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DYNAMIC SIMULATION OF AN EXTRACTIVE
DISTILLATION COLUMN

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DISTILLATION COLUMN

by

DAT TRUNG TRANG, B.A.Sc.

A Thesis

Submitted to the School of Graduate Studies
in Partial Fulfilment of the Requirements
for the Degree
Master of Engineering

McMaster University

MARCH 1976

MASTER OF ENGINEERING (1976)
(Chemical Engineering)

McMASTER UNIVERSITY
Hamilton, Ontario

TITLE: Dynamic Simulation of an Extractive Distillation
Column

AUTHOR: DAT TRUNG TRANG,
B.A.Sc., Ecole Polytechnique, Montreal, Quebec

SUPERVISOR: Dr. J.D. Wright

NUMBER OF PAGES: vii, 147

ABSTRACT

A mathematical model, based on heat transfer, mass transfer and fluid dynamics principles, has been developed to represent the dynamics of an extractive distillation column. The column simulation subroutine was incorporated into the recent DYNamic System Simulator executive package (DYNSYS 2.1), created at McMaster University, which uses Gear's method of integration.

Simulation runs were performed with step and pulse disturbances in the feed composition, feed flowrate and reflux ratio variables. Calculated results were compared with available experimental data obtained from a laboratory-scale (2 inch diameter), fifteen-stage extractive distillation column which used distilled water as the solvent to separate a binary mixture of acetone-methanol. Fairly good consistency was found within the normal operating conditions of the column.

A preliminary simulation study of the dynamics of the column (overhead composition transient behaviour) subject to controlled-cycling of the feed flowrate showed a substantial improvement in the separation efficiency of the column.

ACKNOWLEDGEMENTS

I would like to express my sincere gratitude to Dr. J.D. Wright, Dr. M.H.I. Baird and Dr. J.F. MacGregor for their guidance, encouragement and many discussions throughout this period of the project.

I would like to express my appreciation to my parents for their moral and financial support and also to the following individuals and organizations for their contributions:

Dr. T.W. Hoffman for the time spent discussing about the feed system.

Mr. J.P. Tremblay for his help associated with computer problems.

Mrs. Debbie McCreath for her careful and conscientious work in typing this dissertation.

McMaster University and the Chemical Engineering department for providing financial assistance.

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CHAPTER 1
INTRODUCTION

Because of economic pressure, any industrial company is forced towards greater efficiency and productivity. In many areas, processes can be improved resulting in a favourable return on investment. One area for potential improvement is in process control.

Advances have been slow in industry because of the lack of mathematical techniques to analyze complex control systems and also because of the costly, sometimes impossible, implementation of advanced control schemes.

With the introduction of digital computers into the chemical process industries, more efficient control strategies have been investigated by major chemical companies. However, the approach, if it is to be widely used, has to be simple and fundamental in nature for practical application.

1.1 Computer control of distillation columns

Distillation has been one of the particular processes which attracted the many industrial control designers as well as university research control groups. Distillation can be simply understood as the process of vaporizing then condensing a mixture of components. Precise control of distillation is difficult to achieve because:

(1) Factors affecting separation are not readily interpreted in terms of control system requirements.

(2) Distillation processes are known to interact, sometimes severely.

(3) Measurements used for control may be non-existent or difficult to incorporate into the control strategy.

(4) Distillation units are usually the last in a chain of unit operations, therefore subject to upstream upsets.

(5) Towers with many trays respond very slowly, thus conventional negative feedback control does not seem to be the most efficient solution.

Poor control of a distillation column reduces the throughput capacity, makes the recovery of product difficult and results in excessive utility consumption.

The following sections will present a very practical approach to distillation control resulting from the study of Bojnowski (6).

1.1.1 Relative gain concept

Distillation is a multivariable, highly interactive process. From the control standpoint, a multivariable process is known to have a number of input variables called manipulators such as reflux rate, steam rate or bottom rate, and a number of output variables called controlled variables such as distillate product composition, column pressure or bottom composition.

In such a complex process, in order to achieve low operating cost, good operability and high product quality, the question should be "what variables do I want to control?". The answer is not so evident, the reason is that the controllers interact. Therefore, when looking at a multivariable process, often the question is asked: "If I change a manipulator, what

essential will change in the system?". Obviously, the problem is to determine the best pairing of controlled and manipulated variables. The expert control engineer can often choose the right pairs by experience, but sometimes intuitive solutions can lead to dangerous consequences.

The technique of relative gain is commonly used to find the best pairing of variables. The approach bases the selection on a steady-state analysis which is probably the only drawback, since results must be checked against dynamic considerations. As said by Bojnowski (6), for most systems, the results are consistent with dynamic considerations.

The relative gain is defined as:

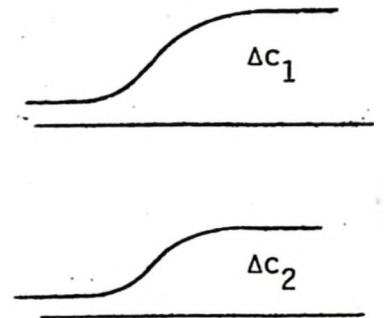
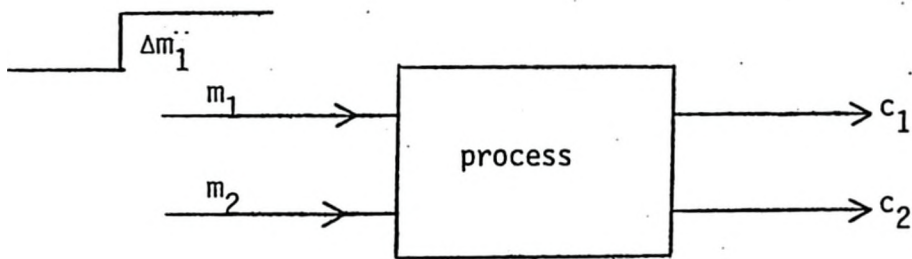
$$\lambda_{ij} = \frac{\partial c_i / \partial m_j |_m}{\partial c_i / \partial m_j |_c} = \frac{\text{open loop gain}}{\text{closed loop gain}} \quad (1.1)$$

Physical meaning for a system of 2×2 can be found on fig.1.1. A change is forced in m_j by keeping all other m 's constant, then the change in c_i is measured. This is the open-loop gain. The same change is applied to m_j , but all the c 's, except c_i , are kept constant by closed-loop control; the change in c_i is observed then the closed-loop gain results.

