used to indicate the nature of the error condition. From a loader map, the user may directly identify the source of the error.

KEYED - Keyboard Input Buffering

A number of utilities and functions process buffered character strings. The buffering of keyboard input is performed by this subroutine. When calling it, the maximum number of characters to be buffered must be specified. If, on input, the character input count

exceeds this number, the input string is ignored and a restart occurs. Striking the "ESC" key causes an abnormal return to the calling task. The normal return occurs only after a carriage return and in this case the actual character input count is passed to the calling task. A null is appended to the buffered string.

ENCOD - String Encoding

A convenient means of characterizing a string of characters is to translate it into a unique numerical quantity. The recognition of symbols by the GOSEX executive follows this principle. Following the convention defined by the Data General Corporation assembler, buffered strings of up to five alphanumeric characters are encoded into two integers. The technique is illustrated by the following example.

To encode the string "ABCDE", the coding value of each character of the string is determined from Table 4-2. These are then combined in the following way:

```
[A] = 11        (([A]·40+[B])·40+[C]) = 10093.
[B] = 12
[C] = 13

[D] = 14        (([D]·40+[E])·32) = 18400.
[E] = 15
```

After performing the above calculation on a character string, the ENCOD subroutine compares the resulting numbers with those found in a symbol table. This table is prepared off-line and consists of a series of three word entries. Two of the words in each entry are the coded representation of a symbol. The third word is the symbol's value.

TABLE 4-2

CHARACTER CODING VALUES

CHARACTER	CODING VALUE	CHARACTER	CODING VALUE
NULL	0	I	19
Ø	1	J	20
1	2	K	21
2	3	L	22
3	4	M	23
4	5	N	24
5	6	O	25
6	7	P	26
7	8	Q	27
8	9	R	28
9	10	S	29
A	11	T	30
B	12	U	31
C	13	V	32
D	14	W	33
E	15	X	34
F	16	Y	35
G	17	Z	36
H	18	DOT	37

Usually, this value is established by the loader and specifies the core address which the symbol defines. Upon a successful comparison, the symbol's value is recovered. This and the core address of the symbol's table entry are passed to the calling task. If an illegal character was found in the buffered string or the string was not defined in the symbol table, the abnormal return to the task is used.

DECOD - Symbol Decoding

Headings for data outputs may be readily generated from information found within the symbol table. By passing to the DECOD subroutine the address of the appropriate symbol table entry, the coded representation of the symbol is recovered and decoded into a buffered string of five alphanumeric characters, preceeded and followed by a space.

BDEC - Binary to Decimal Convert

This utility translates a single precision signed binary integer into a string of ASCII decimal digits. The string is buffered so that lines of output may be prepared. The form of the seven character buffered text string produced by this routine is illustrated below:

```
(SPACE)DDDDD(SPACE)      for positive integers,
     -DDDDD(SPACE)       for negative integers,
```

where "D" indicates any decimal digit.

BOCT - Binary to Octal Convert

If translation from binary to ASCII octal is required, this utility subroutine is used. Like BDEC, it also produces a buffered text string of seven characters. The form of the string is

```
(SPACE)00000(SPACE)      for integers less than 100000,
      100000(SPACE)      for integers greater than 77777,
```

where "O" indicates any octal digit.

BFLT - Binary to Floating Point Convert

Where floating point outputs are desired, this utility produces a base ten exponential representation of a single precision binary floating point number. The ASCII string of fourteen characters is buffered so that lines of output may be generated. The form of the text string is given below:

```
(SPACE).DDDDDDDE±NN(SPACE)   for positive numbers,
     -.DDDDDDDE±NN(SPACE)    for negative numbers,
```

where "D" and "N" denote any decimal digit.

DBIN - Decimal to Binary Convert

The conversion of a string of decimal digits into a single precision signed binary integer is accomplished by this utility subroutine. The string of up to six ASCII characters (including a sign) must be buffered. Illegal characters cause an abnormal return to the caller.

OBIN - Octal to Binary Convert

This utility translates a buffered string of up to six ASCII octal characters (including an optional sign) into a single precision binary integer. As with DBIN, illegal characters in the string cause an abnormal return to the calling routine.

FBIN - Floating Point to Binary Convert

Buffered inputs of fixed point or base ten exponential numbers are converted into single precision binary floating point numbers by this utility. ASCII strings may not exceed thirteen characters. Illegal characters or formats cause an abnormal return to the calling routine.

MTPLY, MTPLA - Single Precision Unsigned Multiply(*)

The MTPLY utility provides the facility to multiply two single precision unsigned integers. The result is a double precision unsigned integer. When it is desired to add a single precision unsigned integer to the product, utility MTPLA is used instead.

DIVID, ROUND - Single Precision Unsigned Divide (*)

Utility DIVID is called to divide a double precision unsigned integer by a single precision unsigned integer. The quotient is a single precision unsigned integer. If required, rounding of the result is achieved by the ROUND utility routine.

LOCAT, RETRV - Buffered Character Storage and Retrieval

A compact means of buffering ASCII character strings is to pack two characters to each 16-bit computer word or one character per byte. The LOCAT and RETRV utilities assume that character strings are stored in sequential words of memory and packed left to right within each word. When called, the LOCAT utility places a character into a byte without affecting the other byte of the word. Conversely, the RETRV utility retrieves a character from a byte. These routines are guided to the byte of interest by a byte pointer.

LNEAR, LNVRS - Linear Integer Polynomial (*)

User application software written in assembler language must often convert data from one set of units to another using a linear polynomial. For instances where integer arithmetic is precise enough, a linear equation and its inverse are available. The expressions are:

$$y = a*x+b \qquad (4\text{-}1)$$

$$x = \frac{y-b}{a} \qquad (4\text{-}2)$$

Coefficients "a" and "b" must be scaled quantities.

QUAD, QNVRS - Quadratic Integer Polynomial (*)

These utility routines are very much like LNEAR and LNVRS above except that these are quadratic routines. The expressions are:

$$y = a \cdot x^2 + b \cdot x + c \qquad (4\text{-}3)$$

$$x = \frac{-b + \sqrt{b^2+4 \cdot a \cdot (y-c)}}{2\ a} \qquad (4\text{-}4)$$

Coefficients "a", "b", and "c" must be scaled quantities.

NUMBS - Single Precision Signed Integer Compare (*)

The magnitude of two single precision signed integers may be compared using this utility. The routine returns to the caller by one of two routes.

RANGE -- Absolute Address Testing

This utility establishes the relative position of an absolute core address. Three separate returns from this routine are possible. The argument address may lie within user address space in page one, the symbol table space in page one or anywhere else in memory.

MFINT, MFENT, MFEXT - Access to the Floating Point Interpreter in a Multitask Environment (*)

For instances where all user application software is written in assembler language, access to the Floating Point Interpreter in a multitask environment is provided by this utility. Quite simply, the utility performs the swapping of the Interpreter pointers that would normally have to be performed by the user software. It does not expand the capabilities of the Interpreter. It is still necessary to ensure

that parallel tasks accessing the Interpreter operate at different priority levels. Attempts at output from the interpretive mode are thwarted by the utility.

A call to MFINT initializes a work area. Entrance and exit from the interpretive mode occur upon MFENT and MFEXT calls respectively.

DSKMG - Disk Message File Access

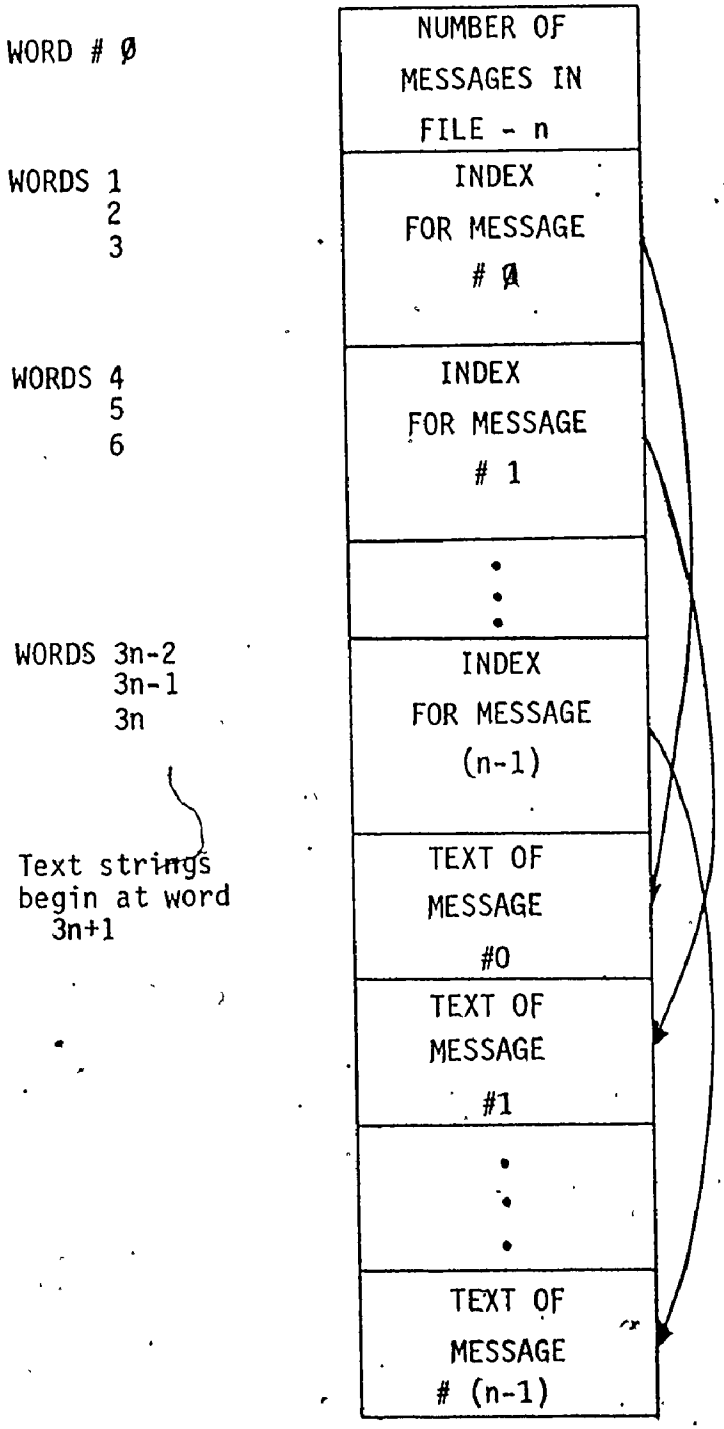
It was previously indicated in Section 1 of this chapter that a specially formatted disk file was accessed to output alarm messages to the keyboard. In addition to this, all messages used in dialogue with the operator are also kept in another disk file. This utility subroutine accesses these disk message files, recovers the message of interest and outputs it to the keyboard.

The structure of a disk message file is shown in Figure 4-3. The first word in the file indicates the number of messages stored within the file. Following this entry is a message directory consisting of three word index blocks. Each block position refers to a given message number. The first index block in the directory refers to message #0, the second to message #1, and so on. Each index block provides the starting position of the message in the file and its character count. The messages proper are stored end to end in the disk file following the message directory. The disk message files are produced off-line using the SORT assembler developed for this work. The use of the SORT assembler is outlined in Section 5.

FIGURE 4-3

STRUCTURE OF A DISK

MESSAGE FILE



Utility DSKMG requires a 7 word extension to the basic 10 (decimal) word work area.

CONTL - Three Term (PID) Position Type Controller (*)

A three term position type controller is available for single input-single output systems. It may be called from routines written in FORTRAN IV. To do this, the user must be familiar with the FORTRAN IV run-time stack. Input data is filtered (see utility FLTER) before being used to compute a control action. The control algorithm is based on the following expressions:

$$P = Pm + K_p \cdot \varepsilon(t) + K_D \cdot \frac{\Delta\varepsilon}{\Delta t} + K_I \cdot \Delta t \cdot \Sigma\varepsilon \qquad (4\text{-}5)$$

$$\frac{\Delta\varepsilon}{\Delta t} = \frac{11 \cdot \varepsilon(t) - 18 \cdot \varepsilon(t-1) + 9 \cdot \varepsilon(t-2) - 2 \cdot \varepsilon(t-3)}{6 \cdot \Delta t} \qquad (4\text{-}6)$$

where P = output control action

P_m = mean value of the output control action

$\varepsilon(t)$ = measurement's deviation from the setpoint at time t

K_p = proportional gain

K_D = proportional-derivative gain, $K_p \cdot \tau_D$

K_I = proportional-integral gain, K_p/τ_I

$\frac{\Delta\varepsilon}{\Delta t}$ = approximate time derivative of the error

Δt = control interval

$\Sigma\varepsilon$ = approximate integral of the error

The approximate time derivative is computed from the expression given above. Computation of a derivative based on differenced data is sensitive to measurement error.

The use of integral action in a control loop may lead to serious reset windup whenever load disturbances or set point changes occur. This effect is reduced by an anti-reset windup algorithm incorporated in this controller. If the controller indicates that action should be outside the bounds specified by the controller's output limit parameters, then the integral sum is not augmented for the current control interval.

The CONTL utility requires an extension of 39 words to the basic 10 (decimal) word work area. Certain entries in this extended area may be examined and changed at run-time by envoking the TUNER executive function (see Section 4).

FLTER - First Order Filter (*)

A first order filter may be used to smooth input data. Data is modified by the following algorithm:

$$\bar{y}(t) = \alpha \cdot \bar{y}(t-1) + (1-\alpha) \cdot y(t) \qquad (4\text{-}7)$$

where $\bar{y}(t)$ = filtered data at time t
$y(t)$ = raw data at time t
α = filter constant, $0 \leq \alpha < 1$

Only positive integer data is accepted by this utility and the filter constant must be scaled.

4.3 Executive Tasks

The executive tasks INTRP, MNITR and MTPLX listed in Table 4-1 are the only tasks which are active initially. All other executive tasks perform data output and must be created at run-time by the operator. Although only five data output routines are indicated, more than five output tasks may exist in practice. For example, individual data log outputs are controlled by independent tasks but are generated by the routine LOGER. Consequently, all output formats and display intervals may be different.

INTRP - Main Program

At run-time, the operator communicates with the main program via the operator's console. However, alarming and data output activity also require access to the keyboard. Since three different GOSEX tasks are competing in real time for the same device, some control is required. The operator must be able to gain access to the main program regardless of the activity on the keyboard. To gain access to the operator's console, an operator interrupt character or password must be transmitted to the main program. This action guarantees the operator uninterrupted use of the keyboard. Upon the release of the keyboard, the alarm monitor is offered access to it once every second. If neither the operator nor the alarm monitor are using the keyboard, access is granted to an active data output executive task.

The main program establishes primary communication with

the operator. Its sole purpose is to obtain the name of an executive function. This is used to call a routine which establishes further dialogue with the operator. The routine which allows the operator to display and change parameter values is an example of an executive function. In all, twenty standard functions are available, and custom user defined functions may be added to the GOSEX executive.

MNITR - User Alarm Monitor

To provide user tasks with the means of outputting messages to the keyboard in an orderly manner, the alarm monitor was devised. Once every second, the alarm monitor scans a table of alarm flags provided by the user. Whenever a flag is raised, an appropriate message stored in a specially formatted disk file is recovered and outputed to the operator's console. A user task may inform the operator of alarm conditions by simply raising flags in the table of alarm flags. The disk message file created for the alarm monitor is produced by a program known as the SORT assembler. This program was developed so that test messages would not have to be stored in computer memory.

MTPLX - Interface Handler

If any one thing characterizes a given installation, it is the type of hardware that exists between the computer and the field. To accommodate the possibility that changes in this interface will eventually be required, the handlers for custom peripheral devides have been assembled as a separate executive task. At run-time, this

task is automatically activated at a user specified frequency. This task would for example initiate the sequential scan of analog to digital convert inputs. This single executive task controls the inputs and outputs of the hardware interface. It operates from a series of information blocks comprising a portion of the link between user tasks and GOSEX. The use of buffers to exchange information between user tasks and GOSEX provides two things. Transfers of data between user tasks and the plant are simplified. Hardware reconfigurations result in minimal source modifications to GOSEX.

Executive Data Output Tasks

Five different types of data output may be generated at run-time. Details on the initiation of the executive output tasks are given in Section 4. A logged output provides a display of data in decimal integer or floating point format. The plot, profile and chart data outputs display data in graphical form. The exchange of data between peripherals -- such as the printing of the contents of a disk file on a line printer -- is accomplished by a copy output.

Logged outputs may be to any of the output devices listed in Section 1. Databases may be produced in either ASCII or binary format. Plot and profile outputs may only be directed to teleprinters and line printers. The copy outputs may be to any output device except a teleprinters. Whereas the log, plot, profile and copy outputs are to standard peripherals, the chart output is to the computer's analog

outputs. Displays on strip chart recorders or storage oscilloscopes are then possible. Samples of log, plot and profile outputs have been reproduced in Figures 4-4, 4-5 and 4-6 respectively.

4.4 Standard GOSEX Functions

The standard GOSEX executive functions are listed in Table 4-1. All executive functions are loaded together into an overlay file prior to run time. At run time and upon operator request, the appropriate portion of the overlay file is brought into memory for execution of a function. GOSEX also allows individual users to write special purpose executive functions. These become part of the executive and consequently they must resemble the standard executive functions with respect to structure and linkage to the various utilities.

The operator interrupt or password -- teletype code <CTRL E> must be given before any function may be envoked. After the password has been given, the executive suspends all outputs to the operator's console. The operator is then prompted to enter the name of a function. Naming errors are reported. If the name was that of an executive function, further dialogue is established by the function itself. Once, the function has completed its operations, suspended outputs to the operator's console are reactivated.

Four groups of standard GOSEX functions are described below. The description for each group is in two parts. The first briefly relates

FIGURE 4-4

FORMAT OF THE LOG OUTPUT

DATE OF RECORD II JJ Th RECORD ID LOG-FORMAT

TIME	TOTER	T1	T2	T3	T4	T5	T6	T7
SELCS								
05 57 10	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 15	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 20	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 25	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 30	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 35	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 40	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 45	[illegible]	00003	00010	00015	00020	00015	00010	00005
05 57 50	[illegible]	00003	00010	00015	00020	00015	00010	00005

FIGURE 4-5

FORMAT OF THE PLOT OUTPUT

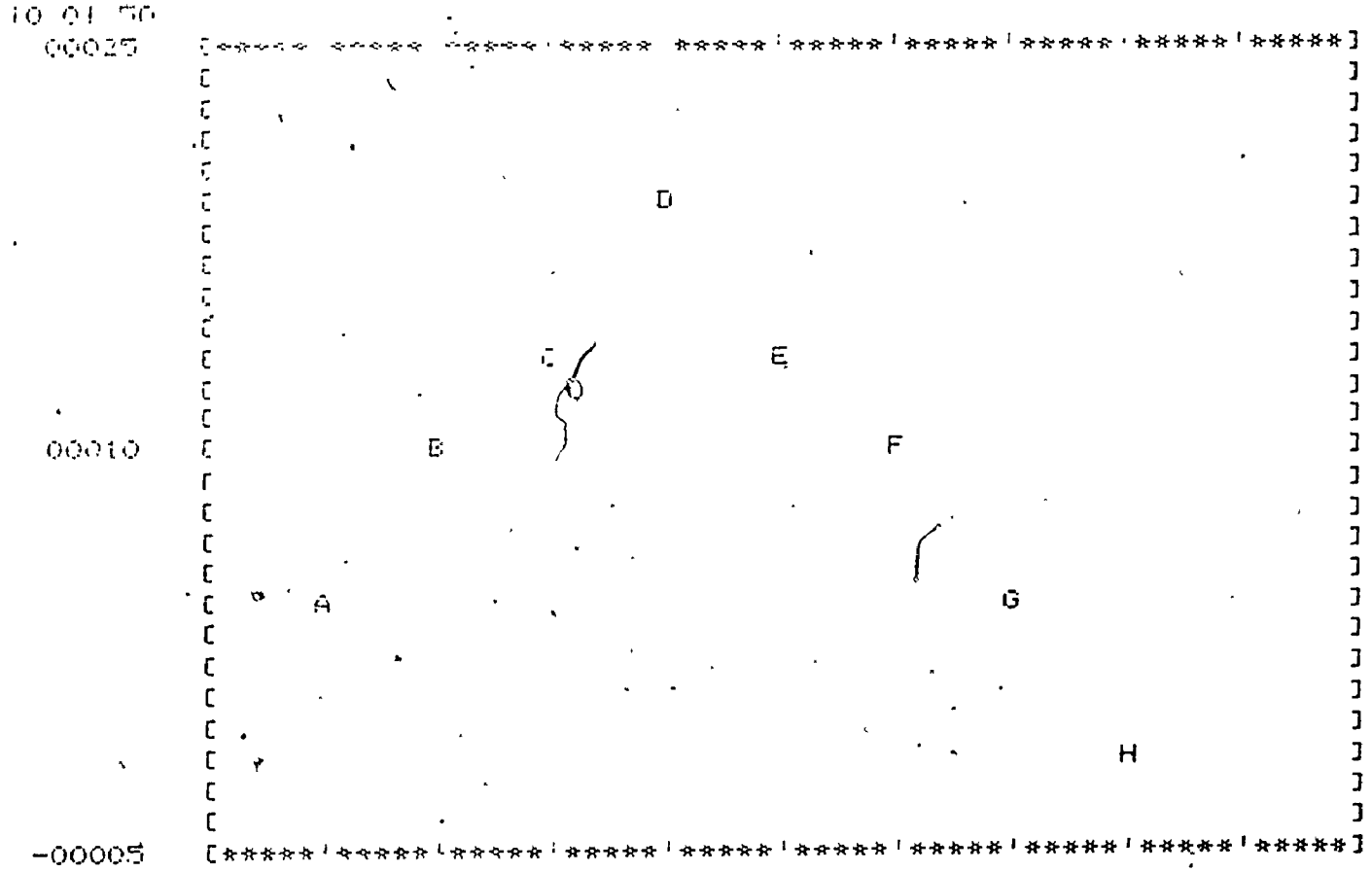
```
DATE OF REPORT  [illegible]  RECORD-ID  PLOT-FORMAT

VARIABLE SYMBOL SCALE FACTOR
   T1        A      -00002
   T2        B       00001
   T3        C       00001
   T4        D       00001
   T5        E       00001
   T6        F       00003
   T7        G       00001

                                         00010                           00050
09 5[illegible]  [****** ****** ***A** ****** *G***B***E* *D***!**F**!*****!*****]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
09 5[illegible] [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
                         A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
09 5[illegible] 45 [          A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
10 00 1[illegible] [          A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
          [              A         G   B   E   D      F              ]
```

FIGURE 4-6

FORMAT OF THE PROFILE OUTPUT

DATE OF RECORD 11/22/78, RECORD ID PROFL-FORMAT

VARIABLE	SYMBOL	AXIAL POSITION
T1	A	00010
T2	B	00020
T3	C	00030
T4	D	00040
T5	E	00050
T6	F	00060
T7	G	00070
T8	H	00080



the purpose and operation of the various functions within that group. The second part outlines the run-time operating procedure. In these portions, the text in italics is generated by the computer. All other text except the comments is provided by the operator. The GOSEX functions (except ENDAL, CLOCK and RETRN) may be prematurely terminated by striking the "ESC" key at the operator's console.

START, CEASE, STATS - User Task Control Functions

These three functions provide the operator with control over the user tasks. The START function as the name implies is used to initiate a user task. To kill an active user task, the CEASE function is envoked. The status -- active or inactive -- of a user task is determined by the STATS function. Each function operates from information provided in the "user task definition table" (see Section 5). Entries in this table identify the user tasks by specifying a task priority, identification and starting address. Tasks may be written in FORTRAN IV or assembler language. A task kill flag is also assigned to each user task. It indicates to the CEASE function whether the task may be killed directly by a scheduler command or if the task must be informed to kill itself. The latter mode is used when a user task is using overlays or has opened read/write disk channels.

START - Start a User Task

```
<CTRL E>
START
TASK NAME:  CSTR
```

Operator is prompted to specify a

user task name defined in the "user task definition table".

Possible messages:

NOT A USER TASK	Either the task name was not defined in the symbol table or it was not defined in the "user task definition table". The prompt is reissued.
TASK IS ALREADY ACTIVE	User task was found to be active. Function terminates.
USER TASK CREATED	User task was created. Function terminates.

CEASE - Kill a User Task

<CTRL E>
CEASE
TASK NAME: CSTR

Operator is prompted to specify a user task name defined in the "user task definition table".

Possible messages:

NOT A USER TASK	Either the task name was not defined in the symbol table or it was not defined in the "user task definition table". The prompt is reissued.
TASK IS ALREADY INACTIVE	User task was found to be inactive. Function terminates.
USER TASK KILLED	User task was killed. Function terminates.

STATS - Provide the Status of a User Task

<CTRL E>
STATS
TASK NAME: CSTR

Operator is prompted to specify a

	user task name defined in the "user task definition table".

Possible messages:

NOT A USER TASK	Either the task name was not defined in the symbol table or it was not defined in the "user task definition table". The prompt is reissued.
TASK IS ACTIVE	User task was found to be active. Function terminates.
TASK IS INACTIVE	User task was found to be inactive. Function terminates.

LOG, MYLOG, PLOT, PROFL, COPY, CHART, ENDIO, ENDAL, CHNGE - Executive Data Output Task Control Functions

The recording of process data for use in off-line studies is an essential operation in any data acquisition and control application. At run time, other forms of data display such as data trending or profiling usually are more useful to the operator. These facts necessitate the generation of multiple outputs. To meet these requirements, GOSEX provides six standard functions to initiate five types of executive data output tasks. Functions which terminate or alter the display rate of these tasks are also provided.

The LOG and MYLOG functions create outputs to any of the output peripheral devices listed in Section 1. Besides the usual ASCII text output format, a binary format may be generated. Data may be displayed in either decimal integer or floating point. Both functions begin by requesting the name of the logging device. If the device is not a

teletype or a disk, the device unit number is also requested. If the device has been configured in the system and is not already active, a record identification is accepted from the operator. The choice of ASCII or binary output must be made if output is to a high speed paper tape punch, magnetic tape transport, cassette transport or disk (if binary output is selected, the binary data may be translated into ASCII by an off-line program). The only differences between the LOG and MYLOG functions appear at this point. With LOG, the operator must specify at the keyboard those variables to be logged and whether in integer or floating point format. On the other hand, MYLOG reads this information from a disk file produced by the SORT assembler described in Section 5. An example of a file's source format is given in Figure 4-7. MYLOG will report errors if any of the following conditions arise:

- a variable is not defined in the user symbol table
- a variable name contains more than five characters
- the character appended to the variable name is not "@" or "#".

Integer format is specified by the "@" character and floating point by "#". Once the variable list is completed, the operator must input the logging interval. If necessary, he also must input the disk file for output to a disk or the tape file number for output to cassette or magnetic tape transports. Logging begins once this data is provided.

The trend plotting of data is initiated by function PLOT and the profiling of data by function PROFL. These outputs may be directed to teletypes and line printers only to provide the operator with a

FIGURE 4-7

FORMAT OF THE MYLOG LIST SOURCE

```
T1@
T2@
T3@
T4@
OBJ#
TFLOW#
NOISE@
RTRDP@
PUFO#
@
```

The "@" appended to a variable name selects integer format on output. Floating point format is selected by the "#" character. The lone "@" at the end of the list is the SORT assembler pseudo-op indicating the end of list. Refer to section 5 for details on the SORT assembler.

graphical display of data. The dialogue of the PLOT and PROFL functions follows that of the LOG function except for the following differences. Only integer data is acceptable for output. The PLOT function requests a scale factor for each variable, thus permitting the trending of data with orders of magnitude difference. With PROFL, input of the data's spacial position (or similar dimension except time) is necessary. The minimum and maximum values of the plotting range must be specified. Output begins upon completion of the data input.

It is frequently necessary to transfer information from one peripheral device to another. An example of this would be the transfer of a file from cassette to disk for use by function MYLOG. The executive tasks which perform these transfers are initiated by the COPY function. The function begins by requesting the name of the device to which the transfer is to be made. All output devices listed in Section 1 except the teletypes may be used. The device unit number is also requested if the device is not a disk. If a disk was specified for output, the disk filename must be given. A tape file number is requested if output is to cassette or magnetic tape. Finally, the RDOS filename of the source must be provided before the executive task is created. All executive output tasks created by the COPY function operate at the lowest software priority level possible.

Where data output to strip chart recorders or storage oscilloscopes is desired, the CHART function must be used. Since the computer

analog outputs are non-standard peripheral devices, only one executive output task is created for output to them. Because of this special circumstance, the creation and killing of this executive task is performed by function CHART itself. Aside from this point, CHART's operation closely parallels the PLOT function. Instead of specifying a scale factor for each variable, the minimum and maximum of the plotting range is required.

Three GOSEX functions allow the operator to alter the operation of active executive output tasks at run-time. They however cannot affect the operation of the output task created by the CHART function. The display interval of all executive data output tasks not created by the COPY function may be altered by the CHNGE function. Executive output tasks not created by function CHART may be killed by functions ENDIO and ENDAL. With ENDIO, a selected output task may be terminated. The device in question is selected in the manner described for the LOG and MYLOG functions above. The ENDAL function kills all active output tasks.

LOG, MYLOG - Data Logging Initiators

```
<CTRL E>
LOG [MYLOG]
DEVICE NAME:  MAGTP
```

Operator is prompted to select an output device name. Those given in Section 1 are acceptable.

Possible messages:

NOT A DEVICE NAME — Device name was not one of those listed in Section 1. The prompt is reissued.

DEVICE NOT PART OF SYSTEM — Specified device was not configured for the application. Function terminates.

DEVICE IN USE — An active output task already exists on the teletype device. Function terminates.

ALL BUFFERS IN USE — All device buffers configured for use are already in use. Function terminates.

If the device is not a disk or a teletype, the following query appears:

DEVICE UNIT #: 3 — An integer, as indicated in Section 1 is expected.

Possible message when unit # is accepted:

DEVICE IN USE — An active output task already exists on the indicated device unit #. The prompt is reissued.

Once the output device has been selected, the following appears:

RECORD ID: GOSEX-OUTPUT
Any 20 character string is accepted.

If the selected output device is not a teletype or a line printer, the following appears:

ASCII OR BINARY OUTPUT: A
Only characters "A" and "B" are accepted.

The following applies to the LOG function only.

VARIABLES LIST-MAX: *00040*

The number is specified when the GOSEX package is configured by the user.

00001 VRBL 1
FORMAT F

Any variable name defined in the symbol table or any octal address in user page one is accepted. Duplicated entries are ignored. Only characters "I" for integer and "F" for floating point are accepted for the format.

00040 GOSEX
FORMAT I
END OF LIST

Requests continue until the maximum number of variables have been entered.

A partial list is obtained by striking the carriage return when a variable name is requested. If this is done for the first request, the following message appears before the prompt is reissued:

NO LIST

The following applies to the MYLOG function only.

PREFORMATTED LIST DISK FILENAME: LOGLIST. LT

The name of the disk file which contains variable name and formatting information must have been produced by the SORT assembler. If the filename is in error or if the selected device buffer cannot accommodate the full list of variable names in the file, the prompt is reissued.

If errors are detected when reading the file, the following message, one for each error found in the file appears:

LIST ERROR, ENTRY #00005

The number indicates the line # in error. Function terminates.

The following is common to the LOG and MYLOG functions:

LOGGING INTERVAL(SECONDS): 60

Operator is prompted to select the logging interval.

Possible messages:

INTERVAL IMPROPERLY SPECIFIED
Specified interval was in error. The prompt is reissued.

If the output is to a magnetic tape device, the following appears:

TAPE FILE #: 8 — Operator is prompted to specify the file # on the selected tape unit. The number must be between 0 and 99.

If output is to a disk, the following appears:

DISK DIRECTORY AND FILENAME: GOSEX. GX
The operator is prompted to specify the RDOS filename or a disk file to be used for the logged output.

If either function is unable to initiate the executive output task, the following appears:

UNABLE TO INITIATE OUTPUT TASK

If the output task was created and it was not to the operator's console, the following appears:

OUTPUT TASK CREATED

PLOT, PROFL - Data Plotting Initiators

<CTRL E>
PLOT [PROFL]
DEVICE NAME: PRINT — Operator is prompted to select an output device name. Only acceptable names are CONSL, TTYPE or PRINT.

Possible messages:

NOT A DEVICE NAME — Device name was not one of those listed in Section 1. The prompt is reissued.

DEVICE NOT PART OF SYSTEM — Specified device was not configured for the application. Function terminates.

DEVICE NOT EQUIPPED FOR PLOTTING — Plot or profile outputs are not permitted on the selected device.

DEVICE IN USE — An active output task already exists on the teletype device. Function terminates.

ALL BUFFERS IN USE — All device buffers configured for use are already in use. Function terminates.

If the device is a line printer, the following query appears:

DEVICE UNIT #: 0 — Integers 0 or 1 are accepted.

Possible message when unit # is accepted:

DEVICE IN USE — An active output task already exists on the indicated device unit #. The prompt is reissued.

Once the output device has been selected, the following appears:

RECORD ID: GOSEX-OUTPUT
Any 20 character string is accepted.

VARIABLES LIST-MAX: 00040
The number is specified when the GOSEX package is configured by the user.

The following applies to the PLOT function only.

00001 VRBL 1
SCALE FACTOR: 6
Any variable name defined in the symbol table or any octal address in user page one is accepted. Duplicated entries are ignored. All non-zero scale factors are accepted.

00040 GOSEX
SCALE FACTOR: -3
END OF LIST
Requests continue until the maximum number of variables have been entered.

The following applies to the PROFL function only.

00001 VRBL
AXIAL POSITION: 24

Any variable name defined in the symbol table or any octal address in user page one is accepted. Duplicated entries are ignored. Acceptable axial positions are integers from 1 to 99 inclusive.

00040 GOSEX
AXIAL POSITION: 87
END OF LIST

Requests continue until the maximum number of variables have been entered.

The following is common to the PLOT and PROFL functions.

A partial list is obtained by striking the carriage return when a variable name is requested. If this is done for the first request, the following message appears before the prompt is reissued:

NO LIST

PLOTTING INTERVAL(SECONDS): 60

Operator is prompted to select the plotting interval.

Possible messages:

INTERVAL IMPROPERLY SPECIFIED

Specified interval was in error. The prompt is reissued.

The lower and upper range of the data to be plotted must be specified. The following queries appear:

MIN RANGE OF PLOT: -2
MAX RANGE OF PLOT: 10

Possible message:

?

Specified range is unacceptable. Prompts are reissued.

If either function is unable to initiate the executive output task, the following appears:

UNABLE TO INITIATE OUTPUT TASK

If the output task was created and it was not to the operator's console, the following appears:

OUTPUT TASK CREATED

COPY - Data Transfer Initiator

<CTRL E>
COPY

DEVICE NAME: MAGTP	Operator is prompted to select an output device name. Those given in Section 1 are acceptable except for CONSL and TTYPE.

Possible messages:

NOT A DEVICE NAME	Device name was not one of those listed in Section 1. The prompt is reissued.
DEVICE NOT PART OF SYSTEM	Specified device was not configured for the application. Function terminates.
NO COPY TO TTY DEVICE	The device name indicated a teletype device. Function terminates.
ALL BUFFERS IN USE	All device buffers configured for use are already in use. Function terminates.

If the device is not a disk, the following query appears:

DEVICE UNIT #: 3	An integer, as indicated in Section 1 is expected.

Possible message when unit # is accepted:

DEVICE IN USE	An active output task already exists on the indicated device unit #. The prompt is reissued.

If the output is to a magnetic tape device, the following appears:

TAPE FILE #: 8 — Operator is prompted to specify the file # on the selected tape unit. The number must be between 0 and 99.

If the output is to a disk, the following appears:

DISK DIRECTORY AND FILENAME: GOSEX GX — The operator is prompted to specify the RDOS filename of a disk file to be used for the transfer.

The RDOS filename of the source for the data transfer must be provided:

SOURCE FILENAME: CTO:2

If the function is unable to initiate the executive output task, the following appears:

UNABLE TO INITIATE OUTPUT TASK

If the output task was created, the following appears:

OUTPUT TASK CREATED

CHART - Analog Output Task Initiator

<CTRL E>
CHART

Possible messages:

NO ANALOG OUTPUTS — The GOSEX package was not configured for data charting.

CHART IN USE. KILL? [Y/N]: Y — The analog outputs are currently being used by an active output task. "Y" for yes and "N" for no are the acceptable responses. If the reply is "N", the function terminates. "Y" kills the task. The function then prepares to initiate another output task.

The list of variables for plotting must be entered.

VARIABLES LIST-MAX: 00004
The number is specified when the GOSEX package is configures by the user.

00001 VRBL
MIN RANGE OF PLOT: -2
MAX RANGE OF PLOT: +10
Any variable name defined in the symbol table or any octal address in user page one is accepted. Duplicated entries are ignored. If the selected range is unacceptable, the prompts are reissued.

00004 GOSEX
MIN RANGE OF PLOT: 3
MAX RANGE OF PLOT: +8
END OF LIST
Requests continue until the maximum number of variables have been entered.

A partial list is obtained by striking the carriage return when a variable name is requested. If this is done for the first request, the following message appears before the prompt is reissued.

NO LIST

PLOTTING INTERVAL (SECONDS): 60
Operator is prompted to select the plotting interval.

Possible messages:

INTERVAL IMPROPERLY SPECIFIED
Specified interval was in error. The prompt is reissued.

If the function is unable to initiate the executive output task, the following appears:

UNABLE TO INITIATE OUTPUT TASK

If the output task was created, the following appears:

OUTPUT TASK CREATED

ENDIO -- Kill a Selected Executive Output Task

<CTRL E>
ENDIO
DEVICE NAME: MAGTP — Operator is prompted to select an output device name. Those given in Section 1 are acceptable.

Possible messages:

NOT A DEVICE NAME — Device name was not one of those listed in Section 1. The prompt is reissued.

DEVICE NOT PART OF SYSTEM — Specified device was not configured for the application. Function terminates.

SPECIFIED OUTPUT INACTIVE — No active output task was found on the teletype device. Function terminates.

If a disk was selected, the RDOS filename is requested:

DISK DIRECTORY AND FILENAME: GOSEX.GX

If the device is not a disk or a teletype, the following query appears.

DEVICE UNIT #: 3 — An integer, as indicated in Section 1 is expected.

Possible messages:

SPECIFIED OUTPUT INACTIVE — No active output task was found on the selected device. Function terminates.

SPECIFIED OUTPUT KILLED — An active output task to the selected device was killed. Function terminates.

ENDAL - Kill all Active Executive Output Tasks

<CTRL E>
ENDAL

This function kills all active output tasks (except the analog output task), then outputs the message:

ALL OUTPUTS KILLED

CHNGE - Change Display Rate of an Active Executive Output Task

<CTRL E>
CHNGE

DEVICE NAME: MAGTP	Operator is prompted to select an output device name. Those given in Section 1 are unacceptable.

Possible messages:

NOT A DEVICE NAME	Device name was not one of those listed in Section 1. The prompt is reissued.
DEVICE NOT PART OF SYSTEM	Specified device was not configured for the application. Function terminates.
SPECIFIED OUTPUT INACTIVE	No active output task was found on the teletype device. Function terminates.

If a disk was selected, the RDOS filename is requested:

DISK DIRECTORY AND FILENAME: GOSEX.GX

If the device is not a disk or a teletype, the following query appears:

DEVICE UNIT #: 3	An integer, as indicated in Section 1 is expected.

Possible messages:

SPECIFIED OUTPUT INACTIVE
No active output task was found on the selected device. Function terminates.

If an active output task was found, the following appears:

CURRENT DISPLAY INTERVAL(SECONDS): 00060
RESET DISPLAY INTERVAL(SECONDS): 00030
The operator is informed of the current display interval on the selected device. He must enter the new display interval.

Possible messages:

INTERVAL IMPROPERLY SPECIFIED
Specified interval was in error. The prompt is reissued.

CHANGE CONFIRMED. The display interval for the selected device is changed and is in effect within ten seconds of the change. Function terminates.

PARAM, TUNER - On-Line Parameter Display and Change

A facility for displaying and changing user task parameters while on-line is absolutely essential in any real-time computer application. Two standard functions are available for this requirement. The contents of any location in user address space may be examined and if necessary altered. These locations may be accessed symbolically or numerically using the PARAM function. Octal integer, decimal integer and floating point formats may be selected for display. Although the PARAM function is very general, this generality makes it unsuitable for the display and alteration of PID controller parameters. The TUNER function provides data conversion and magnitude checking necessary for

these parameters. Constants such as gains and control intervals must be limited to certain ranges. Set points, mean outputs and test limits must be converted between internal and engineering units. TUNER only allows access to predefined controller data blocks, and through TUNER, block entries may be examined and altered. Since neither function has a normal termination sequence, the operator must specifically request dismissal of the function.

PARAM - General Parameter Display and Change

<CTRL E>
PARAM

The operator must command the function using the set of control characters listed below. Numbers and parameters defined in the user symbol table are acceptable inputs.

ESC - Terminate the function.

RUB - Ignore the current input line.

/ - Default display of the contents of the memory address given by the address register.

← - Alter contents of the memory address displayed by the "/" control character.

↵ - Close any opened registers and install a change if the "←" control character was used.

LINE FEED - As ↵ , but move up to next memory address and simulate a "/" control character.

↑ - As *LINE FEED*; but move down in memory.

\+ - Add following entry to sum register.

\- - Subtract following entry from sum register.

= - Display sum register as a decimal integer. When the first character of a line, causes the default display to be integer decimal.

: - Display sum register as an octal integer. When the first character of a line, causes the default display to be integer octal.

@ - When the first character of a line, causes the default display to be floating point.

. - Indicates a decimal number.

Input errors are indicated by the following message:

?

TUNER - PID Controller Parameter Display and Change

<CTRL E>
TUNER
LOOP NAME: LEVEL — The operator is prompted to select one of the predefined controller data blocks.

Possible messages:

NOT A CONTROLLER LOOP — Either the loop name was not defined in the symbol table or it was not a predefined controller data block.

LIQUID LEVEL CONTROL — A message describing the controller loop appears when the loop name is accepted.

The operator must command the function using the set of control characters and parameter names listed below.

ESC - Terminate the function.

RUB - Ignore the current input line.

/ - Display the indicated parameter value.

← - Alter the indicated parameter value.

↵ - Close the current input line and install a change if the "←" control character was used.