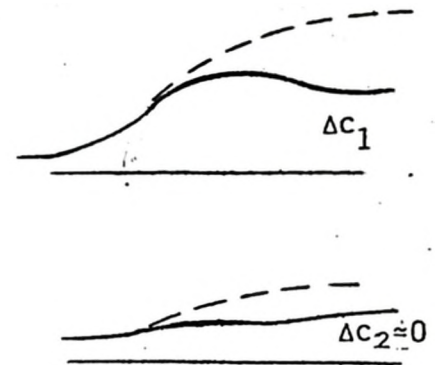
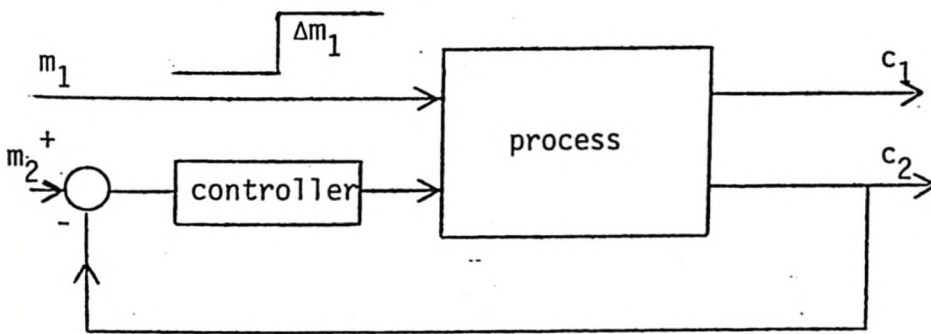
Therefore, for a multivariable process, the relative gain matrix can be obtained:

$$\begin{array}{c} c_1 \\ c_2 \\ c_j \end{array} \begin{bmatrix} m_1 & m_2 & m_j \\ \lambda_{11} & \lambda_{12} & \\ \lambda_{21} & \lambda_{22} & \\ & & \lambda_{ij} \end{bmatrix} \quad (1.2)$$

Fig. 1-1 PHYSICAL MEANING OF THE RELATIVE GAIN
IN THE MULTIVARIATE PROCESS



$$\left. \frac{\partial c_1}{\partial m_1} \right|_{m_2} = \left. \frac{\Delta c_1}{\Delta m_1} \right|_{m_2} = \text{open loop gain}$$



$$\left. \frac{\partial c_1}{\partial m_1} \right|_{c_2} = \left. \frac{\Delta c_1}{\Delta m_1} \right|_{c_2} = \text{closed loop gain}$$

One property of the matrix is that the algebraic sum of any row or column is one. One must note that when λ_{ij} is one, m_j controls c_i and no interaction exists.

One does not have to perform both open-loop and closed-loop experiments. Obtaining the open-loop gains is sufficient since matrix manipulation will give the whole relative gain matrix. Techniques and examples are described in reference 6.

Applications can be based on the following rules:

(1) The pairs with the largest positive numbers should be selected for closed-loop control.

(2) Relative gain values approaching 0.5 indicate strong mutual coupling and will be extremely difficult to control.

(3) Negative numbers indicate a divergent control system, and if these pairs are chosen, control is impossible.

(4) One operating condition for which the c-m pairs were chosen may not be valid for another operating condition.

1.1.2 Factors affecting distillation performance

The control strategy should keep a column functioning as designed, despite various upsets. Two very important facts must be retained for control design objectives:

(1) the composition of the distillate and bottoms streams are intimately affected by the product flowrates. If 100 lbs. of a component is fed to a column, 100 lbs. must be withdrawn. If the 100 lbs. is not withdrawn in the correct amount in each product stream, the desired composition cannot

be obtained even though the column is capable of making the separation. This is called the material balance problem.

(2) Energy is required for separation. If there is not enough energy available to carry out a separation, even though the material flows are correct, the desired compositions will not be obtained. This is known as the separation problem.

Usually, control of the material balance is done with flow variables, and control of separation is achieved with reflux rate variable or feed point location. Unfortunately, in most cases, these two control loops severely interact. The problem is then to decouple the interaction by choosing the right pairs of controlled and manipulated variables.

Applying the relative gain technique and checking the performance on many industrial columns, Bojnowski mentioned many general rules for control of distillation:

(1) When only one product quality is to be controlled closely, the material balance must be manipulated.

(2) The lesser of two product streams should be manipulated to control product quality.

(3) The material balance should be manipulated to control the quality of the less pure product, and the separation should be manipulated to control the quality of the more pure product.

(4) The pressure must be tightly controlled for two reasons. If the pressure is increased, the liquid on the trays and in the reboiler is below its boiling point; the vapor is condensed to heat the liquid to its

boiling point; once at its boiling point, the vapor rate snaps back causing an increase in pressure. This causes column instability. Furthermore, if the column pressure is not held constant, measurements for control purposes are invalid. Suggested control schemes are described in reference 6.

1.1.3 Special features for extractive distillation control

In extractive distillation, the solvent is fed near the top of the column and entrains one or more heavy components on the way down the column. Light components concentrate up and are removed near the top. Heavy components and the solvent are withdrawn at the base and sent to a recovery column to recover the solvent which is recycled back to the extractive column.

When dealing with extractive distillation, one must take into account the following facts:

(1) Since the solvent is an extractant, the correct ratio between feed and solvent must be maintained. Insufficient solvent will cause poor separation while excessive solvent will result in the dilution of light components.

(2) Reflux greatly influences the separation. With higher reflux, better separation occurs, but excessive reflux dilutes the solvent thus causing poor separation. Thus a designer must try to control the solvent concentration at the solvent addition tray.

(3) Usually, extractive distillation is most sensitive to the solvent composition and temperature. Since the heat content of the solvent is a large percentage of total heat requirements, control of solvent temperature

is critical.

1.1.4 Conclusion

In summary, many methods of control other than feedback control have been used in distillation processes with certain special features. One example which can be mentioned is that of ultra high reflux and high reflux ratio separations; because of the extremely long response times, bang-bang control is the recommended control strategy since it is inexpensive, it gives extremely tight control, it gives fast responses to disturbances, it eliminates non-linearity problems such as sticking control valves and it eliminates tuning problems.

Feedforward control is usually applicable where:

- (1) one column is noticeably limiting the capacity of the entire unit.
- (2) a small improvement in recovery efficiency on a large refining column can mean substantial additional production.
- (3) feed rate and composition changes upset a column early in a distillation train and cause problems in the rest of the operation.
- (4) safety considerations demand that compositions stay within certain limits.

A fairly detailed presentation of different control schemes along with discussions can be found in reference 6.

1.2 Project objectives

In general terms, the present project is actually based on a fifteen stage column with thirteen trays and condenser and reboiler systems. Two feed streams enter the column: water, used as an extractant, enters near the top of the column, and a mixture of acetone-methanol is fed near the bottom. Simple binary distillation to separate acetone from methanol is not possible since the mixture forms an azeotrope of .8 mole fraction acetone at atmospheric pressure. As mentioned by D.O'Neill (10), at approximately 0.3 mole fraction water, the azeotrope is completely broken.

1.2.1 Long term objective on the equipment

A complete extractive distillation process must include two columns in series. The first one, usually called the extractive column, extracts the light component, in this case acetone. The second one, often called solvent recovery column, recovers the solvent which is recycled back to the extractive column.

The long term objectives will consist of building the second column, and studying some advanced control configurations on the complete process and checking the performance of each control scheme.

However, before doing any investigation of this kind on such a complex process, one must do more specific work to obtain the minimum requirements, e.g. to find out suitable models at different levels of sophistication, to achieve some simple control of input stream variables such as temperature or flowrate, and to understand the dynamic behavior of the process.

1.2.2 Summary of previous work

Jackson (11) undertook the initial step of this project. His work consisted of building the fifteen stage extractive column, evaluating its steady-state performance, interfacing basic column instrumentation to the mini-computer and developing a basic real time software package mainly for data logging and input stream temperature control. The software was made using the original version of the Real Time Operating System. Major operating problems occurred, due to tray priming at the solvent recovery section and tray weeping near to the bottom of the column.

D.O'Neill (10) rebuilt the column completely and evaluated its operating range as well as its steady-state performance. A steady-state simulation was also developed to better understand the process. A preliminary study on the dynamic behavior was made by disturbing input variables, such as feed composition and feed rate, by conventional step change and pulse change. Transient responses of overhead and bottom compositions were analyzed and satisfactorily fitted by first order transfer models with dead time.

1.2.3 Present objectives

The agreed long term objective was to investigate different control strategies to obtain the best separation performance. Digital computers become more and more an important tool for process designers. Industrial practice tends to use digital simulation to estimate roughly the performance of operations, rather than carrying out experiments on pilot plants. This,

results in substantial time and research cost savings. Therefore, before investigating experimentally a control strategy, it is always economic to obtain a rough result by simulating this strategy on a computer. Obviously, the next step will be to develop a suitable mathematical model which can dynamically represent the extractive column since one needs process models to do any simulation work.

As far as the dynamic study is concerned, input disturbances must be achieved manually. With this technique, the study of oscillatory disturbances or random disturbances is difficult. Therefore, one of the main experimental steps will be to connect control valves into the two feed-streams. Consequently, input flowrates can be controlled automatically by the computer, or can be disturbed, as programmed, by the computer.

A summary of the present objectives is:

- (1) To develop a dynamic model representing the extractive distillation column
- (2) To compare calculated step and pulse responses with available experimental data
- (3) To perform a rough study with oscillatory disturbances, given the flexibility offered by the installation of the control valves.

CHAPTER 2

PROCESS EQUIPMENT AND FACILITIES

As briefly mentioned in chapter 1, section 1.2, the column was totally rebuilt by D.O'Neill with the aim of eliminating liquid priming in the solvent recovery section, due to tray weeping and also due to technical problems caused by the vibrostaltic feed pumps during the operation.

The present chapter will give a brief description of the process equipment followed by the specific modifications made to improve the flexibility of the column for the dynamic study. Control software alterations will also be described as well as the specific possibilities of the modified process arrangement.

2.1 Previous apparatus

The complete details of the apparatus could be found in reference 10 chapter 4. A general description of the experimental equipment will be presented in this section.

2.1.1 Description

Fig. 2.1 shows the arrangement of the extractive distillation process (10) before the modifications.

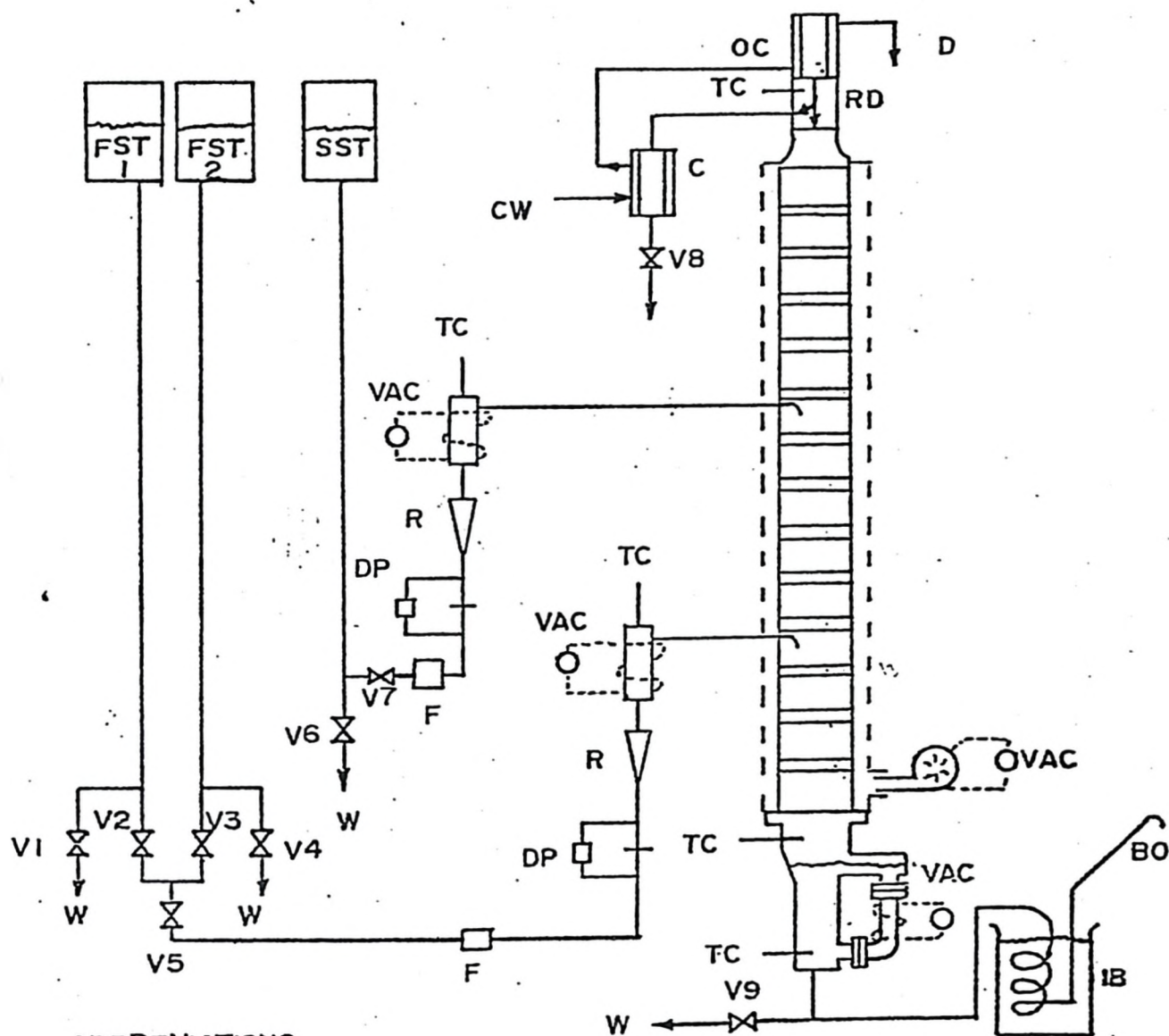
Two storage tanks of 10 liters each, made of glass and located on the second floor of the chemical engineering laboratory, were used to supply

the feed, at two different proportions of acetone-methanol, to the column through 0.63 cm O.D. stainless steel tubing. A system of on/off valves (V1, V2, V3, V4) allowed the sampling of the feed stream and the switching from one storage tank to the other. The tanks were in contact with the ambient atmosphere, therefore the feed just flowed down by gravity. A needle valve (V5) was used to adjust the flowrate manually. A filter prevented the penetration of foreign material to the glass orifice which was used in conjunction with a Dynascience Corporation differential pressure cell to measure the flowrate; the small signal from the DP cell was sent to a Dynascience Corporation Carrier-Demodulator which converted it into a 0-10 volts DC signal used for control purposes. A $F \propto P$ precision flowrator indicated the current flowrate. Before entering the column, the feed was electrically heated by a preheater made from a 30.5 cm \times 1.27 cm O.D. tube wound with resistance wire. A thermocouple measured the outlet temperature from the preheater for control purposes, and a powerstat transformer could be used to vary the power input to the preheater. The feed line was connected to tray 11 from the top.