! - When the first character of a line, the name request is reissued.

- When the first character of a line, complements the caption flag.

The acceptable parameter names and corresponding captions for display are given below.

FILTR/*FILTER CONSTANT (0 TO +1000)/*
INHI/*INPUT HIGH ALARM LIMIT-*
INLO/*INPUT LOW ALARM LIMIT-*
SETPT/*CURRENT SET POINT-*
KP/*PROPORTIONAL GAIN(+VE)/*
KPD/*PROPORTIONAL-DERIVATIVE GAIN(+VE)/*
KPI/*PROPORTIONAL-INTEGRAL GAIN(+VE)/*
SCALE/*SCALE FACTOR & DIRECTION OF ACTION/*
DELAY/*CONTROL INTERVAL(SECONDS)/*
OUTHI/*OUTPUT HIGH LIMIT-*
OUTLO/*OUTPUT LOW LIMIT-*
MEAN/*OUTPUT MEAN-*

In addition, a small set of captions are output regardless of the state of the caption flag. These must be provided in the executive disk message file and they specify the engineering units of the set point, mean output and their limits.

Input errors are indicated by the following messages:

?	
CONVERSION ERROR	An error was detected while attempting to convert data between internal and engineering units.

DIALG, CLEAR, READY, RELSE, CLOCK, RETRN - Miscellaneous Functions

The fourth group of GOSEX functions consists of six functions which satisfy a variety of needs. Reports on a plant's operation may be prepared by the operator at run-time. The DIALG function writes lines of text accepted from the operator's console to a disk file. The contents of the report file may be examined at run-time by copying it to a line printer (see COPY function). It is occasionally necessary to delete disk log files produced by dormant executive output tasks. The CLEAR function is used for this purpose and is programmed to delete only those files created by the GOSEX executive output tasks.

For applications where cassette or magnetic tape transports or disk subdirectories are to be accessed by executive data output tasks, the READY and RELSE functions are needed. The magnetic tape devices or disk subdirectories are initialized by function READY and are released by function RELSE. Everytime a user alarm is output to the operator's console, the time of day and date are appended to the alarm by the CLOCK function. This function may also be envoked by the operator. Finally, when a data acquisition or control experiment is completed, the RETRN function will return control to the RDOS CLI. Before the return occurs however, a user subroutine is called to set user operations at rest, if necessary.

DIALG - Operator Report Generation

```
<CTRL E>
DIALG
DISK DIRECTORY & FILENAME:  REPORT.GX
```

The operator is prompted to specify the RDOS filename of the disk file to accept the report. If the file does not already exist, it is created. If it exists, input text is appended to the file.

```
14:23:57, 07/04/76
```

DIALG automatically writes the time of day and the day's date to the disk file and the operator's console. The operator then enters his report. Input is terminated by the teletype code <CTRL Z>.

```
GOSEX REPORT BY OPERATOR JPT.
ALL IS WELL
<CTRL Z>
```

After the <CTRL Z> code has been entered, the following message appears before the function terminates.

END OF REPORT

CLEAR - Delete a Disk Log File

<CTRL E>
CLEAR
DISK DIRECTORY AND FILENAME: GOSEX.GX
The operator is prompted to specify the RDOS filename of the disk file to be deleted.

Possible messages:

FILENAME ERROR — The specified filename was not an entry in the RDOS directory, the file was in use or the file did not have the appropriate attributes. The prompt is reissued.

DELETION CONFIRMED — The specified disk file was deleted.

READY - Initialize a Magnetic Tape Device or Disk Subdirectory

<CTRL E>
READY
DIRECTORY OR DEVICE NAME: CTO
The operator is prompted to enter the RDOS filename of the directory or device to be initialized.

Possible messages:

DIRECTORY OR DEVICE INITIALIZED
DIRECTORY OR DEVICE ALREADY INITIALIZED
INITIALIZATION NOT POSSIBLE, CODE 00015
The initialization of the directory or device was not possible. The RDOS error code is output before the function terminates.

RELSE - Release a Magnetic Tape Device or Disk Subdirectory

<CTRL E>
RELSE

DIRECTORY OR DEVICE NAME: MT1

The operator is prompted to enter the RDOS filename of the directory or device to be released.

Possible messages:

DIRECTORY OR DEVICE RELEASED
DIRECTORY OR DEVICE IN USE

Directory or device could not be released since it was in use: The function terminates.

RELEASE NOT POSSIBLE, CODE 00015

The release of the directory or device was not possible. The RDOS error code is output before the function terminates.

CLOCK - Display Time of Day and the Day's Date

```
<CTRL E>
CLOCK
15:34:23, 07/27/76
[H: M: S,  M/ D/ Y ]
```

This function generates a text indicating the time of day and the day's date before it terminates.

RETRN - Return to RDOS CLI

```
<CTRL E>
RETRN
```

Once the user shutdown sequence is completed and the RETRN function has done the necessary bookkeeping, the following appears before a return to the RDOS CLI occurs.

USER SPACE RELEASED

4.5 Interface Between GOSEX and User Software

Users of the GOSEX package must provide a link between GOSEX

and the user application software. The format of the software interface which forms the basis of the link is outlined in this section. The example provided here is designed to illustrate several aspects of the linkage. Because the example is limited in scope, readers seeking more details should refer to Section 5 of Appendix C. A listing of the reactor Model Reference Adaptive Control software interface is provided there.

Portions of the software interface must exist in central memory, but others must reside on disk as specially formatted files. These files are produced by the SORT assembler and their structure has already been presented in Section 2 and Figure 4-3. Two of these files are messages files: one contains the text messages used in dialogue with the operator and the other supplies the messages for reporting user alarms. Their RDOS filenames must be "OPCOM.MG" and "MESSG.MG" respectively. The other files are required by function MYLOG and provide data for the initiation of logged outputs (see Section 4). These may be given any acceptable RDOS filename.

Sources for the SORT assembler must be disk files written in ASCII with even parity. A source file may contain any number or text strings and individual strings may not exceed 132(decimal) characters. All ASCII characters are permitted. Nulls, line and form feeds are ignored by the SORT assembler and only a carriage return will terminate a particular line of text. All other ASCII characters except "<" and ">"

are passed directly to the output file. The angle brackets are used to specify an ASCII character by its octal number equivalent. The last line of a source file must contain a lone "@" character followed by a carriage return. The listing of a source and the SORT assembler report of this source are given in Figure 4-8. Lines with syntax errors are flagged in the report.

The core resident portion of the interface consists of tables and constants which permit direct links between user and GOSEX software. It must be written in assembler language. Since it consists primarily of data, users will not experience serious difficulty. All user symbols to be recognized by GOSEX must be appended to the table of executive symbols. This constitutes the symbol table and the format of the user supplied section of this table is outlined in Figure 4-9. The technique described in Section 2 (see utility ENCOD) served in its preparation. All other information needed to complete the interface is illustrated in Figure 4-10. At run-time, GOSEX analyzes all of the information provided in this section of the interface. Errors and omissions are reported at the operator's console. Fatal errors cause the program to abort.

The byte pointer to the RDOS disk filename of the overlay file which contains all of the executive functions and user overlays must be provided at label "OVLAY".

The messages contained in the user alarm disk message file are tied to the entries of an alarm table defined at label "ALARM". When a

FIGURE 4-8

SOURCE FORMAT FOR THE SORT ASSEMBLER

```
<15><12>
<12>NOT AN EXECUTIVE FUNCTION
<12EXECUTIVE FUNCTION NOT AVAILABLE
<12>TASK NAME:
<12>NOT A USER TASK<15>
<A>USER TASK CREATED
<12>TASK IS ALREADY ACTIVE
<12>USER TASK KILLED
<12>TASK IS ALREADY INACTIVE
     .
     .
     .
/ALL ASCII CHARACTERS ARE ACCEPTABLE/
     .
     .
     .
/ANY NUMBER OF TEXT MESSAGES/
@
```

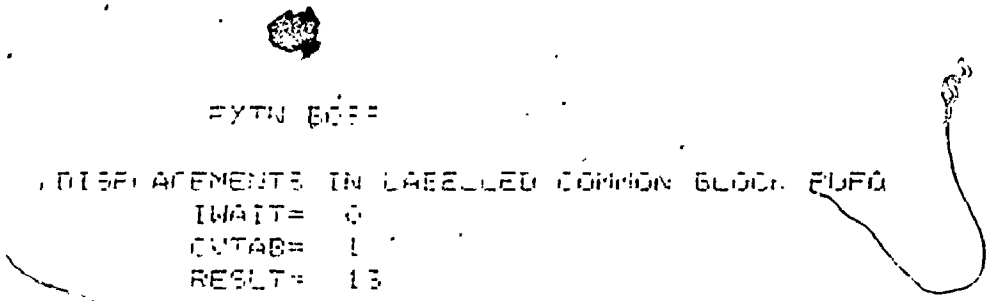
SORT ASSEMBLER REPORT

```
 LINE #  LINE AS READ FROM SOURCE FILE
 00000   <15><12>
 00001   <12>NOT AN EXECUTIVE FUNCTION
 00002 E <12EXECUTIVE FUNCTION NOT AVAILABLE
 00003   <12>TASK NAME:
 00004   <12>NOT A USER TASK<15>
 00005 E <A>USER TASK CREATED
 00006   <12>TASK IS ALREADY ACTIVE
 00007   <12>USER TASK KILLED
 00008   <12>TASK IS ALREADY INACTIVE
 00009       .
 00010       .
 00011       .
 00012   /ALL ASCII CHARACTERS ARE ACCEPTABLE/
 00013       .
 00014       .
 00015       .
 00016   /ANY NUMBER OF TEXT MESSAGES/

ERRORS IN SOURCE:PASS 2 ABORTED
```

FIGURE 4-9

FORMAT OF THE TABLE OF

USER SYMBOLS



```
          FYTN BASE

,DIFFERENTS IN LABELLED COMMON BLOCK FIFO
          IWAIT=  0
          CVTAB=  1
          RESLT=  13

          BASE
          23 *40 +0 *3I
          12 *40 +25 *40 +24
           DADD FIFO, IWAIT          ,EQUIVALENCE FOR IWAIT
          19 *40 +20 *3I
          19 *40 +33 *40 +11
           DADD FIFT, CVTAB          ,EQUIVALENCE FOR THE FIRST
          11 *40 +17 *3I             ,ELEMENT OF ARRAY CVTAB
          13 *40 +3I *40 +30
           DADD FIFO  RESLT          ,EQUIVALENCE FOR THE FIRST
          22 *40 +30 *3I             ,ELEMENT OF VECTOR RESLT
          28 *40 -15 *40 +23

          SST=      -1
          NEST=    SST
          USST=    SST

           END
```

FIGURE 4-10

CORE RESIDENT PORTION OF THE SOFTWARE INTERFACE

```
          TITL INFCE

          ENT OVLAY, ALARM, DATUM, ANALG, RELAY
          ENT SENSE SCAN, CLOOP, SUPRS, TASKS
          ENT TRAP
          EXTN BOSS
          TXTM 1

          NREL

OVLAY     OVLAY+1*2          ,BYTE POINTER TO THE OVERLAY FILENAME
          TXT @PUFO OL2      ,OVERLAY FILENAME

ALARM     4                  ,NUMBER OF FLAGS IN THE ALARM TABLE
          BLK 4              ,RESERVE AREA FOR 4 FLAGS

DATUM     BLK 6              ,RESERVE AREA FOR 6 ANALOG INPUT DATA

ANALG     BLK 2              ,RESERVE AREA FOR 2 ANALOG OUTPUT DATA

RELAY     BLK 5              ,RESERVE AREA FOR 5 RELAY OUTPUT FLAGS

SENSE     TRAP               ,CONTACT SENSE INPUT DISPATCH TABLE
TRAP      0

SCAN      5                  ,ACTIVATE MTFLX FIVE TIMES PER SECOND

CLOOP     1B0                ,END OF TABLE INDICATION-NO PID CONTROL LOOPS

SUPRS     JMP 0,3            ,USER SHUTDOWN SEQUENCE-NONE PROVIDED HERE

TASKS     BOSS               ,TASK STARTING ADDRESS
          100                ,TASK PRIORITY
          200                ,TASK IDENTIFICATION
          1B0                ,TASK KILL FLAG
          0                  ,FORTRAN IV TASK
          1B0                ,END OF TABLE INDICATION

UDEF      0                  ,NO USER DEFINED FUNCTIONS

          END
```

table entry is made non-zero, the alarm monitor (see Section 3, MNITR) copies the corresponding text from a disk message file onto the operator's console.

Depending on the type of hardware interface handler (see Section 3, MTPLX) prepared for a particular GOSEX package, buffers for the analog and digital input and output data must be reserved. For example, analog input and output data are stored in tables "DATUM" and "ANALG" respectively. Similarly, tables "RELAY" and "SENSE" are used for relay outputs and contact sense inputs respectively. The frequency at which executive task MTPLX is activated is given at label "SCAN".

All single variable controller loops are identified in the control loop definition table at label "CLOOP".

The user shutdown routine at label "SUPRS" allows the user to prepare for a return to the RDOS CLI. This routine must be in assembler.

The user task definition table is at label "TASKS". The definition of a user task includes a task priority, identification, starting address, kill flag and mode (assembler or FORTRAN IV). All user tasks to be controlled by the operator must be defined in this table.

If any user functions are to be used, these must be inserted into the executive function list extension at label "UDEF". Each entry must include a function name, starting address and overlay code.

Finally, the essence of the linkage between user and GOSEX soft-

ware lies within the user software itself. For tasks written in assembler language, the usual extended assembler pseudo-ops for inter-program communication are used. However, in applications where some user tasks are written in FORTRAN IV, special techniques for exchanging data between FORTRAN and non-FORTRAN areas are required. Those described below are illustrated in Figure 4-11. For further information, the reader is urged to consult Data General Corporation's FORTRAN IV User's and Run-Time Library manuals.

Access to non-FORTRAN data by FORTRAN routines is accomplished by the use of FORTRAN external declarations. Conversely, non-FORTRAN routines can access FORTRAN data declared in labelled common. If required, access to a FORTRAN routine's run-time stack frame is also possible. For this, assembler language statements referencing the stack are inserted into the FORTRAN program itself. Equivalencing of FORTRAN IV stack variables and parameters for assembly results when the compiler global switch "F" is used. The parameters specify the displacements above the bottom of a stack frame where the FORTRAN variables are kept. Each element of a stack frame is addressed relative (-200 to +177) to the stack pointer (AC3) where relative address -200 is the bottom of the stack frame.

The need to exchange data between FORTRAN and non-FORTRAN space arises for three reasons. These are:

FIGURE 4-11

LINKAGE TECHNIQUES BETWEEN

FORTRAN AND NON-FORTRAN AREAS

```
      PARAMETER NDATA=3
      TASK DATA
C-----LABELED COMMON DEFINITIONS-LINKED THROUGH SYMBOL TABLE, FIGURE 4-10
      COMMON /FIFO/ IWAIT,CVTAB(2,NDATA),RESLT(NDATA)
C-----EXTERNAL DECLARATION TO LINK FORTRAN AND NON-FORTRAN AREAS
      EXTERNAL DATUM
C-----INITIALIZE CYCLE INTERVAL AND CONVERSION DATA ARRAY
      DATA IWAIT /VTOP 5,1 0,2 0,3 0,4 0,5 0,6.0/
C-----SUBROUTINE TASK TO ESTABLISH LINK
    1 CALL TRANS(DATUM,CVTAB,RESLT)
C-----WAIT 'IWAIT' SECONDS
      DO 2 I=1 IWAIT
      CALL WAIT(1,2,IER)
      IF (IER .NE. 1) CALL KILL
    2 CONTINUE
      GO TO 1
      END


      PARAMETER NDATA=3
C-----INTERFACE SUBPROGRAM TRANSLATES INTEGER DATA IN EXTERNAL VECTOR
C-----DATUM INTO REAL DATA RESLT FOUND IN LABELLED COMMON
      SUBROUTINE TRANS(DATUM,CVTAB,RESLT)
      DIMENSION DATUM(NDATA),CVTAB(2,NDATA),RESLT(NDATA)
      INTEGER DATUM
      DO 1 I=1 NDATA
      RESLT(I)=FLOAT(DATUM(I))*CVTAB(1,I) + CVTAB(2,I)
    1 CONTINUE
C-----OUTPUT CONVERTED DATA TO DISK FILE
      CALL ASSIGN(1,'DATAFILE',8,IER)
      IF (IER .NE. 1) CALL KILL
      WRITE BINARY(1) (RESLT(I),I=1,NDATA)
      CALL CLOSE(1,IER)
      IF (IER .NE. 1) CALL KILL
      RETURN
      END
```

- All pilot plant input/output data are stored in non-FORTRAN user space data tables.

- All GOSEX functions require that parameters and variables be located in non-FORTRAN user space.

- User assembler language tasks must store their data in non-FORTRAN user space.

Generally speaking, FORTRAN parameters and variables to be accessed by GOSEX and assembler language user tasks should be located in labelled common blocks. GOSEX itself must be linked to the elements of the labelled common blocks through the table of user symbols. Any FORTRAN routine which requires data located in non-FORTRAN user space may access it by external declarations. Under FORTRAN IV, external declarations are usually used to define subroutines or functions appearing as arguments in a routine's subroutine or function calls. As shown in Figure 4-11, they may also define the address of constants or the starting address of arrays. Direct access to data in non-FORTRAN user space by any FORTRAN routine is then possible.

In order to prepare GOSEX for operation, the user must determine the hardware configuration needed for his application. This will allow the user to prepare the appropriate hardware interface handler (see executive task MTPLX) and to assemble the GOSEX programs. The objectives of the user software must be stated and assembler or FORTRAN IV programs developed to meet these aims. Finally, as outlined in this section, links between GOSEX and user software must be established. Links are

an integral part of the user software and without them, GOSEX and user operations are not possible.

A prerequisite for proper use of GOSEX is an understanding of the hardware and software events associated with real time GOSEX operations. Without this understanding, many GOSEX features will be misused and the usual consequence of this is overly complex and inflexible user software.

CHAPTER 5

MODEL FITTING AND MODEL REFERENCE ADAPTIVE CONTROL STUDIES

5.1 Introduction

The formulation of a model reference adaptive control algorithm in Chapter 2, Section 3 presumed the existence of a suitable reference model. The essential characteristic of the model was asymptotic stability. Practical considerations also suggested, although theoretically not required, that the reference model exhibit dynamic properties resembling those desirable of the process under closed loop control.

An empirical approach to obtain a suitable reference model begins with the collection of dynamic data. This phase is described in Section 2. The parameters of measurement Equation 2-21 and of the dynamic Equation 2-19 are fitted to these data. For convenience, these two equations are repeated as Equations 5-1 and 5-2 respectively.

$$y(k) = Et(k) + Gu(k-1) \qquad (5\text{-}1)$$

where y: vector of estimated reaction extents in the reactor effluent, nx1
t: vector of functions of temperature data, mx1
u: vector of inputs, rx1
E: correlation matrix, nxm
G: correlation matrix, nxr

$$x(k+1) = Ax(k) + Bu(k) \qquad (5\text{-}2)$$

where x: state vector of the effluent stream reaction extents
A: transition matrix, nxn
B: control matrix, nxr

n = 3
m = 3
r = 2

The form of these two equations eliminated many difficulties which normally arise in state space control systems when it is not possible to synchronize the acquisition of relevant plant data. The estimation of real matrices E, G, A and B defined by Equations 5-1 and 5-2 is described in Section 3. The reference model is also derived by applying a constrained optimal controller to the fitted dynamic model. The discrete time Lyapunov matrix Equation 2-37 is then solved given the stable closed loop transition matrix obtained by optimal control. Finally, model reference adaptive control studies based on the reference model of Section 3 are presented in Section 4.

In all, seven experimental runs are examined here and are summarized by Table 5-1. As shown, Run #1 provided the data needed to obtain a reference model essential for the model reference adaptive control studies. The ability of measurement Equation 5-1 to predict reactor effluent stream extents is verified by Run #2. Discussions of the properties of the model reference adaptive control algorithm derived in Chapter 2 are based on the results of Runs 3 to 7.

TABLE 5-1

SUMMARY OF REACTOR EXPERIMENTS

Run #	DATE	TYPE OF CONTROL	OBJECTIVES	APPLICABLE FIGURES
1	Sept 13/76	Univariate: Hot Spot temperature maintained by n-butane manipulation.	Obtain sufficient data to estimate parameters of Equations 5-1 and 5-2.	5-3 to 5-7
2	Oct 24/76	Univariate: Reactor effluent propane extent maintained by n-butane manipulation.	Verification of Equation 5-1 to predict reactor effluent stream extents.	5-8 to 5-12
3	Nov 15/76	MRAC: Proportional action only. Coolant temperature load upsets.	Test basic regulatory properties of MRAC.	5-13, 5-14 to 5-18
4	Oct 21/76	MRAC: Proportional and integral actions combined. Coolant temperature load upsets.	Test expanded MRAC properties.	5-13, 5-19 to 5-23
5	Oct 22/76	MRAC: Proportional and integral actions combined. Reference model retriggering. Coolant temperature load upsets.	Evaluate the relative importance of the reference model states with respect to the other terms of the MRAC algorithm.	5-13, 5-24 to 5-29
6	Nov 16/76	MRAC: Proportional and integral actions combined. Propane extent setpoint load changes.	Evaluate the MRAC algorithm's servo mechanism. Integral action as the only driving force.	5-13, 5-30 to 5-35
7	Nov 14/76	MRAC: Proportional, integral and setpoint actions combined. Propane extent setpoint load changes.	Evaluate the MRAC algorithm's servo mechanism. Both the integral and setpoint actions provide the driving force.	5-13, 5-36 to 5-41

It must be emphasized that the estimation process of Section 3 is directed at finding a set of parameters that yield a reasonable dynamic model of the process. The issue here is not one of estimation, but rather one of arriving at a dynamic model which may be used for model reference adaptive control.

All experiments described in this chapter were supported by a nucleus of assembler language user tasks and user defined executive functions which operated certain components of the n-butane hydrogenolysis pilot plant reactor. These routines were designed for use with the GOSEX executive program developed for this work. Although the various operations performed by the basic reactor software have been described in Section 4 of Appendix C, no description of the linkage that must be established between this and the user's reactor control software is provided. For this reason, it is useful to digress for a moment and discuss the linkage.

User tasks VISOR and CSCON are designed to perform the following real-time operations:

- -Proportional-integral control of the n-butane and hydrogen reactant flow rates. The executive's univariate DDC controller was envoked once every second. Measurement of the reactor pressure drop was also performed.
- -The actuation of a field multiplexer for the acquisition of reactor temperature data. On-off control of the reactor coolant was also performed once every six seconds.
- -The acquisition and correction of reactor effluent stream analysis data.

Corresponding to these functions, certain data were available to the user.

These included temperatures, flow rates and effluent stream composition.

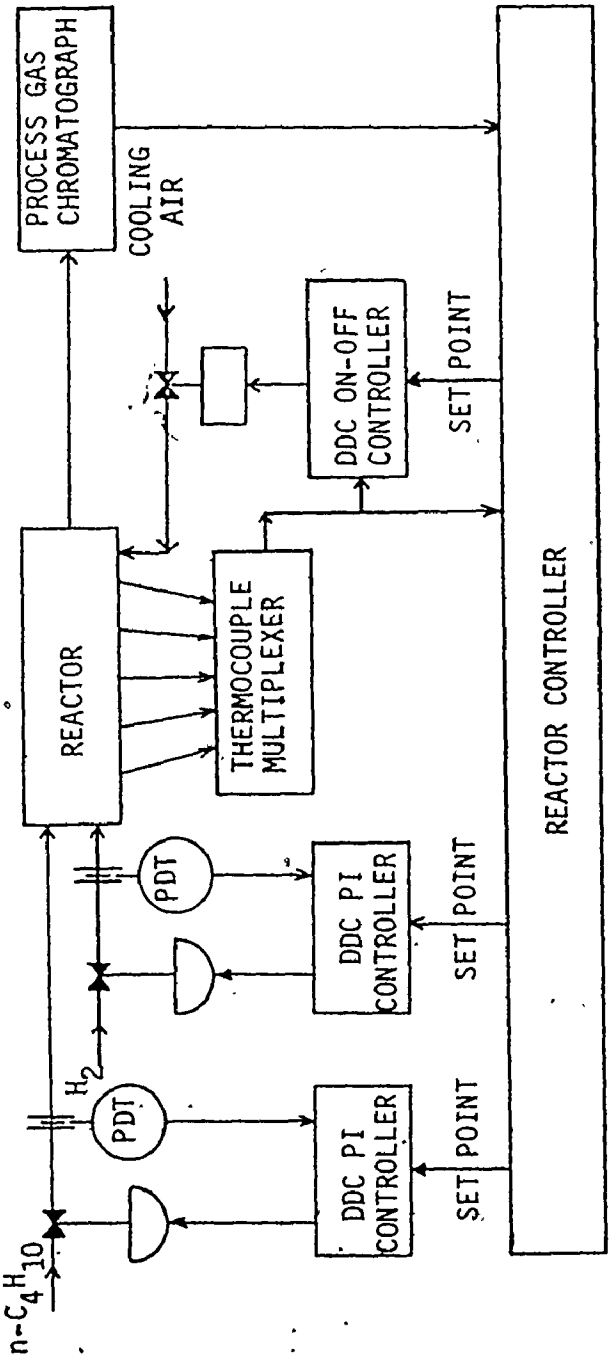
The user's reactor control software may access any of these data in the manner described in Section 5 of Chapter 4. Based on these, it could choose to modify the coolant temperature on-off controller setpoint or the reactant flow controller setpoints as illustrated by Figure 5-1. For this work, reactor control relied on the adjustment of the reactant flow setpoints and disturbances were usually introduced manually by step changes in the coolant temperature on-off controller setpoint.

The precision of the chromel-alumel thermocouples used throughout the pilot plant reactor was reported by the manufacturer to be $\pm$ 2.5^{o}C at the reactor operating temperatures. Because of certain factors including multiplexing techniques and transmission noise, the signal variation was possibly as large as $\pm$ 5^{o}C. All temperature data were filtered to remove the high frequency variations. Low frequency noise was unaffected by the first order filter and explains the fluctuations in the temperature data reported here.

Flowrate data were also smoothed by a first order filter. Variations in the data were numerically small and did not affect the flow data appreciably. The flowrate data presented here consist of the flow controller setpoints instead of the actual flow data. It was assumed (without serious error) that the actual flowrates closely followed the

FIGURE 5-1

BASIC STRUCTURE OF THE REACTOR CONTROL SOFTWARE



variations in the controller setpoints.

Analysis data from the gas chromatograph were corrected on-line using flow controller setpoint data. The exact algorithm has been described in Chapter 3, Section 5. Because of assumptions used in the correction and inaccuracies in the raw chromatographic data, errors in the corrected effluent stream composition data were approximately 10% of the corrected data.

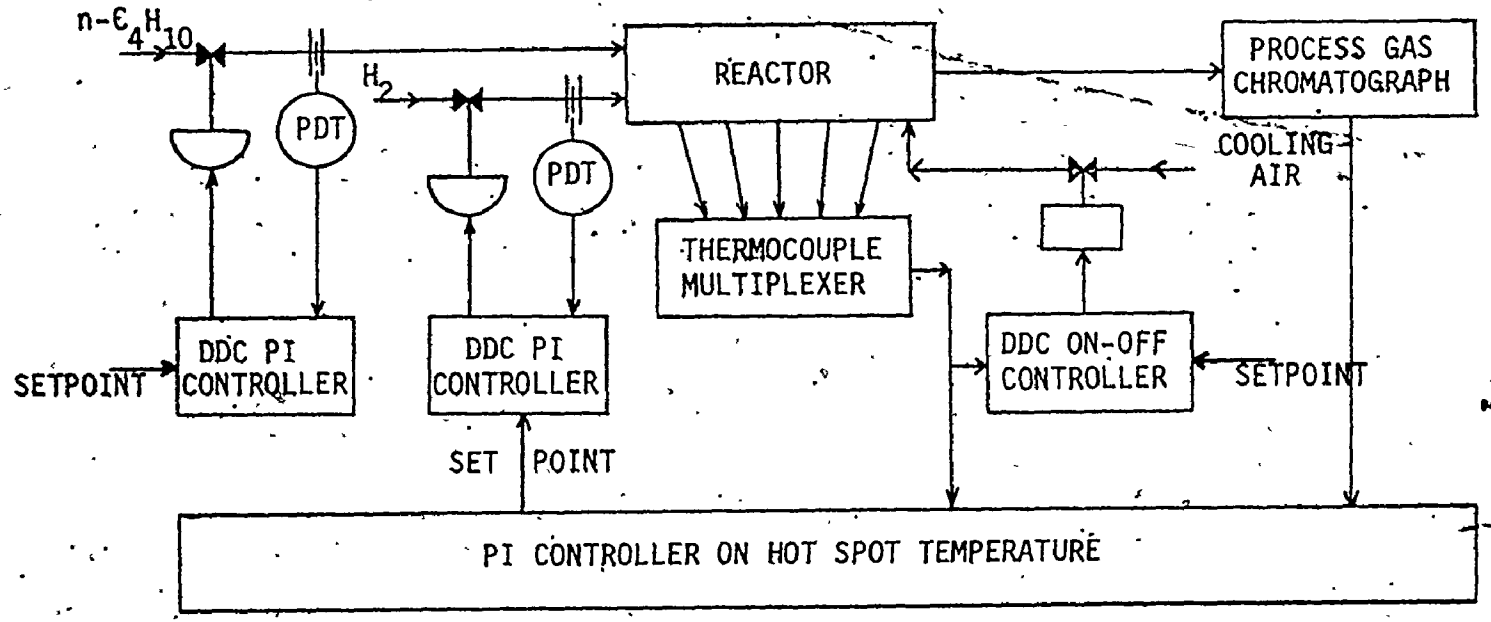
5.2 Acquisition of Data for Estimation

Before model reference adaptive control of the butane hydrogenolysis reactor could be attempted, reactor model matrices E, G, A and B defined by Equations 5-1 and 5-2 had to be estimated from actual plant data. Estimates of all the elements of these low order matrices were easily determined from dynamic data. Because the reactor could not be operated under open loop conditions -- the reactor is open loop unstable -- it was necessary to collect all dynamic data about an operating level using some control action. A conventional single variable proportional-integral (PI) controller was used to maintain the reactor hot spot temperature constant through manipulation of an input feed rate. Since both inputs were believed to be equally good, it was arbitrarily decided to manipulate the hydrogen feed rate. A schematic diagram of the reactor system for the exploratory stage of the experimental program is shown in Figure 5-2.

FIGURE 5-2

HOT SPOT TEMPERATURE CONTROL

BY HYDROGEN MANIPULATION



From previous experience, it was known that the hot spot temperature was a very sensitive measurement for single variable control purposes. Since this temperature was related to the model state variables through a complex set of reaction mass and energy balances, a suitable operating level had to be located experimentally. Several operating conditions were investigated and the following summary of observations resulted:

- -Reactor control was very difficult when the coolant temperature was above 255°C;
- -Insufficient reactivity was found for coolant temperatures below 245°C;
- -The maximum hot spot temperature setpoint that could be properly maintained was 280°C when the coolant temperature was 250°C;
- -Significant amounts of propane but only traces of ethane were observed for butane conversions between 10 and 30%;
- -When butane conversions exceeded 35%, the hot spot temperature exceeded 300°C;
- -For conversions above 40%, the selectivity of propane fell rapidly;
- -Frequent action (at least once every minute) was required to control the reactor at an elevated hot spot temperature;
- -Whenever the conversion of n-butane exceeded 35%, the reactor became completely uncontrollable.

Two things were very evident from the preliminary investigation. At all feasible operating conditions, little or no ethane was produced and because of this, none of the servo-control studies presented here involved ethane directly. The presence of only trace amounts of ethane in the reactor effluent stream has been explained in subsequent work by Wong [1977]. Results of a canonical analysis of reactor data showed that

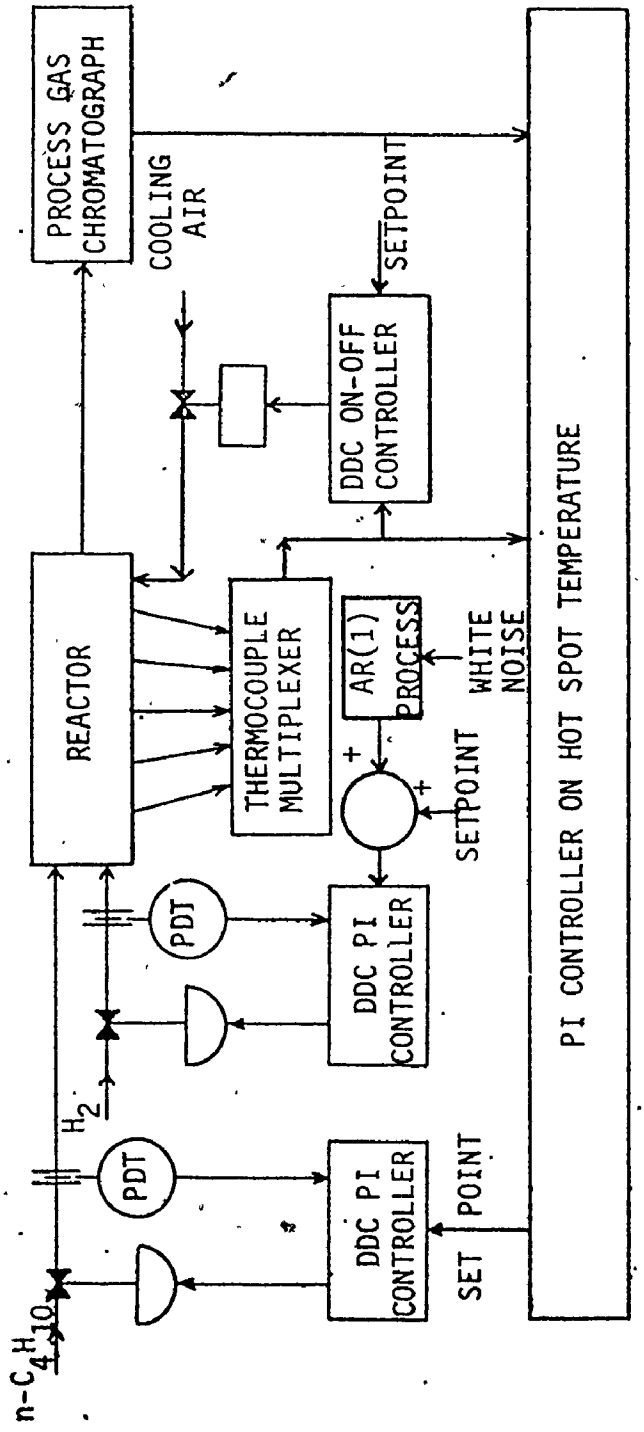
in fact only two chemical reactions are significant at the feasible operating conditions. Although theoretically three independent reactions exist (the reader is referred to Chapter 2, Section 2 and Equations 2-3, 2-4 and 2-6), in practice only two are found to be independent. It was also observed that the manipulation of the hydrogen feed rate was a very weak control. Typically, very large changes in hydrogen feed flow rates were needed to maintain control of the hot spot temperature. These large actions aggravated the control problem by altering the effective time constant of the thermal wave. Severe cyclic operation resulted which would not be stabilized by changes in controller parameters.

It was noted during the course of the investigation that the reactor was very sensitive to changes in n-butane feed rate. Slight variations of this input were sufficient to affect the amount of heat released by reaction. This in turn manifested itself by a rapid change in the reactor's axial temperature profile. In view of the reactor's sensitivity to the n-butane input, single variable control based on n-butane manipulations was investigated. A schematic diagram of the reactor system for this stage is shown in Figure 5-3. In this particular case however, the auto-regressive disturbance generator was not used to perturb the hydrogen flow controller setpoint. The study demonstrated that control about a wide range of suitable operating conditions was feasible. Furthermore, the reactor could be controlled about an operating hot spot temperature of 300^{o}C. The excursions in input and output variables obtained using the n-butane flow rate as the manipulated input

FIGURE 5-3

HOT SPOT TEMPERATURE CONTROL

BY n-BUTANE MANIPULATION - Run #1



were far less severe than those which occurred using the hydrogen flow rate for control.

Preliminary experimentation also indicated that a discrete control interval of about thirty (30) seconds was desirable. A somewhat greater interval ultimately resulted in reactor instability. A shorter interval offered no practical advantages principally because thermocouple response times were about thirty seconds. Based on this information and the fact that flowrates and temperature data were renewed at one and twelve second intervals respectively, the decision was made to perform all experimental studies with a discrete control interval of thirty seconds. Because chromatographic data were only available at 361 second intervals, it was not directly used in any of the control algorithms, but used instead for recursive updates of measurement equation parameters.

Identification of the underlying process dynamics was not an objective of this study since a model of the n-butane hydrogenolysis reactor had been developed from mechanistic arguments. Experience gained during the preliminary study indicated that data suitable for the estimation of dynamic model parameters could be gathered if the pilot plant was operated under univariate closed loop control with n-butane as the manipulated input. Estimation of open loop model parameters from closed loop data is simplified if that data has been properly collected (Box et al [1976]). Disturbances of suitable intensity and frequency to excite the process sufficiently to yield information about the parameters to be

estimated were introduced through variations in the hydrogen feed rate. Perturbation of the n-butane feed rate would make controlled operation extremely difficult and consequently was not implemented. It was decided that an autoregressive process of order one -- AR(1) -- would be used to perturb the hydrogen flowrate about an appropriate operating level. The data shown in Figures 5-4, 5-5 and 5-6 were collected during a six hour experiment (Run #1) using the control scheme illustrated in Figure 5-3. Operating conditions are listed in Table 5-2. During the course of the experiment, the magnitude of the hydrogen disturbance was increased to cover a wider range of operating conditions.

Subsequent analysis of the data from Run #1 exposed a fault in the random number generator used to synthesize the AR(1) disturbance to the hydrogen flow controller setpoint. This was manifested by the highly periodic nature of the hydrogen feedrate plotted in Figure 5-4. However, the data for Run #1 were still useful and estimation of model parameters from this data was not adversely affected.

From Figure 5-4, it is apparent that the simple univariate PI controller had considerable difficulty containing the excursions of the hot spot temperature plotted in Figure 5-5. Although it appears that the n-butane control was always at either of two boundaries, in fact there are several values of this input which lie between them. It is interesting to note that in Figure 5-6 the measured propane extent also seemed to lie most often on either of two levels.

TABLE 5-2

OPERATING CONDITIONS OF THE

DATA ACQUISITION EXPERIMENT - Run #1

Coolant Temperature: 250°C

Mean Operating Value of the Hydrogen Input

95 cm^3/sec, 1 ATM, 25°C

$\Phi = 0.6$ $2\sigma_{H_2} = 3.5$ cm^3/sec initially

8.0 cm^3/sec finally

Controller Settings*

Hot Spot Temperature Setpoint: 300°C

Control Interval: 30 seconds

Proportional Gain: +4.00

Proportional-Integral Gain: +0.05

Operating Limits of the n-butane Input

13 to 21 cm^3/sec, 1 ATM, 25°C

* Parameters of the GOSEX DDC PI controller (see Chapter 4, Section 2)

FIGURE 5-4
RUN # 1

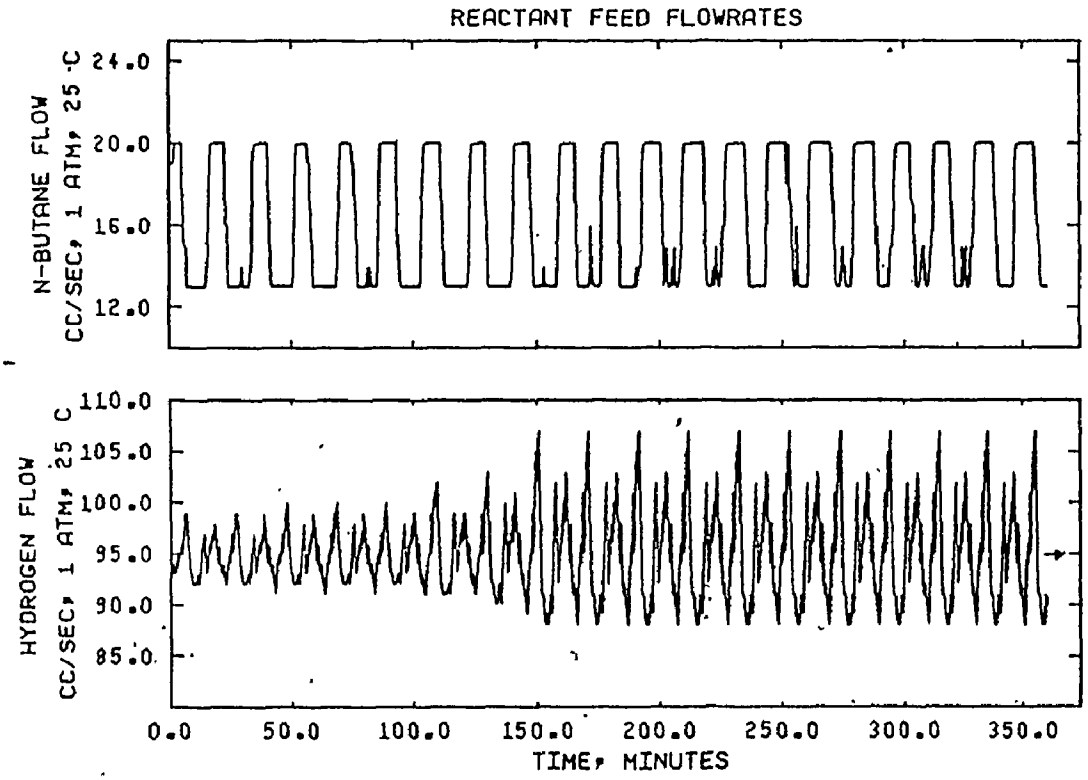
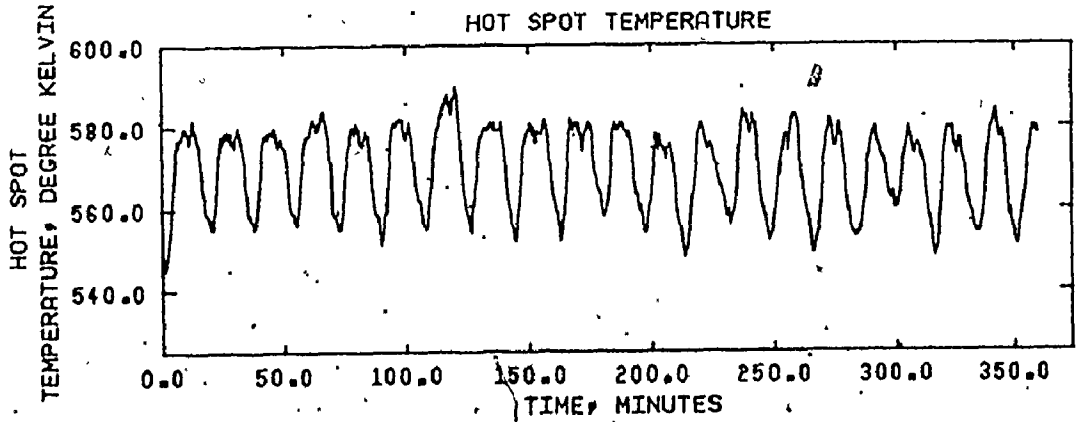


FIGURE 5-5
RUN # 1



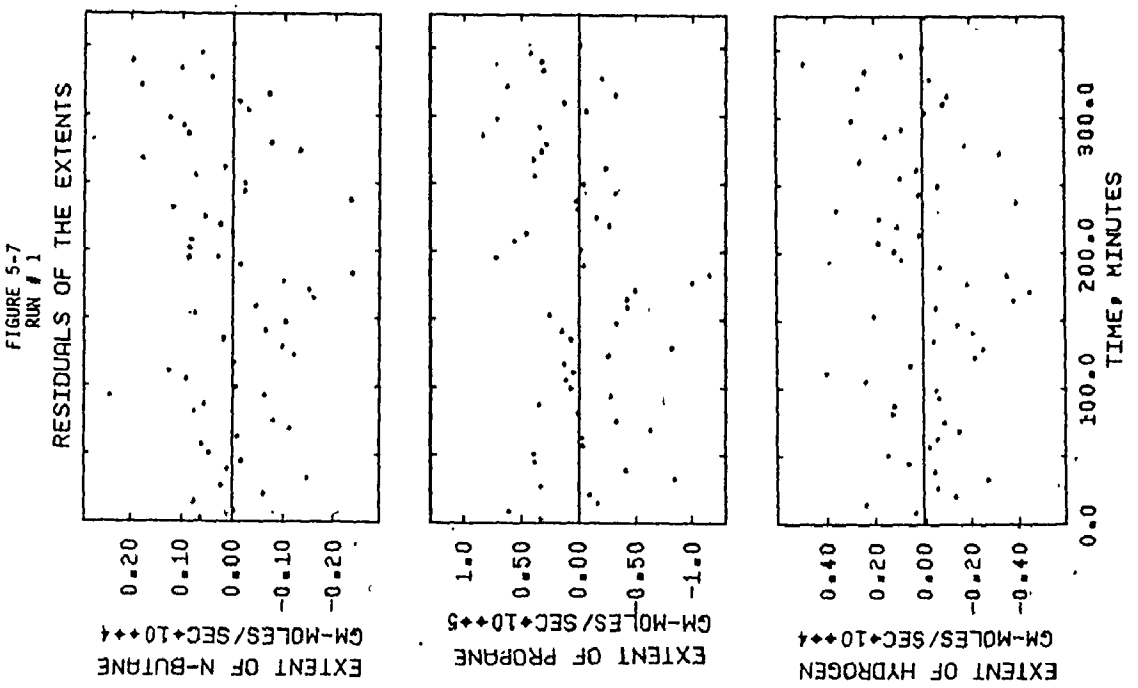


FIGURE 5-7
RUN # 1
RESIDUALS OF THE EXTENTS
EXTENT OF N-BUTANE
GM-MOLES/SEC*10**4
0.20
0.10
0.00
-0.10
-0.20
EXTENT OF PROPANE
GM-MOLES/SEC*10**5
1.0
0.50
0.00
-0.50
-1.0
EXTENT OF HYDROGEN
GM-MOLES/SEC*10**4
0.40
0.20
0.00
-0.20
-0.40
0.0
100.0
200.0
300.0
TIME, MINUTES

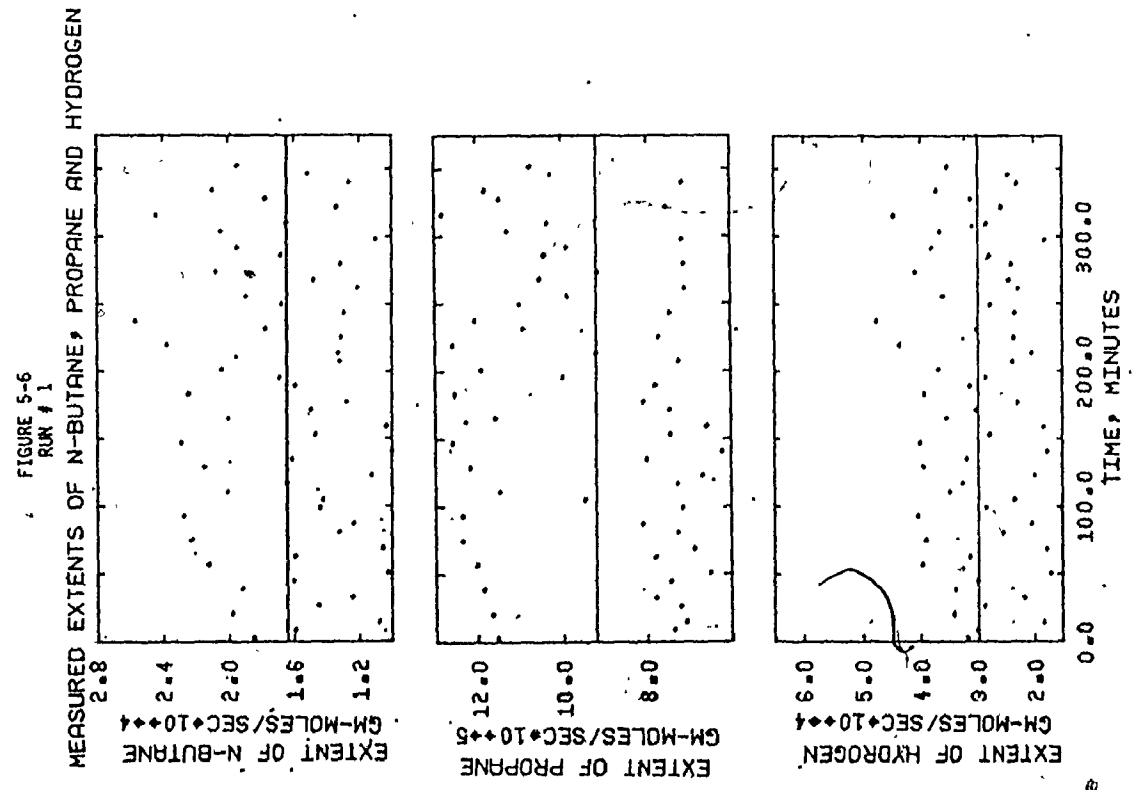


FIGURE 5-6
RUN # 1
MEASURED EXTENTS OF N-BUTANE, PROPANE AND HYDROGEN
EXTENT OF N-BUTANE
GM-MOLES/SEC*10**4
2.8
2.4
2.0
1.6
1.2
EXTENT OF PROPANE
GM-MOLES/SEC*10**5
12.0
10.0
8.0
EXTENT OF HYDROGEN
GM-MOLES/SEC*10**4
6.0
5.0
4.0
3.0
2.0
0.0
100.0
200.0
300.0
TIME, MINUTES

Run #1 yielded 60 usable sets of chromatographic data and 724 sets of control action data.

5.3 Estimation of the Measurement and Dynamic Model Equation Matrices

A prerequisite for the fitting of the dynamic model Equation 5-2 was the fitting of measurement Equation 5-1. To accomplish the latter, a suitable set of functionals of reactor axial temperature data had to be discovered.

Although time filtering of temperature data was provided by the application software (see Appendix C, Section 4), it was also advantageous to consider spacial smoothing of the reactor axial temperature data. A low order polynomial fitted over a short reactor length could be used for interpolation to suitable axial locations.

It has been shown by Jutan [1976] that a seventh order orthogonal polynomial can be used to approximate the reactor axial temperature profile. For this reason, only functionals of axial collocation point temperatures have been examined. Each collocation temperature was interpolated by a quadratic polynomial fitted by least squares over four points containing the collocation point. The normalized axial collocation points are listed in Table 5-3.

Several different functionals of the axial collocation point temperatures were examined. These are described in subsequent paragraphs.

TABLE 5-3

7^{th} ORDER ORTHOGONAL COLLOCATION

POLYNOMIAL CONSTANTS

COLLOCATION POINTS	QUADRATURE WEIGHTS FOR INTEGRATION
0.0	$-0.46306479 \times 10^{-1}$
0.034	+0.15972577
0.169	+0.13151664
0.381	+0.27334790
0.619	+0.19811371
0.831	+0.21824414
0.960	+0.33944621
1.0	+0.31413692

Normalized axial position

When finally selected, the rows of matrices E and G were estimated independently of each other by linear least squares. This practice was consistent with the on-line recursive updating of these matrices previously described in Chapter 2, Section 2. The convergence of matrices E and G while on-line would be enhanced if correlations between functionals were small. It was equally important that the functionals reflect true variations in plant operation.

Analytical data to be used in the estimation of matrices E and G were available at six minute intervals only. The chromatographic determination of a particular sample not only included composition data but also the reactant feed flow rates of hydrogen and n-butane and the reactor axial temperatures which prevailed at the time of sample injection. The temperature and flow rate data between successive composition measurements were not used. It was assumed for fitting purposes that the feed flow rates had been set for one control interval (30 seconds) prior to sample injection. In actual fact, this assumption was frequently erroneous because of the cycle time of the process gas chromatograph. Application task CSCON (described in Appendix C) which monitored the instrument could only verify that the reactant flow rates were constant for the duration of the three second "start-of-analysis" sequence which preceeded sample injection. If the flow rates had changed due to controller or operator action during this short interval, the data from the analysis of that sample were not used to estimate matrices E and G.

A first attempt at fitting Equation 5-1 was to correlate the reactor effluent extents with the reactor axial collocation point temperatures and reactants feed flow rates. The flowrates were corrected to the reactor pressure (1.65 ATM) and the coolant temperature. Several parameters of this model were very highly correlated (0.9999), particularly those associated with temperatures near the location of the hot spot. These results suggested that a more parsimonious form could be used.

The use of canonical correlations was considered by Wong [1977]. This technique forms a set of new variables which are linear combinations of the original variables with maximum correlation. These new variables are orthogonal.

Wong successfully applied the techniques to a set of reactor data but despite his success it was felt that large excursions from operating levels or reactor disturbances not present in the data would require off-line re-evaluation of the functionals, a technique not suitable for servo-control.

An empirical approach was considered. It is known that the composition of a packed bed reactor's effluent depends very much on the magnitude and location of the hot spot temperature. In order to reflect this dependence, it was believed reasonable to consider the definition of new variables which were simple functionals of the reactor axial collocation point temperatures. The three that were selected are:

-area of the temperature profile above the coolant temperature (essentially an energy balance);

-the difference between the hot spot temperature and the coolant temperature (a measure of kinetic activity);

-the normalized axial position of the hot spot temperature.

The area under the temperature profile was considered to be a good measure of the extent of the reaction. A large area would indicate a high conversion of reactants whereas a small area would suggest very little chemical activity. The area could be easily estimated by the application of quadrature weights (tabulated in Table 5-3) to the temperature data at the collocation points. By itself, the area estimated by this method would not reflect the effect of a very large hot spot temperature. Because the process of integration is in fact a filtering operation, it was decided that the value and location of the hot spot temperature would complement the integral information very well.

The value and location of the hot spot temperature could be determined by either of two possible alternatives. The analytical approach was to extract the information from the derivative of the seventh order orthogonal polynomial fitted to the temperature data at the axial collocation points. Of the real zeroes of the derivative which were located within the reactor, the one that gave the largest value of the maximum was assumed to specify the location of the hot spot. Although the algorithm developed to determine this information functioned reasonably well in most situations, it failed when the hot spot temperature was at the end of the reactor bed. This situation generally arose when the

reactor temperature profile was levelling out. False extrema resulted when the seventh order orthogonal polynomial was fitted to this profile. For this reason and because the algorithm was very time consuming on a minicomputer, another approach was investigated.

The location and magnitude of the hot spot temperature could be roughly determined by simply scanning the axial collocation point temperatures. Although this approach yielded only approximate values, the algorithm would be reliable and its execution time on a minicomputer negligible.

The manner by which the three functionals of the axial collocation point temperatures were to be evaluated was finally determined. The elements of matrices E and G of Equation 5-1 were then fitted by linear least-squares to the analytical data of Run #1. As mentioned earlier, the rows of matrices E and G were assumed to be independent. The results of this fit are shown in Table 5-4 and were considered to be acceptable if one considers the following remarks.

The reader is reminded that the purpose of Equation 5-1 is the prediction of reactor effluent extents given the reactants' feed flow rates and the reactor axial collocation point temperatures. Provided that normal reactor operation is contained within a narrow range of conditions, precise estimates of matrices E and G of Equation 5-1 are possible. This was not the case with Run #1 described in the previous section. For reasons already

stated, wide excursions in plant operation were required to obtain data suitable for the fitting of a dynamic model of the reactor. Because of this, it was not surprising that the parameters of Equation 5-1 have very wide confidence limits, as demonstrated in Table 5-4. In fact, most could be labelled insignificant. Regardless of this, Equation 5-1 predicted the chromatographic data reasonably well. The residuals defined as the difference between the predicted and measured extent data have been plotted in Figure 5-7. In all plots, the range of the ordinate is six standard deviations of the residuals. One standard deviation is defined by Equation 5-3.

$$s = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n(n-1)}} \qquad (5\text{-}3)$$

where s: standard deviation
x_i: residual value
$\bar{x}$: mean value of the residuals, assumed zero for plotting purposes
n: sample size

The analytical data of Run #1 have been used to estimate the values of the elements of matrices E and G of Equation 5-1. This equation was an empirical correlation predicting reactor effluent extents given the axial collocation point temperatures and the reactant feed rates. In order to fit Equation 5-2 to the dynamic data of Run #1, Equation 5-1 was used to predict the reactor effluent stream extents at the control intervals. The matrices of Equation 5-2 were then fitted to these newly transformed data. Because Equation 5-2 was dynamic in nature, a multi-

TABLE 5-4

MEASUREMENT EQUATION MATRICES

ESTIMATES

$$E = \begin{bmatrix} +0.599 \pm 0.486 \times 10^{-5} & -0.222 \pm 2.53 \times 10^{-6} & -0.353 \pm 1.65 \times 10^{-4} \\ +0.137 \pm 0.257 \times 10^{-5} & -0.537 \pm 1.333 \times 10^{-6} & -0.811 \pm 8.683 \times 10^{-5} \\ +0.137 \pm 0.093 \times 10^{-4} & +0.686 \pm 4.820 \times 10^{-6} & -0.728 \pm 3.140 \times 10^{-4} \end{bmatrix}$$

$$G = \begin{bmatrix} +0.103 \pm 0.067 \times 10^{-4} & -0.188 \pm 0.234 \times 10^{-5} \\ +0.417 \pm 0.353 \times 10^{-5} & -0.864 \pm 1.24 \times 10^{-6} \\ +0.202 \pm 0.127 \times 10^{-4} & -0.355 \pm 0.447 \times 10^{-5} \end{bmatrix}$$

CORRELATION MATRIX =

$$\begin{bmatrix} 1.0 & -0.611 & +0.738 & -0.297 & -0.246 \\ & 1.0 & -0.400 & +0.850 & +0.173 \\ & & 1.0 & -0.132 & -0.272 \\ & & & 1.0 & +0.0755 \\ & & & & 1.0 \end{bmatrix}$$

MEAN VALUE OF DATA =

$$\begin{bmatrix} 0.164 \times 10^{-3} \\ 0.929 \times 10^{-4} \\ 0.298 \times 10^{-3} \end{bmatrix} = \begin{bmatrix} \text{Extent of n-butane} \\ \text{Extent of propane} \\ \text{Extent of hydrogen} \end{bmatrix} \quad \text{gm-moles/sec}$$

$$\begin{bmatrix} 16.5 \\ 94.8 \end{bmatrix} = \begin{bmatrix} \text{Feed rate of n-butane} \\ \text{Feed rate of hydrogen} \end{bmatrix} \quad \text{cm}^3\text{/sec, 1 ATM, } 25^\circ\text{C}$$

$$\begin{bmatrix} 21.5 \\ 47.4 \\ 0.836 \end{bmatrix} = \begin{bmatrix} \text{Area of axial temperature profile above coolant temperature} \\ \text{Difference between hot spot temperature and coolant temperature.} \\ \text{Position of hot spot temperature, normalized axial location} \end{bmatrix}$$

response parameter estimation program (Jutan [1976a]) was used to estimate the values of the elements of matrices A and B. The estimation program was based on Bayesian arguments.

To execute properly, the multiresponse parameter estimation program required an initial estimate of matrices A and B. Since no prior information about the values of these matrices was available, a set of arbitrary quantities was selected. Realizing the numerical difficulties which could arise if these estimates were outrageous, a diagonal matrix with small diagonal elements (10^{-3}) was used for matrix A and all elements of matrix B were set quite small (10^{-4}). Also aware that the estimation program would have to labour to obtain reasonable estimates, preliminary estimation was performed with only limited data. Because the last 3½ hours of Run #1 contained the greatest information (the perturbation in the hydrogen flow controller setpoint was at its greatest for the entire run), the run's last 60 data sets (0.5 hr.) of control action data were used.

Some difficulty in the convergence of the B matrix was encountered and it appeared that improper parameter scaling was the cause. Preliminary fitting of matrices A and B was eventually successful once the elements of the B matrix were scaled down by three orders of magnitude. These prelim-

inary estimates were then used as initial parameter values for a final estimation using the last 240 data sets (2 hrs.) of control action data from Run #1. The final estimates of the A and B matrices listed in Table 5-5 were allowed to converge to a relative accuracy of 10^{-5}. Each parameter has been listed with a confidence region of four standard deviations of the parameter.

It was observed that the final values of the elements of the A and B matrices did not change significantly from their initial values. This suggested that the reactor characteristics remained largely unchanged over the two hour period over which the dynamic model Equation 5-2 was fitted.

The eigenvalues of transition matrix A have been provided in Table 5-5 and it is observed that all magnitudes of the eigenvalues are less than unity. Because of the large variance in the elements of the transition matrix, it is not possible to conclude from these eigenvalues that the process itself is open loop stable. In fact, experience with this pilot plant reactor indicates otherwise. What they do indicate however, is that at least two states have dynamics comparatively slower than the third.

It is sometimes possible to partially predict the performance of a fitted open loop system such as the one just fitted here under high gain feedback control by examining its transmission zeroes. Transmission zeroes of the state space system

TABLE 5-5

DYNAMIC MODEL (OPEN LOOP)

MATRICES ESTIMATES

$$A = \begin{bmatrix} +10.8 \pm 1.86 & -8.55 \pm 1.30 & -3.48 \pm 0.640 \\ +3.70 \pm 0.462 & -2.45 \pm 0.322 & -1.31 \pm 0.169 \\ +21.1 \pm 4.44 & -17.9 \pm 3.10 & -6.48 \pm 1.62 \end{bmatrix}$$

$$B = \begin{bmatrix} (+0.105 \pm 0.009)\times 10^{-4} & (-0.160 \pm 0.009)\times 10^{-5} \\ (+0.483 \pm 0.012)\times 10^{-5} & (-0.715 \pm 0.024)\times 10^{-6} \\ (+0.203 \pm 0.011)\times 10^{-4} & (-0.311 \pm 0.023)\times 10^{-5} \end{bmatrix}$$

Eigenvalues of the A matrix: $+0.171$

$+0.850 \pm 0.184i$

$$x(k+1) = A\,x(k) + B\,u(k) \qquad (2\text{-}19)$$

$$y(k) = I\,x(k) \qquad (2\text{-}20)$$

where x: state vector of effluent stream : [extent of n-butane; extent of propane; extent of hydrogen]
reaction extents, nx1

u: vector of inputs, rx1 : [n-butane flow; hydrogen flow]

y: vector of measured reaction extents, nx1
A: transition matrix, nxn
B: control matrix, nxr
I: identity matrix, mxm
n = 3
m = 3
r = 2

are defined to be the set of complex numbers λ which satisfy the inequality

$$\text{rank} \begin{bmatrix} A - \lambda I & B \\ \bar{I} & 0 \end{bmatrix} < n + \min(r,m) \qquad (5\text{-}4)$$

where λ: transmission zero of the system of Equations 2-19 and 2-20.
n,r,m: ranks of matrices A, B and $\bar{I}$ respectively
I,$\bar{I}$: identity matrices of rank n amd m respectively

If a system is not degenerate (i.e. has a finite number of transmission zeroes), then the transmission zeroes will coincide with a subset of the same system under high gain feedback. However, the maximum number of transmission zeroes our system may possess is equal to

$$n - \max(r,m) = 0 \qquad (5\text{-}5)$$

Thus, in this case the fitted system has no transmission zeroes and conclusions about its behaviour under high gain feedback control are not possible (Davison et al [1974]).

Matrices A and B of Equation 5-2 were fitted to the control

action dynamic data of Run #1. These matrices were then used to form the augmented matrices A_m and B_m of Equation 2-28.

$$x_m(k+1) = A_m x_m(k) + B_m u(k) + D_m \Delta\bar{x} \qquad (2\text{-}28)$$

where x_m: $\begin{bmatrix} x \\ z \end{bmatrix}$, augmented state vector, (n+s)x1

A_m: $\begin{bmatrix} A & 0 \\ F & I \end{bmatrix}$, transition matrix, (n+s)x(nxs)

B_m: $\begin{bmatrix} B \\ 0 \end{bmatrix}$, control matrix, (n+s)xr

D_m: $\begin{bmatrix} 0 \\ I \end{bmatrix}$, (n+s)xs

This equation was then an open loop model of the reactor system. A stable closed loop model of the reactor system was then obtained by application of optimal feedback control for use in the derivation of a model reference adaptive control algorithm. In essence, the optimal closed loop model became a reference model for reactor control.

A quadratic performance index with a penalty for control action was defined for Equation 2-28. The penalty for control action was required to constrain the reactant input flow rates within fixed boundaries determined by the reactor's normal operating conditions. The method of dynamic programming was selected for the minimization problem. Details of the procedure have been provided in Appendix C, Section 2.

A set of typical operating values of the reactor states was taken from the control action data of Run #1 to begin the optimal feedback controller calculation. Only a narrow range of Lagrange multiplier (λ) values led

to reasonable solutions of an optimal feedback controller. Of these, the only acceptable result was selected on the basis of the greatest excursions in reactant feed rates which remained within boundaries determined by the reactor's normal operating conditions. The data relevant to the selected case are provided in Table 5-6. With a value for matrix A_m^* of Equation 2-29 (the fitted reference model), a model reference adaptive control algorithm was derived in the manner outlined in Chapter 2, Section 3. The properties of the controller were then investigated in a series of on-line control experiments.

5.4 Model Reference Adaptive Control Studies

Runs 2 to 7 summarized by Table 5-1 are discussed in this section. The control objective of all controllers examined here was to maintain the molar flow rate or extent of propane in the reactor effluent at a given setpoint. For the regulatory controllers (Runs 2, 3, 4 and 5), the propane extent setpoint was the operating value 0.929×10^{-4} gm-moles/sec determined from the estimation data of Run #1. For the runs involving servo control (Runs 6 and 7), setpoint load changes were limited to 30% of the above operating value. All controllers acted on the deviation of the extent of propane in the reactor effluent from this operating value. The propane extents were predicted by Equations 5-1 from reactor axial temperature and reactant flow rate data at the control intervals (30 seconds). Equation 5-1 had previously been fitted to the analytical data

TABLE 5-6

OPTIMAL FEEDBACK CONTROLLER

COMPUTATION DATA

SENSITIVITY TO LAGRANGE MULTIPLIER

LAGRANGE MULTIPLIER $\times 10^{+12}$	$\Delta n\text{-}C_4H_{10}$ MIN	$\Delta n\text{-}C_4H_{10}$ MAX	ΔH_2 MIN	ΔH_2 MAX	MEAN VALUES OF REACTANT	
					$n\text{-}C_4H_{10}$	H_2
0	-30.8	43.6	-183.1	321.6	16.5	94.8
0.001	-17.3	17.5	- 95.0	140.9		
0.005	- 8.51	6.73	- 37.2	61.0		
0.01	- 5.61	5.01	- 18.1	43.8		
0.0125	- 4.83	4.50	- 13.0	40.3		
0.015	- 4.25	4.11	- 9.17	37.7		
0.0175	- 3.79	3.81	- 6.17	35.6		
0.02	- 3.42	3.56	- 5.28	33.9		
0.025	- 2.86	3.17	- 4.69	31.2		
0.05	- 1.52	2.24	- 3.64	24.7		
0.075	- 1.00	1.86	- 3.14	22.0		
0.1	- 0.72	1.64	- 2.81	20.9		
0.5	- 0.24	0.91	- 1.54	17.1		
1.0	- 0.39	0.71	- 1.11	16.0	16.5	94.8

cm^3/sec, 1 ATM, 25^oC

TABLE 5-6

(continued)

Initial Values of the states (gm-moles/sec)

$$\begin{bmatrix} -0.553 \times 10^{-4} \\ -0.267 \times 10^{-4} \\ -0.101 \times 10^{-3} \\ 0 \\ 0 \end{bmatrix}$$

Lagrange Multiplier Value: 2.0×10^{-14}

Optimal Gain Matrix $= D_N^T =$

$$\begin{bmatrix} -0.557 \times 10^{+7} & -0.437 \times 10^{+8} \\ +0.528 \times 10^{+7} & +0.398 \times 10^{+8} \\ +0.169 \times 10^{+7} & +0.134 \times 10^{+8} \\ +0.519 \times 10^{+6} & +0.323 \times 10^{+7} \\ -0.420 \times 10^{+6} & -0.295 \times 10^{+7} \end{bmatrix}$$

Stability Matrix $= A_m^* =$

$$\begin{bmatrix} -0.868 & +0.0410 & +0.360 & -0.250 & -0.331 \\ -0.637 & +0.551 & +0.139 & -0.194 & -0.0807 \\ -1.90 & -0.919 & +1.07 & -0.463 & -0.662 \\ 0 & +1 & 0 & +1 & 0 \\ +3 & -2 & -1 & 0 & +1 \end{bmatrix}$$

from Run #1. The matrices of Equation 5-1 were re-estimated recursively as new analytical data became available at six minute intervals. The recursive algorithm has been outlined in Chapter 2, Section 2. The pilot plant reactor was operated under closed loop for at least one hour before the data presented in Figures 5-9 to 5-12 and 5-14 to 5-41 were recorded.

Run #2 was an attempt to employ a univariate DDC PI controller to maintain constant the propane extent in the reactor effluent when the reactor was subjected to coolant temperature load changes. Simultaneously, the ability of Equation 5-1 to predict reaction extents while on-line could be evaluated. Runs 3 to 7 were designed to investigate certain aspects of the model reference adaptive controller derived according to the procedure described in Chapter 2, Section 3.

The control scheme configuration for Run #2 is given in Figure 5-8. As illustrated, the hydrogen feed rate was manually adjusted and the n-butane feed rate altered by cascade action from the propane extent PI controller. As expected, this control scheme was found to be inherently unstable. In order to get suitable data for illustrative purposes, it was necessary to fix the hydrogen flow controller setpoint at 125 cm^3/sec, 1 ATM, 25°C. When compared to the data from Run #1, this level was significantly higher. The propane extent PI controller settings used throughout Run #2 are provided in Table 5-7. The data for Run #2 are given in Figures 5-9 to 5-12.

The reactor was operated for one hour at a coolant temperature

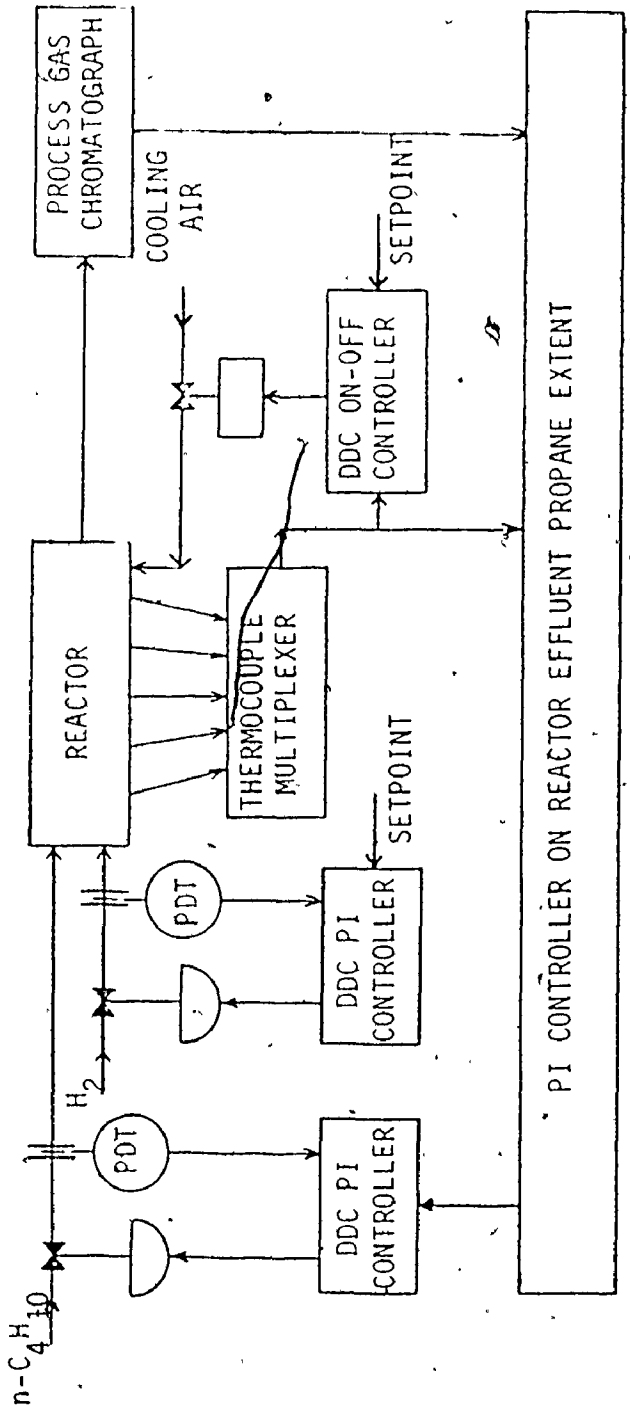


FIGURE 5-8

REACTOR EFFLUENT

PROPANE EXTENT CONTROL BY

n-BUTANE MANIPULATION - Run #2

TABLE 5-7

PROPANE EXTENT PI CONTROLLER

SETTINGS* - RUN #2

Proportional Gain (K_p) = 200.

Proportional Integral Gain (K_{PI}) = 2.

Scale Factor : +1000.

Control Interval: 30. seconds

Cascaded n-butane setpoint low limit: 12 cm^3/sec, 1 ATM, 25°C

Cascaded n-butane setpoint high limit: 25 cm^3/sec, 1 ATM, 25°C

* Parameters of the GOSEX DDC PI controller (see Chapter 4, Section 2).

FIGURE 5-9
RUN # 2

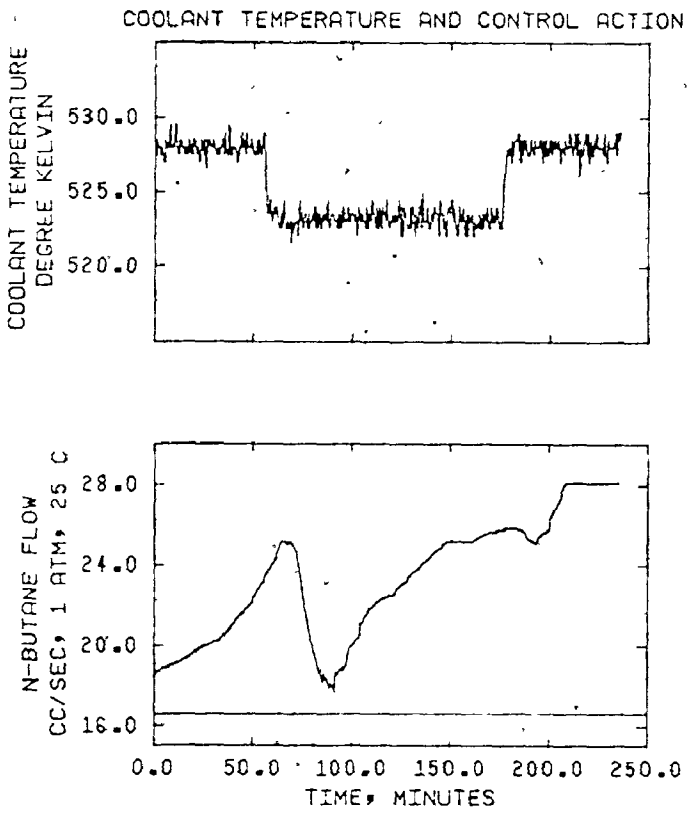
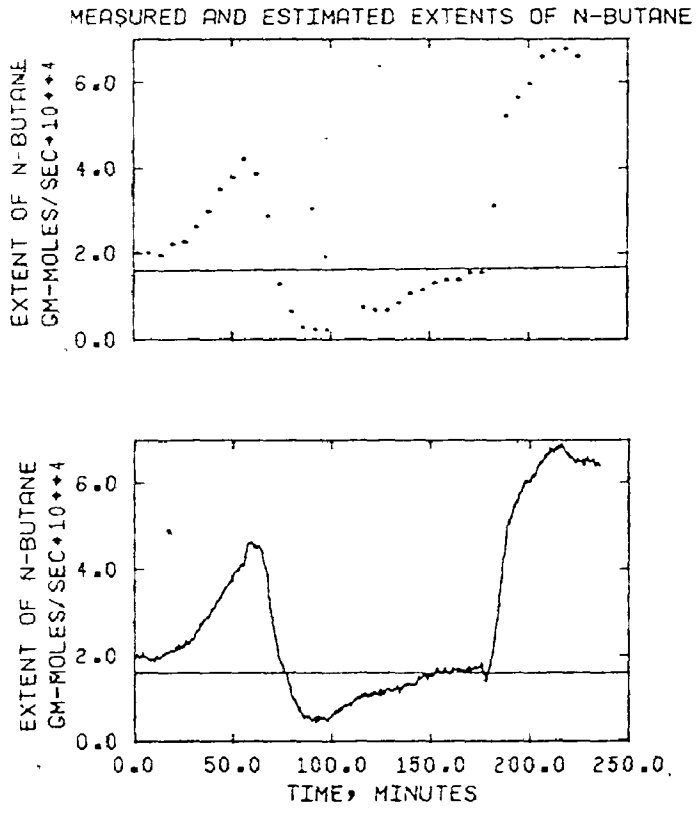


FIGURE 5-10
RUN # 2



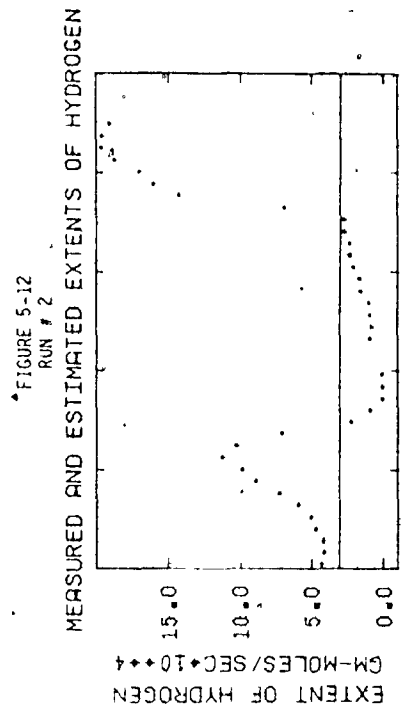
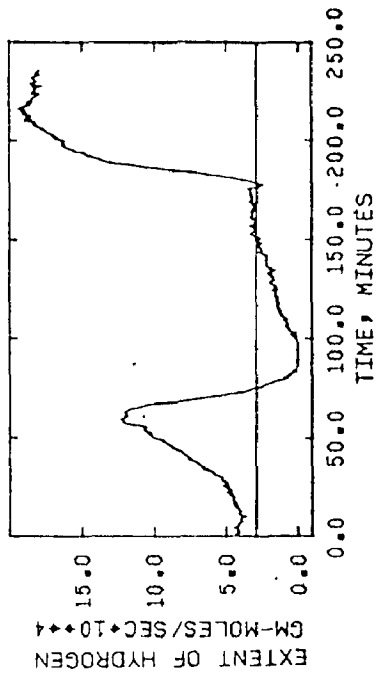


FIGURE 5-12
RUN # 2



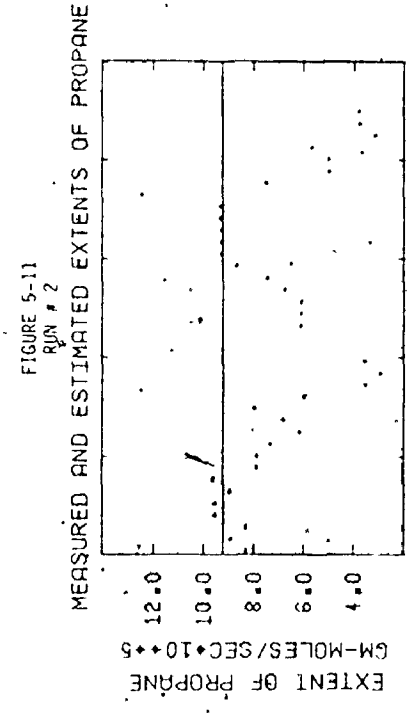
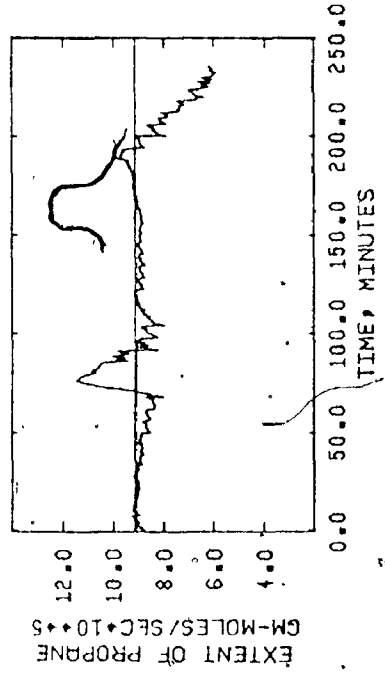


FIGURE 5-11
RUN # 2



of 255°C before the setpoint of the coolant temperature on-off controller was reduced to 250°C. Operation continued for another two hours followed by a return of the setpoint to 255°C. The experiment was ended after another hour of operation at this condition. The actions of the controller when subjected to these coolant temperature load changes are presented in Figure 5-9. Plots of the time variation of the measured and estimated extents of n-butane, propane and hydrogen are shown in Figures 5-10, 5-11 and 5-12 respectively. The ability of Equation 5-1 to predict effluent extents is confirmed by a study of these three figures. The predictions of the n-butane and hydrogen extents are somewhat better than those of propane.

Despite the reasonable predictions of the effluent extents, the single variable PI controller could not hold the propane extent at its setpoint. Before the first coolant temperature load change, the n-butane feed rate increased continuously, thereby moving the reactor into a regime where bed temperatures in excess of 700°K occurred, As indicated by the measured extents of propane data (Figure 5-11), a susbstantial decrease of the controlled variable occurred during this interval. This situation was clearly unstable in view of the monotonic rise of the n-butane flow rate shown in Figure 5-9. The sudden and relatively large drop of the n-butane feed rate just after the first coolant temperature load change was attributed to the erroneous values of the propane extents predicted at that time. These abnormally large estimates were partly due to the sudden changes in the values of the functionals of the reactor

axial collocation temperatures which arose upon the load changes. They also may have resulted from poorly converged estimates of the matrices of Equation 5-1. Because of the unstable characteristics of Run #2, this explanation is most likely.

The unstable behaviour of the control system persisted until the end of the experiment. In fact, instability was very evident before any load changes were even attempted.

The failure of the univariate PI controller may be attributed to a single cause. Although inaccuracies in the predicted propane extents over certain intervals were detrimental to the controller's actions, the control system was underspecified since numerous operating conditions could feasibly yield the desired propane extent. The use of a multiloop or multivariable control scheme is indicated when the objective of control is the regulation of the propane extent in the reactor effluent stream.

Confident that the measurement Equation 5-1 provided reasonable estimates of the effluent stream extents, software to implement the model reference adaptive control theory which has been developed in Chapter 2 was prepared. The structure of this software has been described in Appendix C, Section 6, and is schematically represented by Figure 5-13.