The same arrangement was used for the solvent stream, except that only one 10 liter storage tank was present. The tubing from the tank to the preheater input was in Tygon.

The column was made of thirteen sieve plates, a condenser system and a reboiler system. The sieve plates were separated by 15.25 cm \times 5.08 cm I.D. Q.V.F. glass pipes. The weir limited the holdup of liquid on a tray; the overflow flowed down the downcomer to the tray below. Each sieve plate

fig. 2.1 FLOW DIAGRAM -
EXTRACTIVE DISTILLATION COLUMN



ABBREVIATIONS

BO	bottom overflow	OC	overhead condenser
C	cooler	R	rotameter
CW	cooling water	RD	reflux divider
D	drain	SST	solvent storage tank
DP	differential pressure	TC	thermocouple
F	filter	V	valve
FST	feed storage tank	VAC	variable AC power
IB	ice bath	W	waste

was 0.16 cm thick and had 93 holes of 0.89 cm diameter; a feed port, vapor sampler, a thermocouple port and a liquid sampler were provided. A hot jacket surrounding the column to prevent heat loss to the ambient atmosphere was made from two sections of 13.34 cm I.D. perspex plastic pipe. A hot air gun blew the heated air upward in the jacket.

A stainless steel reboiler of 327 ml capacity was used with an overflow arrangement as shown in fig. 2.1; the liquid flowed by gravity or column pressure through the ice bath and went out by the tube exit which was maintained at a certain height that one can adjust to obtain the desired reboiler liquid level. The holdup of liquid from the output of the reboiler to the tube exit was 25 ml.

The condenser was equipped with a water-cooled system and a reflux divider electrically activated by a timing device made by Eagle Signal Corporation.

A more detailed description could be found in the work of Jackson (11) and of O'Neill (10).

2.1.2 Problems in operation and restrictions on dynamic study

The above equipment presented some problems encountered at different stages of the operation.

(1) Before doing any dynamic investigation on the process, one must bring the column to a steady-state level. From that point, perturbations can be put into the desired input variables. A practical question would be "when is the column at steady-state?"

Until the present investigation, temperature readings at the stages and overhead flowrate measurements were used to determine experimentally whether the column is at steady state or not. Very often, when the samples were analyzed later on, it was found that a trend still existed as far as the composition is concerned, showing lack of steady-state reaching. If one wants to study the dynamic of the column due to a certain kind of input disturbance, this fact becomes crucial, since the response depends intimately upon the trend existing at the initial time of perturbation.

(2) It was noticed that during a run, it could happen that the air gun which blows heated air through the jacket, stopped for a significant period of time. This will undoubtedly cause an upset in the negligible heat loss assumption made in the simulation work.

Since each run usually requires at least 10 hours, the presence of electrical devices is very undesirable in the sense that the whole time for the experiment could be wasted if an electrical problem occurs at the last period of the planned run. The feed stream preheater, solvent stream preheater and reboiler heater are locations where electrical devices have been used.

(3) The needle valves on the feed and solvent streams were used to adjust the flowrates to the desired values. When a flowrate, as measured by the DP cell, exceeded the tolerance limits, the computer sent a signal to the process site and the adjustment had to be carried out manually by checking the readings on the flowrators.

This technique of manual control is very inaccurate. From the dynamic point of view, since the operating range for the flowrates are small,

the possible perturbation amplitude is relatively small, therefore, this technique of controlling or varying the flowrate would not be recommended.

(4) Furthermore, oscillatory disturbances like sine wave, square wave or random disturbance, cannot be used as long as the computer is not arranged to do such perturbation. This is due to the inaccuracy of the manual adjustment and lack of time available for it since one must take samples quite often during a dynamic run.

Given the problems pointed out in the last two parts, some modifications were made in order to assist the investigator in obtaining better results as well as to give more versatility to the experimental dynamic work. The two next sections will present modifications on the equipment and on the computer control software.

2.2 Modifications to apparatus

2.2.1 Feed and solvent system

The needle valves V5 on the feed line and V7 on the solvent line were replaced by two control valves, 1/4 in. stainless steel body, trim 0, air to open type with neoprene diaphragm, manufactured by Badger Meter Inc. Fisher electro-pneumatic transducers, type 546, were used to receive a 1-9 VDC input signal from the D/A converter and to convert it into a pressure from 3-15 psi on the control valve diaphragm. An air line at 25 psig supplied the input to the transducers.

One problem occurred when replacing the needle valves by the control valves. The liquid coming from the storage tanks located about 15

feet above, flowed down just by gravity, and it was found that there was not enough head to push the liquid through the control valve orifice at the required rate even if it was fully opened. Two solutions were possible:

(1) One could design an electrical pump, and without altering the storage system, introduce it before the control valve location.

(2) One could replace the glass storage tanks by pressurized tanks and apply a pressure to create additional head on the liquid.

After considering the difficulties encountered while using electrical devices and the economic point of view, the second alternative was chosen.

2.2.2 Storage tank system

Three stainless steel storage tanks were purchased from AC Tanks Co. two for the feed line and one for the solvent line. They could handle a maximum pressure of 200 psi and had a maximum capacity of about 25 liters. A nitrogen cylinder was used to exert the necessary pressure. The hardware connections are presented on fig. 2.2.

Such an arrangement implies that the pressure should be the same in the three tanks. Calibration curves for the feed line and the solvent line are presented in Appendix A. A safety valve (SV) was used for safety purposes and for clearing the pressure at the end of each run.

However, some operational difficulties occurred:

(1) One has to set the gas cylinder valve at the pressure where the calibration was obtained, before each run, which is very difficult with the accuracy given by the actual pressure gauge; therefore calibration

must be checked at every run.

(2) Filling the tanks requires a very substantial amount of time and caution since the mixture acetone-methanol is inflammable and usually a large amount of feed material is used. The feeding should be made from the top hole of the tanks. One must be extremely careful in estimating the quantity of material needed for the run since the tanks can be fed only before the run and not during the run.

The next section will present the modifications made to the computer program developed to assist the experimenter when operating the column.

2.3 Software facilities

2.3.1 Previous control package

D. Jackson (11) has developed a computer program to aid in the manual operation of the column. The software was created within a Real Time Operating System (RTOS) provided by the computer manufacturer. Computer-process interfacing allowed the function of input-output hardware devices according to a criterion which minimized the average time devices must wait for servicing.

Many tasks were created to initiate or terminate the operation, to perform parameter changes, to measure and display process temperatures, and input stream flowrates, to control the input stream temperatures according to an on/off scheme and to create a signal at the process site for manual correction of the input stream flowrates to desired values.

The tasks were scheduled for execution by the operating system depending on their respective priority and the availability of the peripheral devices for input-output tasks.

Complete details of the software package as well as listings of programs and algorithms can be found in the work of D. Jackson (11). Since the software has to be entirely modified, no further description of the previous package is given in this work.

2.3.2 Modifications and new facilities

The actual computer system in the Chemical Engineering department is operating under the Real time Disk Operating System (RDOS) supplied by the computer manufacturer. References 23, 24, 25 are useful to understand how to use commands. All tasks developed to assist the operation of the column have been changed to be used with the Generalized Operating System Executive created by P. Tremblay (22). This executive offers a large number of facilities as well as a lot of flexibility for control purpose programs. Reference (22) must be regarded as the most important source of information on the actual control package for the distillation column.

Several programs were created:

(1) The program INFCE interfaces the user program which consists of a number of independent tasks, to the GOSEX.

(2) Tasks FEETC and SOLTC perform the control of the input feed and solvent temperatures by turning on or off the preheaters, and also

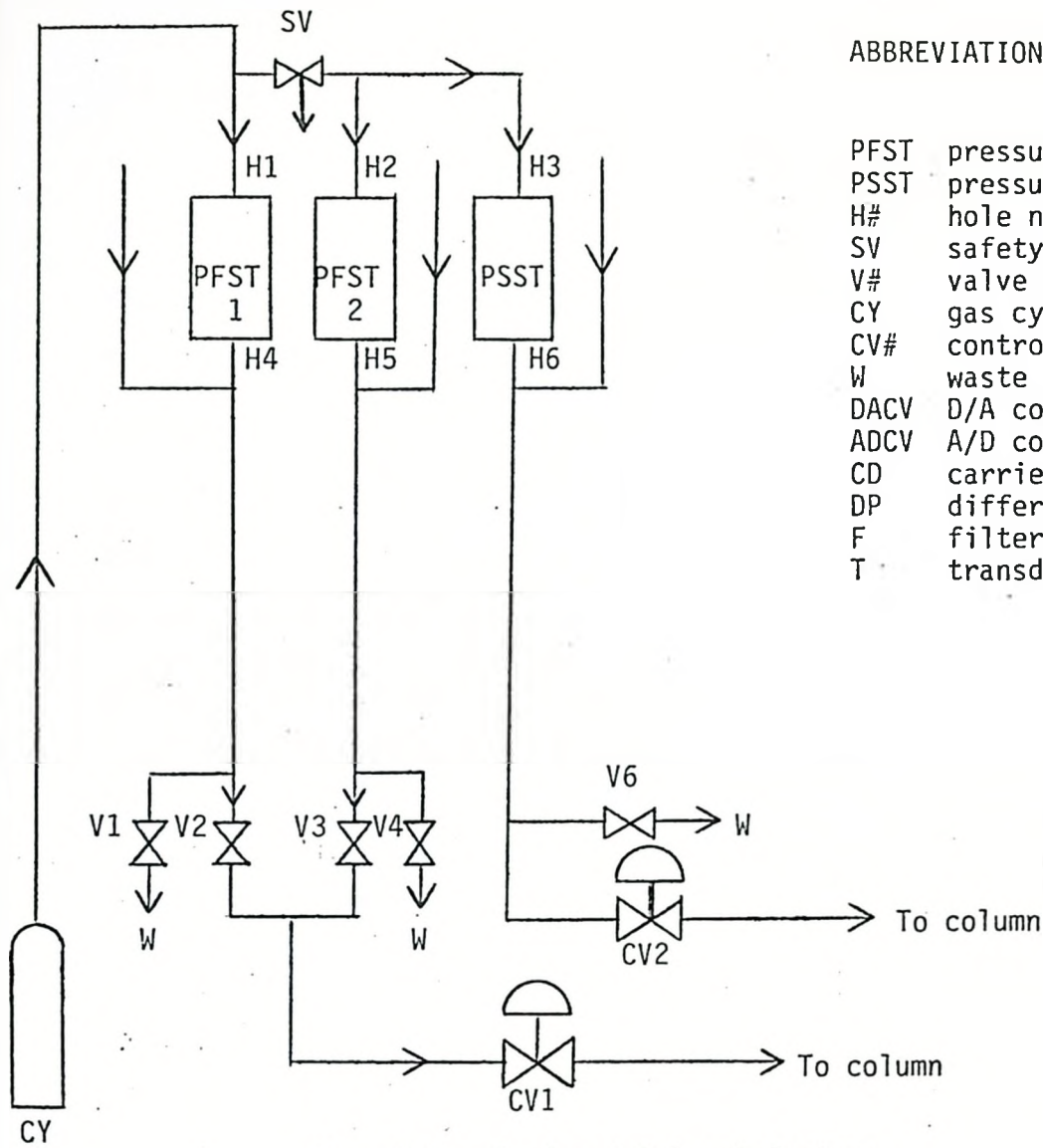
measure up to five temperature locations, convert into engineering units for displaying. There are many possible modes of display. The user should refer to reference (22) to be able to issue correct commands for these display modes.

(3) The introduction of the two control valves in the feed and solvent lines required additional software to actuate the valves via the computer. Two tasks were created, FEEFM and SOLFM, to calculate the control action to the valve based on the flowrate reading from the D.P. cell and based on a PID control algorithm performed by the GOSEX utility routine CONTL. Instructions for using this routine could be found in detail in ref. 22. FEEFM and SOLFM also convert the raw data, i.e. the stream flowrate, and the control action which is the percentage-opening of the valve, into engineering units for display. The simple control loop for the two flowrates on the feed and solvent lines is presented on fig. 2.3.

(4) Task SSAMP was used to acknowledge at the computer site any change occurring at the process site by using the contact senses, for instance the taking of a sample by the operator.

(5) A program to input a square wave to the feed rate variable was also developed. Task FEEFT shifts the feed flowrate set point from a high level (FHL) to a low level (FLL) according to a half period determined by TWAIT. These parameters could be changed on-line by using the GOSEX function PARAM. (see ref. 22)

Algorithms and listings of the programs as well as the loading procedure are presented in Appendix G.