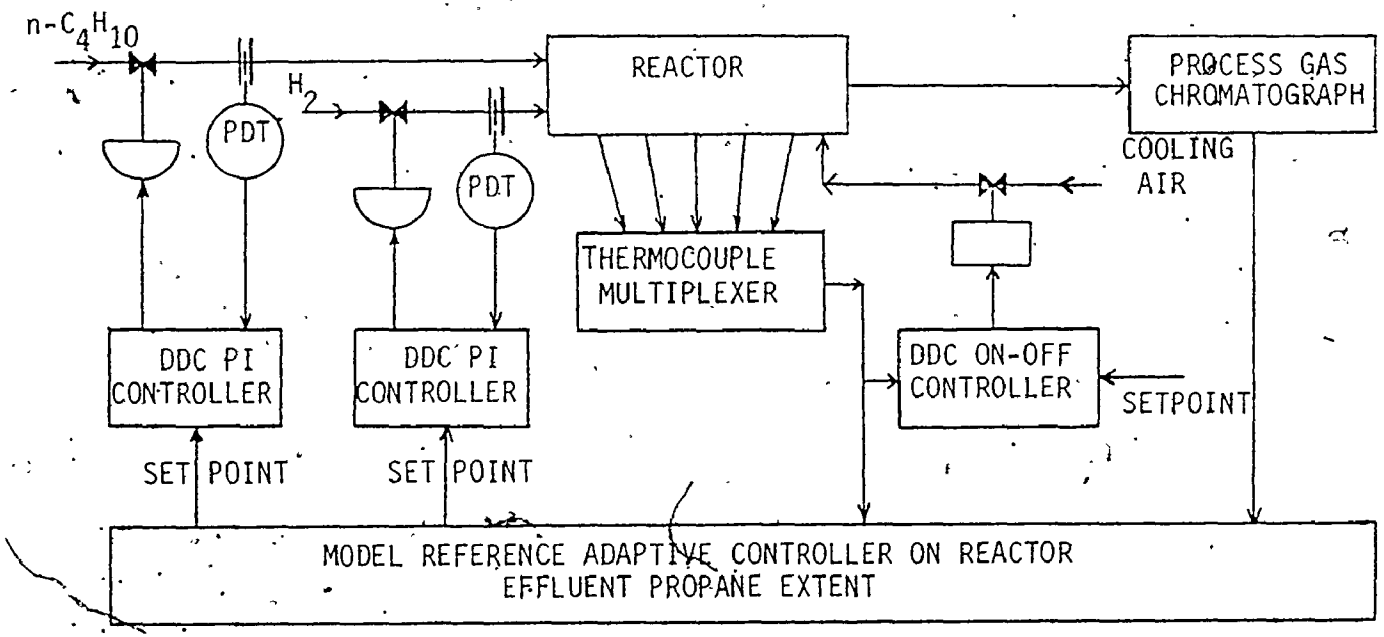
Initial values of $\Phi(k-1)$, $\Psi(k-1)$, $\Gamma(k-1)$ and $\Omega(k-1)$ (Equations 2-51 and 2-52) are required to begin the recursive adaptive control algorithm. A few experiments (not recorded here) were undertaken to provide

FIGURE 5-13

MODEL REFERENCE ADAPTIVE CONTROL

OF THE REACTOR EFFLUENT

PROPANE EXTENT - Runs #3 to 7



reasonable initial values of these matrices for Runs 3 to 7. A feasible estimate for $\Phi(k-1)$ was determined by differencing two reasonable candidates for the reference model. These candidates were byproducts of the optimal controller calculations performed earlier to produce an acceptable closed loop stable reference model. Since no information about $\Psi(k-1)$ was available, all elements were set to a small value (10^{-4}). It was also decided that the initial control policy determined by $\Gamma(k-1)$ and $\Omega(k-1)$ would be open-loop. With these set to the null matrix, exploratory experiments with the model reference adaptive controller were done. The objective was essentially to arrive at converged values of $\Phi(k)$, $\Psi(k)$, $\Gamma(k)$ and $\Omega(k)$ once suitable values of the adaptive loop gains (ξ_{ij} and γ_{ij}) were discovered. Because no estimates of these gains were available at the start of the exploratory experiments, all were initialized to zero. The converged matrices and stable adaptive loop gains would then be available for Runs 3 to 7.

It is perhaps useful at this time to digress momentarily to explain precisely how a typical model reference adaptive control experiment was performed. To begin, the n-butane hydrogenolysis pilot plant reactor was manually brought up to the normal operating conditions of Run #1 listed in Tables 5-2 and 5-4. The detailed startup procedure is available (Wright et al [1977]).

While the startup occurred, the process minicomputer (details have been provided in Chapter 3) was also prepared for the experiment. The real time application programs operating under the GOSEX executive were acti-

vated. The structure of the model reference adaptive control software has been explained in Appendix C, Section 6. Listings of the programs themselves are available (Tremblay [1977b]).

Once the normal reactor conditions were reached, the model reference adaptive control task was executed. Initial conditions of the states (model and process) and inputs were obtained by on-line sampling of the current reactor operating conditions. Starting values of the adaptive controller matrices and scalars were taken from a special data file prepared before the start of the experiment. After initialization of the adaptive controller software, it was possible to alter constants such as the adaptive loop gains.

It was not altogether unexpected to discover that the first few trials of the model reference adaptive controller with only proportional action led to unstable reactor operation. It was stated in Chapter 2 that the use of the pseudo-inverse approximation to arrive at the final gain matrices of the linear multivariable control law (Equation 2-31) was an approximation that could possibly result in an unstable closed loop system. Although there was the possibility of finding another pseudo-inverse which would be adequate, a search for an appropriate candidate was out of the question. Another plausible cause for the instability of the reactor is the fact that the control system does not specifically deal with the non-minimum phase characteristics of the reactor. A careful study of the behaviour of the unstable control system pointed out the

fact that the action of the hydrogen input was always in the wrong direction. Since the adaptive algorithm calculated the actions as deviations of the inputs about their operating levels, the malfunction was corrected by simply negating the contribution of the proportional and integral controller terms to the hydrogen action. This solution proved successful for several experimental conditions and was essential to the model reference adaptive control studies of Runs 3 to 7.

Preliminary studies with the modified model reference adaptive control algorithm indicated that suitable values for the proportional action adaptive loop gains (columns 1, 2 and 3 of ξ) were 0.5×10^{-2}. Smaller values of 0.25×10^{-4} were needed for the integral action adaptive loop gains (columns 4 and 5 of ξ). When setpoint action was attempted, the adaptive loop gains (matrix γ) were set to 0.1×10^{-3}. Setting to zero a given column of the ξ or γ matrices would effectively disable adaptation with respect to the particular state or setpoint. The values of the adaptive loop gains used in Runs 3 to 7 have been listed in Table 5-8. Only a very narrow range in the values of the adaptive loop gains would result in stable reactor operation. Consequently, this constraint made it impractical to explore the effects of the adaptive loop gains on adaptive controller properties.

Five different experiments with the modified model reference adaptive controller were undertaken and are reported here. Of those that were successful, the reactor clearly exhibited non-minimum phase behaviour.

TABLE 5-8

ADAPTIVE LOOP GAINS

	Proportional Action $\xi(1)$, $\xi(2)$, $\xi(3)$	Integral Action $\xi(4)$, $\xi(5)$	Setpoint Action $\gamma(1)$, $\gamma(2)$
Adaptive Loop Gains	0.5×10^{-2}	0.25×10^{-4}	0.1×10^{-3}
Applicable Runs	3,4,5,6,7	4,5,6,7	7

Run #3 (the first of the five) was with all but the proportional feedback actions disabled and when compared to Run #4 was meant to verify the necessity of the integral action term to remove offset. Run #5 with the integral action term enabled was designed to investigate the importance of the model reference states in the adaptive algorithm. The controllers for these three experiments were subjected to severe coolant temperature load changes and were evaluated in part on their ability to maintain the effluent stream propane extent at its setpoint.. Step changes of 5 and 10 ^{o}K are severe upsets for the n-butane hydrogenolysis reaction since its reaction rate doubles for $2^{o}K$ temperature rises. Runs #6 and #7 were two other experiments which were undertaken to test the servo-mechanisms of the model reference adaptive controller.

Although the use of integral action in a model reference adaptive controller may not be required for all systems (Oliver et al [1973]), the results of Runs 3 and 4 suggest that indeed it is needed for the control of the n-butane hydrogenolysis reactor. The behaviour of the closed loop system under simple multivariable proportional feedback adaptive control was recorded during Run #3 and the data is presented in Figures 5-14 to 5-18. The data for Figures 5-19 to 5-23 was collected during Run #4 and serves to demonstrate the marked improvement in control by the addition of multivariable integral action to the proportional action previously employed. Both Runs 3 and 4 were conducted at essentially the same conditions, each being subjected to similar coolant

FIGURE 5-14
RUN # 3
COOLANT TEMPERATURE

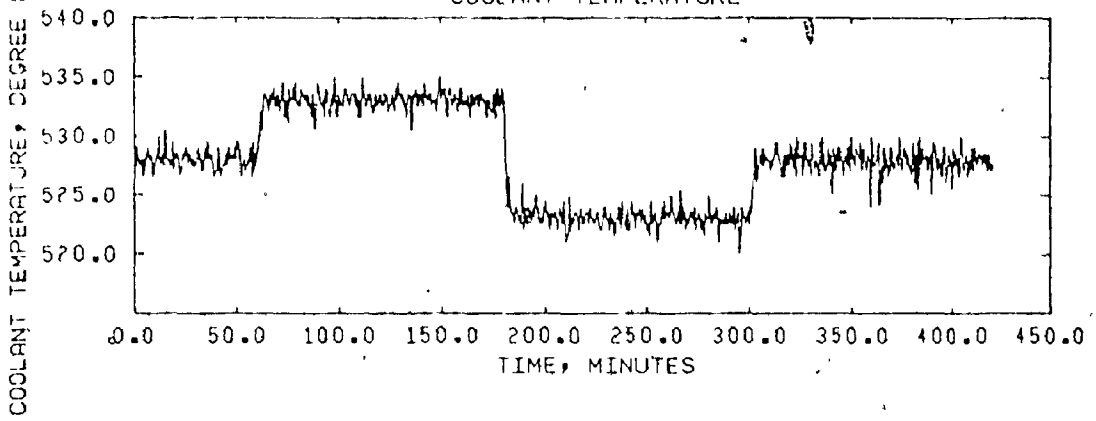


FIGURE 5-15
RUN # 3
CONTROL ACTION - FLOWRATES OF N-BUTANE AND HYDROGEN

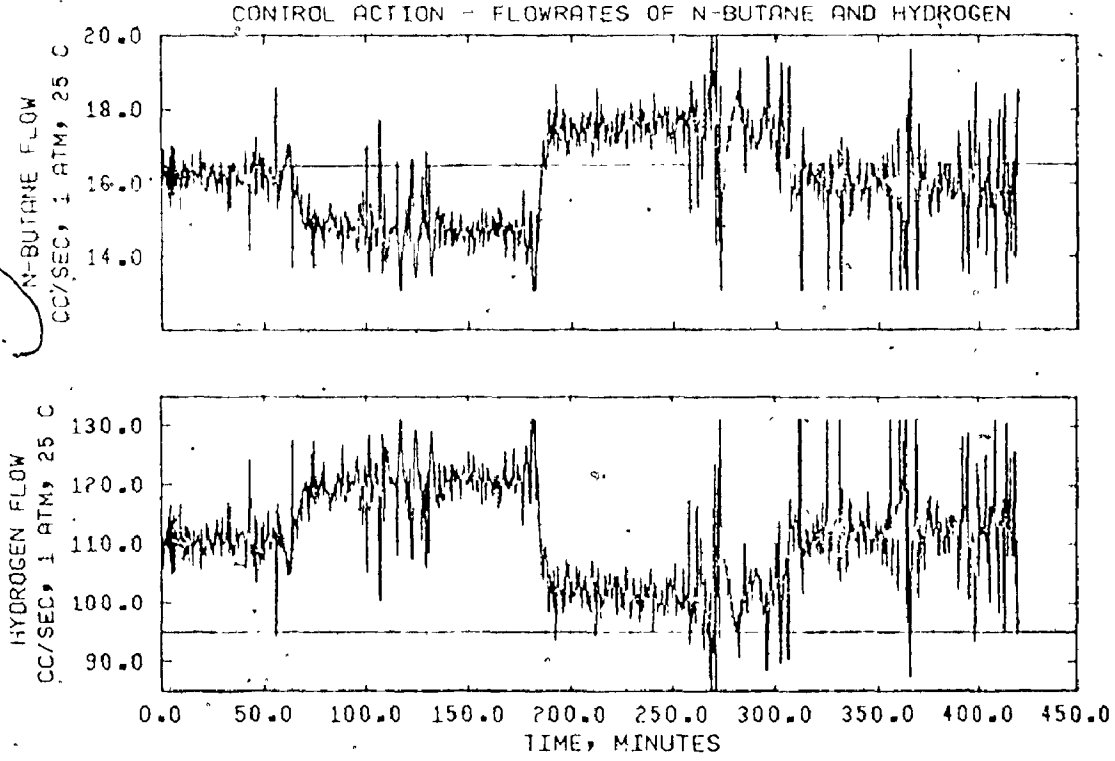


FIGURE 5-16
RUN # 3

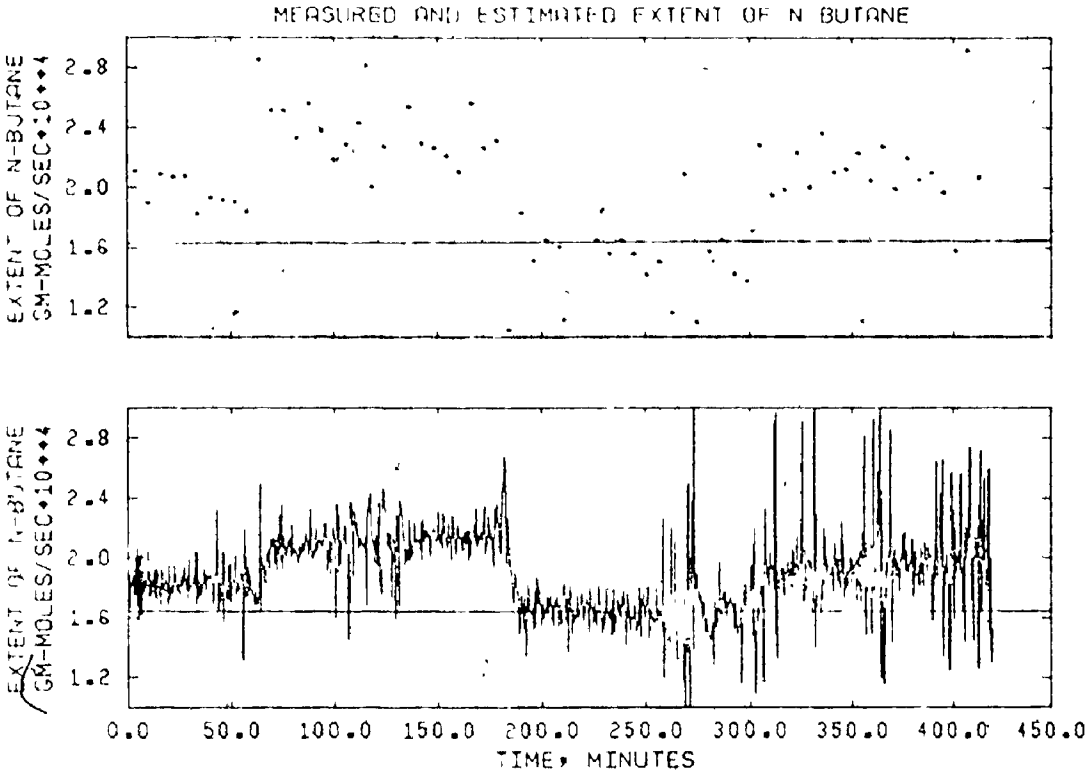
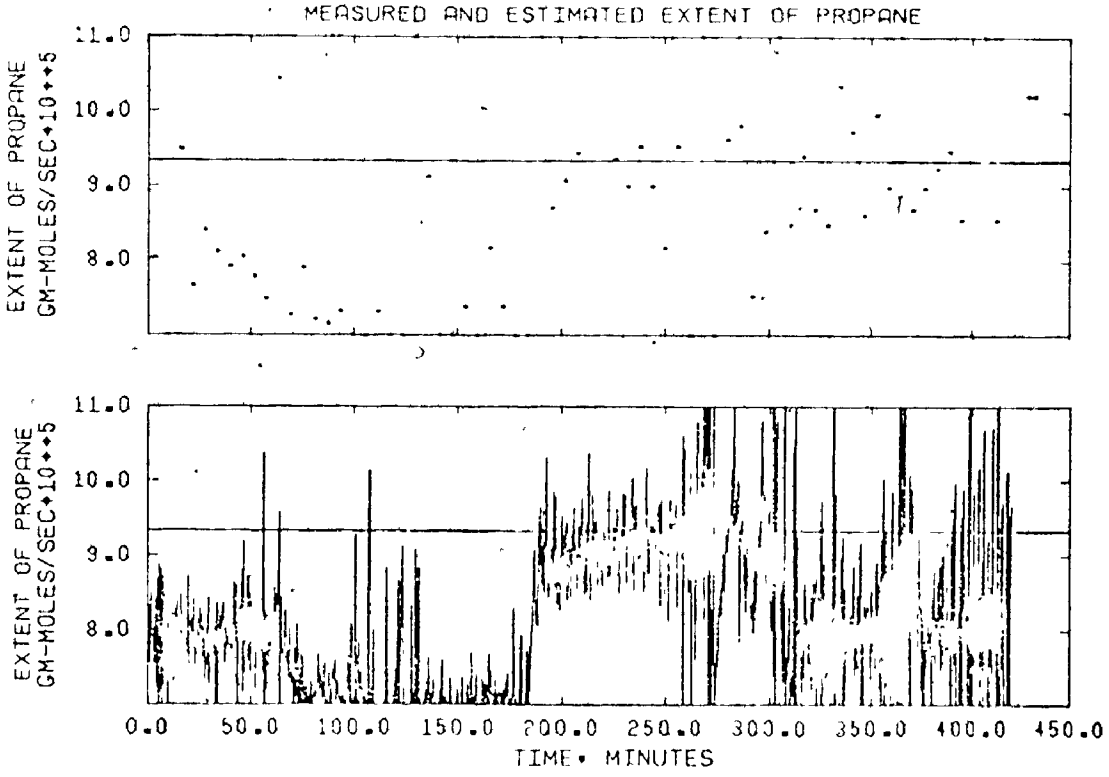


FIGURE 5-17
RUN # 3



temperature load changes as illustrated by Figures 5-14 and 5-19. The first of the changes was an increase of the coolant temperature by five degrees Kelvin. After two hours at this condition, the coolant temperature was dropped by ten degrees Kelvin. The final disturbance was another increase of the coolant temperature by five degrees Kelvin. This upset also occurred approximately two hours after the previous one. The coolant temperature load changes were unmeasured disturbances and consequently only sudden changes in the states could reflect the upsets.

The control actions in response to these disturbances were considerably more violent for Run #3 than for Run #4 although both did exhibit similar characteristics. As expected, a rise in coolant temperature induced a reduction in the n-butane feed flow rate and an increase in the hydrogen feed flow rate. When the coolant temperature fell, the actions were reversed. In both runs, the movement in the feed flowrates was in the direction most likely to maintain the extent or propane in the reactor effluent at constant value. These observations are also applicable to the results of Run #5 to be analyzed shortly.

A consequence of the rapid changes in feed flow rates during Run #3 was a large scatter in the measured extents of n-butane, propane and hydrogen of the reactor effluent. The estimates of these extents which were essential to the calculation of the control action were reasonably accurate but by no means as noise free as those of Run #4. It appears that the presence of integral action during Run #4 dampened the large

FIGURE 5-18
RUN # 3
MEASURED AND ESTIMATED EXTENT OF HYDROGEN

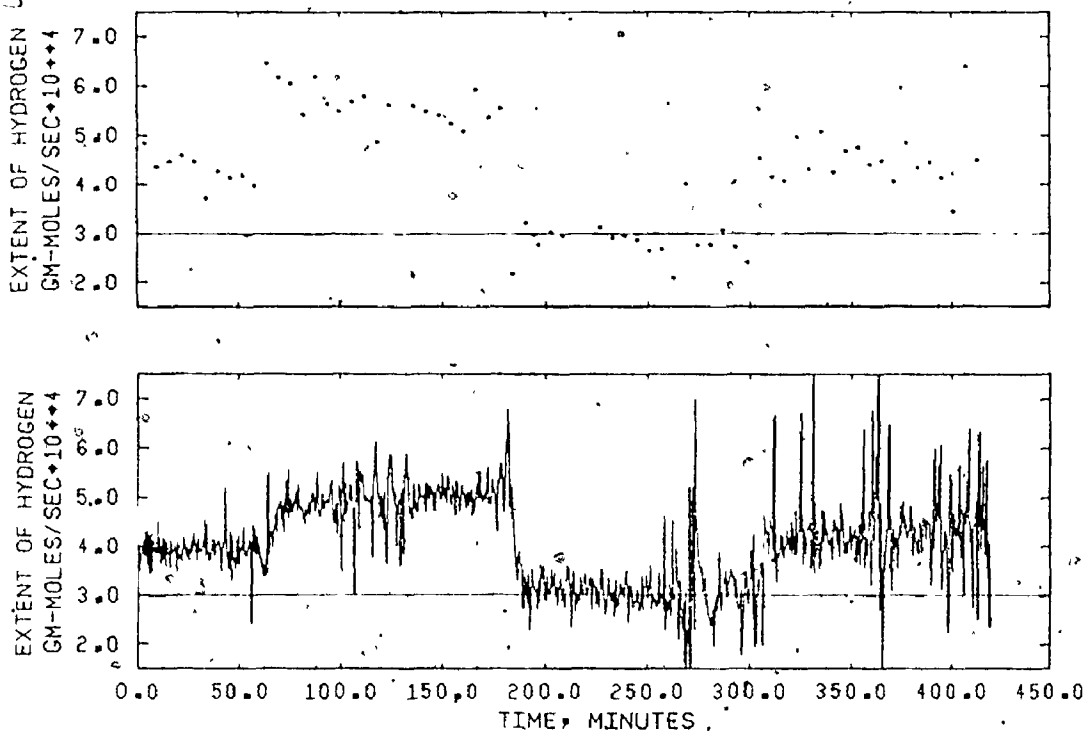


FIGURE 5-19
RUN # 4
COOLANT TEMPERATURE

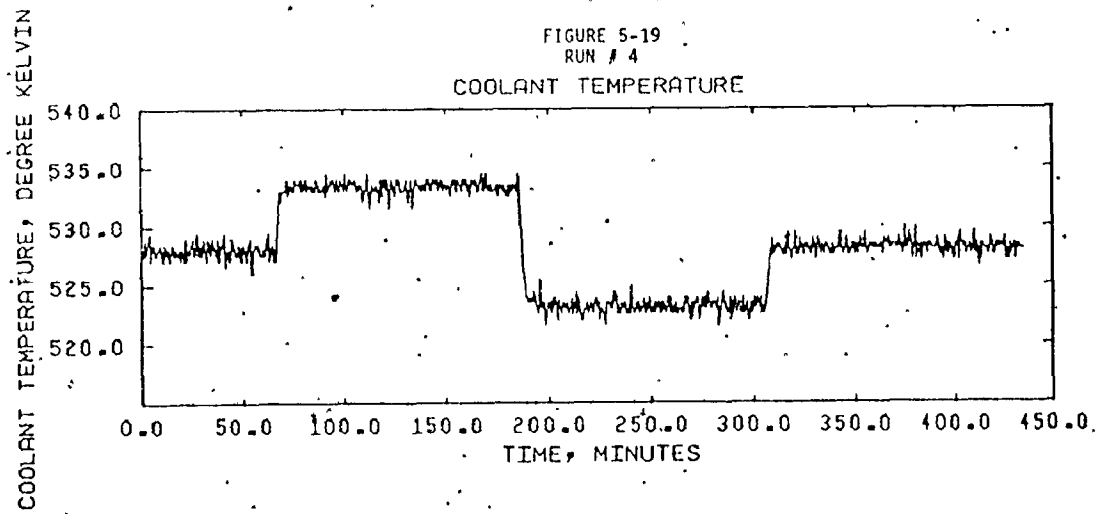


FIGURE 5-20
RUN # 4

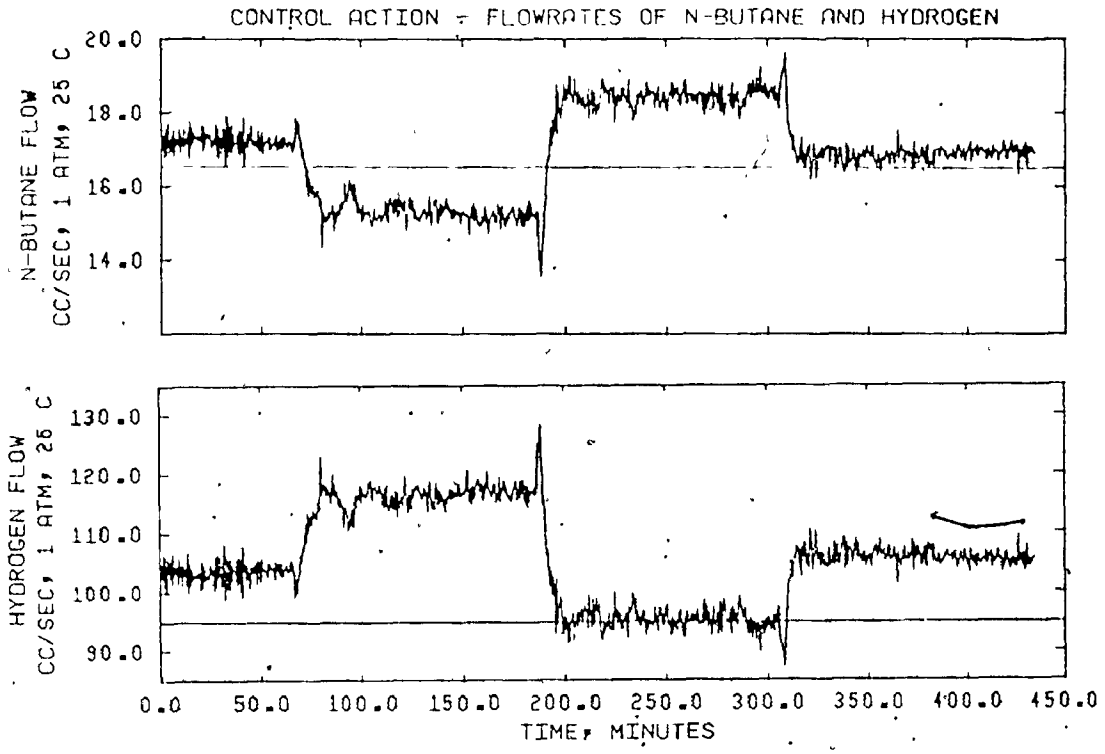


FIGURE 5-21
RUN # 4

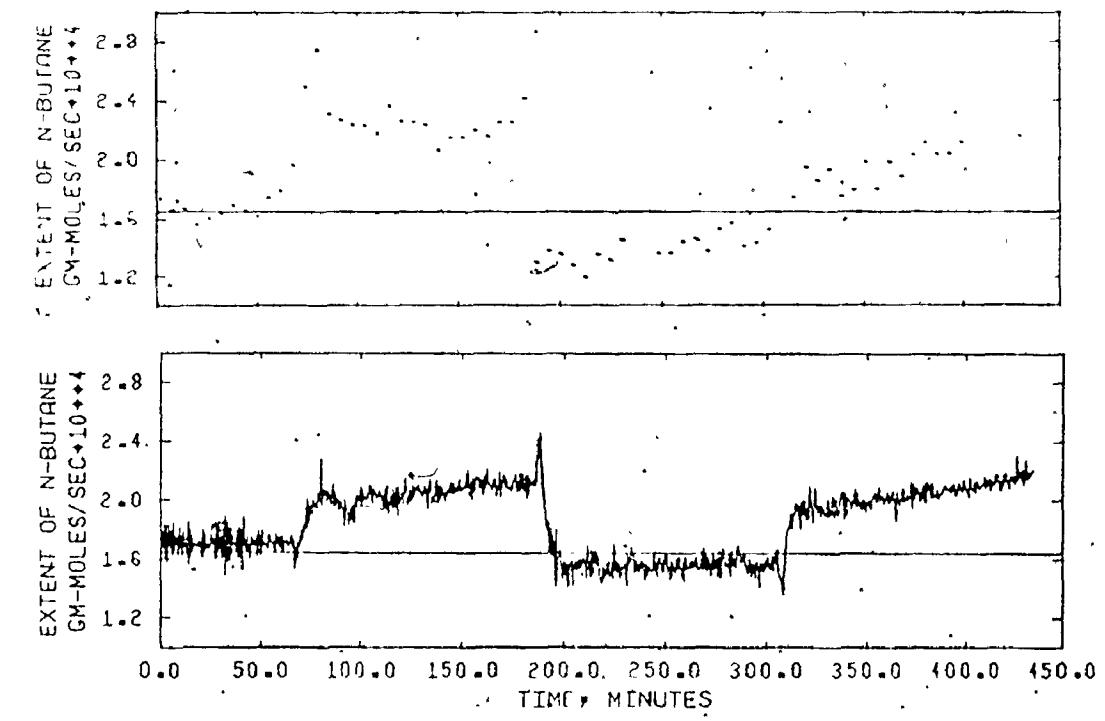


FIGURE 5-22
RUN # 4
MEASURED AND ESTIMATED EXTENT OF PROPANE

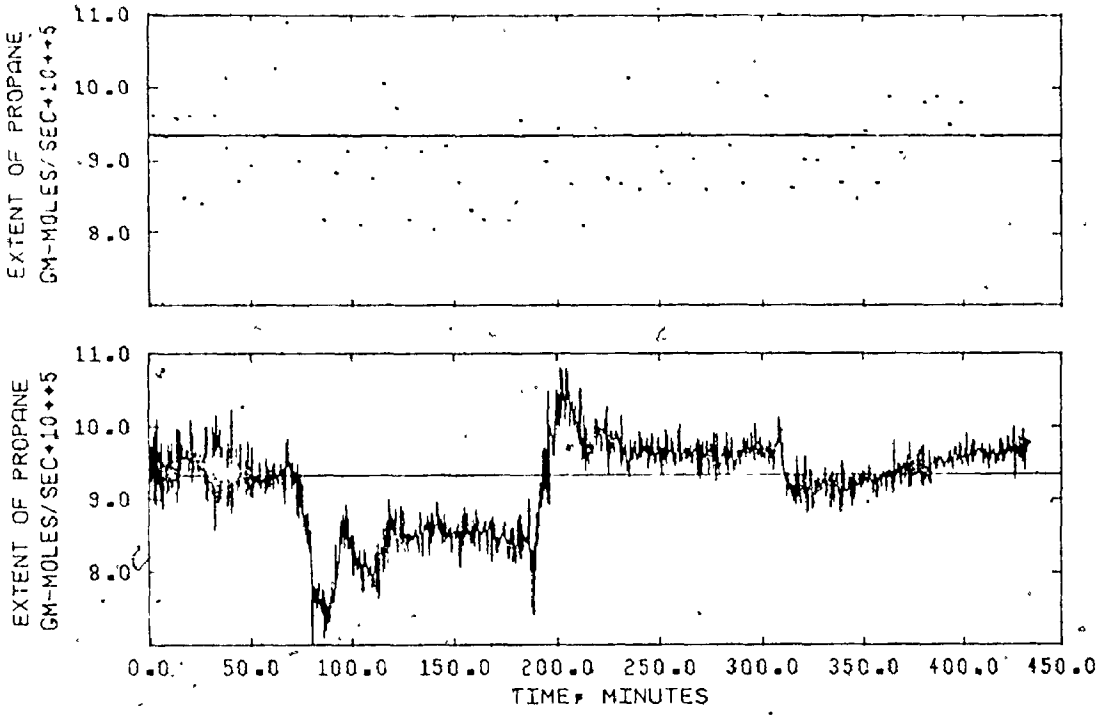
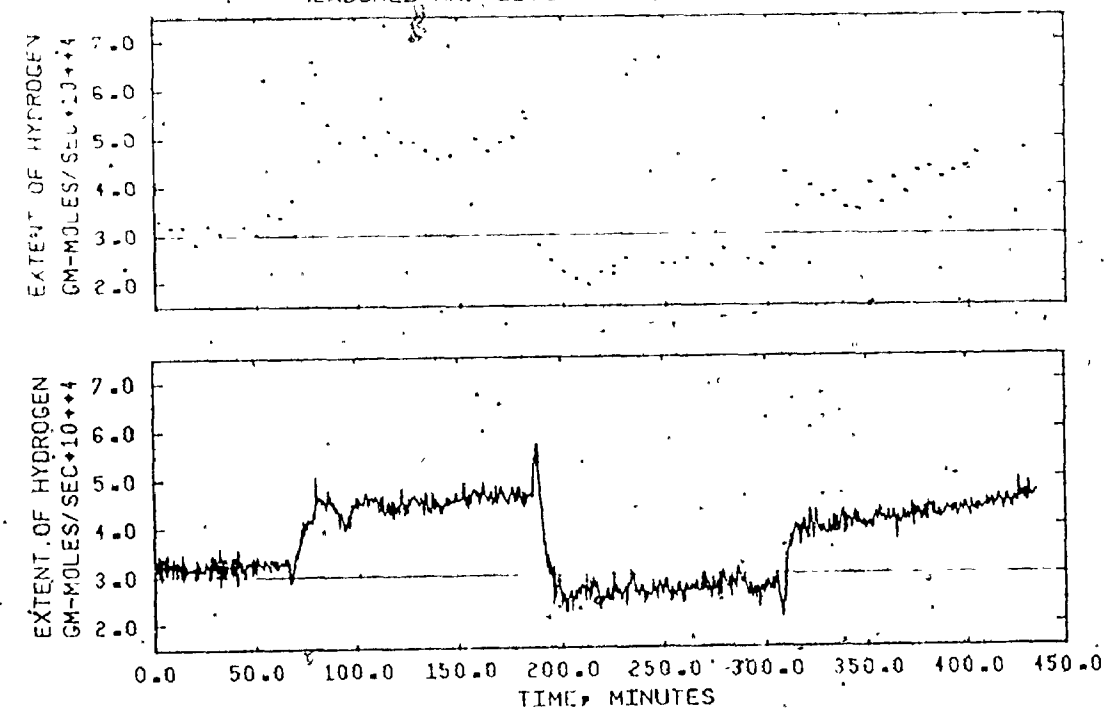


FIGURE 5-23
RUN # 4
MEASURED AND ESTIMATED EXTENT OF HYDROGEN



excursions of the inputs which were characteristic of Run #3. A result of this was clearly more stable effluent extents. Quite unlike Run #3, it was possible during Run #4 to maintain the extent of propane about the controller's setpoint (9.29×10^{-5} gm-moles/sec) with only moderate deviations (10%) from this value. In spite of the empirical correction which was made to this model reference adaptive controller, it has been demonstrated that for this system integral action is needed to keep the reactor effluent propane extent at its normal operating value.

The influence of the reference model states on the stability and convergence properties of the adaptive controller needed to be determined. Data from Runs 3 and 4 indicated that the reference model states were several orders of magnitude smaller than the process states for the duration of the runs. Since the reference model was inherently stable, it was expected that its state variables asymptotically approached zero deviation after some time. But as this occurred, their influence on the adaptive algorithm also vanished. This could be prevented if it were possible to remove the stochastic components of the output signals and pass them to the reference model as unregulated inputs. But since the adaptive control algorithm as derived and implemented assigns all differences between reference model and process states to improper control of the process, disturbances were induced artifically. Run #5 was performed to examine the effects of perturbation of the reference model on the control of the pilot plant reactor. The data from this run are plotted

in Figures 5-24 to 5-29. The only way of introducing reasonable disturbances into the reference model was to reset the model states to the actual process states whenever the model states became significantly smaller than the process states. With this in mind, the model reference adaptive control software was modified to reset the values of the model states to those of the process states whenever all of the values of the model states fell below 25% of the values of the process states. At this level, reference model retriggering occurred at a rate which permitted the system to stabilize after each upset.

Except for the software changes needed to implement reference model retriggering, the same software and experimental conditions used for Run #4 were used for Run #5. The data from Run #5 are plotted in Figures 5-24 to 5-29 with plots of the reference model states given in Figure 5-25. During the course of the experiment, the reference model was retriggered more than a dozen times. Due to its dynamic characteristics, the model states rose to values considerably larger than possible in the plant, but quickly returned to normal values. The optimal controller inherent in the reference model was selected on the basis of the excursions of the open-loop model inputs and not its states. For this reason, the reference model states are observed upon retriggering to rise to large values before the closed-loop model inputs are able to reduce the reference model states to normal values. A comparison of the control actions of Runs 4 and 5 in response to coolant temperature load changes shows them to be similar except for the larger variations which are present in the data of Run #5. These variations are also present in the extent data.