ABBREVIATIONS

- PFST pressurized feed storage tank
- PSST pressurized solvent storage tank
- H# hole number #
- SV safety valve
- V# valve number #
- CY gas cylinder
- CV# control valve number #
- W waste
- DACV D/A converter
- ADCV A/D converter
- CD carrier-demodulator
- DP differential pressure cell
- F filter
- T transducer

fig. 2.2 Feed and Solvent Systems

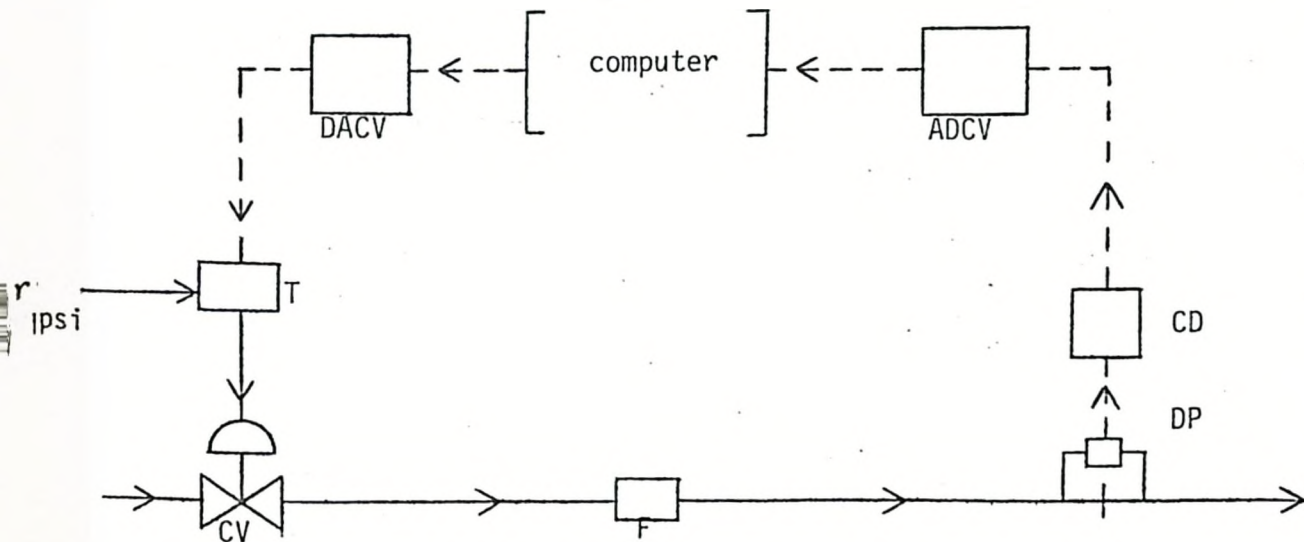


fig. 2.3 Elementary Flowrate Control Loop

2.4 Capabilities of modified apparatus and software

With the present apparatus, the study of the dynamics of the extractive distillation column could be extended to the introduction of oscillatory disturbances such as square wave and sine wave in the feed flowrate variable. The solvent flowrate variable could be investigated in the same way. A good variable to be studied will be the ratio of the feed to the solvent. Random disturbances, whether at two levels or according to a statistical distribution, could also be input into the input stream flowrates. With some modifications on the software, these disturbances could be realized under open-loop or under closed-loop control.

CHAPTER 3

DYNAMIC SIMULATION

As discussed in chapter 1, simulation on a digital computer has become and has been proven to be an efficient and economic tool in the design work of an engineer. Steady state simulation has been used intensively in university research as well as in industrial engineering work, especially to design new equipment, to conceive or improve processes, or to optimize the operating conditions for a better product quality at a minimum cost.

Dynamic simulation finds its importance, for example, in the study of optimal start-up of a process, in the investigation of the effects and the policy to be followed in the case of an equipment failure, and recently, especially in the transient study of process equipment and the design of different control strategies.

Before doing any simulation work, the first step must be to represent the real chemical equipment or process by an adequate mathematical relation. The cost of such model development will obviously increase with the degree of accuracy of the mathematical model; therefore such investment must be related to the objective of the simulation work.

3.1 Literature review on dynamic simulation of distillation

The literature contains many references to the study of the transient behavior of the distillation column which represents a complex and non-linear

chemical process.

Marshall and Pigford (7) presented a tentative modelling approach for packed columns. The continuity equation was applied to a differential unit length of the bed to yield differential material balance equations. A linear equilibrium relationship, constant molal holdup per unit length and constant molal overflow were the main assumptions.

Montroll and Newell (8) investigated the exact solution of a set of non-linear differential material balance equations for multistage separation of binary mixtures. On an IBM 701, Jackson and Pigford (9) tried to obtain a numerical solution for the differential material equations by approximating with finite difference equations. Total reflux, a relative volatility equilibrium relationship, a constant Murphree efficiency and a zero condenser hold-up were assumed. Also, the initial liquid compositions on the trays were considered as equal.

Huckaba and Danly (4) have done intensive studies on binary batch distillation which is basically a time dependent process. Besides the differential mass balance equations normally used by previous investigators, differential energy equations were introduced for the first time to take into account the inequality of the liquid flowrates between plates. The relaxation of the equality of flow assumption obviously contributed to a better representation of the real process.

Rosenbrock (5) developed mathematically a method of calculation of the unsteady state behavior of continuous distillation columns. The results for a step change in the feed composition were obtained for binary mixtures, based on total reflux assumption. Several non-linear equilibrium relationships

and a Murphree efficiency different from 100% were considered. Rosenbrock's calculated results were compared to the experimental data of Armstrong and Wilkinson (1), and it was found that the method was only acceptable for the initial transient period; fairly substantial divergences in the comparison appeared at later times. However, the use of a digital computer to handle complex and time-consuming calculation was found to be very promising.

An analytical exact solution to a step change in the feed composition was attempted by Voetter (12) using a linear equilibrium relationship. The introduction of the various simplifying assumptions was shown to yield up to 40 percent error in the results.

Acrivos (2) and Katz (3) have extended the dynamic study by introducing randomly fluctuating input conditions in a linear stagewise system with binary mixtures.

Franke (13) has modeled in detail the behaviour of a continuous experimental distillation column using a binary mixture, with a step change in the input feed composition.

The simulation of distillation with more than two components requires a much more powerful method to handle a large number of equations within a reasonable computer time. A typical problem could involve more than 50 components and columns with more than 100 stages.

A new technique of handling differential equations was used in the present study, with a ternary system and a fifteen stage column. Also, a new approach of using the energy balance equations to adjust the liquid and

vapor flowrates was investigated.

3.2 General features of the executive package DYN SYS 2.1

In chemical engineering, stiff systems of ordinary differential equations describing the process occur widely in reaction kinetics and in multistage processes. Stiff systems are defined as systems where the time constants differ greatly in magnitude. To be able to study the transient behaviour of such a system, the integration time step size is limited by the smallest time constant. Therefore the prediction of the entire dynamic response of such a system requires a large computer time and cost if conventional numerical techniques are used. An interesting investigation of different existing techniques was presented by Barney (14).

In the past few years, several executive packages have been developed especially for chemical engineers. These are more problem-oriented and use variations of what is known as the modular approach.

In 1970, Brobow, Johnson and Ponton have developed at McMaster University an executive package known as DYNamic SYStems Simulator, using a third order Adams-Moulton-Shell routine to integrate ordinary differential equations. This method proved to be insufficient to handle stiff systems. The integration technique was revised by Barney in 1974 and finally Gear's integration algorithm in conjunction with Key's technique of solving linear algebraic equations was implemented into the new version called DYN SYS 2.1. An option for stiff systems with a tridiagonal Jacobian matrix is also included since this case generally occurs when one deals with counter current stagewise processes.

The principal features of the executive DYNYSYS 2.1 used in this project will be outlined in the following sections.

3.2.1 Modularity

A chemical plant is usually made up of processing equipment such as reactors, columns, heat exchangers, etc., with control devices such as analyzers, control valves, etc., connected by material flows and control or measuring signals.

Each equipment item or device can be represented by a mathematical equation or set of equations which form a unit computation or computation module. Then a mathematical model of a plant can be seen as a network of modules in which information will flow in a manner analogous to the material flow or control signals in the real plant. Therefore, the dynamic information flow diagram is very similar to the process flow diagram.

This simulation approach, known as the modular approach, is very convenient and flexible when one wants to study the combinations or configurations of physical equipment or to design control strategies on a digital computer. It is not as efficient computationally as the equation-oriented approach since it involves more information transfer, but it helps the user to visualize his process, and especially it presents a great flexibility and an easy adaptability to different control and operational policies.

As a library of equipment and control modules gradually becomes available, the programming effort for new plant studies is reduced. However, the routines should be made general enough for further use. Another feature

is that real variables are used in the modular approach, rather than transformed variables. The modules may be quite non-linear in behavior.

A detailed presentation of the concept can be found in reference 14.

3.2.2 Gear's method of integration

One of the most important features in a dynamic simulation executive is the numerical technique of integration. DYNYSYS 2.1 adopted the method developed by C.W. Gear in 1971 to solve ordinary differential equations.

The subroutine is called DIFSUB(30) and uses a variable-order, variable step, linear, predictor-corrector algorithm. To be more flexible in handling a variety of types of chemical processes, the subroutine offers two options, one for stiff systems and one for nonstiff systems.

3.2.2.1 Nonstiff option

When the whole process comprises non-stiff modules, this option must be chosen. Basically, the predictor step is described by the Adams-Bashforth explicit equation:

$$y_{n+1} = y_n + h \sum_{i=1}^k \beta_i \dot{y}_{n+1-i} \quad (3.2.a)$$

The corrector step uses the Adams-Moulton equation:

$$y_{n+1} = y_n + h \sum_{i=0}^k \beta_i \dot{y}_{n+1-i} \quad (3.2.b)$$

The coefficients β_i and β_i' may be found in reference 15, and the order may vary from 1 to 7.

3.2.2.2 Stiff option

When the whole process comprises just stiff modules, or both stiff and non-stiff modules, this option must be chosen. Obviously, the degree of stiffness is a matter for the judgement of the investigator.

The following approximations are used:
for the predictor pass:

$$y_{n+1} = h \beta_1 \dot{y}_n + \sum_{i=1}^k \alpha_i y_{n+1-i} \quad (3.2.c)$$

for the corrector pass:

$$y_{n+1} = h \beta_0^* \dot{y}_{n+1} + \sum_{i=1}^k \alpha_i^* y_{n+1-i} \quad (3.2.d)$$

The coefficients in the predictor equation can be found in reference 15. Values of the corrector coefficients are given in reference 16. The order may vary from 1 to 6. The corrector equation has been found stable for stiff equations for order up to 6. Further details concerning accuracy, stability and stiffness coefficient determination are discussed in reference 14.

Since the corrector equation is implicit, a method of iteration is required for convergence of the solutions. Two methods of iteration are available for the stiff option: the direct Jacobi iteration is used for

non-stiff modules in a stiff process, and the Newton-Raphson iteration is used for stiff modules. In the latter case, the Jacobian matrix is needed and may be user-supplied or evaluated numerically. Descriptions of the two iterative techniques can be found in reference 14. The application to the distillation column simulation is presented in section 3.3.

3.2.3 Algebraic equation solver

Since the corrector equation is implicit, a set of algebraic linear equations will be obtained. An important factor in saving computer time cost is the choice of the method to solve these simultaneous equations, since one deals generally with large systems of ordinary differential equations in a plant simulation.

The coefficient matrix of the linear equations was shown to be a function of the Jacobian matrix for the system. In general, in a counter-current stagewise process such as the distillation column, the Jacobian matrix has many zeros. Such a matrix is called a sparse matrix, and using a technique which just operates on the non-zero elements will reduce greatly the computer time used.

The routine called SIMULT developed by Key (28) in 1973 was adapted and implemented in DYNYSYS 2.1. Seven pivoting options are available, but, the option of minimum row-minimum column was chosen for this project: the coefficient matrix is searched to find the row with the least number of non-zero coefficients; then for the non-zero elements in this row, the column with the most zeros is chosen as the pivotal column. If more than one row or

column are chosen, the row or column with the smallest index is used.

The storage scheme is illustrated by the following example:

Let the matrix:

$$\underline{P} = \begin{bmatrix} 0 & 1 & 2 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 3 \end{bmatrix}$$

P is stored as:

$$\underline{A} = \begin{bmatrix} 1 & 2 \\ 1 & 1 \\ 0 & 1 \\ 1 & 3 \end{bmatrix} \quad \underline{ICOL} = \begin{bmatrix} 2 & 3 \\ 3 & 4 \\ 0 & 5 \\ 1 & 4 \end{bmatrix}$$

One must refer to reference 14 for more details and explanations.

3.2.4 Adaptation of a new module to DYNSSYS 2.1

This section will present the main features of how to construct a subroutine representing a unit computation and to adapt it to the main executive. This will be useful for future work when the simulation of the solvent recovery column must be made or when investigation on different control schemes is undertaken.

3.2.4.1 Main components of the DYN SYS 2.1 executive

Basically, the executive consists of the following programs:

- DYN 1: this subroutine reads in data such as initial values of the variables, parameters of the equipment, characteristic values, etc., and prints out for checking, when called by the main program.
- DYN 2: this subroutine establishes the logical sequence of execution of the modules, when called by the main program.
- OUTPUT: this subroutine handles all outputs at each time interval specified by the user, when called by DYN 1 or by the main program.
- PROPS: this function reads in the properties of each component in the material flow when called by DYN 1.
- DIFSUB: this subroutine uses the Gear's method to perform the integration and is called by the modules.
- SIMULT: this subroutine solves the set of linear algebraic equations, simultaneously, when called by DIFSUB.
- TRIDAG: this subroutine solves the set of linear algebraic equations simultaneously, when called by DIFSUB, if the Jacobian matrix is tridiagonal.
- DYN SYS: the main program of the executive.

The listings of the above subroutines can be found in reference 14. Fig. 3.1 shows the interactions between the different components involved in the simulation work in this project.