FIGURE 5-24
RUN # 5
COOLANT TEMPERATURE

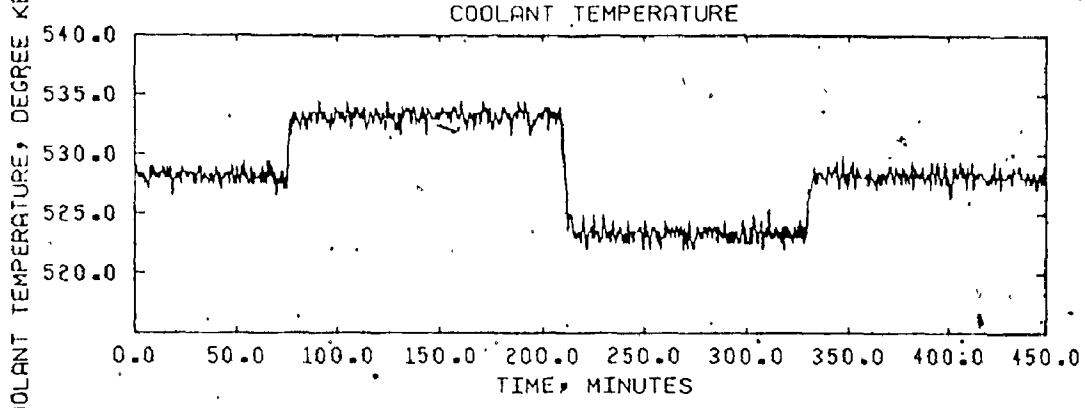


FIGURE 5-25
RUN # 5
REFERENCE MODEL RETRIGGERING

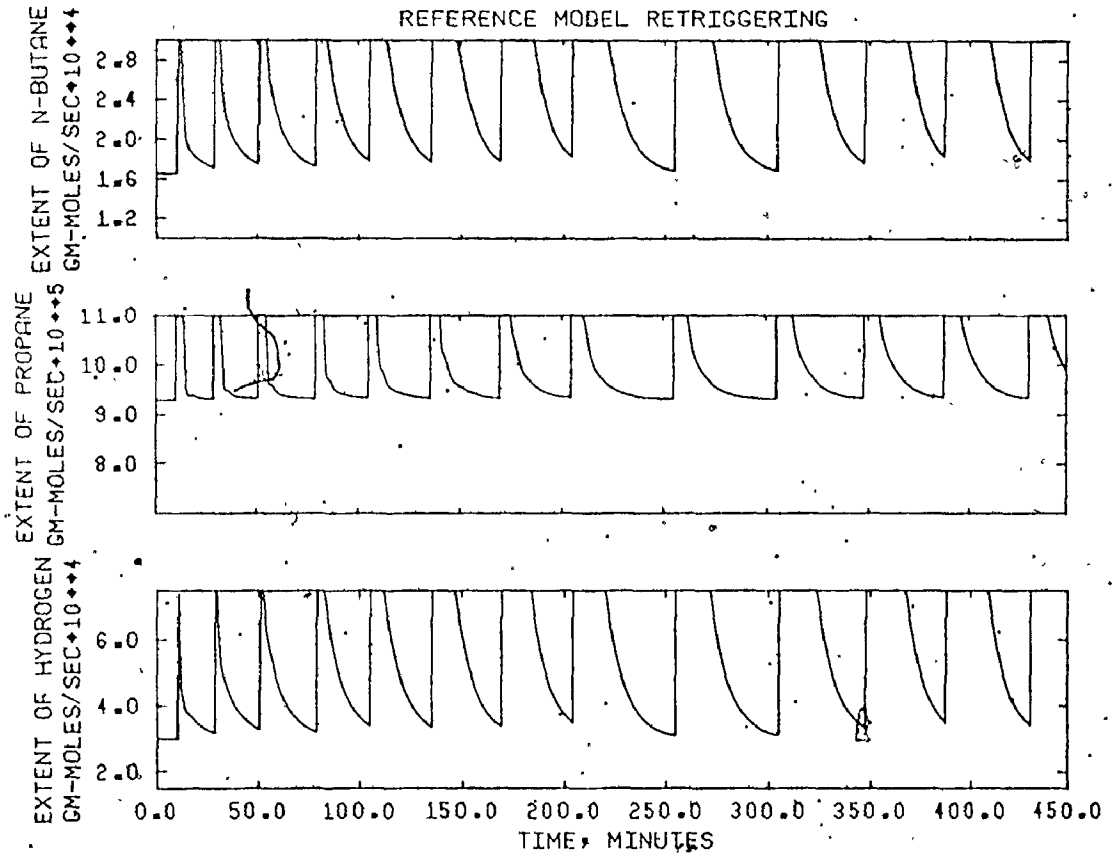


FIGURE 5-26
RUN # 5
CONTROL ACTION - FLOWRATES OF N-BUTANE AND HYDROGEN

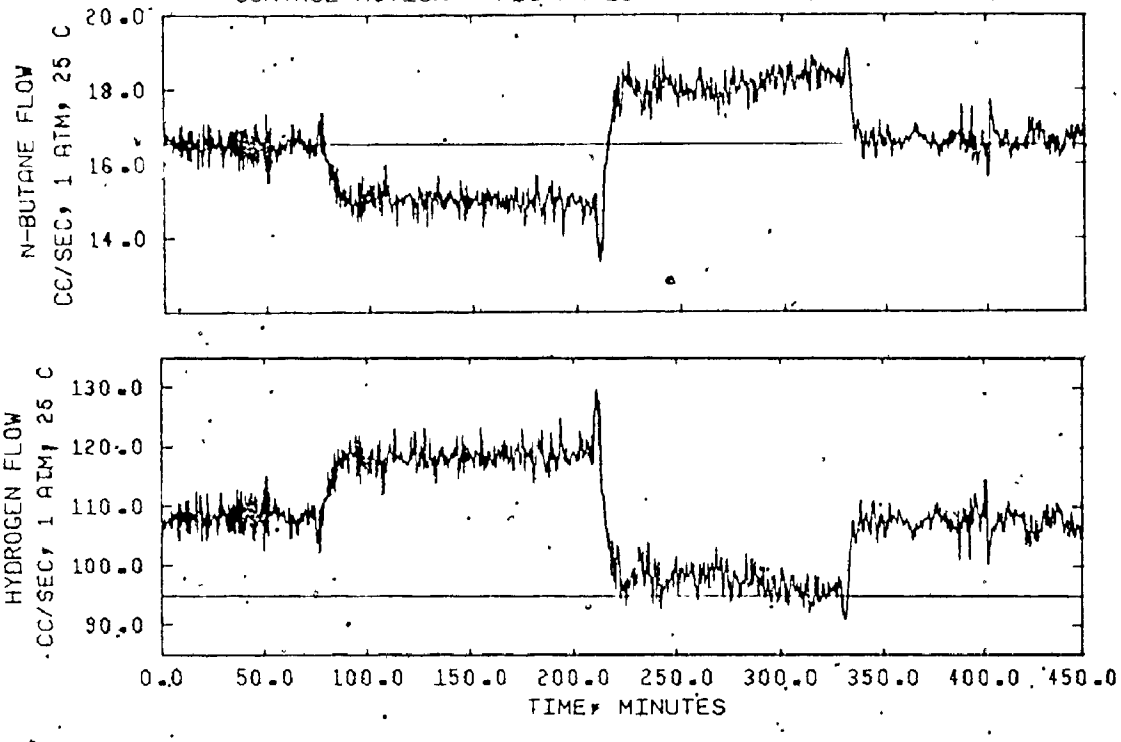


FIGURE 5-27
RUN # 5
MEASURED AND ESTIMATED EXTENT OF N-BUTANE

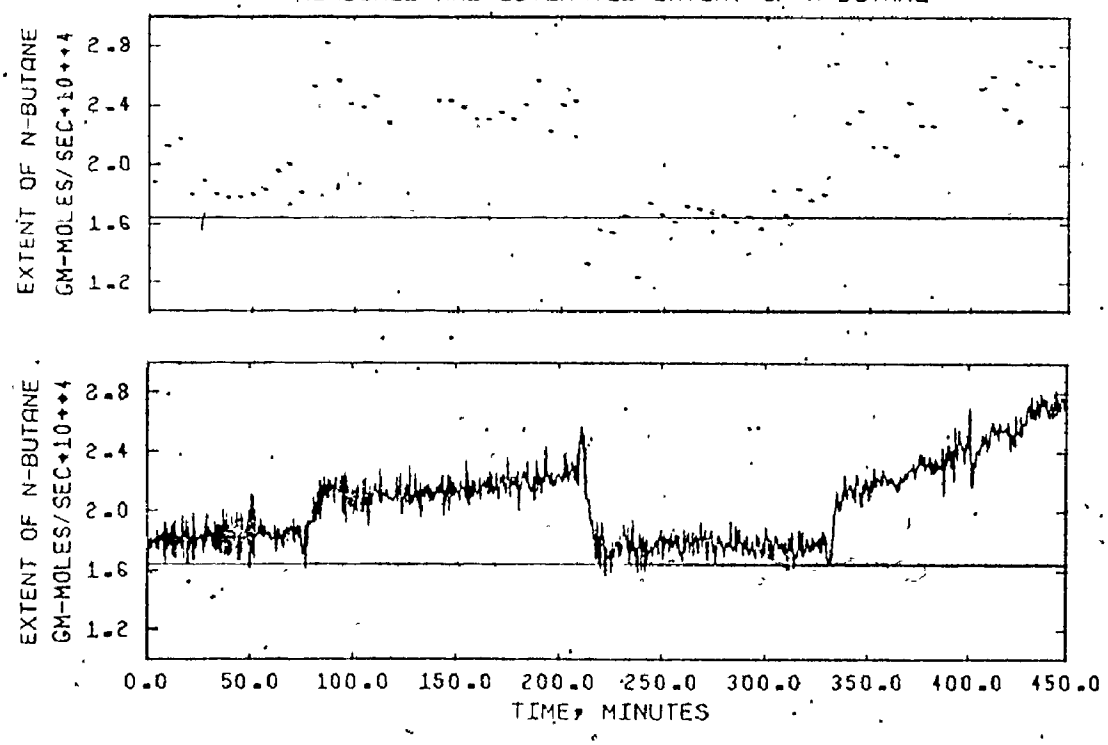


FIGURE 5-28
RUN # 5
MEASURED AND ESTIMATED EXTENT OF PROPANE

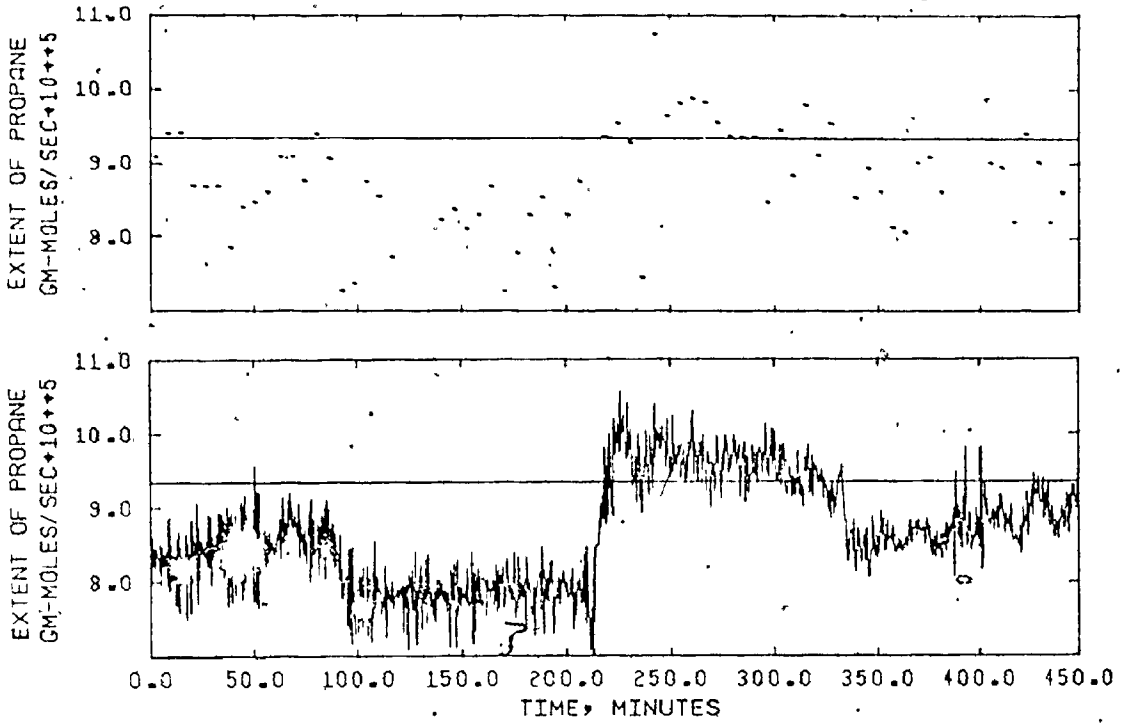
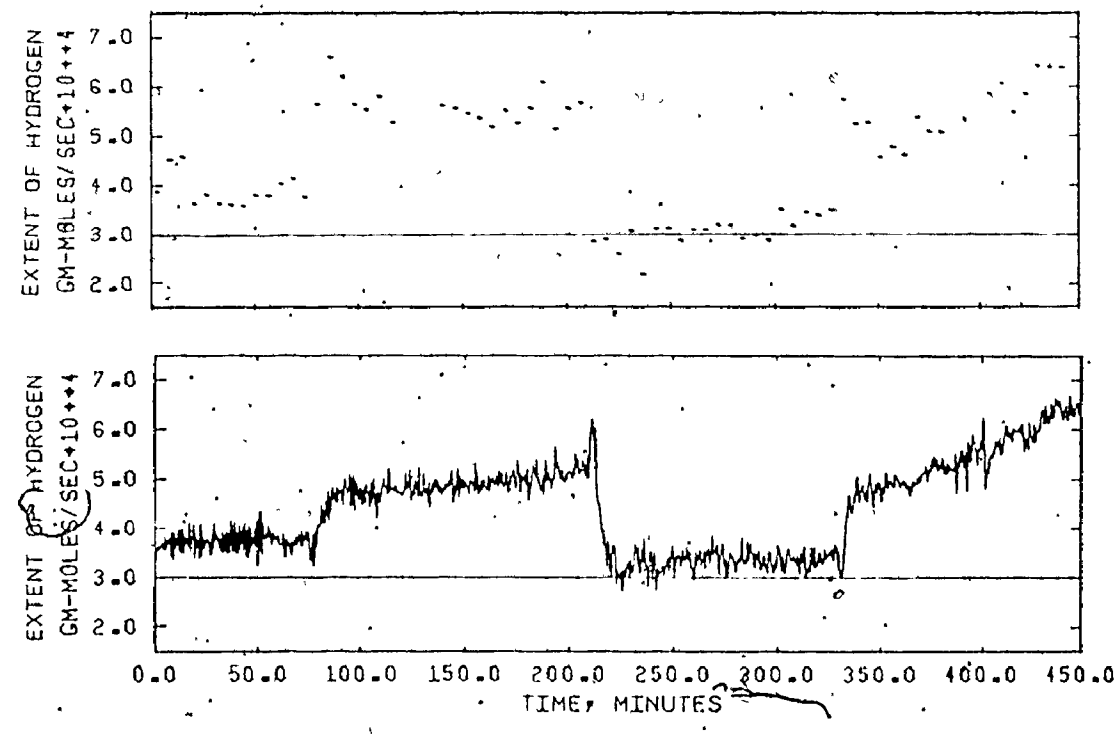


FIGURE 5-29
RUN # 5
MEASURED AND ESTIMATED EXTENT OF HYDROGEN



More importantly, there is significantly more scatter in the measured propane extent data of Run #5 than in Run #4. This difference in performance suggests that in this situation, model perturbations may be undesirable, particularly since the model state variables rise to such large values.

From the data for Runs 3, 4 and 5, it has been possible to conclude that the addition of integral action to the basic proportional feedback action adaptive control algorithm is desirable. By contrast, the retriggering of the reference model has induced poorer control and for this reason perturbation of the reference model may be detrimental to the control objectives.

The adaptive controller gain matrix $[K_{FB}(k) \mid K_I(k)]$ defined by Equation 2-31 was recorded at certain times during Runs 3, 4 and 5. Visual inspection of these matrices indicated that the elements appeared to vary monotonically in time, apparently converging to their ultimate values. For the duration of the different experiments (usually a minimum of 9 hours), the variation in the value of the gain matrix elements was typically less than 10%, with the greatest change occurring during the early moments of the experiments. It was not practical to operate the reactor for a period of time long enough to ensure convergence of the gain matrix.

Runs 6 and 7 were intended to test the servo-mechanisms designed into the model reference adaptive control algorithm. Setpoint action was incorporated in two very distinct ways. The definition of the integral

states of Equation 2-27 provided an implicit mechanism which was explored by Run #6. An explicit mechanism arises from the definition of the linear multivariable controller, Equation 2-31. The behaviour of the control system including both the implicit and explicit setpoint mechanisms was evaluated with the data from Run #7.

Both Runs 6 and 7 were conducted in essentially the same way, subjecting the model reference adaptive control algorithm to step changes in the propane extent setpoint. The reference model states were also reset to the process states upon a setpoint change. The changes in the propane extent setpoint were 30% of the steady state value 0.929×10^{-4} gm-moles/sec listed in Table 5-4 and were in fact the largest that were attempted successfully. Too large a change resulted in unstable operation. For the duration of both experiments, the coolant temperature was maintained at $250^{\circ}C$. For the first two hours of recorded operation, the propane extent setpoint was kept at an elevated value of 1.21×10^{-4} gm-moles/sec. The setpoint of propane extent was then reduced to its mean value of 0.929×10^{-4} gm-moles/sec for another two hours followed by a return to the previous value. The only real difference between runs was in the fact that the setpoint adaptive loop gains were zero for Run #6 and 0.1×10^{-3} for Run #7.

The data for Run #6 are presented in Figures 5-30 to 5-35. The control actions in response to the setpoint changes shown in Figure 5-30 are given in Figure 5-32. The reference model states are plotted in

FIGURE 5-30
RUN # 6

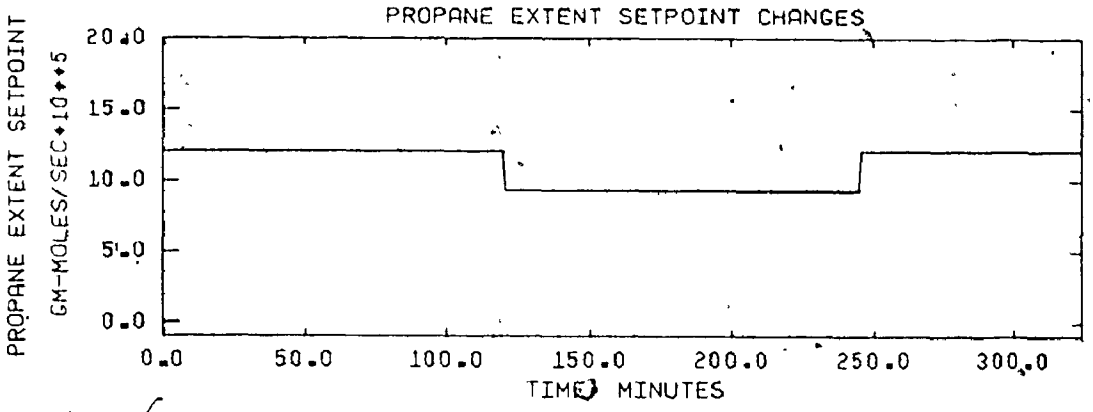


FIGURE 5-31
RUN # 6

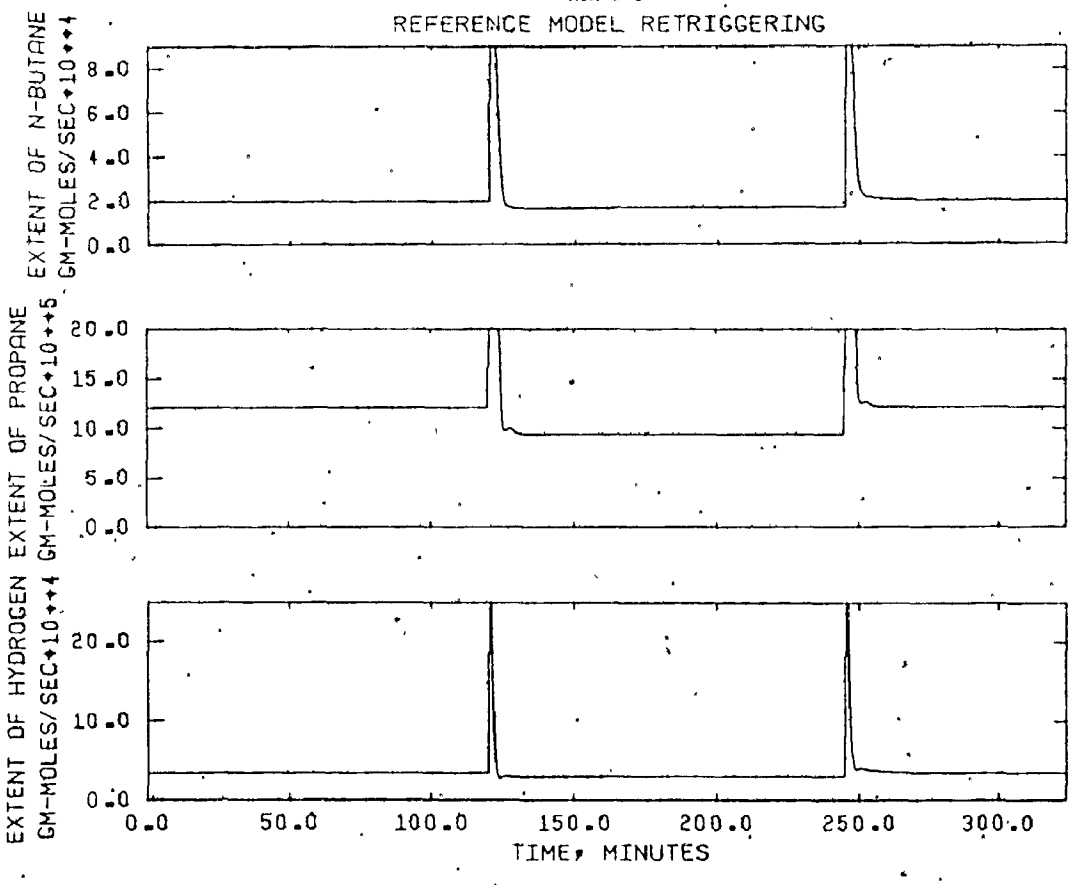


FIGURE 5-32
RUN # 6

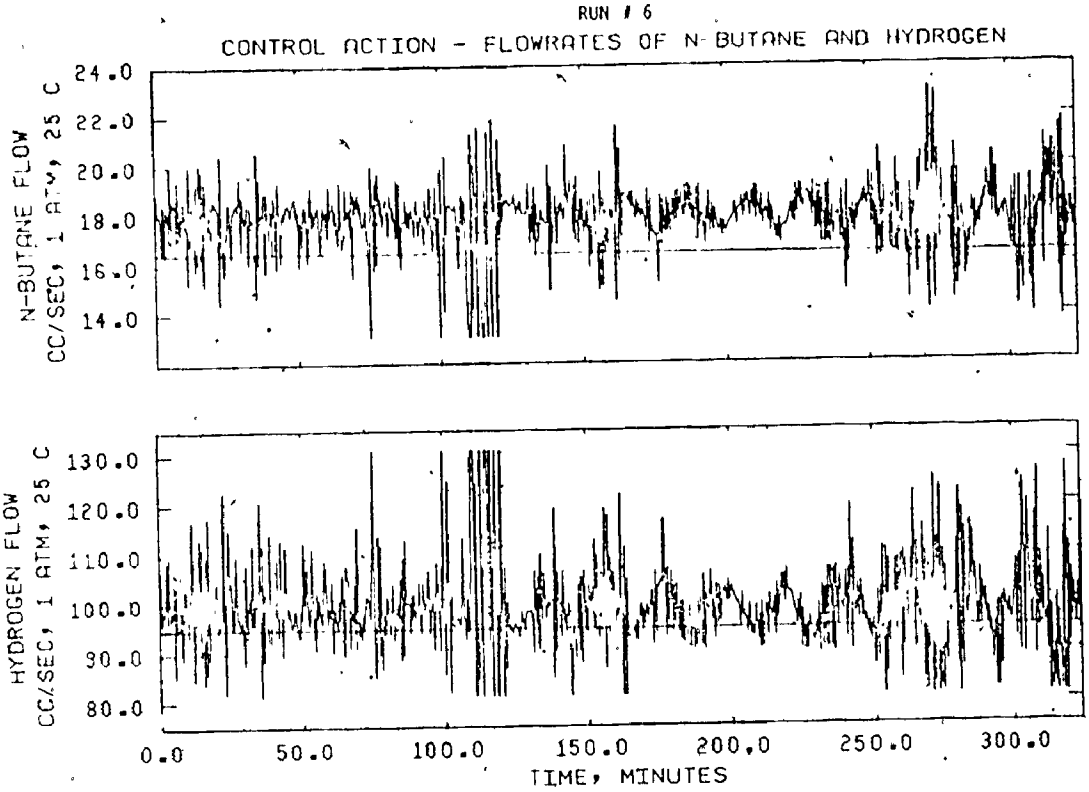


FIGURE 5-33
RUN # 6

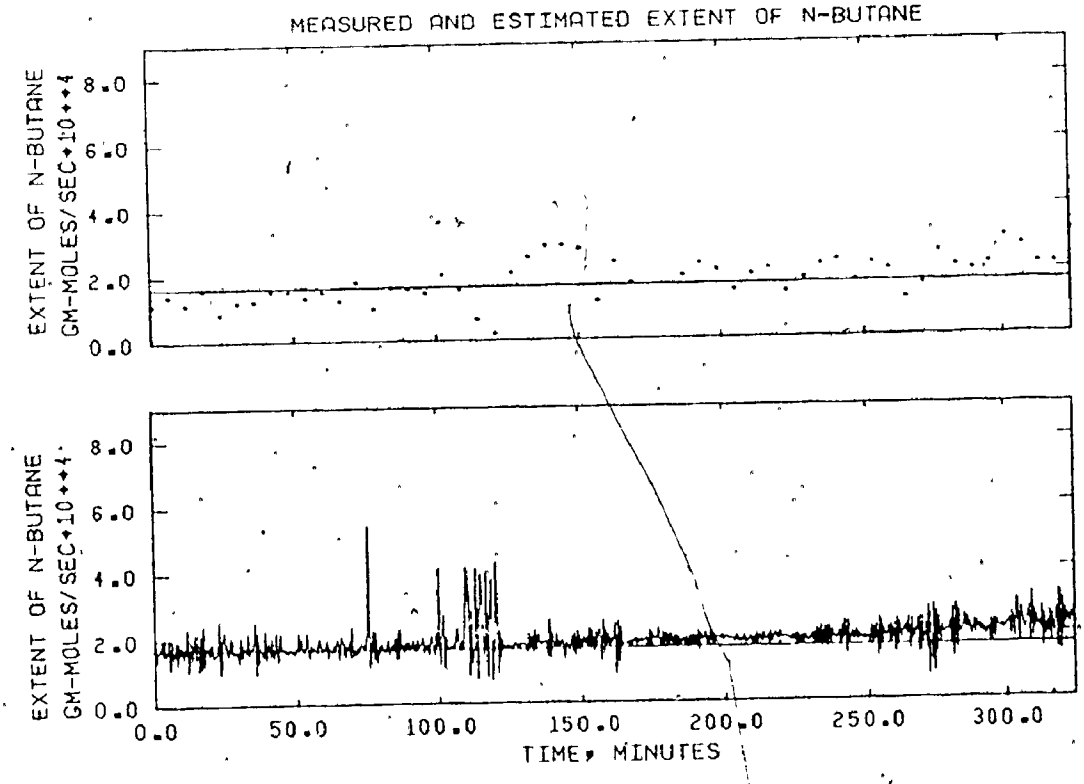


FIGURE 5-34
RUN # 6

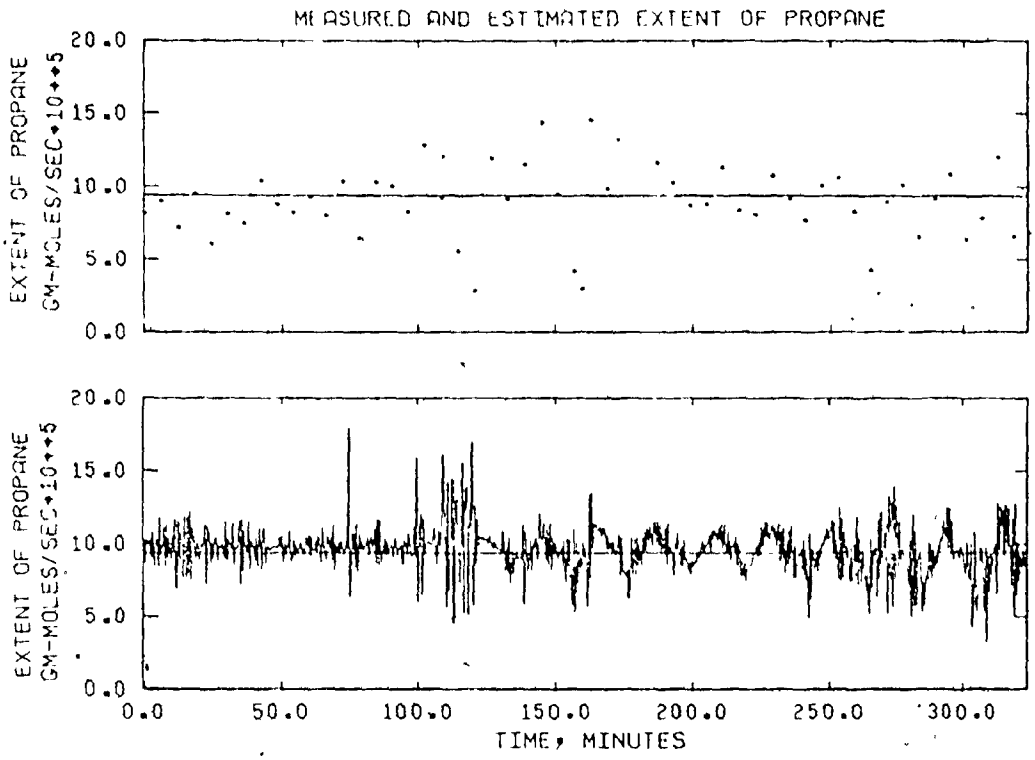


FIGURE 5-35
RUN # 6

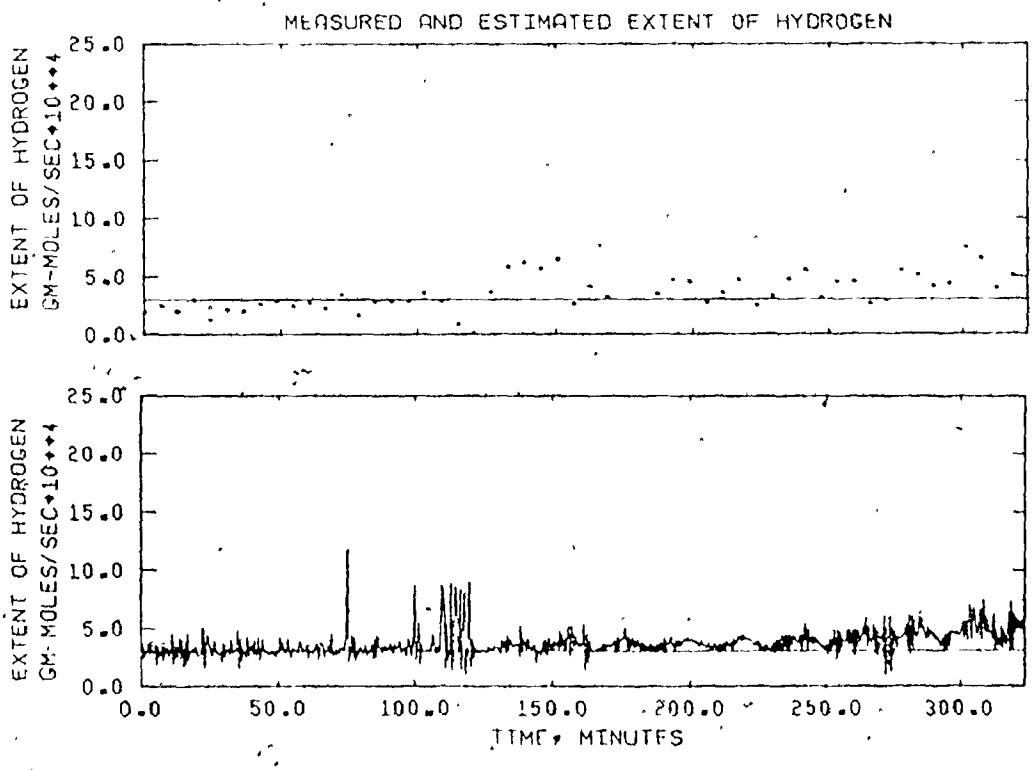


Figure 5-31. This figure shows the resetting of the reference model states upon a setpoint change. In spite of the very large upsets caused by setpoint changes, the adaptive control algorithm could not respond positively to produce the desired responses. No marked level changes in either the control actions or effluent extents were observed. In fact, it appeared that the controller did experience some difficulty maintaining the propane extent constant in the reactor effluent. This is reflected by the large variations in the reactant feed flowrates.

The use of significantly different integral action loop gains (columns 4 and 5 of ξ) resulted in reactor instability as was anticipated. The adaptive controller was incapable of producing the desired propane extent level changes in the reactor effluent stream. Apparently, the integral action term of the model reference adaptive controller was too weak to move the control system any distance away from the operating conditions about which it was fitted. Use of the setpoint action term of the adaptive controller was clearly indicated to achieve the desired results.

Significantly different properties resulted after setting the setpoint action adaptive loop gains (columns 1 and 2 of γ) to non-zero. The data from Run #7 are given in Figures 5-36 to 5-41. Since both Runs 6 and 7 were conducted in essentially the same way, Figures 5-36 and 5-37 provide no new information. The remaining figures illustrate an instability

FIGURE 5-36
RUN # 7

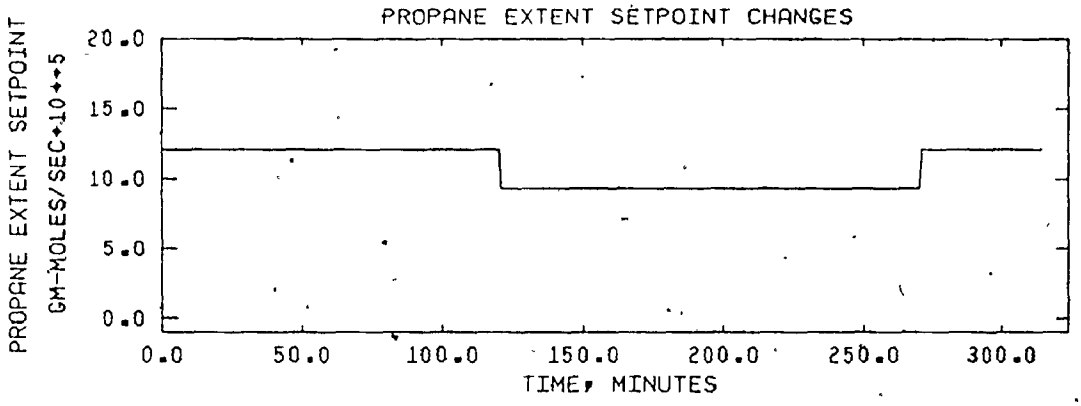


FIGURE 5-37
RUN # 7

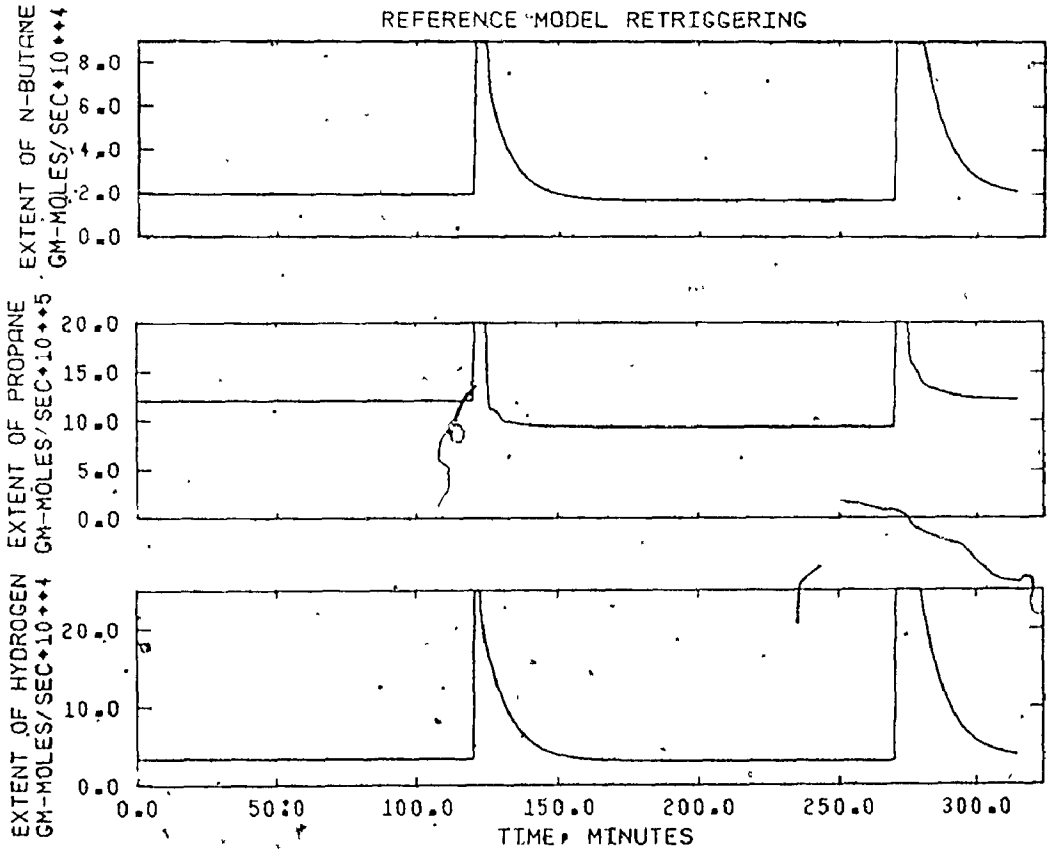


FIGURE 5-38
RUN # 7

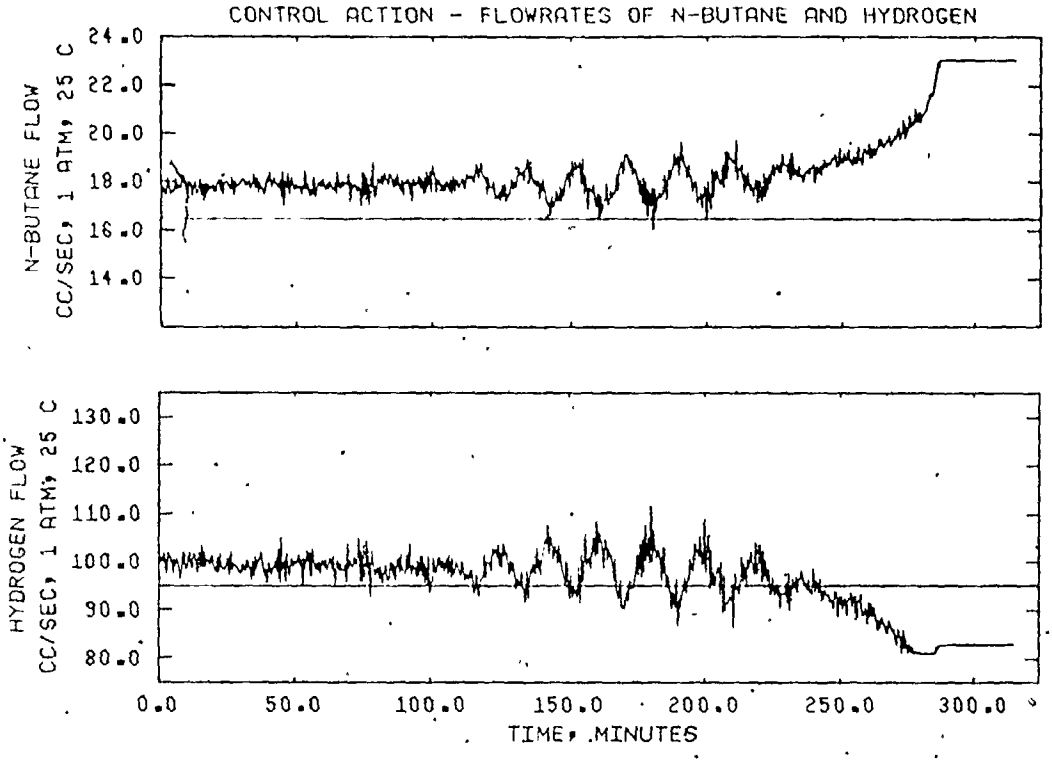


FIGURE 5-39
RUN # 7

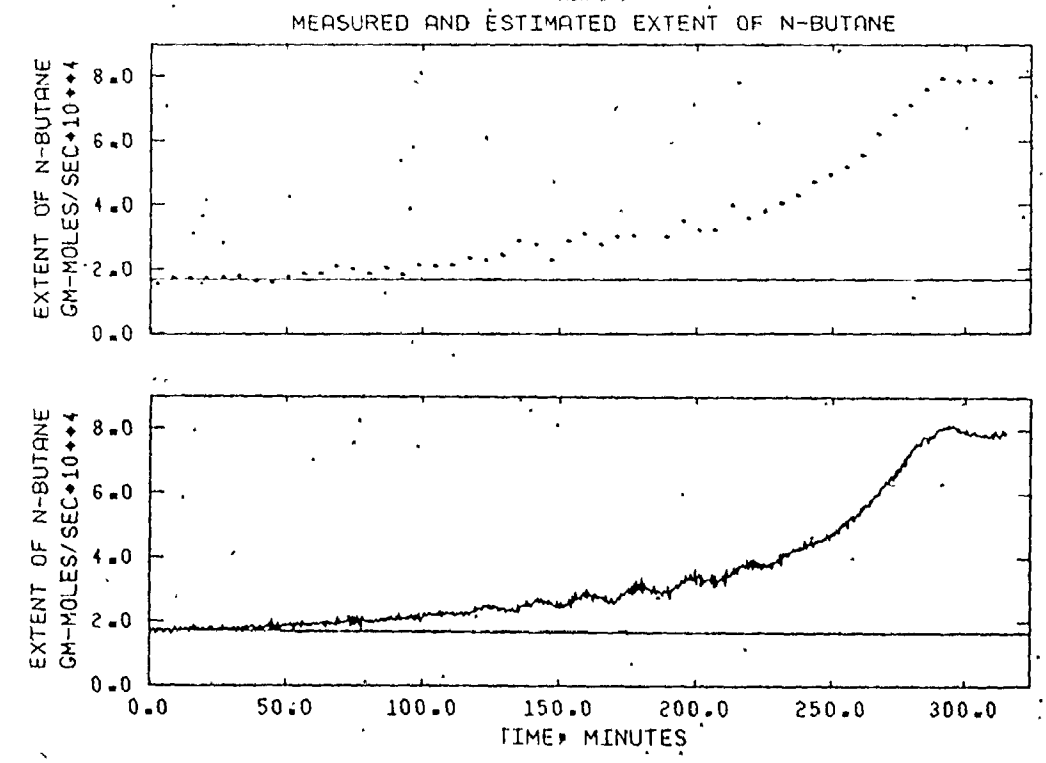


FIGURE 5-40
RUN # 7

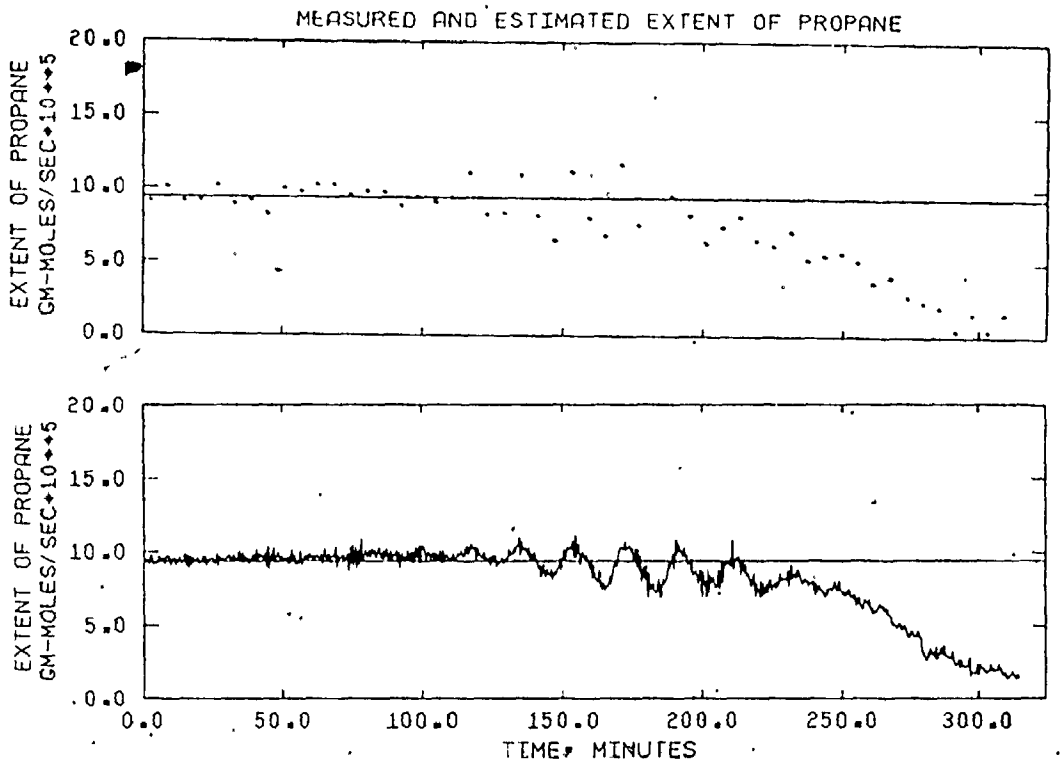
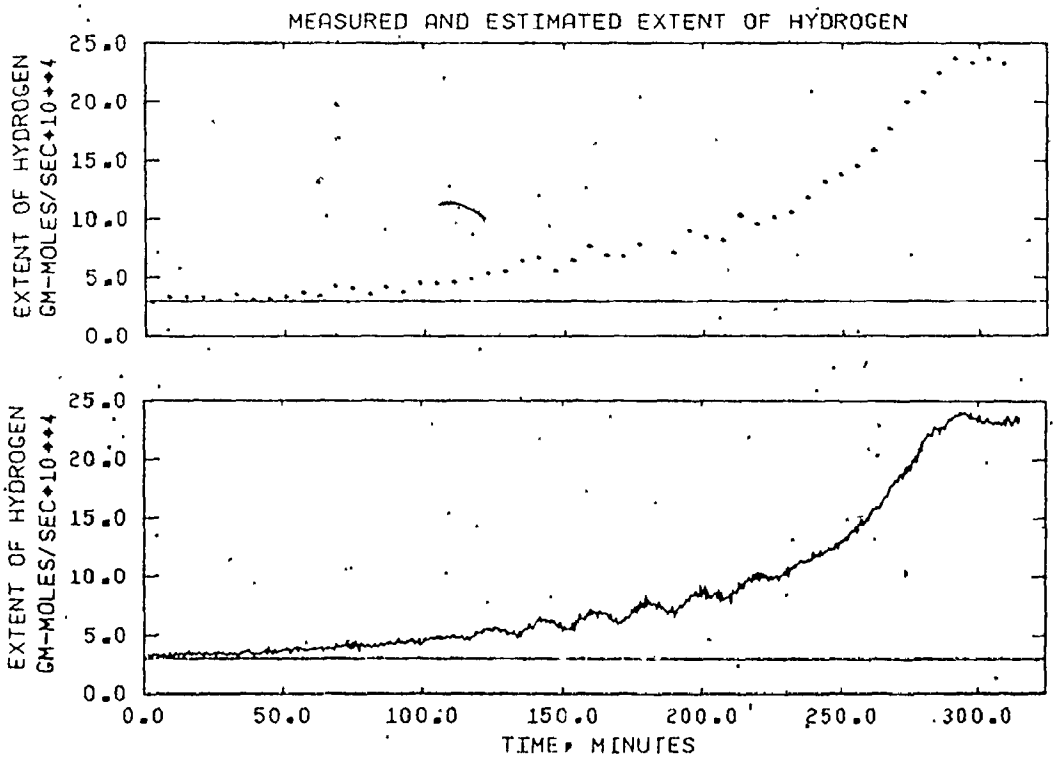


FIGURE 5-41
RUN # 7



due to incorrect signs in the control action. This behaviour resembled that of earlier regulatory runs but because of the larger number of degrees of freedom, no practical solution was found for this particular problem. The controller was stable when much smaller setpoint changes (5% and less) were used but then no noticeable change in the propane extent level was observed. A wide range of adaptive loop gains was used but none could stabilize the reactor system upon 30% setpoint changes. The value of 0.1×10^{-3} was found to delay reactor runaway enough to produce the response figure included herein.

5.5 Discussion

The n-butane hydrogenolysis pilot plant reactor was sufficiently complex to question the value of developing a mathematical model from first principles. Using intuitive arguments based on actual knowledge of the reactor's operating properties, a discrete time state space model form of low order was proposed. This model did not however explicitly account for the non-minimum phase properties typical of catalytic packed bed reactors. The problems associated with the merging process temperatures, flows and composition data were resolved by defining a measurement equation which could be recursively updated while on-line. Data for estimating the parameters of the state space model and measurement equation were obtained experimentally. The parameters of the model were easily estimated from this data using established estimation computer programs. The fitted model unfortunately did not exhibit non-minimum

phase behaviour and this significant difference between process and model could account for the model reference adaptive controller's tendency to move in the wrong direction.

Given a model of the reactor, a stable reference model was derived by application of a standard optimization technique. The stable system formed the basis for a formulation of a model reference adaptive control algorithm designed to satisfy Lypunov's second theorem of stability. It was however necessary to jeopardize the stability of this system by introducing a pseudo-inverse into the calculation of the multivariable feedback controller gain matrices. The approximation which results from this pseudo-inverse could lead to gain matrices causing instability. A loss of information arises by virtue of the fact that a 5 x 5 system must be reduced to a 5 x 2 system.

Another consideration is the true order of the reaction system at the operating conditions used for this study. In Section 2 of this chapter, it was stated that the system should be of third order considering the chemical reactions involved. However, examination of the fitted dynamic model transition and control matrices listed in Table 5-5 indicates that the system may be of second order only. Subsequent to this work, Wong [1977] has demonstrated that this should be the case. If in fact the fitted third order model should be singular, this could also account for the odd behaviour of the model reference adaptive controller employed for this study.

In this experimental study, changing the sign of the hydrogen control action term led to stable operation when the proportional and integral actions of the model reference adaptive controller were used. It was not possible to stabilize the system when explicit setpoint action was attempted. Because of the very small amount of ethane produced at the normal reactor operating conditions, the objective of the model reference adaptive controller was limited to controlling the extent of propane in the reactor effluent. For those cases which were successful, only a very limited range of adaptive loop gains could maintain stability. The use of integral action was found to provide adquate control characteristics in a regulatory environment. The implicit and explicit servo-action of the adaptive controller was totally incapable of performing its designed function and generally resulted in unstable behaviour.

CHAPTER 6

CONCLUSION

The primary and secondary objectives of this thesis as defined in Chapter 1, Section 1 have been fulfilled. A non-adiabatic, catalytic packed bed pilot scale reactor has been designed, constructed and commissioned. This apparatus has been shown to exhibit properties of commercial scale reactors and consequently can be used to experimentally evaluate the performance of various control schemes. To facilitate experimentation, the apparatus was interfaced to a minicomputer. A real time executive program was developed and has proved to be extremely valuable to most computer based research programs presently undertaken within the Department. This executive program largely eliminates the assembler language programming that is generally required in most data acquisition and control applications.

With the secondary objectives of this thesis satisfied, work was begun to satisfy the primary one. The modelling of complex chemical systems such as packed bed reactors has been a major obstacle for the application of model-based control theories. In this work, a low order model form for an n-butane hydrogenolysis reactor was postulated using mechanistic arguments. This approach to modelling was reasonable since the process was reasonably well understood. The parameters of the low order model were fitted to dynamic plant data. An efficient means of combining reactor effluent stream analysis data with reactant feed rates

and reactor internal temperatures has also been examined. On-line updating of the parameters of a measurement equation made it possible to track reactor excursions due to measured or unmeasured upsets. The low order model was the basis of a derivation of a model reference adaptive controller. The design method was based on Lyapunov's second theorem of stability. The objective of the controller was to regulate the production rates of reaction intermediates of the n-butane hydrogenolysis pilot scale reactor. Both regulatory and servo control action terms were included in the controller design and were tested experimentally.

The discussion in Section 5 of Chapter 5 has identified three possible explanations for the model reference adaptive controller's inability to function properly. An empirical fix however resulted in stable operation for the regulatory portion of the controller, whereas proper servo action was never truly successful. Results from the regulatory runs indicate that integral action is desirable in that it dampens variations and eliminates offset.

Several avenues for future work have been identified as a result of this study. The adaptive algorithm should be designed by methods which do not rely upon the pseudo-inverse. This approximation may lead to unstable operation particularly if the difference in the number of states and inputs is great. Great care must be exercised when formulating the process model. If a reactor is to be modelled, the decision of whether or not to include non-minimum phase characteristics must be

made. Whether or not the effect is actually modelled, the controller must be designed to account for it. In this work, no attempt has been made to separately model the noise of the reactor. This should be done and incorporated into an adaptive control algorithm.

Associated with these investigations are a few minor modifications to the apparatus. The thermocouple multiplexer described in Chapter 3 should be redesigned to improve its reliability and accuracy and increase the scan speed. Electrical power to the reactor feed preheater and the six coolant heaters should be placed under regulatory control. Reactant and coolant temperatures could then be used as effective manipulated inputs. Any or all of these changes would necessitate slight software modifications to the GOSEX source (refer to Chapter 4).

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APPENDIX A

CATALYST SYNTHESIS AND CONDITIONING

Preparation of the nickel catalyst involved impregnation of silica gel with a solution of nickel nitrate followed by reduction of the absorbed nickel nitrate to pure nickel.

The silica gel used for the synthesis was manufactured by the Davison Chemical Division of the W.R. Grace & Co. and was distributed by Canadian Industries Limited. The manufacturer claimed a particle size distribution between 12 and 28 mesh, (1.4 to 0.6 mm) for its Grade 408 silica gel. Tests indicated that 1 gm of the silica gel at room temperature -- previously dried at 200^{o}C for 24 hours -- could absorb 0.33 cm^3 of distilled water. It was assumed that 1 gm of silica gel would also absorb 0.33 cm^3 of aqueous nickel nitrate solution. The bulk density of the silica gel was found to be 0.75 gm/cm^3.

The nickel nitrate used in the synthesis was obtained from the Fisher Scientific Company (Chemical Stock Number N-62). The molecular formula of the nickel nitrate crystals was specified by the manufacturer to be $Ni(NO_3)_2 \cdot 6H_2O$, which corresponds to a formula weight of 291. This implies that the nickel content of the nickel nitrate is 20.2%.

A reactor charge of catalyst (approximately 300 gm or 400 cm^3) was prepared by mixing 5 volumes of inert silica gel with one volume of catalyst. The nickel content of the catalyst was 2.5%.

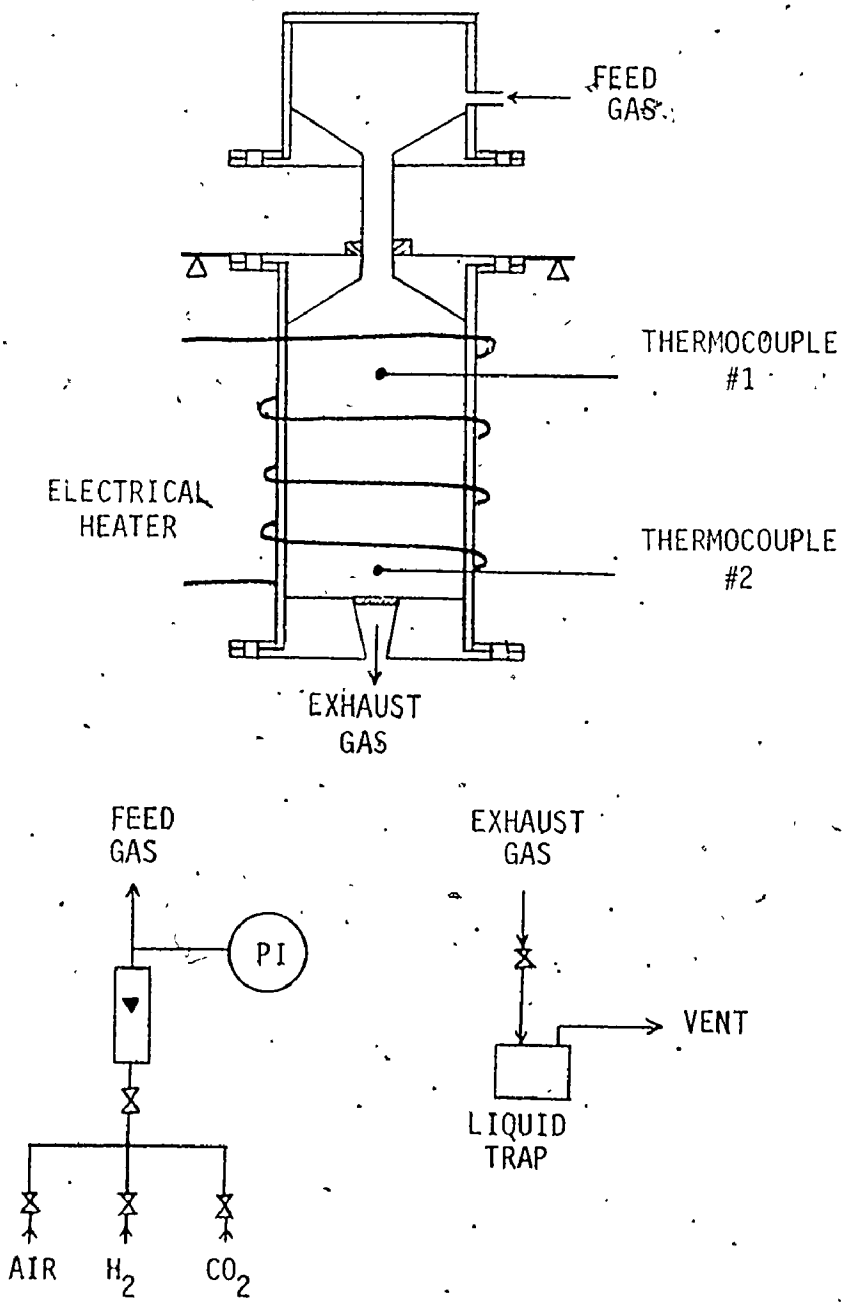
A batch of catalyst was synthesized in the following manner. A large amount of silica gel was washed with distilled water and dried at 200°C for 24 hours. A 300 gm sample of this silica gel was then used in the synthesis; the remaining material was used to dilute the pure catalyst. In order to produce a 2.5% Ni catalyst, 38. 1 gm of nickel nitrate was dissolved in distilled water to form a 100 cm^3 solution. The aqueous solution was then used to impregnate the 300 gm of dried silica gel. The saturated silica gel was then dried at 200°C for about 24 hours followed by reduction of the nickel nitrate to nickel metal in the catalyst conditioning unit.

The nickel catalyst used for the hydrogenolysis of n-butane had to be conditioned for use. Nickel was present in the nitrate form after the first stage of the catalyst synthesis. This was transformed into nickel oxide by heating at high temperature in the presence of air. However, further reduction to nickel metal required the presence of hydrogen, also at high temperature. After conditioning, the catalyst could not be exposed to the atmosphere since the oxidation of nickel metal is virtually instantaneous. An apparatus has been designed for catalyst conditioning and transferring of the reduced catalyst to the reactor without contact with the atmosphere.

A schematic of the apparatus is given in Figure A-1. The apparatus consisted of two basic parts:

FIGURE A-1

CATALYST CONDITIONER



-conditioning reactor
-charging bottle

The conditioning reactor was fabricated from 3 inch Schedule 40 stainless steel pipe with flanged ends. The bottom flange supported the material within the reactor. A porous stainless steel disk mounted within the flange allowed flowing gas to leave the reactor. The top flange supported the charging bottle and due to the taper design on the reactor interior also helped discharge the reactor after catalyst conditioning. An electrical heater was wrapped around the body of the reactor and was powered by a variable power supply. The conditioner was insulated with about two inches of ceramic wool. Two chromel-alumel thermocouples provided measurements of the conditioner's inside temperature.

The charging bottle was also fabricated from 3 inch Schedule 40 stainless steel pipe. It accomplished two very important functions. During the nickel reduction steps, it preheated the feed gases to the conditioning reactor. Once the nickel had been reduced to its metallic form, the charging bottle was used to transfer the active catalyst to the process reactor.

The apparatus was mounted so that it could pivot to facilitate the discharge of conditioned catalyst. To charge the reactor, the dried synthesis catalyst was funnelled into the reactor and the charging bottle attached to the top flange of the reactor. The initial reduction was

performed at 450°C with flowing air and the reactor pressure was maintained at 5 PSIG. After about 8 hours of heating, the air was turned off and the unit allowed to cool to room temperature. A flow of hydrogen was then established -- about 10 cm^3/sec at a reactor pressure of 5 PSIG -- and the unit reheated to 450°C for 4 hours. The apparatus was again cooled to room temperature.

At this point, the catalyst was conditioned for use. The following procedure was used to ensure that the catalyst was transferred to the process reactor without being contacted with air. The reader is referred to Figure 3-4 for precise location of the valves mentioned below.

STEP A - Preliminary Procedure

Disconnect power leads to conditioner heating coil.
Reactor bypass 3-way ball valve: set to bypass.
D/P cell calibration station pressure ports: all set to atmosphere.
Reactor inlet valve: open wide.
Reactor exit valve: open wide.
3-way solenoid valves: de-energized.
Reactor product stream vent: open wide.
Reactor and bypass restrictor valves: open wide.
Reactor CO_2 feed valve: closed.
Conditioning station CO_2 feed valve: closed.
Disconnect reactor feed line and remove gas inlet thermocouple.
Remove reactor feed section and mount new moistened gasket onto it.
Remove old catalyst with vacuum apparatus and insert reactor charging sleeve.
Pour into the reactor approximately 20 cm of dried silica gel. This causes reactor thermocouple #12 to be at the end of the catalytic portion of the bed.
Turn on CO_2 bottle to provide a 12 PSIG supply.

STEP B - Conditioner Discharging and Catalyst Blanketting

Turn off hydrogen flow through conditioner and vent hydrogen lines.

Conditioning station pressure adjust valve: open wide.
Establish low flow of CO_2 through conditioner for about one minute.
Turn off CO_2 flow through conditioner and flip unit to discharge catalyst into charging bottle.
Establish low flow of CO_2 through charging bottle and disconnect it from reactor.

STEP C - Reactor Flushing

With hand over top of reactor, open reactor CO_2 feed valve slightly to flush all lines upstream of the reactor exit valve.
Shut reactor exit valve to flush reactor itself.

STEP D - Process Reactor Charging and Isolation

Pour catalyst from charging bottle into process reactor and spoon out any catalyst above the bottom of the charging sleeve.
Close conditioner CO_2 feed valve.
Remove reactor charging sleeve.
Replace reactor feed section. Reconnect feed line and replace thermocouple.
Allow to flush. Pressurize reactor to 12 PSIG with CO_2 by shutting reactor inlet valve.

Once this procedure was completed, the conditioned catalyst was transferred without contacting the atmosphere. The active catalyst was stored inside the reactor for long periods by maintaining the carbon dioxide pressure at 12 PSIG. To ensure that air did not enter the process reactor, all reactor feed lines were flushed with hydrogen prior to reactor startup. The reactor carbon dioxide feed valve must be closed when operating the reactor.

APPENDIX B

CALIBRATION OF INSTRUMENTS

B.1 Introduction

Before the startup of the butane hydrogenolysis pilot plant, it is necessary to verify the calibration of the thermocouple and differential pressure transmitters and of the process gas chromatograph. The checkout procedure outlined in this appendix should only be attempted after the instruments have operated for at least 24 hours. Note also that these instruments should be connected to the process computer's plant interface during calibration. The coeffecients of the polynomials fitted to the calibration data have been tabulated in Table B-1.

B.2 Calibration of the Thermocouple Transmitters

Before applying power to the thermocouple transmitters, the transmitter inputs must be shorted and a 200 ohm (¼ watt, 1%) resistance connected across their outputs. For this work, the thermocouple transmitters were calibrated for temperatures between 0 and 415^{0}C. This range corresponds to a 0 to 17 millivolt input from a chromel-alumel thermocouple. To produce the 17 millivolt input needed for calibration, an accurate potentiometer was required. Calibration was effectively a two step procedure.

The transmitter input was shorted and the "ZERO" adjustment was

TABLE B-1

CALIBRATION COEFFICIENTS OF THE FITTED POLYNOMIALS

FITTED SYSTEM	APPLICABLE FIGURE	RANGE AND UNITS OF INDEPENDENT VARIABLE	RANGE AND UNITS OF INDEPENDENT VARIABLE	FITTED POLYNOMIAL
Thermocouple Transmitter	B-1	102 → 511 ADC units	$0 \leq T \leq 415$ ^{o}C	$T = 1.015\ R - 1.035 \times 10^{+2}$
Flowmeter Differential Pressure Transmitter	B-2	$107 \leq R \leq 511$ ADC units	$0 \leq \Delta P \times 10^{+4} \leq 2417$ atmospheres $\times 10^{+4}$	$\Delta P \times 10^{+4} = +5.991\ R - 644.7$
Reactor Differential Pressure Transmitter	B-3	$107 \leq R \leq 511$ ADC units	$0 \leq \Delta P \times 10^{+4} \leq 1400$ atmospheres $\times 10^{+4}$	$\Delta P \times 10^{+4} = +3.441R - 358.6$
Hydrogen Flowmeter	B-4	$107 \leq R \leq 511$ ADC units	$5 \leq F \leq 161$ cm^3/sec at 1 ATM, 25°C	$F = -0.300 \times 10^{-3}R^2 + 0.591R - 0.546 \times 10^{+2}$
n-Butane Flowmeter	B-5	$107 \leq R \leq 511$ ADC units	$4 \leq F \leq 37$ cm^3/sec at 1 ATM, 25°C	$F = -0.171 \times 10^{-3}R^2 + 0.190R - 0.141 \times 10^{+2}$

TABLE B-1
(continued)

FITTED SYSTEM	APPLICABLE FIGURE	RANGE AND UNITS OF INDEPENDENT VARIABLE	RANGE AND UNITS OF INDEPENDENT VARIABLE	FITTED POLYNOMIAL
Process Gas Chromato-graph	B-6			
Methane		$76 \leq R \leq 511$ ADC units	$0 \leq M \times 10^{+1} \leq 1000$ Mole Percent $\times 10^{+1}$	$M \times 10 = -0.339 \times 10^{-3} R^2 + 0.2482 \times 10^{+1} R - 0.1849 \times 10^{+3}$
Ethane		$85 \leq R \leq 511$ ADC units	$0 \leq M \times 10^{+1} \leq 500$ Mole Percent $\times 10^{+1}$	$M \times 10 = -0.118 \times 10^{-3} R^2 + 0.1247 \times 10^{+1} R - 0.1062 \times 10^{+3}$
Propane		$77 \leq R \leq 511$ ADC units	$0 \leq M \times 10^{+1} \leq 250$ Mole Percent $\times 10^{+1}$	$M \times 10 = +0.191 \times 10^{-3} R^2 + 0.468 R - 0.376 \times 10^{+2}$
n-Butane		$37 \leq R \leq 511$ ADC units	$0 \leq M \times 10^{+1} \leq 250$ Mole Percent $\times 10^{+1}$	$M \times 10 = -0.992 \times 10^{-4} R^2 + 0.586R - 0.234 \times 10^{+2}$

used to obtain a 2.00 VDC drop across the output impedance. The 17 millivolt source was then applied to the transmitter input and the "SPAN" adjustment used to obtain a 10.00 VDC drop. This two step technique was repeated until the amplifier "ZERO" and "SPAN" converged to the desired values. The instrument's calibration curve was then determined by applying a series of known potentials to the input.

Calibration of the two thermocouple transmitters used for this work indicated that they were effectively identical. The calibration data are presented graphically in Figure B-1. A linear relation was found to fit the data well.

B.3 Calibration of the Differential Pressure Transmitters

The "SPAN" adjustment of the hydrogen and n-butane flowmeter differential pressure transmitters was preset at 100 inches of water by its manufacturer. The "SPAN" of the differential pressure transmitter across the process reactor was preset at 52.5 inches of water. With this adjustment already made, only the "ZERO" of the instrument needed to be verified. Before applying power to the differential pressure transmitters, a 200 ohm (¼ watt, 1%) resistance was connected across their outputs. Before adjustment was attempted, the input of the instruments was set to atmospheric pressure. This was done at the differential pressure transmitter calibration station (see Figure 3-5). The "ZERO" adjustment of the instruments was used to arrive at a 2.10 VDC drop

FIGURE B-1

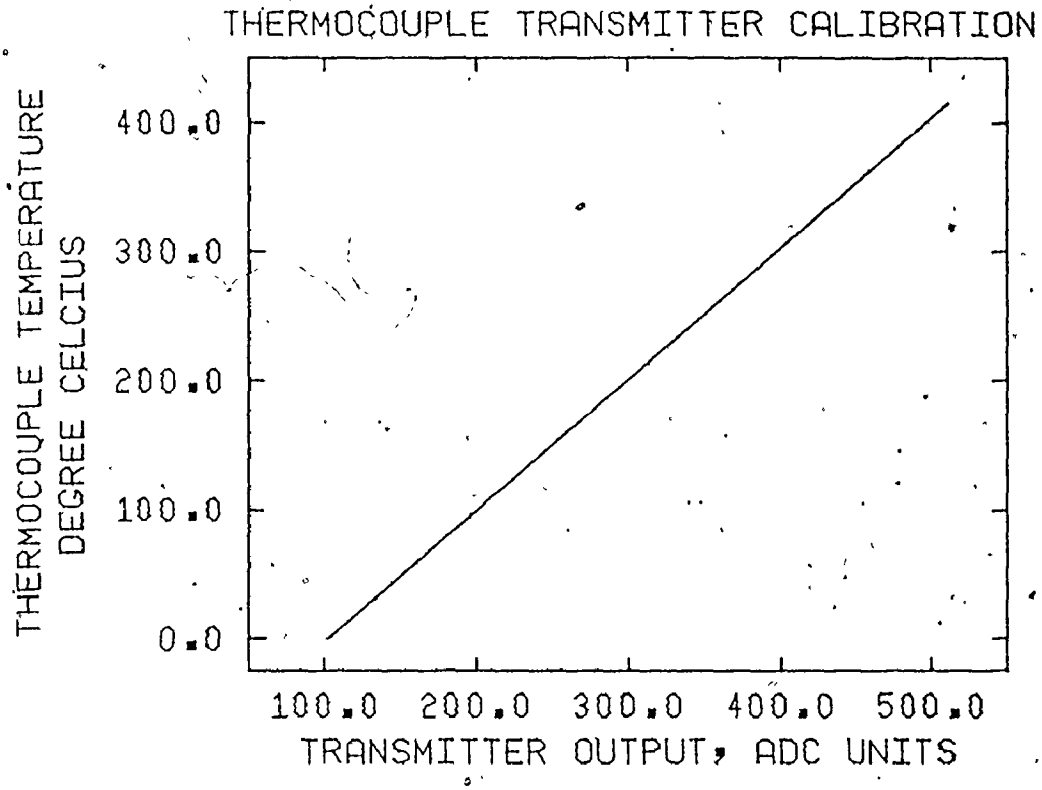
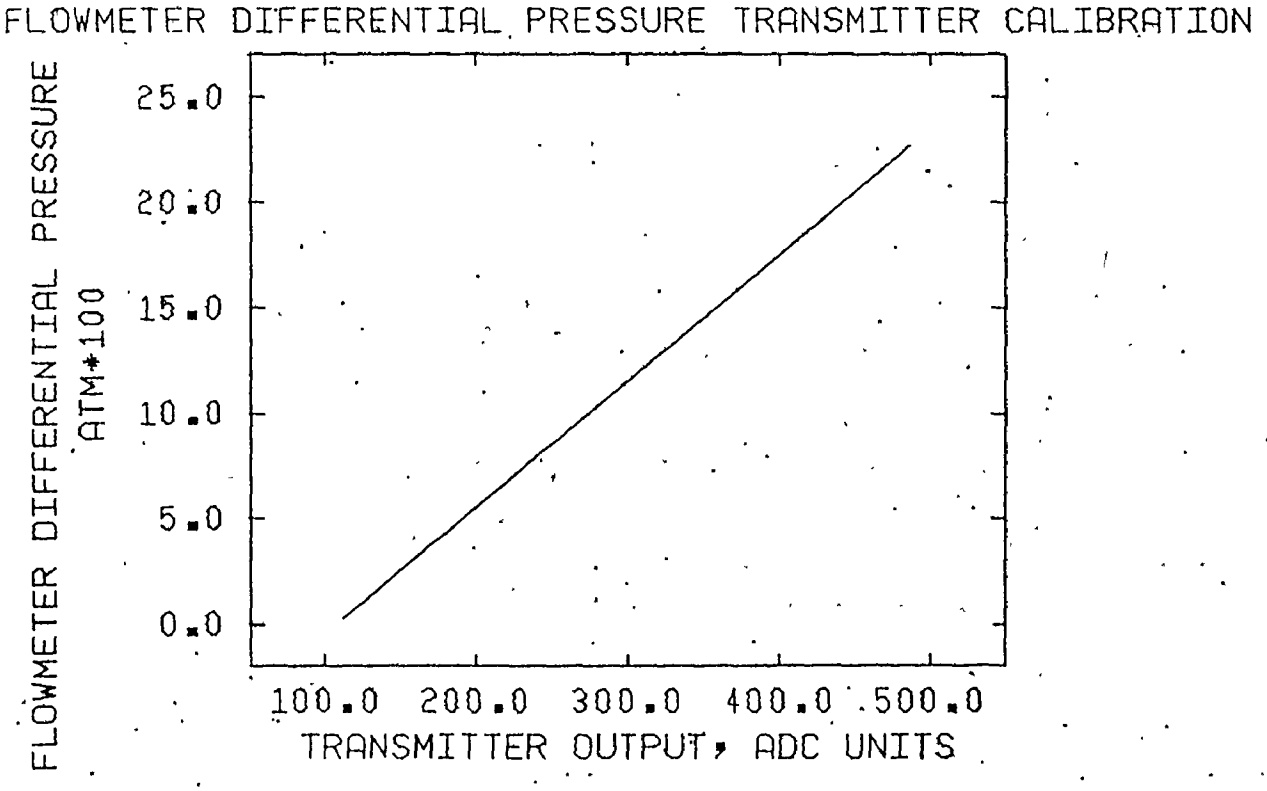


FIGURE B-2



across the output impedance.

Calibration of the hydrogen and n-butane flowmeters and differential pressure transmitters was done simultaneously. Results suggested that the differential pressure transmitters were identical. The data given in Figure B-2 were fitted by a linear relation. The calibration curve of the differential pressure transmitter across the pilot plant reactor was obtained by simply measuring the instrument's reponse to a series of known differential pressures. The data are represented in Figure B-3.

B.4 Calibration of the Gas Flowmeters

In the calibration of flowmeters for gas service, it is customary to fix the downstream pressure at some value. Hence the variation through the flowmeter results from a change in the upstream pressure only. In this work, a back pressure regulator maintained the downstream pressure of both the hydrogen and n-butane flowmeters constant at 10 PSIG. The pressure upstream of a flowmeter was varied by altering the diaphragm pressure of a control valve. The flowmeters were fabricated from Type 316 stainless steel needle tubing. The precise dimensions and lengths of tubing that were used are given in Table B-2. Hydrogen was supplied at 28 PSIG and n-butane at 18 PSIG.

To calibrate the flowmeters, it was necessary to vary the control valve diaphragm pressure. For accuracy, an output of the computer's

FIGURE B-3

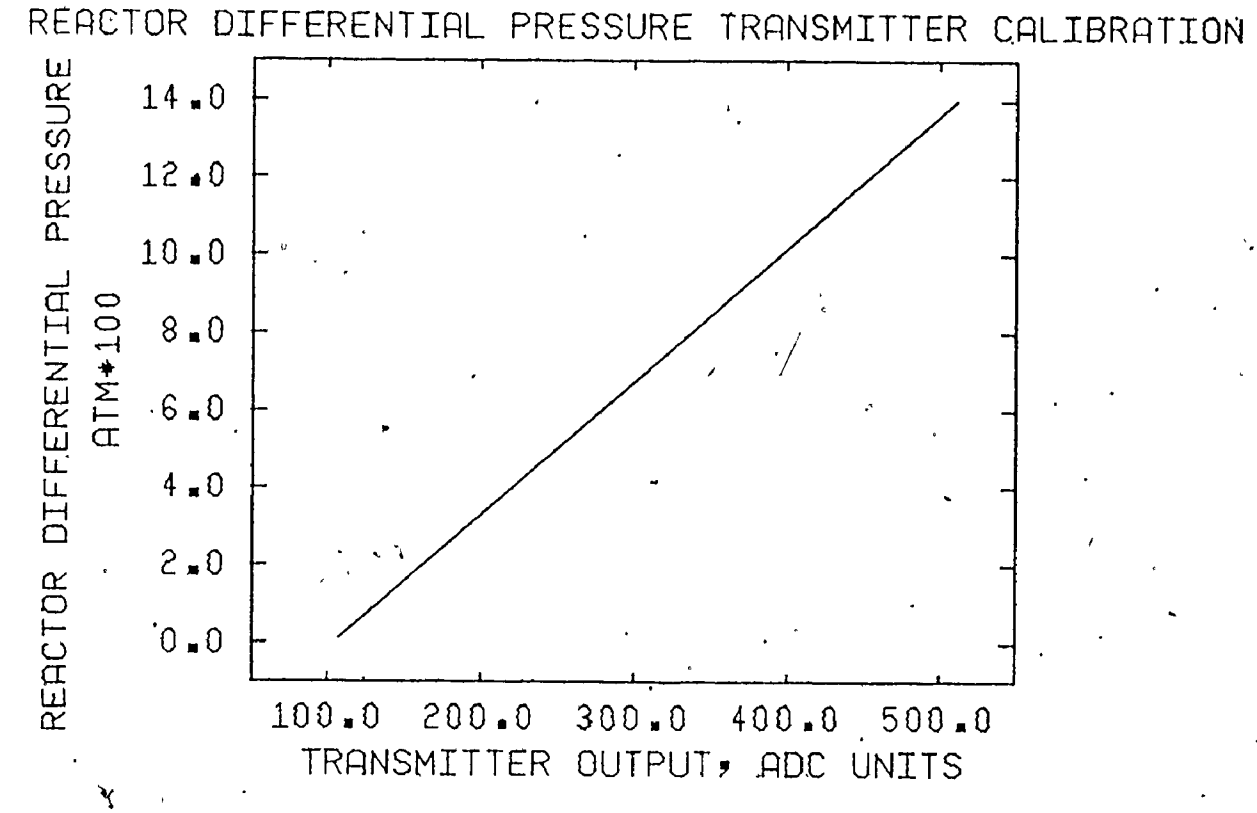


FIGURE B-4

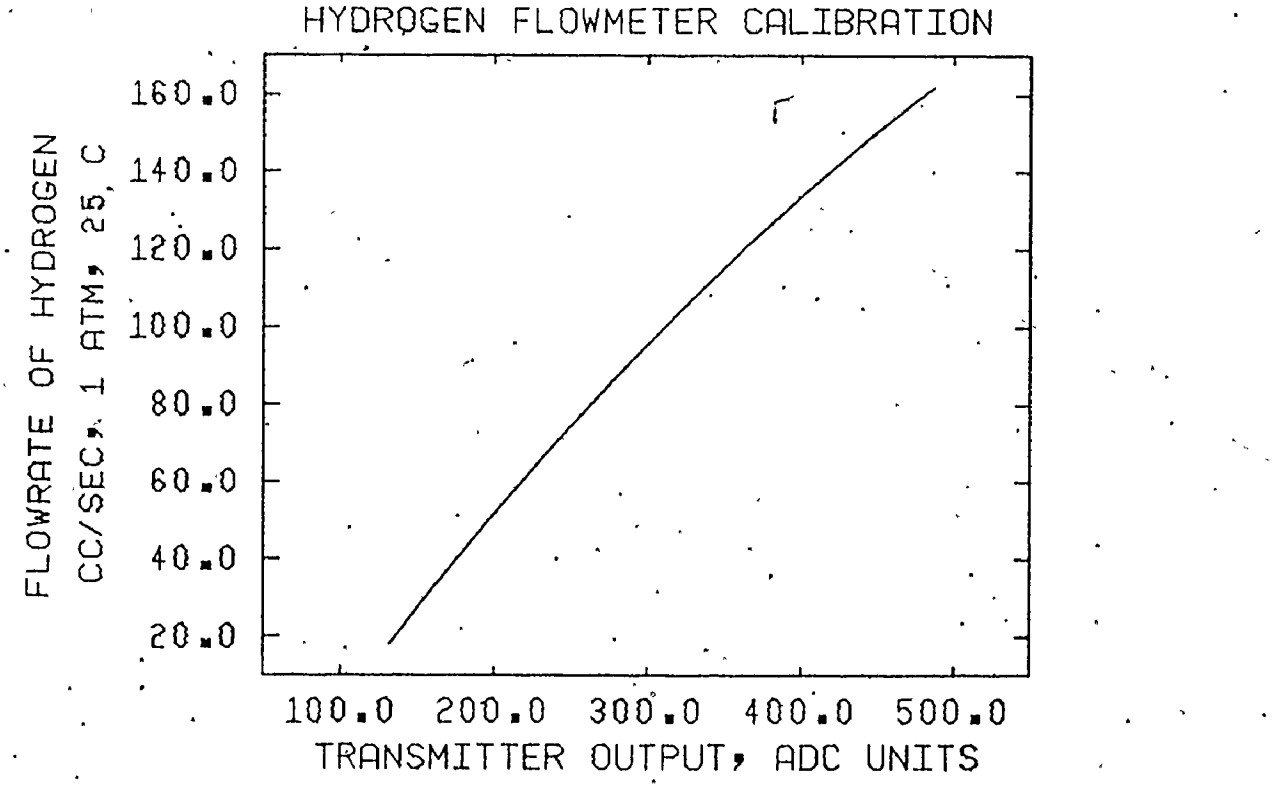


TABLE B-2

DIMENSIONS OF FLOWMETER

NEEDLE TUBING+

GAS	TUBE ID (cm)	TUBE LENGTH (cm)
Hydrogen	0.137	162
n-Butane	0.0838	19

+ 316 Stainless Steel from Atlas Alloys Inc.

DAC was used instead of the manual adjustment that was available. At a particular setting of the diaphragm pressure, the flowrate of gas as measured using a bubble flowmeter or a wet test meter was obtained. Several measurements were taken at each setting. The pressure drop across the flowmeter was determined from the voltage drop at the appropriate differential pressure transmitter output. In addition, the manometer located at the differential pressure transmitter calibration station (see Figure 3-5) was also used. The calibration data and fitted quadratic polynomial are presented in Figure B-4 for hydrogen and Figure B-5 for n-butane.

B.5 Calibration of the Process Gas Chromatograph

A Beckman Model 6700 Process Gas Chromatograph was used to perform the analysis of the butane hydrogenolysis reactor product stream. The instrument design was conceptually innovative. Unfortunately, serious shortcomings in implementation forced the user to tailor his analysis scheme to the limitations of the instrument. Couple this with insufficient and often incorrect documentation, users uninitiated in the field of analog and digital electronics will find it awkward to set up this process gas chromatograph. Regardless of these pitfalls, the instrument was very reliable once it had been calibrated for service. To assist future users of this process gas chromatograph, a procedure for instrument set up is provided. This procedure should be used only after the reader is

FIGURE B-5

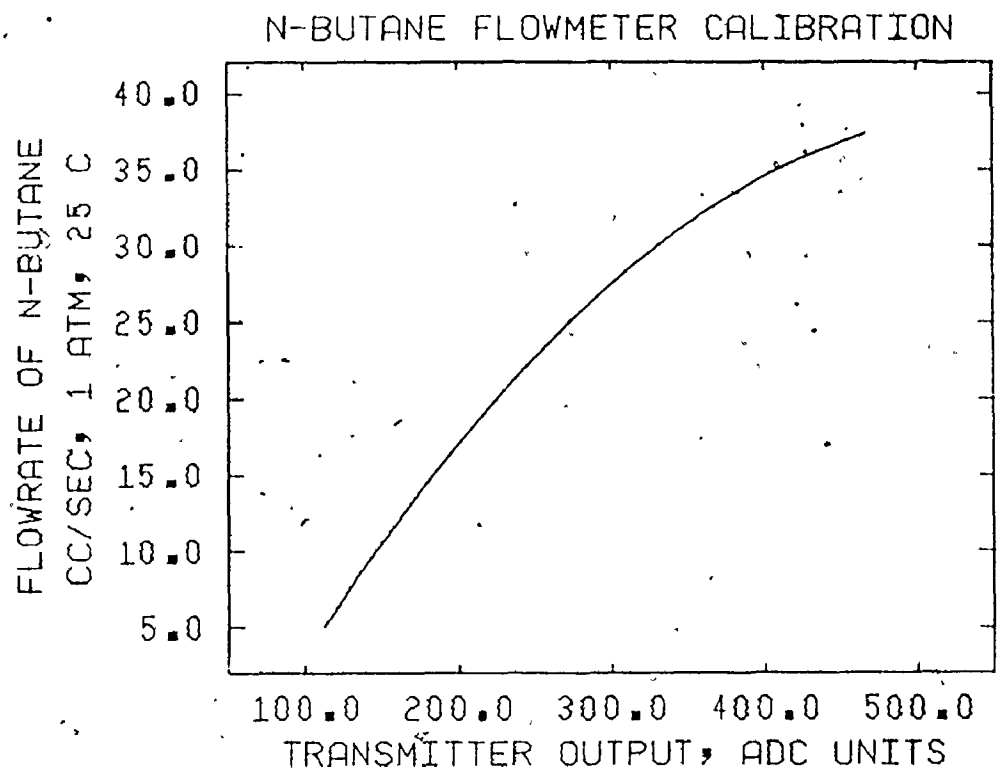
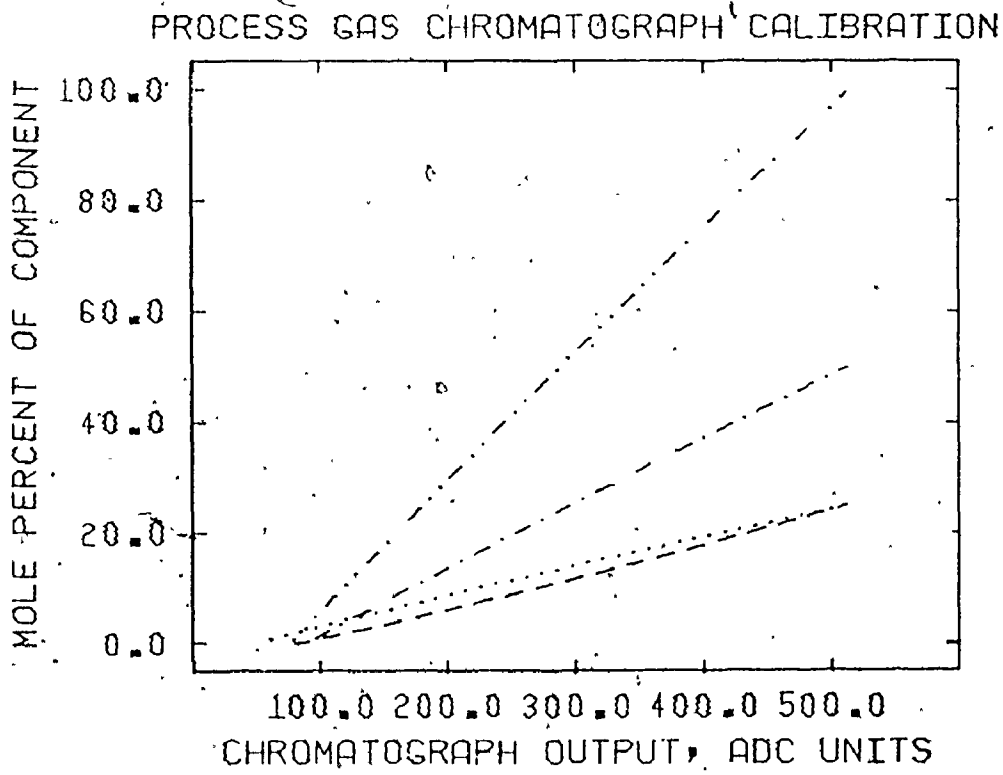


FIGURE B-6



familiar with the manufacturer's documentation.

STEP 1 - Analyzer Check-out

The contents of the analyzer must be inspected first. The 10-port valves, needle valves, columns and detector must be connected in the manner illustrated in Figure 3-15. The analyzer air supply must be at 55 PSIG and regulated instrument air at 20 PSIG. The carrier gas (hydrogen) supply pressure must be at 50 PSIG and the regulated carrier gas at about 14 PSIG.

Carrier flow through both sides of the detector should be roughly set at 60 cm^3/min by adjusting the appropriate needle valves. All programmer front panel switches should be in the left most position. In the rear of the programmer, 500 ohm (¼ watt, 1%) resistors should be connected across the current outputs. With the filament power switch at "OFF" and the programmer/analyzer interconnecting cable in place, power may be applied to the programmer and analyzer. The preregulated and regulated bridge voltages should be about 30 and 26 VDC respectively. The analyzer oven temperature should then rise to 110°C (by mercury thermometer) and remain there. With valves A and B energized, the bypass needle valve is adjusted for a carrier flow of about 60 cm^3/min. Valves A and B are de-energized and carrier is permitted to flush the system for one hour. Power is then applied to the filaments. At this point, the gas chromatograph must be allowed to stablilize for 24 hours. After this time, the filament current is adjusted to 150 ma and the

carrier and reference flows accurately set to 60 cm^3/sec. It is good practice to first set the reference flow by adjustment of the regulated carrier gas pressure.

R2 of the thermal conductivity detector power supply and amplifier (634106 & 634103) enables adjustment of the filament current. If the difference between the preregulated and regulated bridge voltage exceeds 5 VDC, the preregulated voltage from the programmer must be reduced for a difference of 4.5 VDC. With TB1-1, TB1-5 and TP11 all shorted together and a voltmeter between TP9 and TP11, R6 is adjusted for zero reading. Move the jumper from TB1-1 to TP10 and adjust R21 for +0.7 VDC reading. Finally, the jumper at TP10 is moved to TB1-7 and R7 adjusted for zero reading. All jumpers are removed. The "AUTO ZERO" switch on the programmer front panel is set to the "ON" position and the voltage monitor to the "AUTO ZERO" position. R21 is adjusted for a midrange display on the voltage monitor. The "AUTO ZERO" switch is then returned to the "AUTO" position. The detector amplifier is now ready for service. Note that adjustment of R2, R6, R21 and R7 must be repeated periodically.

STEP 2 - Zeroing of Programmer Amplifiers

On the back plane of the basic terminal assembly (632151), the inputs to amplifier AR1 are shorted to ground. R5 is adjusted for zero reading between TP1 and TP2.

Inside the programmer, connect a voltmeter between TP1 and TP2 of the master control assembly (632160). With the manual polarity reverse switch at "ON", the output amplifier AR1 is adjusted for zero reading with R10. The short on the basic terminal assembly must now be removed and manual polarity reverse set to "OFF".

STEP 3 - Zeroing of Integrator Amplifier

All front panel switches must be in the left most position. The digital timer board (632196) is set for a cycle time of 360 seconds in one second increments. For this step, all other cards except one universal component board (632181) must be removed from the programmer chassis. This one component board with integrator control option (632148) must be programmed in the following way:

-component on time: 020
-component off time: 340
-readout: on
-integrate: on
-calibrate/auto: calibrate
-R4 of the integrator control at clockwise limit.

The integrator board (632184) "AUTO/CALIB" switch must be at "CALIB" and the calibrate/adjust switch on the master control board at "ON". R18 on the master control board is adjusted for zero reading between the center pin of the "AUTO/CALIB" switch and TP3 of the integrator board. The "AUTO/CALIB" switch is placed in the "AUTO" position and the programmer allowed to run. R8 on the integrator board is adjusted for constant output between TP2 and TP3. The universal component board must be removed once the integrator has been zeroed.

STEP 4 - Adjustment of Component Area Long Term Memory Amplifier Gains

In addition to the digital timer board already present in the programmer chassis, five other boards must be programmed for analysis of methane, ethane, propane and butane. These boards include a dual valve board (632166) and four universal component boards with integrator control and long term memory (635037) options. The six boards which control the analysis must be programmed according to Table B-3 before adjustment of the long term memories is possible.

The "CALIBRATE/ADJUST" switch on the master control board must be at "ON" and the "AUTO/CALIB" switch on the integrator board at "CALIB". Adjust R18 on the master control board for a +5 VDC reading between the center pin of the "AUTO/CALIB" switch and TP3 of the integrator board. Selecting one universal component board at a time, remove the board cover and insert the board into the programmer chassis. Set the component switch to manual. On the long term memory option, adjust R6 for -10 VDC output between the amplifier output side of R5 and the ground side of R10. Connect a voltmeter across the appropriate current output in the rear of the programmer. R7 on the long term memory is adjusted for a +10 VDC reading. Return the component switch to "AUTO". Remove the universal component board from the programmer chassis and replace the board cover.

Once all long term memories have been adjusted, the dual valve

board and the four programmed universal component boards are inserted into the programmer chassis.

STEP 5 - Adjustment of the Component Area Amplifier

The adjustment must be done dynamically using mixtures containing the maximum feasible amount of each component. These amounts must be determined from the desired operating conditions of the reactor. One day before this adjustment, a mixture containing suitable proportions of ethane, propane and n-butane must be prepared at the calibration mixture preparation station (Figure 3-14). Analysis of the mixture is then performed with all programmer automatic functions enabled. After the component off times of ethane, propane and butane, the corresponding output voltages are noted. R1 of each component integrator control is adjusted until a reading of +10 VDC is maintained. Once this is achieved, the procedure is repeated with samples of methane.

STEP-6 - Component Calibration

The calibration curves for methane, ethane, propane and butane are determined by simply noting the instrument responses to a series of known mixtures. The responses should be linear with respect to component mole fraction. This indicates that the relative molar responses of any three components relative to the fourth is a constant.

Six sets of data were obtained to establish the calibration curves presented in Figure B-6. Variations in the chromatograph responses over the entire range of operation were so small (minor fluctuations in the

least significant figure) that calibration errors were virtually nill. Quadratic polynomials were used to fit the data.

TABLE B-3

PROGRAMMER BOARD SETTINGS

DIGITAL TIMER

CYCLE TIME: 360 seconds
by one second steps

DUAL VALVE BOARD

VALVE	ON TIME	OFF TIME
A	2	85
B	40	200

UNIVERSAL COMPONENT BOARDS

COMPONENT	ON TIME	OFF TIME	AUTO ZERO	MEMORY
CH_4	43	80	ON	1
C_2H_6	106	199	OFF	2
C_3H_8	213	280	OFF	3
$n\text{-}C_4H_{10}$	294	345	OFF	4

A difference of two seconds between programmed time on and actual time on exists when Auto Zero is not used. When Auto Zero is used, the difference increases to four seconds. All component boards are programmed with the X1, X10 and POLARITY REVERSE at OFF and amplifier range at low. The integrator function is set for readout, integrate and automatic operation. At the memory select, the selected memory is not enabled.

APPENDIX C

MODEL REFERENCE ADAPTIVE CONTROL APPLICATION SOFTWARE

C.1 Direct Solution of Lyapunov's Matrix Equation For Continuous and Discrete Time Systems

The square matrix $\bar{P}$ defined by Lyapunov's matrix equation

$$A_c^T \bar{P} + \bar{P} A_c = -Q_c \qquad (C\text{-}1)$$

where A_c: continuous time system transition matrix, nxn
Q_c: positive definite, symmetric matrix, nxn
$\bar{P}$: positive definite symmetric matrix, nxn, the solution of Equation C-1.

may be obtained by a variety of techniques. If A_c has only negative eigenvalues and $Q_c = I$, it has been shown (Bellmann et al [1960]) that $\bar{P}$ will be a positive definite symmetric matrix. The direct method of computing matrix $\bar{P}$ is to solve a set of $\frac{1}{2} n(n+1)$ simultaneous linear equations derived by rearrangement of Equation C-1. An algorithm due to MacFarlane [1963] provides a systematic way of forming this system of equations. The listing of the FORTRAN IV subroutine to calculate matrix $\bar{P}$ based on this algorithm is given in Figure C-1.

Stability analysis of the discrete time linear system

$$x(k+1) = A_d\, x(k) \qquad (C\text{-}2)$$

where A_d: discrete time system transition matrix, nxn
x: discrete time system state, nx1

by Lyapunov's criteria results in the matrix equation

$$A_d^T P A_d - P = -Q_d \qquad \text{(C-3)}$$

where Q_d: positive definite symmetric matrix, nxn
P: positive definite symmetric matrix, nxn, the solution of Equation C-3

Symmetric matrix P is readily evaluated for systems like Equation C-2 by transforming Equation C-3 into the form of Lyapunov's matrix equation. According to Barnett and Storey [1970], a suitable transformation is

$$A_c^T = (A_d + I)^{-1} \cdot (A_d - I) \qquad \text{(C-4)}$$

If the absolute value of all the eigenvalues of A_d are less than unity, A_c is obtained from Equation C-4 will have only negative eigenvalues. Substituting Equation C-4 into Equation C-1 indicates that

$$Q_d = 2(I - A_c^T)^{-1} \cdot Q_c \cdot (I - A_c)^{-1} \qquad \text{(C-5)}$$

Q_d is a symmetric positive definite matrix if Q_c is symmetric and positive definite.

The FORTRAN IV program listed in Figure C-2 performs the indicated transformation followed by calculation of the P matrix.

FIGURE C-1

SOLUTION OF LYAPUNOV'S EQUATION

CONTINUOUS FORM

```
C*****SOLUTION OF THE LIAPUNOV FUNCTION "AT*P+P*A=-Q"
C*****EQUATION IS OF ORDER NA   SOLUTION ACCORDING
C*****TO MACFARLANE   "AT" MUST BE THE TRANSPOSE OF
C*****THE SYSTEM MATRIX "A"   MATRICES "P" AND "Q" ARE POSITIVE.
C*****DEFINITE SYMMETRIC MATRICES   ELEMENTS OF THE UPPER
C*****TRIANGLE OF "Q" MUST BE PASSED IN VECTOR "Q"   MATRIX "P"
C*****IS PASSED TO THE CALLER IN MATRIX "AT"   ELEMENTS OF
C*****THE UPPER TRIANGLE OF P ARE ALSO PASSED IN
C*****VECTOR "P"   "D" IS USED TO
C*****PASS THE DETERMINANT OF THE REDUCTION MATRIX TO THE
C*****CALLER   IF "D" IS ZERO, THE SOLUTION OF THE LIAPUNOV
C*****FUNCTION WAS NOT POSSIBLE   MATRICES "NMAT" AND "B"
C*****AND VECTORS "P", "L" AND "M" ARE INTERMEDIATES ONLY.
C*****"N" IS DEFINED AS "(NA*(NA+1)/2)".
C*****WRITTEN NOVEMBER 1975 BY J-P TREMBLAY
C
X     COMPILER DOUBLE PRECISION
C
C*****NOTE THAT ALL CALLED SUBROUTINES MUST BE DOUBLE
C*****PRECISION IF THIS PROGRAM IS COMPILED WITH THE
C*****DOUBLE PRECISION OPTION
C
      SUBROUTINE LIAPF(AT,NMAT,NA,B,Q,P,L,M,N,D)
C
      DIMENSION AT(NA,NA),NMAT(NA,NA)
      DIMENSION B(N,N),Q(N),P(N),L(N),M(N)
C
C*****ZERO THE B MATRIX AND THE P VECTOR
C
      CALL GMSET(P,0.0,N,1)
      CALL GMSET(B,0.0,N,N)
C
C*****GENERATE NMAT
C
      K=1
      DO 2 I=1,NA
      DO 1 J=1,NA
      NMAT(I,J)=K
      K=K+1
      IF (I .EQ. J) GO TO 2
      NMAT(J,I)=NMAT(I,J)
    1 CONTINUE
    2 CONTINUE
C
C*****GENERATE ELEMENTAL MATRICES AND ADD THEM TO B
C
      DO 5 I=1,NA
      MR=1
      DO 4 J=1,N
      DO 15 IL=1,NA
```

```
   15 CONTINUE
      GO TO 4
   16 MC=1
      DO 3 I=1,N
      IF (I  NE  NMAT(I,MC)) GO TO 3
      B(J,I)=B(J,I) + AT(MR,MC)
      IF (J  EQ  NMAT(I,I)) B(J,I)=B(J,I) + AT(MR,MC)
      IF (MC  NE  NA) MC=MC+1
    3 CONTINUE
      IF (MR  EQ  NA) GO TO 5
      IF (MC  NE  1) MR=MR+1
    4 CONTINUE
    5 CONTINUE
C
C*****INVERT THE REDUCTION MATRIX
C
      CALL MINV(B,N,D,L,M,$999)
C
C*****CALCULATE SOLUTION VECTOR P
C
      DO 7 I=1,N
      DO 6 J=1,N
      P(I)=P(I) - B(I,J)*Q(J)
    6 CONTINUE
    7 CONTINUE
C
C*****MAP VECTOR P INTO MATRIX AT
C
      DO 11 I=1,NA
      DO 10 J=I,NA
      AT(I,J)=P(I+(J*J-J)/2)
      AT(J,I)=AT(I,J)
   10 CONTINUE
   11 CONTINUE
C
  999 CONTINUE
C
      RETURN
      END
```

FIGURE C-2

SOLUTION OF LYAPUNOV'S EQUATION

DISCRETE FORM

```
X      COMPILER DOUBLE PRECISION
C
C*****SOLUTION OF LYAPUNOV S MATRIX EQUATION FOR DISCRETE
C*****TIME SYSTEMS  "AT*P*A-P=-Q"
C*****METHOD DESCRIBED BY BARNETT AND STOREY, PAGE 79
C*****WRITTEN NOVEMBER 1975 BY J-P TREMBLAY
C
      PARAMETER NA=5, N=15
C
C*****NA          ORDER OF THE LYAPUNOV MATRIX EQUATION
C*****N=NA*(NA+1)/2
C
C*****NOTE THAT ALL CALLED SUBROUTINES MUST BE DOUBLE
C*****PRECISION IF THIS PROGRAM IS COMPILED WITH THE
C*****DOUBLE PRECISION OPTION.
C
      DIMENSION AT(NA,NA),NMAT(NA,NA)
      DIMENSION B(N,N),Q(N),P(N),L(N),M(N)
      DIMENSION BP(NA,NA),BM(NA,NA),BI(NA,NA)
C
C*****OPEN CHANNELS TO DATA FILES
C
      CALL OPEN(0,"LIAPDATA.JP",1,IER)
      IF (IER  NE  1) GO TO 99
      CALL CFILW("PEEMAT.JP",2,IER)
      IF (IER  NE  1) GO TO 99
      CALL OPEN(1,"PEEMAT.JP",3,IER)
      IF (IER  NE  1) GO TO 99
C
C*****READ AND OUTPUT SYSTEM MATRIX AND "Q" MATRIX AS VECTOR
C
      READ(0,501) ((AT(I,J),J=1,NA),I=1,NA),(Q(I),I=1,N)
  501 FORMAT((E12.5))
      WRITE(12,601) ((I,J,AT(I,J),J=1,NA),I=1,NA)
  601 FORMAT(1H ,15X,"SOLUTION OF THE LIAPUNOV FUNCTION",/)
     1 24X,"DISCRETE SYSTEM",///,15X,
     2"SYSTEM MATRIX",/,((15X,"A(",I1,",",I1,") = ",E12.5)))
      WRITE(12,602) (I,Q(I),I=1,N)
  602 FORMAT(1HO,///,15X,"VECTOR Q",/,((15X,"Q(",I2,") = ",E12.5)))
C
C*****GENERATE IDENTITY MATRIX
C
      CALL GMSET(BI,0.0,NA,NA)
      DO 1  I=1,NA
      BI(I,I)=1.0
    1 CONTINUE
C
C*****START OF TRANSFORMATION FOR AT MATRIX
C
      CALL GMADD(AT,BI,BP,NA,NA)
```

```
      CALL GMSUB(AT,BI,BM,NA,NA)
      CALL MINV(BP,NA,D,L,M,$9)
      CALL GMPRD(BP,BM,AT,NA,NA,NA)
C
C*****SOLVE LIAPUNOV FUNCTION FOR MATRIX "P"
C
      CALL LIAPF(AT,NMAT,NA,B,Q,P,L,M,N,D)
      IF (D  EQ  0 ) GO TO 999
C
C*****WRITE OUT DETERMINANT OF REDUCTION MATRIX AND
C*****THE SOLUTION MATRIX "P" BOTH TO LINE PRINTER
C*****AND DISK FILE
C
      WRITE(12,603) D,((I,J,AT(I,J),J=1,NA),I=1,NA)
  603 FORMAT(1HO,///,15X,"DETERMINANT OF REDUCTION MATRIX= ",
     1E12.5,///,15X,"SOLUTION MATRIX P",//,
     2((15X,"P(",I1,",",I1,") = ",E12.5)))
      WRITE(1,604) ((AT(I,J),J=1,NA),I=1,NA)
  604 FORMAT(1H ,E12.5)
      GO TO 9999
C
    9 WRITE(10,607)
  607 FORMAT(1HO,14X,"FAILURE OF DISCRETE TO CONTINUOUS",
     1" TRANSFORMATION")
      GO TO 9999
C
   99 WRITE(10,605) IER
  605 FORMAT(1HO,14X,"INPUT/OUTPUT FILENAME ERROR  CODE= ",I3)
      GO TO 9999
C
  999 WRITE(12,606)
      WRITE(10,606)
  606 FORMAT(1HO,14X,"REDUCTION MATRIX IS SINGULAR")
C
 9999 CALL RESET
C
      STOP
      END
```

C.2 Linear Multivariable Optimal Control of a Discrete Time Linear System

The discrete time linear model of a process is assumed to be of the form

$$x(k+1) = Ax(k) + Bu(k) \qquad \text{(C-6)}$$
$$\text{at } k=0,\ x=x(0)$$

where A: discrete time system transition matrix, nxn
B: discrete time system control matrix, nxr
x: discrete time system states, nx1
r: discrete time system inputs, rx1

Matrices A and B are real and time-invariant. Optimal control of the system will consist of driving the states $x(\infty)$ to zero. A quadratic performance index with a penalty for control is defined to be

$$J = \sum_{k=0}^{N-1} \left[x^T(k+1)Sx(k+1) + \lambda u^T(k)Ru(k) \right] \cdot h \qquad \text{(C-7)}$$

where λ: Lagrange multiplier
h: discrete time interval
S,R: symmetric weighting matrices

Substitution of Equation C-6 into Equation C-7 results in the following objective function:

$$J = \sum_{k=0}^{N-1} \left[\begin{array}{l} x^T(k)Q_1x(k) + u^T(k)Q_2u(k) \\ + u^T(k)Q_3x(k) + x^T(k)Q_3{}^Tu(k) \end{array} \right] \cdot h \qquad \text{(C-8)}$$

where Q_1: A^TSA
Q_2: $B^TSB + \lambda R$
Q_3: B^TSA

According to Noton [1965], the minimization of J by dynamic programming yields the following recursive relationships:

$$D_m = \left[hQ_2 + B^T G_{n-1} B\right]^{-1} \cdot \left[hQ_3 + B^T G_{n-1} A\right] \qquad (C\text{-}9)$$

$$G_n = \left[Q_1 + D_n^T Q_2 D_n - D_n^T Q_3 - Q_3^T D_n\right] \cdot h + \left[A - BD_n\right]^T G_{n-1} \left[A - BD_n\right] \qquad (C\text{-}10)$$

$$D_o = \left[0\right] \qquad (C\text{-}11)$$

$$G_o = Q_1 h \qquad (C\text{-}12)$$

with Equations C-11 and C-12 being used to start the scheme. Matrix D_n will converge to some matrix D_N as $N \longrightarrow \infty$ if a suitable value for "λ" is used. With D_N evaluated the optimal control at initial time is given by

$$u(o) = -D_N\, x(o) \qquad (C\text{-}13)$$

where D_N: optimal gain matrix, rxn

Substitution of Equation C-13 into Equation C-6 provides the closed loop optimal control system

$$x(k+1) = \Phi x(k)$$
$$\Phi = \left[A - BD_N\right] \qquad (C\text{-}14)$$

A listing of the FORTRAN IV routine for optimal control of the reactor model described in Chapter 2 is given in Figure C-3. Typical

FIGURE C-3

OPTIMAL CONTROL OF A DISCRETE STATE SPACE SYSTEM

```
X     COMPILER DOUBLE PRECISION
C
C*****LINEAR MULTIVARIABLE OPTIMAL CONTROL OF THE DISCRETE
C*****REACTOR MODEL BASED ON THE EXTENTS OF BUTANE, PROPANE
C*****AND HYDROGEN AND THE MOLAR FLOWRATES OF PROPANE AND
C*****ETHANE  THE LATTER ARE LINEAR COMBINATIONS OF THE EXTENTS.
C*****THE DYNAMIC PROGRAMMING METHOD USED HEREIN IS
C*****DESCRIBED BY NOTON, PAGES 25 AND 115
C*****WRITTEN APRIL 1976 BY J-P TREMBLAY
C
      PARAMETER NM=5, NR=2, NS=2
C
C*****NM          NUMBER OF STATES
C*****NR          NUMBER OF MANIPULATED INPUTS
C*****NS          NUMBER OF SETPOINT INPUTS
C
C*****NOTE THAT ALL CALLED SUBROUTINES MUST BE DOUBLE
C*****PRECISION IF THIS PROGRAM IS COMPILED WITH THE
C*****DOUBLE PRECISION OPTION
C
      DIMENSION T(NM,NM),V(NM,NR),Q(NM,NS),S(NM,NM),R(NR,NR)
      DIMENSION Q1(NM,NM),Q2(NR,NR),Q3(NR,NM),GN(NM,NM),DN(NR,NM)
      DIMENSION DN1(NR,NM),WK1MM(NM,NM),WK2RM(NR,NM),WK3RR(NR,NR)
      DIMENSION WK4MM(NM,NM),WK5RR(NR,NR),WK6M(NM)
      DIMENSION SUMX(NM),SUMU(NR),UMAX(NR),UMIN(NR)
      DIMENSION L(NM),M(NM),X(NM),U(NR),SP(NS)
C
C*****OPEN CHANNELS TO INPUT AND OUTPUT DISK FILES
C
      CALL OPEN(0,"OPENLOOP JP",1,IER)
      IF (IER .NE. 1) GO TO 99
      CALL CFILW("CLOSEDLOOP JP",2,IER)
      IF (IER .NE. 1) GO TO 99
      CALL OPEN(1,"CLOSEDLOOP JP",3,IER)
      IF (IER .NE. 1) GO TO 99
C
C*****INITIALIZE MATRICES
C
      CALL GMSET(S,0.0,NM,NM)
      CALL GMSET(R,0.0,NR,NR)
      CALL GMSET(SUMX,0.0,NM,1)
      CALL GMSET(SUMU,0.0,NR,1)
C
C*****READ OPEN LOOP MATRICES A,B AND D AND DIAGONAL ELEMENTS
C*****OF WEIGHTING MATRICES S AND R.  READ INITIAL
C*****VALUES OF THE STATES AND OPERATING SETPOINTS
C
      READ(0,500) ((T(I,J),J=1,NM),I=1,NM),
     1((V(I,J),J=1,NR),I=1,NM),
     2((Q(I,J),J=1,NS),I=1,NM),
```

```
     4(X(I), I=1, NM), (SP(I), I=1, NS)
C
C*****GET
C*****(1) CONVERGENCE TEST VALUE- MINIMUM ACCEPTABLE RELATIVE
C*****    CHANGE BETWEEN SUCCESSIVE ESTIMATES OF GAIN MATRIX
C*****(2) LAGRANGE MULTIPLIER VALUE
C*****(3) DISCRETE TIME INTERVAL IN SECONDS
C
      ACCEPT 'CONVERGENCE TEST VALUE= ', TEST,
     1"LAGRANGE MULTIPLIER VALUE= ", WGHT,
     2"DISCRETE TIME INTERVAL= ", HDT
C
C*****ENSURE THAT INPUTS ARE POSITIVE
C
      TEST=ABS(TEST)
      WGHT=ABS(WGHT)
      HDT=ABS(HDT)
C
C*****GENERATE Q1, Q2 AND R3 MATRICES
C
      CALL GMPRD(S, T, WK1MM, NM, NM, NM)
      CALL GTPRD(T, WK1MM, Q1, NM, NM, NM)
      CALL GTPRD(V, WK1MM, Q3, NM, NR, NM)
      CALL GTPRD(V, S, WK2RM, NM, NR, NM)
      CALL GMPRD(WK2RM, V, Q2, NR, NM, NR)
      CALL GMMPK(R, WGHT, WK3RR, NR, NR)
      CALL GMADD(WK3RR, Q2, Q2, NR, NR)
C
C*****INITIALIZATION OF GN AND DN1 MATRICES AND
C*****INDICATION OF THE STARTING TIME OF CALCULATION
C
      CALL GMMPK(Q1, HDT, GN, NM, NM)
      CALL GMSET(DN1, 0 0, NR, NM)
      LPCNT=0
      CALL FGTIM(JH, JM, JS)
      WRITE(10, 600) JH, JM, JS
C
C*****BEGINNING OF RECURSIVE SOLUTION FOR OPTIMAL
C*****CONTROL MATRIX DN   ENDS WHEN DIFFERENCE BETWEEN
C*****DN AND DN1 IS SMALL
C
    4 CONTINUE
      EMAX=0.0
      DO 7 K=1, 50
      LPCNT=LPCNT+1
C
C*****CALCULATE ESTIMATE OF DN
C
      CALL GTPRD(V, GN, WK2RM, NM, NR, NM)
      CALL GMPRD(WK2RM, V, WK5RR, NR, NM, NR)
      CALL GMMPK(Q2, HDT, WK3RR, NR, NR)
      CALL GMADD(WK3RR, WK5RR, WK3RR, NR, NR)
      CALL MINV(WK3RR, NR, D, L, M, $999)
      CALL GMPRD(WK2RM, T, DN, NR, NM, NM)
      CALL GMMPK(Q3, HDT, WK2RM, NR, NM)
      CALL GMADD(WK2RM, DN, WK2RM, NR, NM)
      CALL GMPRD(WK3RR, WK2RM, DN, NR, NR, NM)
C
C***      FOR          ICE OF DN
```

```
      ERROR=0.0
      DO 6 I=1,NR
      DO 5 J=1,NM
      ERRS=ABS((DN(I,J)-DN1(I,J))/DN(I,J))
      IF (ERRS  GE  TEST) ERROR=AMAX1(ERROR,ERRS)
      DN1(I,J)=DN(I,J)
    5 CONTINUE
    6 CONTINUE
      IF (ERROR  EQ  0.0) GO TO 8
      EMAX=AMAX1(EMAX,ERROR)
C
C*****GAIN MATRIX NOT CONVERGED YET COMPUTE NEW GN MATRIX AND
C*****RETURN TO CALCULATE NEW ESTIMATE OF DN
C
      CALL GMPRD(V,DN,WK1MM,NM,NR,NM)
      CALL GMSUB(T,WK1MM,WK1MM,NM,NM)
      CALL GTPRD(WK1MM,GN,WK4MM,NM,NM,NM)
      CALL GMPRD(WK4MM,WK1MM,GN,NM,NM,NM)
      CALL GTPRD(D3,DN,WK1MM,NR,NM,NM)
      CALL GMTRA(WK1MM,WK4MM,NM,NM)
      CALL GMADD(WK1MM,WK4MM,WK4MM,NM,NM)
      CALL GMPRD(D2,DN,WK2RM,NR,NR,NM)
      CALL GTPRD(DN,WK2RM,WK1MM,NR,NM,NM)
      CALL GMSUB(WK1MM,WK4MM,WK1MM,NM,NM)
      CALL GMADD(D1,WK1MM,WK1MM,NM,NM)
      CALL GMMP4 (WK1MM,HDT,WK1MM,NM,NM)
      CALL GMADD(WK1MM,GN,GN,NM,NM)
    7 CONTINUE
      CALL FGTIM(IH,IM,IS)
      WRITE(10,601) LPCNT,IH,IM,IS,EMAX
      IF (LPCNT  GE  5000) STOP - NO CONVERGENCE AFTER 5000 ITERATIO
      GO TO 4
C
C*****DN MATRIX CONVERGED-OUTPUT INFO TO LINE PRINTER
C
    8 CALL FGTIM(IH,IM,IS)
      WRITE(10,602) IH,IM,IS,LPCNT
      PAUSE TURN ON LINE PRINTER
      WRITE(12,603) TEST,WGHT,HDT,JH,JM,JS,IH,IM,IS,LPCNT,
     1((I,J,T(I,J),J=1,NM),I=1,NM)
      WRITE(12,604) ((I,J,V(I,J),J=1,NR),I=1,NM)
      WRITE(12,605) ((I,J,Q(I,J),J=1,NS),I=1,NM)
      WRITE(12,606) (I,I,S(I,I),I=1,NM)
      WRITE(12,607) (I,I,R(I,I),I=1,NR)
      WRITE(12,616) (I,X(I),I=1,NM)
      WRITE(12,617) (I,SP(I),I=1,NS)
      WRITE(12,608) ((I,J,DN(I,J),J=1,NM),I=1,NR)
C
C*****CALCULATION OF STABILITY A MATRIX AND WRITTING OF
C*****THIS TO LINE PRINTER AND DISK
C
      CALL GMPRD(V,DN,WK1MM,NM,NR,NM)
      CALL GMSUB(T,WK1MM,WK1MM,NM,NM)
      WRITE(12,610) ((I,J,WK1MM(I,J),J=1,NM),I=1,NM)
      WRITE(1,609) ((WK1MM(I,J),J=1,NM),I=1,NM)
C
C****EVALUATE PERFORMANCE OF OPTIMAL CONTROL
C
      DO 11 I=1,25
```

```
      CALL GMPRD(DN, X, U, NR, NM, 1)
      DO 9 J=1, NM
      SUMX(J)=SUMX(J) + X(J)*X(J)
    9 CONTINUE
      DO 10 J=1, NR
      IF (I  GT.  1) GO TO 12
      UMAX(J)=U(J)
      UMIN(J)=U(J)
   12 CONTINUE
      IF (U(J)  GT  UMAX(J)) UMAX(J)=U(J)
      IF (U(J)  LT  UMIN(J)) UMIN(J)=U(J)
      SUMU(J)=SUMU(J) + U(J)*U(J)
   10 CONTINUE
      CALL GMPRD(T, X, WORK6M, NM, NM, 1)
      CALL GMPRD(V, U, X, NM, NR, 1)
      CALL GMSUB(WORK6M, X, X, NM, 1)
      CALL GMPRD(Q, SP, WORK6M, NM, NS, 1)
      CALL GMADD(WORK6M, X, X, NM, 1)
   11 CONTINUE
      WRITE(12,614) (I, SUMX(I), I=1, NM)
      WRITE(12,615) (I, SUMU(I), I=1, NR)
      WRITE(12,618) (I, UMAX(I), I, UMIN(I), I=1, NR)
      GO TO 9999
C
   99 WRITE(10,612) IER
      GO TO 9999
C
 999 WRITE(10,613)
C
9999 CALL RESET
      STOP
C
  500 FORMAT('(E12.5)')
  600 FORMAT(1HO,"STARTED OPTIMAL CONTROLLER CALCULATION AT ",
     1I2," ",I2," ",I2)
  601 FORMAT(1H ,"TIME AT ITERATION",I5," IS ",I2," ",I2," ",I2,
     1/,10X,"MAXIMUM RELATIVE ERROR= ",E12.5)
  602 FORMAT(1H ,"ENDED OPTIMAL CONTROLLER CALCULATION AT ",
     1I2," ",I2," ",I2,/,5X,"TOTAL ITERATIONS REQUIRED= ",I4,/)
  603 FORMAT(1HO,14X,"LINEAR MULTIVARIABLE OPTIMAL CONTROL",/,
     119X,"OF A DISCRETE CONTROL SYSTEM",//,15X,
     2"CONVERGENCE TEST VALUE= ",E12.5,/,15X,
     3"LAGRANGE MULTIPLIER= ",E12.5,/,15X,
     4"DISCRETE TIME INTERVAL= ",F6.1," SECONDS",/,15X,
     5"STARTING TIME= ",I2," ",I2," ",I2,/,15X,
     6"STOPPING TIME= ",I2," ",I2," ",I2,/,15X,
     7"TOTAL ITERATIONS REQUIRED= ",I4,///,15X,
     8"DISCRETE A MATRIX",//,((15X,"A(",I1,",",I1,") = ",E12.5)))
  604 FORMAT(1HO,14X,"DISCRETE B MATRIX",//,
     1((15X,"B(",I1,",",I1,") = ",E12.5)))
  605 FORMAT(1HO,14X,"DISCRETE D MATRIX",//,
     1((15X,"D(",I1,",",I1,") = ",E12.5)))
  606 FORMAT(1HO,14X,"DIAGONAL OF S MATRIX",//,
     1((15X,"S(",I1,",",I1,") = ",E12.5)))
  607 FORMAT(1HO,14X,"DIAGONAL OF R MATRIX",//,
     1((15X,"R(",I1,",",I1,") = ",E12.5)))
  608 FORMAT(1HO,14X,"OPTIMAL GAIN MATRIX",//,
     1((15X,"DN(",I1,",",I1,") = ",E12.5)))
  609 FORMAT(1H ,E12.5)
  610 FORMAT(1HO,14X,"STABILITY A MATRIX",//,
```

```
     1((          I1,",",I1,") = ",E1_ 5)))
 612 FORMAT(1HO,5X,"INPUT/OUTPUT FILENAME ERROR  CODE= ",I3)
 613 FORMAT(1HO,5X,"CALCULATION ABORTED  INVERSION ERROR")
 614 FORMAT(1HO,14X,"CONTROLLER PERFORMANCE REPORT",//,
     1((15X,"SSX(",I1,") = ",E12 5)))
 615 FORMAT(1H ,/,((15X,"SSU(",I1,") = ",E12 5)))
 616 FORMAT(1HO,14X,"INITIAL VALUES OF THE STATES",//,
     1((15X,"X(",I1,") = ",E12 5)))
 617 FORMAT(1HO,14X,"SETPOINT INPUTS",//,
     1((15X,"SP(",I1,") = ",E12 5)))
 618 FORMAT(1H ,/,((15X,"UMAX(",I1,") = ",E12.5,
     1X,"UMIN(",I1,") = ",E12 5)))
     END
```

execution time for a fifth order model is about 4.5 minutes for 145 iterations on the NOVA 2/10 minicomputer when $\lambda = 2 \times 10^{-14}$ and the convergence test value is 1×10^{-8}. The double precision option was used.

C.3 Steady State Reactor Mass Balance

Equations 2-3 to 2-6 -- repeated below -- form the basis of a steady state mass balance around an n-butane hydrogenolysis packed bed catalytic reactor.

$$n\text{-}C_4H_{10} + H_2 \xrightarrow{F} C_3H_8 + CH_4 \qquad (2\text{-}3)$$

$$n\text{-}C_4H_{10} + H_2 \xrightarrow{1-F} 2C_2H_6 \qquad (2\text{-}4)$$

$$C_3H_8 + H_2 \longrightarrow C_2H_6 + CH_4 \qquad (2\text{-}5)$$

$$C_2H_6 + H_2 \longrightarrow 2CH_4 \qquad (2\text{-}6)$$

Assuming that inlet and outlet conditions of the reactor are identical and that only hydrogen and n-butane are in the feed, the following steady state mass balance arises:

$$Gc_{n\text{-}C_4H_{10}} = Gc^{I}_{n\text{-}C_4H_{10}} - (e_1 + e_2) \qquad (C\text{-}15)$$

$$Gc_{C_3H_8} = e_1 \qquad (C\text{-}16)$$

$$Gc_{C_2H_6} = 2e_2 - e_3 \qquad (C\text{-}17)$$

$$Gc_{CH_4} = e_1 + 2e_3 \qquad (C\text{-}18)$$

$$Gc_{H_2} = Gc^{I}_{H_2} - (e_1 + e_2 + e_3) \qquad (C\text{-}19)$$

where G: total volumetric flowrate, cm^3/sec

c_i, c_i^I: concentration of component i, at exit and inlet respectively, gm-moles/cm^3

e_1, e_2, e_3: extent of reaction for Equations 2-3, 2-4 and 2-6 respectively in terms of the amount of product formed per unit time, gm-moles/sec

With the definitions

$$\begin{aligned} f_{n\text{-}C_4H_{10}} &= e_1 + e_2 \\ f_{C_3H_8} &= e_1 \qquad (C\text{-}20) \\ f_{H_2} &= e_1 + e_2 + e_3 \end{aligned}$$

where f_i: extent of reaction for component i, gm-moles/sec

applied to Equations C-15 to C-19, Equations 2-7 to 2-11 are formed.

$$Gc_{n\text{-}C_4H_{10}} = Gc^{I}_{n\text{-}C_4H_{10}} - f_{n\text{-}C_4H_{10}} \qquad (2\text{-}7)$$

$$Gc_{C_3H_8} = +f_{C_3H_8} \qquad (2\text{-}8)$$

$$Gc_{C_2H_6} = +3f_{n\text{-}C_4H_{10}} - 2f_{C_3H_8} - f_{H_2} \qquad (2\text{-}9)$$

$$Gc_{CH_4} = -2f_{n\text{-}C_4H_{10}} + f_{C_3H_8} - 2f_{H_2} \qquad (2\text{-}10)$$

$$Gc_{H_2} = Gc^{I}_{H_2} - f_{H_2} \qquad (2\text{-}11)$$

where G: total volumetric flowrate, cm^3/sec

c_i, c_i^I: concentration of component i at exit and inlet respectively, gm-moles/cm^3

f_i: extent of reaction for component i, gm-moles/sec

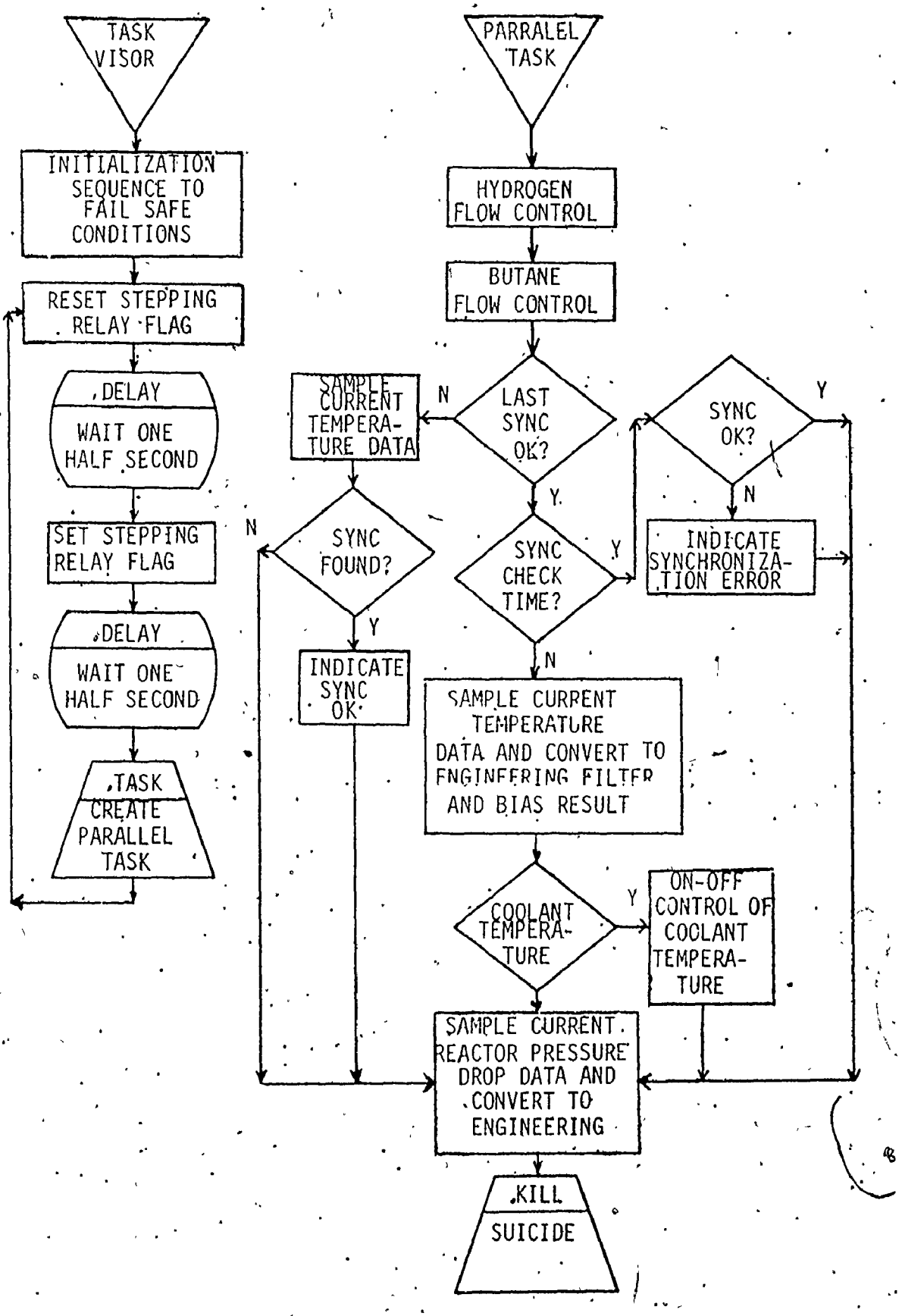
C.4 Basic Reactor Operating Software

Five assembler language routines written for use with the GOSEX executive formed the nucleus of all software developed for control of the butane hydrogenolysis pilot plant reactor. Two of these were user tasks and the remaining three were special purpose user defined executive functions. Listings of these routines are included in the pilot plant operating instructions manual (Wright et al [1977]).

Except for the effluent stream composition data, all data to or from the pilot plant was controlled by the user task VISOR. Its functional diagram is provided in Figure C-4. Once every second, VISOR sequenced the acquisition of temperature and differential pressure data. To obtain new temperature data from the plant, the thermocouple multiplexer (described in Chapter 3, Section 4) rotary relay was advanced one position at the start of each one second interval. At the end, a parallel task was created to process all new plant data provided by the executive. The differential pressures across the hydrogen and n-butane flowmeters were converted into equivalent flowrates and based on these data, the executive's PI control algorithm was used to maintain the flowrates at specified setpoints. These setpoints could be altered by the GOSEX executive function TUNER or by any user software. Provided that the rotary relay synchronization check did not occur, the data from the thermocouple transmitters was converted into temperatures. The temperature data was corrected for bias, smoothed by a first order filter and saved. If the temperature was

FIGURE C-4

TASK VISOR FUNCTIONAL DIAGRAM



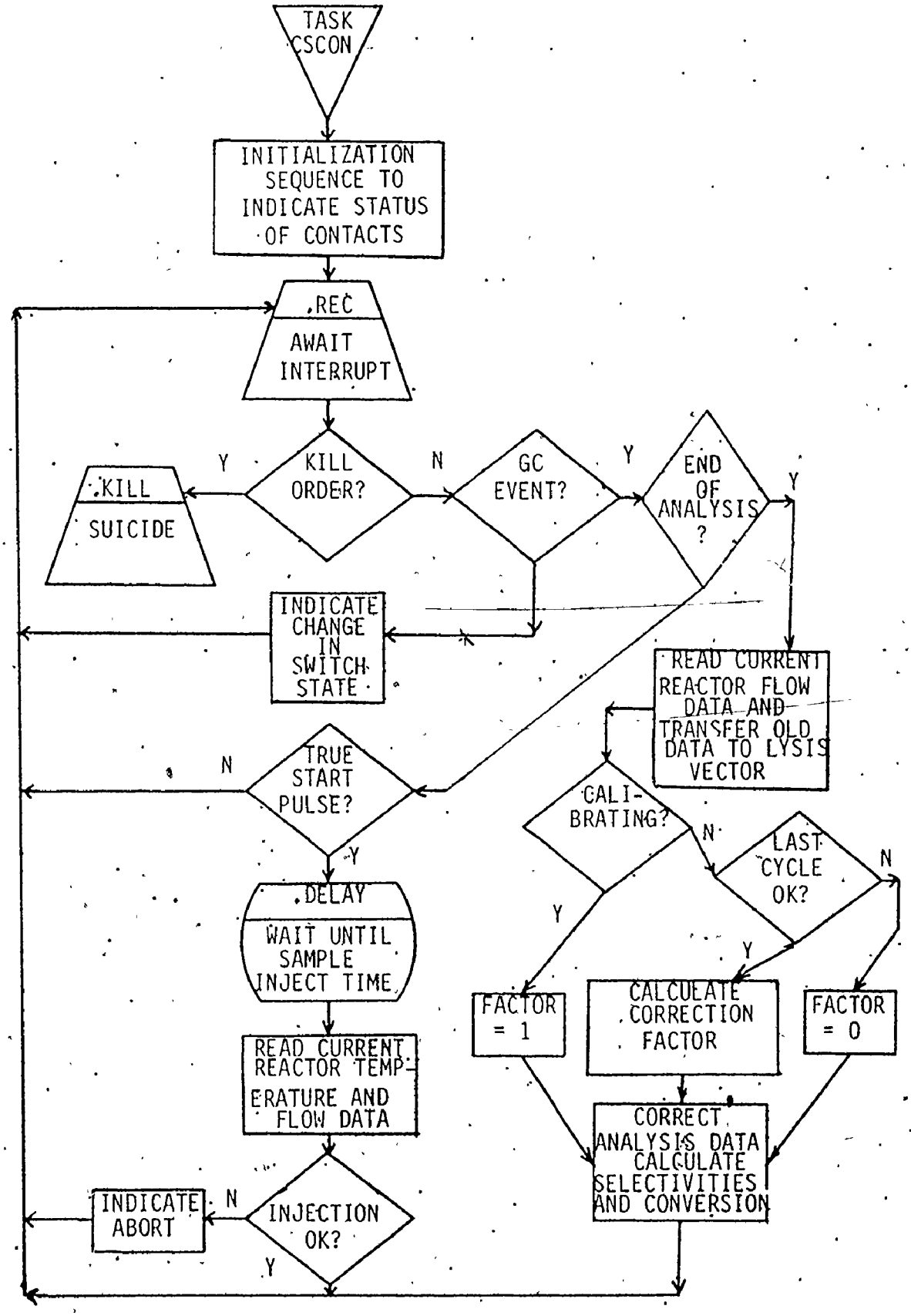
that of the reactor coolant, a thermostat controller was envoked. Cooling was provided when this temperature exceeded the desired setpoint. Two types of biases were used to correct temperature data. One of these was continuously updated by task VISOR and the other was specified by the user. At each rotary relay synchronization check (which occurred at every twelvth multiplexer reading), the thermocouple transmitter "ZERO" level was determined. Provided that this reference value was within certain limits, it was used to correct data obtained during the next cycle of the multiplexer. If the "ZERO" level was found to be in error, an alarm was flagged and a hunt for the synchronization point began. In addition to the transmitter bias, the user was able through executive function PARAM to specify a bias for each thermocouple, thereby accounting for differences between individual thermocouples. Finally, before the parallel task aborted, the reactor differential pressure transmitter data was converted into a pressure drop and saved.

Quite unlike task VISOR, task CSCON was only activated by a change in state of any of the computer's contact sense inputs. This task's functional diagram is provided in Figure C-5. If any of the pilot plant operating switches was moved between the manual and automatic positions, a suitable alarm would be output to the operator's console. If the process gas chromatograph caused the activation of task CSCON, the resulting operations would be determined by which contact sense input had changed state. If the process gas chromatograph were placed "IN-SERVICE", CSCON

FIGURE C-5

TASK CSCON FUNCTIONAL

DIAGRAM



did not inhibit the processing of analysis information. This information became available on the "END-OF-ANALYSIS" pulse generated by the process gas chromatograph at the end of an analysis cycle. At this time, component peak areas provided by the executive were converted to mole fractions and corrected by the algorithm described in Section 5 of Chapter 3. These results and the reactor conditions which prevailed at the time of sample injection were saved in tabular form -- vector LYSIS. A flag indicating the availability of new information was set provided that the process gas chromatograph was not in the "CALIBRATION MODE" or an analysis failure had not been detected. CSCON omitted the correction of mole fractions when the process gas chromatograph was in the "CALIBRATION MODE". An analysis failure occurred only if the feed flow rates to the reactor changed during the three second "START-OF-ANALYSIS" sequence. If a change did occur, CSCON caused the output of an alarm to the operator's console. Upon a proper "START-OF-ANALYSIS", an alarm was output at the operator's console and normal operations were resumed.

User defined executive functions SETUP, QENCH and PANIC performed specialized operations when envoked by the operator. SETUP was used to initialize data for tasks VISOR and CSCON. Rapid quenching of the reactor was possible by envoking the QENCH function. Function PANIC was available for an emergency shutdown of the pilot plant.

C.5 Interface Between GOSEX and the Model Reference Adaptive Control Software

The interface which is presented in this section was used to link GOSEX and the model reference adaptive control software described in Section 5. It is typical of any interface that must be prepared when an application of GOSEX is considered.

As mentioned in Section 5 of Chapter 4, the interface between GOSEX and user software is in two parts. One portion of the interface must reside on disk as specially formatted files. The contents of the executive message file OPCOM.MG and the user message file MESSG.MG have been listed in Figure C-6 and C-7 respectively. The core resident portion of the interface consists of a table of symbols and a series of communication buffers. The basic reactor and model reference adaptive control symbols have been combined with those of the executive in Figure C-8. The remainder of the interface is found in Figure C-9. Functions QENCH and PANIC do not kill any of the user's control tasks. For this reason, user tasks which alter the flow or coolant temperature controller set-points should be dormant when these functions are envoked.

C.6 Model Reference Adaptive Control Software

The software to implement the model reference adaptive control theory developed in Chapter 2 and actually employed in experiments described in Chapter 5 is outlined here. Listings of the routines whose titles appear in Table C-1 are available (Tremblay [1977b]).

FIGURE C-6

EXECUTIVE MESSAGE FILE

```
 15: 12:
 1: NOT AN EXECUTIVE FUNCTION
 12:EXECUTIVE FUNCTION NOT AVAILABLE
 12:TASK NAME
 12:NOT A USER TASK 15:
 12:USER TASK CREATED
 12:TASK IS ALREADY ACTIVE
 12:USER TASK FILLED
 12:TASK IS ALREADY INACTIVE
 12:TASK IS INACTIVE
 12:TASK IS ACTIVE
 12:DEVICE NAME.
 12:NOT A DEVICE NAME<15>
 12:DEVICE NOT PART OF SYSTEM
 12:SPECIFIED OUTPUT FILLED
 12:SPECIFIED OUTPUT ALREADY INACTIVE
 12:ALL OUTPUTS FILLED
 12:DISK DIRECTORY & FILENAME
 12:DELETION CONFIRMED
 12:FILENAME ERROR 15:
 12:CURRENT DISPLAY INTERVAL(SECONDS)
 12:RESET DISPLAY INTERVAL(SECONDS)
 12:CHANGE CONFIRMED
 12:INTERVAL IMPROPERLY SPECIFIED<15>
 15: 12: END OF REPORT
 15: 12: 40: *?*
 15: 12: 40:
 15: 12:LOOP NAME
 12:NOT A CONTROLLER LOOP 15:
FILTER CONSTANT(0 TO +1000 )/ 40>
INPUT HIGH ALARM LIMIT-
INPUT LOW ALARM LIMIT-
CURRENT SET POINT-
PROPORTIONAL GAIN(+VE)/ 40>
PROPORTIONAL-DERIVATIVE GAIN(+VE)/<40>
PROPORTIONAL-INTEGRAL GAIN(+VE)/<40>
SCALE FACTOR & DIRECTION OF ACTION/<40>
CONTROL INTERVAL(SECONDS)/ 40>
OUTPUT HIGH LIMIT-
OUTPUT LOW LIMIT-
OUTPUT MEAN-
<15: 12: CONVERSION ERROR
 15:<12: 40>*?*<15:<12>
<12>FILE IN USE
<12>DELETION NOT POSSIBLE, CODE<40>
<12>VARIABLES LIST-MAX
<12>DEVICE IN USE<15>
<12>ALL BUFFERS IN USE
 12:FORMAT:40>
<12>NO LIST<15>
<12>END OF LIST<15>
```

```
<12>OUTPUT TASK CREATED
<12>UNABLE TO INITIATE OUTPUT TASK
<12>DEVICE UNIT #:
<12>DEVICE NOT EQUIPPED FOR PLOTTING
<12>SCALE FACTOR
<12>PLOTTING INTERVAL(SECONDS):
<12>MIN RANGE OF PLOT:
<12>MAX RANGE OF PLOT.
<15><12><40>GOSEX - BACKGROUND OPERATION
<15><12><40>GOSEX - FOREGROUND OPERATION
<15><12>USER BUILT SYMBOL TABLE LENGTH ERROR<15><12>
<15><12>RELAY BIT STATUS TABLE NOT DEFINED<15><12>
<15><12>A/D READ DATA STORAGE NOT DEFINED<15><12>
<15><12>USER CLOCK SET TO RTC FREQUENCY<15><12>
<15><12>USER CLOCK NOT DEFINED<15><12>
<15><12>CONTACT SENSE DISPATCH TABLE NOT DEFINED<15><12>
<15><12>USER SHUTDOWN ROUTINE NOT DEFINED<15><12>
<15><12>USER TASK DEFINITION TABLE NOT DEFINED<15><12>
<15><12>ERROR DETECTED IN USER TASK DEFINITION TABLE<15><12>
<15><12>USER ALARM DEFINITION TABLE NOT DEFINED<15><12>
<15><12>USER MESSAGE FILE NOT DEFINED<15><12>
<15><12>EXECUTION ABORTED<15><12>
<15><12>AOK-TO RUN, STRIKE ANY KEY<15><12>
<12>DIRECTORY OR DEVICE NAME
<12>DIRECTORY OR DEVICE INITIALIZED
<12>DIRECTORY OR DEVICE ALREADY INITIALIZED
<12>INITIALIZATION NOT POSSIBLE, CODE<40>
<12>DIRECTORY OR DEVICE RELEASED
<12>DIRECTORY OR DEVICE IN USE
<12>RELEASE NOT POSSIBLE, CODE<40>
<15><12>USER SPACE RELEASED<15><12>
<15><12>CONTROL LOOP DEFINITION TABLE NOT DEFINED<15><12>
<15><12>ERROR DETECTED IN CONTROL LOOP DEFINITION TABLE<15><12>
<15><12>ERROR DETECTED IN CONTACT SENSE DISPATCH TABLE<15><12>
<12>AXIAL POSITION
<15><12>UDEF EXECUTIVE FUNCTION LIST EXTENSION NOT DEFINED<15><12>
<12>ASCII OR BINARY OUTPUT.
<12>RECORD ID
<12>TAPE FILE #.
<12>PREFORMATTED LIST DISK FILENAME
<12>OUTPUT BUFFER ERROR
<12>LIST ERROR, ENTRY #
<12>SOURCE FILENAME:
<12>NO COPY TO TTY DEVICE
<12>CHART IN USE - KILL? [Y/N].
<12>NO ANALOG OUTPUTS
<15><12>D/A OUTPUT DATA STORAGE NOT DEFINED<15><12>
<15><12>USER INTERRUPTING DEVICES NOT DECLARED<15><12>
CC/SEC HYDROGEN/<40>
% VALVE OPEN/<40>
<12>HYDROGEN FLOW CONTROL
CC/SEC BUTANE/<40>
<12>BUTANE FLOW CONTROL
<15><12>SUPERVISORY PROGRAM SETUP
<15><12>OIL TEMPERATURE SET POINT:
<15><12>USE FUNCTION TUNER TO SET REACTANTS FLOWRATES
<15><12>REACTOR QUENCHING INITIATED
<15><12>ALL FLOWS OFF  COOLING ON.  FEED VENTING ON.
@
```

FIGURE C-7

USER ALARM MESSAGE FILE

```
<15><12>SYNC ERROR IN MULTIPLEXER UNIT # 1<15>
<15><12>SYNC ERROR IN MULTIPLEXER UNIT # 2<15>
<15><12>COOLING AIR ON, HUNTING FOR SYNC POINT<15>
<15><12>MULTIPLEXER UNIT # 1 OK<15>
<15><12>MULTIPLEXER UNIT # 2 OK<15>
<15><12>THERMOSTAT ACTIVATED<15>
<15><12>HYDROGEN FLOW TOO HIGH<15>
<15><12>HYDROGEN FLOW TOO LOW<15>
<15><12>BUTANE FLOW TOO HIGH<15>
<15><12>BUTANE FLOW TOO LOW<15>
<15><12>HYDROGEN UNDER LOCAL CONTROL<15>
<15><12>HYDROGEN UNDER AUTOMATIC CONTROL<15>
<15><12>BUTANE UNDER LOCAL CONTROL<15>
<15><12>BUTANE UNDER AUTOMATIC CONTROL<15>
<15><12>COOLING AIR UNDER LOCAL CONTROL<15>
<15><12>COOLING AIR UNDER AUTOMATIC CONTROL<15>
<15><12>REACTOR VENT UNDER LOCAL CONTROL<15>
<15><12>REACTOR VENT UNDER AUTOMATIC CONTROL<15>
<15><12>FEED VENT UNDER LOCAL CONTROL<15>
<15><12>FEED VENT UNDER AUTOMATIC CONTROL<15>
<15><12>GC OUT OF SERVICE<15>
<15><12>GC IN SERVICE<15>
<15><12>PROCESS STREAM ANALYSIS ENABLED<15>
<15><12>GC CALIBRATION ENABLED<15>
<15><12><7><7><7>ANALYSIS CYCLE ABORTED<15>
<15><12>ANALYSIS CYCLE OK<15>
<15><12><7><7>MRAC TASK ERROR<15>
<15><12>MRAC AND GC SYNCHRONIZED<15>
<15><12>REFERENCE MODEL RETRIGGERED<15>
@
```

FIGURE C-8

TABLE OF SYMBOLS

```
          TITL SYMBL

,SYMBL TAPE # 1 OF 3
,USER BUILT SYMBOL TABLE
,THIS TAPE-GOSEX SYMBOLS

          ENT USST,UEST

,EXECUTIVE FUNCTION SYMBOLS
          EXTN START,CEASE,STATS,ENDIO,ENDAL,CLEAR,CHNGE,PARAM
          EXTN TUNER,LOG,PLOT,READY,RELSE,RETRN,CLOCK,PROFL
          EXTN MYLOG,COPY,CHART,DIALG

,DEVICE SYMBOLS
          EXTN CONSL,PRINT,TTYPE,PUNCH,DISK,CASET,MAGTP

          NREL

,USER MUST DECLARE THE FOLLOWING AT THE END OF TAPE # 3
,         SST     LAST SYMBOL-CODE WORD # 1
,
,         UEST=   EST
;         USST=   SST

,ALSO, THE USER MUST INCLUDE THE APPROPRIATE  EXTN
,DECLARATIONS FOR TAPE # 3   THIS MAY BE DONE IN TAPE # 3 ITSELF
,IN THIS INSTANCE, IT IS NECESSARY THAT THE EXTERNAL
,ECLARATIONS PRECEED ANY OTHER STATEMENTS

,CODING TABLE FOR RADIX 50 SYMBOLS

,         CHARACTER       VALUE(DECIMAL)
,         NULL            0
,         0               1.
,         1               2.
;         2               3.
;         3               4.
;         4               5.
;         5               6.
;         6               7.
;         7               8.
;         8               9.
;         9               10.
;         A               11.
;         B               12.
;         C               13.
,         D               14.
;         E               15.
;         F               16.
;         G               17.
```

```
;       H       18.
;       I       19.
;       J       20.
;       K       21.
;       L       22.
;       M       23.
;       N       24.
;       O       25.
;       P       26.
;       Q       27.
;       R       28.
;       S       29.
;       T       30.
;       U       31.
;       V       32.
;       W       33.
;       X       34.
;       Y       35.
;       Z       36.
;               37

;EXAMPLE OF CODING:
;SYMBOL "ABCDE" MAY BE ENCODED BY THE USER IN THE FOLLOWING WAY
;       [D]*40.+[E]*32          ;SYMBOL CODE WORD # 2
;       [A]*40.+[B]*40.+[C]     ;SYMBOL CODE WORD # 1

;WHERE [#] DECOTES THE CODING VALUE OF THE CHARACTER AS
;GIVEN IN THE TABLE ABOVE

;WRITTEN OCTOBER, 1974 BY
;       JEAN-PIERRE TREMBLAY
;       DEPARTMENT OF CHEMICAL ENGINEERING
;       MCMASTER UNIVERSITY
;       HAMILTON, ONTARIO, CANADA


EST:

;EXECUTIVE FUNCTIONS LIST
        START           ;SYMBOL VALUE-USUALLY ESTABLISHED AT LOAD TIME
        36800.          ;SYMBOL CODE WORD # 2
        47611           ;SYMBOL CODE WORD # 1
        CEASE
        37600.
        21411.
        STATS
        39328.
        47611.
        ENDIO
        25120.
        24974.
        ENDAL
        14784.
        24974.
        CLEAR
        14976.
        21695.
        CHNGE
        22240.
        21544.
```

```
14816.
42068.
TUNER
20096.
49264.
LOG
0
36217.
PLOT
38400.
42505.
READY
19040.
45411.
RELSE
37600
45422
RETRN
36608
45430.
CLOCK
17312.
21705
PROFL
21184
42745.
MYLOG
32544.
38222.
COPY
44800
21826.
CHART
36800.
21531
DIALG
28704.
23171.

DEVICES LIST
CONSL
37824.
21824.
PRINT
31680.
42739.
TTYPE
33760.
49235.
PUNCH
17216.
42864.
DISK
26880.
23189.
CASET
20160.
21269.
MAGTP
```

```
39232.
37257.

;CONTROLLER PARAMETERS LIST-VALUE SPECIFIED IN PARAMETER TAPE
FILTR
39296.
26382
INHI
24320
31378.
INLO
32000.
31382.
SETPT
34240.
47030
KP
0
34640.
KPD
0
34654.
KPI
0
34659.
SCALE
28640.
46931.
DELAY
15200
23022
OUTHI
23648
41270.
OUTLO
28960.
41270.
MEAN
30720.
37411.

EOT                ;END OF SYMBL TAPE # 1 OF 3


;SYMBL TAPE # 2 OF 3
;REACTOR CONTROL SYMBOLS

 EXTN VISOR, HLOOP, BLOOP, H2FRI, C4FRI
 EXTN H2VAL, C4VAL, VLCON, H2CON, C4CON
 EXTN TPCON, DPCON, RTRDP, T1, T2, T3, T4
 EXTN T5, T6, T7, T8, T9, T10, T11, T12, T13
 EXTN T14, T15, T16, T17, T18, T19, T20
 EXTN T21, T22, OILSP, CSCON, TOTFR
 EXTN C4MFI, C4MFO, C3MFI, C3MFO, C2MFI, C2MFO
 EXTN C1MFI, C1MFO, H2MFI, H2MFO, SELC3, SELC2
 EXTN SELC1, CONV, C3FRI, C2FRI, C1FRI, H2FRO
 EXTN C4FRO, C3FRO, C2FRO, C1FRO
 EXTN SETUP, BENCH, PANIC
 EXTN TF1, TF2, TF3, TF4, TF5, TF6, TF7, TF8, TF9
 EXTN TF10, TF11, TF12, TF13, TF14, TF15, TF16
```

```
        .EXTN TF17,TF18,TF19,TF20,TF21,TF22,ALPHA
        EXTN BT1,BT2,BT3,BT4,BT5,BT6,BT7,BT8
        EXTN BT9,BT10,BT11,BT12,BT13,BT14,BT15
        EXTN BT16,BT17,BT18,BT19,BT20,BT21,BT22
        EXTN CLBC3,CLBC4,CLBC1,CLBC2

;WRITTEN JUNE, 1976 BY
;       JEAN-PIERRE TREMBLAY
;       DEPARTMENT OF CHEMICAL ENGINEERING
;       MCMASTER UNIVERSITY
;       HAMILTON, ONTARIO, CANADA

;WRITTEN IN DGC S NOVA-LINE ASSEMBLER LANGUAGE
;FORMATTED FOR USE WITH THE GOSEX EXECUTIVE

        VISOR
        25. *40. +28. *32.
        32 *40. +19 *40 +29.
        HLOOP
        25 *40 +26. *32.
        18.*40 +22 *40 +25
        BLOOP
        25 *40 +26 *32.
        12 *40 +22 *40. +25.
        H2FRI
        28 *40 +19. *32.
        18 *40 +3. *40. +16.
        C4FRI
        28. *40 +19 *32.
        13. *40 +5 *40. +16
        H2VAL
        11. *40, +22 *32.
        18. *40. +3 *40. +32.
        C4VAL
        11 *40 +22. *32
        13 *40 +5. *40. +32.
        VLCON
        25 *40 +24. *32.
        32 *40 +22 *40 +13.
        H2CON
        25 *40. +24 *32.
        18 *40. +3. *40. +13.
        C4CON
        25. *40 +24. *32.
        13. *40. +5 *40 +13
        TPCON
        25. *40 +24. *32.
        30. *40. +26. *40 +13.
        DPCON
        25. *40. +24. *32.
        14. *40. +26. *40. +13.
        RTRDP
        14. *40. +26. *32
        28. *40 +30. *40 +28.
        T1
        0
        30 *40. +2 *40.
        T2
        0
        30. *40. +3. *40.
```

```
T3.
0
30. *40. +4. *40.
T4
0
30 *40. +5. *40.
T5
0
30. *40. +6. *40.
T6
0
30. *40. +7. *40.
T7
0
30 *40 +8. *40.
T8
0
30. *40. +9 *40.
T9
0
30 *40. +10. *40.
T10
0
30. *40 +2. *40. +1.
T11
0
30. *40. +2 *40. +2.
T12
0
30 *40. +2 *40. +3.
T13
0
30. *40 +2 *40 +4.
T14
0
30 *40. +2 *40 +5.
T15
0
30 *40 +2 *40. +6.
T16
0
30. *40 +2 *40. +7.
T17
0
30. *40 +2. *40. +8.
T18
0
30. *40 +2. *40. +9.
T19
0
30. *40. +2. *40. +10.
T20
0
30. *40. +3. *40 +1.
T21
0
30. *40. +3. *40. +2.
T22
0
30. *40. +3. *40. +3.
```

```
29 *40. +26. *32.
25. *40. +19. *40. +22.
CSCON
25. *40 +24. *32
13 *40 +29 *40. +13.
TOTFR
16 *40 +28. *32.
30 *40. +25. *40 +30.
C4MFI
16. *40 +19. *32.
13. *40 +5 *40 +23.
C4MFO
16 *40 +25 *32
13 *40 +5 *40. +23
C3MFI
16 *40. +19 *32.
13 *40 +4 *40 +23.
C3MFO
16 *40 +25, *32.
13. *40 +4 *40 +23.
C2MFI
16 *40 +19 *32.
13. *40 +3. *40. +23
C2MFO
16 *40 +25 *32.
13. *40 +3 *40. +23.
C1MFI
16. *40 +19. *32.
13. *40 +2 *40 +23.
C1MFO
16. *40 +25. *32.
13 *40. +2 *40 +23.
H2MFI
16 *40 +19 *32
18 *40 +3. *40. +23.
H2MFO
16 *40 +25, *32.
18 *40 +3 *40 +23
SELC3
13 *40 +4. *32.
29 *40 +15 *40 +22.
SELC2
13 *40. +3. *32.
29 *40. +15. *40 +22.
SELC1.
13 *40. +2 *32.
29. *40. +15 *40. +22
CONV
32 *40 +0 *32.
13. *40. +25. *40. +24.
C3FRI
28. *40. +19. *32.
13. *40. +4. *40. +16.
C2FRI
28 *40 +19 *32.
13. *40. +3. *40. +16
C1FRI
28 *40. +19. *32.
13. *40. +2. *40. +16.
```

```
H2FRO
28. *40. +25. *32.
18. *40. +3 *40 +16.
C4FRO
28 *40. +25. *32.
13 *40 +5 *40. +16
C3FRO
28 *40 +25. *32.
13 *40 +4 *40 +16
C2FRO
28 *40 +25 *32
13 *40 +3 *40 +16
C1FRO
28 *40. +25 *32
13 *40 +2 *40 +16.
SETUP
31. *40 +26. *32
29 *40 +15 *40 +30
QENCH
13 *40 +18 *32
27 *40 +15 *40 +24.
PANIC
19 *40 +13 *32
26 *40 +11 *40 +24.
TF1
0
30 *40 +16 *40 +2
TF2
0
30 *40 +16 *40 +3
TF3
0
30 *40 +16 *40. +4.
TF4
0
30. *40 +16 *40 +5.
TF5
0
30. *40 +16. *40. +6.
TF6
0
30 *40 +16. *40 +7.
TF7
0
30 *40 +16. *40. +8.
TF8
0
30 *40 +16 *40. +9
TF9
0
30. *40. +16 *40 +10.
TF10
1 *40. +0 *32
30. *40. +16 *40 +2.
TF11
2 *40. +0. *32
30. *40 +16 *40 +2.
TF12
3. *40. +0. *32.
30 *40. +16. *40. +2.
```

```
4 *40. +0. *32.
30 *40. +16 *40. +2.
TF14
5. *40 +0. *32.
30 *40 +16 *40 +2.
TF15
6 *40 +0. *32.
30 *40 +16 *40. +2
TF16
7 *40 +0 *32
30 *40 +16 *40 +2
TF17
8 *40 +0 *32
30 *40 +16 *40. +2
TF18
9 *40 +0 *32.
30 *40 +16 *40. +2.
TF19
10 *40. +0 *32.
30. *40 +16. *40. +2
TF20
1 *40 +0. *32
30. *40 +16 *40. +3.
TF21
2 *40 +0 *32
30. *40 +16 *40. +3.
TF22
3 *40 +0 *32.
30 *40 +16. *40 +3.
ALPHA
18. *40 +11 *32
11 *40 +22 *40 +26.
BT1
0
12 *40 +30 *40. +2.
BT2
0
12 *40 +30 *40. +3
BT3
0
12 *40 +30 *40 +4
BT4
0
12 *40 +30. *40. +5.
BT5
0
12 *40 +30 *40. +6.
BT6
0
12 *40. +30 *40. +7.
BT7
0.
12. *40 +30. *40. +8.
BT8
0
12 *40 +30 *40. +9.
BT9
0
12 *40 +30. *40 +10.
```

```
BT10
1. *40. +0. *32.
12. *40 +30 *40. +2.
BT11
2 *40. +0 *32.
12 *40 +30 *40 +2
BT12
3 *40. +0 *32
12 *40 +30 *40 +2.
BT13
4 *40 +0 *32
12 *40 +30 *40 +2
BT14
5 *40 +0 *32
12 *40 +30 *40 +2
BT15
6 *40. +0 *32
12 *40 +30. *40 +2.
BT16
7 *40 +0 *32
12 *40 +30 *40 +2.
BT17
8 *40 +0 *32.
12 *40 +30 *40 +2
BT18
9 *40 +0 *32
12 *40 +30 *40 +2
BT19
10 *40 +0 *32
12 *40 +30. *40. +2.
BT20
1 *40 +0 *32
12 *40 +30 *40. +3
BT21
2 *40 +0 *32
12 *40 +30. *40 +3
BT22
3 *40 +0 *32
12 *40 +30 *40 +3.
TF5                 ,EQUIVALENCE FOR TR1
0
30 *40 +28 *40 +2
TF16                ,EQUIVALENCE FOR TR2
0
30 *40 +28 *40 +3
TF13                ,EQUIVALENCE FOR TR3
0
30. *40 +28. *40 +4
TF7                 ,EQUIVALENCE FOR TR4
0
30. *40 +28 *40. +5.
TF9                 ,EQUIVALENCE FOR TR5
0
30. *40 +28 *40 +6.
TF12                ,EQUIVALENCE FOR TR6
0
30. *40 +28. *40 +7
TF18                ,EQUIVALENCE FOR TR7
0
30 *40 +28 *40. +8.
```

```
          0
          30. *40. +28. *40. +9.
          TF6                 ;EQUIVALENCE FOR TR9
          0
          30 *40 +28 *40 +10.
          TF10                ;EQUIVALENCE FOR TR10
          1 *40 +0. *32.
          30 *40 +28 *40 +2.
          TF19                ;EQUIVALENCE FOR TR11
          2 *40 +0. *32
          30 *40 +28 *40 +2
          TF4                 ;EQUIVALENCE FOR TOIL1
          22 *40 +2 *32
          30 *40 +25 *40 +19.
          TF21                ;EQUIVALENCE FOR TOIL2
          22 *40 +3 *32
          30. *40 +25 *40 +19.
          CLBC3
          13 *40. +4 *32
          13 *40 +22 *40 +12
          CLBC4
          13 *40 +5. *32.
          13. *40 +22 *40 +12.
          CLBC1
          13 *40 +2 *32.
          13 *40. +22 *40 +12
          CLBC2
          13 *40 +3. *32.
          13. *40 +22 *40 +12.

           EOT                ;END OF SYMBL TAPE # 2 OF 3

;SYMBL TAPE # 3 OF 3
;MRAC REACTOR CONTROL SYMBOLS

           EXTN MRAC

;WRITTEN AUGUST, 1976 BY
;       JEAN-PIERRE TREMBLAY
;       DEPARTMENT OF CHEMICAL ENGINEERING
;       MCMASTER UNIVERSITY
;       HAMILTON, ONTARIO, CANADA

;WRITTEN IN DGC'S NOVA-LINE ASSEMBLER LANGUAGE
;FORMATTED FOR USE WITH THE GOSEX EXECUTIVE

          MRAC
          13. *40 +0. *32.
          23 *40 +28 *40. +11.
          .GADD PUFO, FORGT
          17 *40 +30 *32.
          16 *40. +25 *40. +28.
          .GADD PUFO, PRDC3
          13 *40 +4. *32.
          26 *40 +28 *40. +14.
          .GADD PUFO, PRDC2
          13. *40. +3. *32.
          26. *40. +28. *40. +14.
          .GADD PUFO, SWTCH
```

```
13. *40. +18. *32.
29. *40 +33 *40. +30.
 GADD PUFO, C4LO
25 *40 +0. *32.
13 *40. +5. *40 +22.
 GADD PUFO, C4HI
19 *40 +0 *32
13 *40 +5. *40. +18.
 GADD PUFO, H2LO
25 *40. +0. *32.
18 *40 +3. *40. +22.
 GADD PUFO, H2HI
19 *40 +0. *32
18. *40 +3 *40 +18.
 GADD PUFO, DIAG
17 *40. +0. *32.
14. *40 +19 *40 +11.
 GADD PUFO, FUDGE
17 *40 +15 *32
16 *40. +31 *40. +14.
 GADD PUFO, NETA1
11 *40. +2. *32.
24 *40. +15 *40. +30.
 GADD PUFO, NETA2
11. *40. +3. *32.
24 *40 +15 *40 +30.
 GADD PUFO, NETA3
11 *40. +4. *32
24 *40 +15 *40 +30.
 GADD PUFO, NETA4
11 *40 +5. *32.
24 *40 +15 *40. +30
 GADD PUFO, NETA5
11 *40. +6. *32.
24 *40. +15. *40. +30
 GADD PUFO, NU1
0
24 *40 +31. *40. +2.
 GADD PUFO, NU2
0
24 *40 +31 *40. +3.
 GADD PUFO, TRIG
17 *40 +0. *32
30 *40. +28 *40 +19.

SST=    -1

UEST=   EST
USST=   SST

FORGT=  0
PRDC3=  2
PRDC2=  4.
SWTCH=  6.
C4LO=   7.
C4HI=   9.
H2LO=   11.
H2HI=   13.
DIAG=   15.
FUDGE=  16.
```

NETA1= 18.
NETA2= 20.
NETA3= 22.
NETA4= 24.
NETA5= 26
NU1= 28.
NU2= 30
TRIG= 32.

END

FIGURE C-9

INTERFACE TO GOSEX

```
          TITL INFCE

 INTERFACE TO THE GOSEX EXECUTIVE FOR REACTOR CONTROL

          ENT OVLAY, ALARM, DATUM, RELAY, SENSE, ANALG
          ENT SCAN, CLOOP, SUPRS, TASKS, UDEF
          ENT SETUP, QENCH, PANIC, JOBFG
          EXTN HLOOP, BLOOP, VISOR, TRAP, CSCON, ERROR
          EXTN UOVY1, UOVY2, UOVY3
          EXTN UEXC1, UEXC2, UEXC3
          EXTD TIMER

          TXTM 1

 DEFINITION OF ENTRY SYMBOLS
 OVLAY   ADDR OF BYTE POINTER TO OVERLAY FILENAME
 ALARM   ALARM TABLE
 DATUM   A/D DATA STORAGE TABLE
 RELAY   RELAY STATUS TABLE
 SENSE   CONTACT SENSE DISPATCH TABLE
 ANALG   D/A DATA STORAGE TABLE
 SCAN    FREQUENCY OF USER CLOCK
 CLOOP   CONTROLLER DEFINITION TABLE
 SUPRS   USER SHUTDOWN ROUTINE
 TASKS   USER TASKS DEFINITION TABLE
 UDEF.   USER DEFINED EXECUTIVE FUNCTION LIST EXTENSION
 SETUP   USER FUNCTION TO SET UP CONDITIONS FOR VISOR TASK
 QENCH   USER FUNCTION TO INITIATE QUENCHING OF THE REACTOR
 PANIC   USER FUNCTION TO KILL ALL REACTOR ACTIVITY WITHOUT
         AFFECTING MONITORING ACTIVITIES
 JOBFG   MRAC TASK KILL FLAG

 DEFINITION OF EXTERNAL SYMBOLS
 HLOOP   HYDROGEN FLOW CONTROLLER BLOCK
 BLOOP   BUTANE FLOW CONTROLLER BLOCK
 VISOR   S. A. OF THE SUPERVISORY PROGRAM
 TRAP.   ADDR OF THE CONTACT SENSE DISPATCH WORD
 CSCON   S. A. OF THE CONTACT SENSE CONTROLLER
 ERROR   GOSEX CALL TO THE ERROR HANDLER
 MRAC.   S A OF THE MRAC FORTRAN IV TASK
 UOVY1:  OVERLAY CODE OF USER FUNCTION SETUP
 UOVY2   OVERLAY CODE OF USER FUNCTION QENCH
 UOVY3.  OVERLAY CODE OF USER FUNCTION PANIC
 UEXC1:  S. A. OF USER FUNCTION SETUP
 UEXC2   S A OF USER FUNCTION QENCH
 UEXC3   S A. OF USER FUNCTION PANIC
 TIMER   GOSEX ENTRY SPECIFYING THE # OF RTC PULSES IN ONE SECOND

 WRITTEN AUGUST, 1976 BY
         JEAN-PIERRE TREMBLAY
```

```
;                OF
;       MCMASTER UNIVERSITY
;       HAMILTON, ONTARIO, CANADA
;
;WRITTEN IN DGC'S NOVA LINE ASSEMBLER LANGUAGE
;FORMATTED FOR USE WITH THE GOSEX EXECUTIVE

        NREL

OVLAY   +1*2            ;BYTE POINTER TO OVERLAY FILENAME
        TXT @REACTOR.OL@

ALARM   ALRMS           ;# ALARMS IN TABLE
        BLK ALRMS       ;ALARM TABLE

DATUM   BLK ATODS       ;A/D DATA STORAGE TABLE

RELAY   BLK RLAYS       ;RELAY STATUS TABLE

SENSE   TRAP            ;CONTACT SENSE DISPATCH TABLE
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP
        TRAP

ANALG   BLK DTOAS       ;D/A DATA STORAGE TABLE

SCAN:   10              ;FREQUENCY OF USER CLOCK

CLOOP   HLOOP           ;CONTROLLER DEFINITION TABLE
        HLOOP
        BLOOP
        BLOOP
        1B0             ;END OF TABLE INDICATION

SUPRS.  LDA 1 C4OFF     ;GET OFF LEVEL FOR BUTANE
        STA 1 ANALG+C4D2A       ;SET LEVEL
        LDA 1 H2OFF     ;GET OFF LEVEL FOR HYDROGEN
        STA 1 ANALG+H2D2A       ;SET LEVEL
        MOV 3 2
        LDA 1 TIMER:
         SYSTM          ;WAIT ONE SECOND
         DELAY
        ERROR
        LDA 0 PATOF     ;GET FINAL RELAY PATTERN
        DOA 0 25        ;SET.IT
        JMP 0 2         ;RETURN TO RETRN

TASKS:  VISOR           ;SUPERVISORY PROGRAM
        100
```

```
          1BO
           IFN FORT4
           -4              ;ASSEMBLER TASK
           ENDC

          CSCON            ;CONTACT SENSE CONTROLLER.
          100
          120
          TRAP
           IFN FORT4
           -4              ;ASSEMBLER TASK
           ENDC

           IFN FORT4
          EXTN MRAC
          MRAC             ;MRAC FORTRAN IV TASK
          360
          200
          JOBFG
          0
           ENDC

          1BO              ;END OF TABLE INDICATION

UDEF      3                ;EXECUTIVE FUNCTION LIST EXTENSION
          SETUP            ;FUNCTION TO SET UP CONDITIONS FOR VISOR TASK
          UOVY1
          UEXC1
          QENCH            ;FUNCTION TO QUENCH THE REACTOR
          UOVY2
          UEXC2
          PANIC            ;FUNCTION TO KILL ALL REACTOR ACTIVITY
          UOVY3
          UEXC3

C4OFF     ANORG/10.
H2OFF     ANORG*2/10
PATOF     040000           ;ALL BUT COOLING RELAY OFF
JOBFG     0

          END
```

TABLE C-1

Summary of MRAC Software

Routine Name	Type	Purpose
MRAC	CORE RESIDENT	Model Reference Adaptive Control Main Program
TIMIG	CORE RESIDENT	Controller Timing
OUTPT	CORE RESIDENT	Implementation of Control Action
JBFG	CORE RESIDENT	Task Kill Flag Check
MRAC1	OVERLAY	Controller Initialization
COLOC	OVERLAY	Collocation Temperature Calculation
TFITS	OVERLAY	Least Squares for Quadratic Polynomial
MRAC2	OVERLAY	Control Algorithm
RECUR	OVERLAY	Measurement Equation Update
RLS	OVERLAY	Recursive Least Squares

Due to the limited core storage of the NOVA 2/10 minicomputer, the RDOS overlay facility was used extensively in the implementation of the model reference adaptive control algorithm. All the software was written in real-time FORTRAN IV. For simplicity, FORTRAN IV parameters to be accessed by GOSEX at run-time were kept in labelled common and blank common storage was used to preserve all constant and variable data needed by all calculations. Temporary storage was provided by the run-time stack.

The start executive function was used to create task MRAC at run-time. This task sequences through an initialization and synchronization procedure before actual control calculations begin. This is performed by subroutine MRAC1 which first reads the data file "MRACFEED.JP" to initialize scalars, vectors and matrices needed by the adaptive controller calculations. Current reactor operating conditions are then used to generate estimates of the reactor states. To ensure that the cycles of the adaptive controller and process gas chromatograph are synchronized, task MRAC pauses until the current chromatograph cycle is completed. Once synchronization occurs, task MRAC enters a thirty second delay loop which repeatedly calculates a new control action. Task MRAC will abort if a fatal error or operator kill command occurs.

Task MRAC enters a thirty second cycle which begins by a call to overlayed subroutine COLOC and TFITS. The new temperature data are passed to overlayed subroutine MRAC2 which actually calculates the model

reference adaptive control action. This action is implemented by subroutine OUTPT. It restricts the flow rates to within adjustable limits. Because of the ever present danger of catalyst deactivation due to contamination by elemental carbon, the hydrogen to n-butane ratio of the feed is kept above 3.5. In addition, the order in which the flow controller setpoints are altered depends on the directions of change of the feed flow rates. To prevent the possibility of the hydrogen to n-butane ratio falling below 3.5 during transients which follow the setpoint changes, the changes are made two seconds apart. The MRAG2 subroutine is programmed to prevent reset windup of the controller's integral action term. Binary output to disk files, MRACOUT1.JP and MRACOUT3.JP is controlled by the "SWICH" parameter.

The interval timing of this controller is performed by subroutine TIMIG. Once every second for the duration of the delay between successive control calculations, the task kill flag is examined by the JBFG subroutine. Should it become set -- indicating a CEASE command from the operator -- task MRAC aborts, leaving the flow controller setpoints at safe levels. As well, the measurement equation (Equation 2-21) parameters are updated whenever the first element of the LYSIS vector becomes set. This event indicates the availability of new analytical data. Each row of the equation matrices are updated by a call to overlayed subroutine RECUR. Recursive least squares updates are performed by subroutine RLS (subroutines RECUR and RLS are loaded into the same overlay segment).

Binary output of analytical data to disk files MRACOUT2.JP and MRACOUT4.JP is controlled by the "SWTCH" parameter. The updating process may be bypassed by setting the "DIAG" parameter to zero. At the end of the thirty second interval -- which includes the time to compute and implement control action and perhaps also the time to update parameters -- the cycle is repeated. A summary of the software switch options is provided in Table C-2.

If at any time a run-time error is detected, an alarm is output to the console and the MRAC task aborts if the error is fatal. The flow controller setpoints are reset to safe levels when this occurs.

At the end of an experiment, a special translator must be used to read the binary output data files and to output their contents in ASCII format. Output must be to the high speed paper tape punch if the data are to be processed at the campus computing center facilities.

The model reference adaptive control software was written in a very general form allowing the adjustment of key parameters while on-line. These parameters included the propane extent setpoint, the proportional, integral and setpoint adaptive loop gains and a few software switches to control the output of results to data files. This programming technique permitted the use of the adaptive controller program in all experimental runs reported in Chapter 5. For example, the adaptive loop gains of Equation 2-38 may not be zero but the software has been structured to

disable a portion of the adaptive algorithm whenever an adaptive loop gain is set to zero.

TABLE C-2

MRAC Software Switch Options

Switch	Value	Effect
DIAG	0	No update of measurement equation matrices.
DIAG	≠0	Update measurement equation matrices.
SWTCH	0	No output to disk data files
SWTCH	1	Output reactor operating conditions to data file "MRACOUT1.JP" and analytical data to data file "MRACOUT2.JP".
SWTCH	2	As SWTCH=1 but output adaptive controller gain matrices to data file "MRACOUT3.JP".
SWTCH	3	As SWTCH=1 but output updated measurement equation matrices to data file "MRACOUT4.JP".
SWTCH	4	As SWTCH=1,2,3