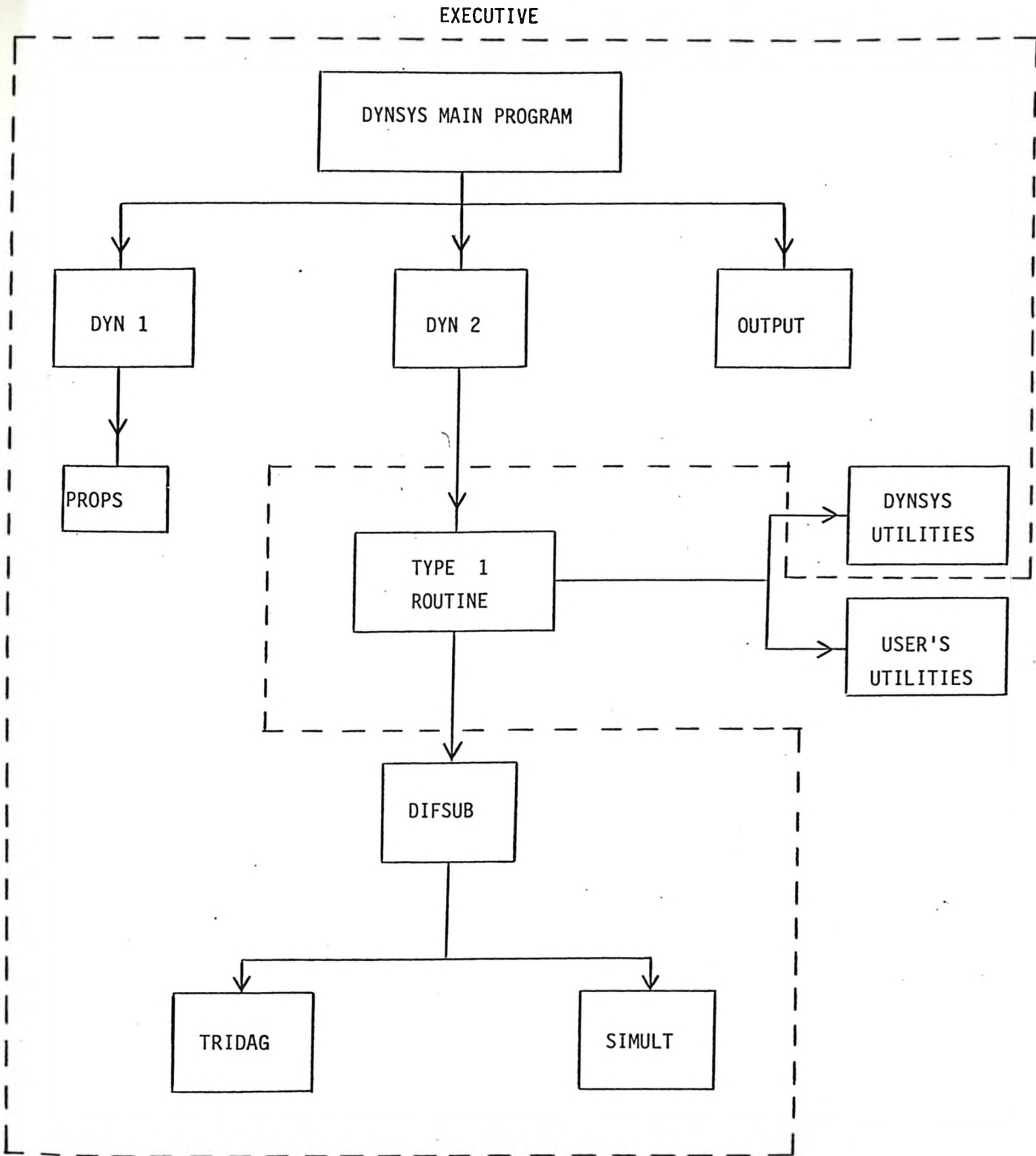


fig. 3.1 INTERACTION BETWEEN DYNYSYS COMPONENTS
AND USER COMPONENTS

3.2.4.2 Construction of a module

Both the stiff and non-stiff options of Gear's method are available. However, the same option must be used for the entire simulation.

When the simulation diagram contains both stiff and non-stiff modules, the stiff option must be used, which means that the stiff coefficients in the approximative equations will be used in the integration. Then, depending on whether the module is stiff or non-stiff, the Newton-Raphson iteration or Jacobi direct iteration will be chosen.

A detailed skeleton of a module is shown in fig. 3.2.

Up to three iterations are allowed in the corrector pass. If convergence within a user-specified tolerance does not appear after the third iteration, the integration step size is reduced to 1/4 of its current size and the step is repeated for all modules.

The user can access to a number of parameters within the executive. A list is given in Appendix B.

3.3 Distillation column dynamic simulation

A tentative mathematical model has been written to represent the dynamic behavior of the experimental extractive distillation column of fifteen stages with a ternary organic system. The module created is used under the executive DYNYSYS 2.1 for further flexibility for future work. The control configuration could be investigated after an appropriate model has been found for the main process.

fig. 3.2 SKELETON OF MODULE FOR DYNYSYS 2.1

SURROUTINE TYPE2.1

COMMENTS DESCRIBING MODULE

THE FOLLOWING COMMON BLOCKS ARE OR MAY BE REQUIRED:

MAT,CON,PTAB,UNIT,GEAR2,MODULE,ROW,COLUMN,JACOB,SUBDI,DIAG,SUPERD

COMMON/MAT/MP(,),EP(,),S(, ,),EX()

COMMON/CON/IG,NCOMP,NC5,H,NE,NS,NPR,NPOL,TMAX,IURDER,NGRAPH

COMMON/PTAB/IGFLAG,PP(,)

COMMON/UNIT/IM,NMP

COMMON/GEAR2/EPS,TIME,KFLAG,JSTART,NBVMAX,ICONV,ISTIFF

COMMON/MODULE/IDERY,ITER,ITRI,MC,IPIVOT

THE ROW DIMENSION OF JCOL AND XJACOB MUST BE THE SAME AS IN DIFSUB
MC IS MAXIMUM NUMBER OF COLUMNS IN XJACOB AND JCOL

COMMON/COLUMN/JCOL(,MC) (NORMAL OPTION)

COMMON/JACOB/XJACOB(,MC) (NORMAL OPTION)

N IS NUMBER OF ODES

COMMON/SUBDI/A(N) (TRIDIAGONAL OPTION)

COMMON/DIAG/B(N) (TRIDIAGONAL OPTION)

COMMON/SUPERD/C(N) (TRIDIAGONAL OPTION)

SECTION #1 : PARAMETER CALCULATIONS

CALCULATE MODULE PARAMETERS : STREAM INPUT,INITIAL CONDITIONS,
VALUES OF ITER ETC.

INPUT STREAM INFORMATION IS OBTAINED FROM S(IG,)
VALUE OF INDEPENDENT VARIABLE (Y) NEED ONLY BE SPECIFIED ON FIRST
INTEGRATION STEP (I.E. INITIAL CONDITIONS)

JSTART=0 ON FIRST INTEGRATION STEP

=CURRENT ORDER OF INTEGRATION TECHNIQUE ON LATER STEPS

IF ISTIFF=0, NONSTIFF COEFFICIENTS WILL BE USED IN INTEGRATION ALGORITHM
(DIFSUB) FOR ALL MODULES,
JACOBIAN MATRIX IS NOT REQUIRED

IF ISTIFF=1, STIFF COEFFICIENTS WILL BE USED FOR ALL MODULES
THEN, IF ITER=0 DIRECT ITERATION OF CORRECTOR WILL BE USED
(NONSTIFF MODULE)

JACOBIAN IS NOT REQUIRED
IF ITER=1 NEWTON-RAPHSON ITERATION OF CORRECTOR WILL
BE USED (STIFF MODULE)

JACOBIAN MATRIX MUST BE SUPPLIED

ITER MUST BE SPECIFIED 0 OR 1
IT IS NOT USED UNLESS ISTIFF=1

IF(IG.EQ.2) GO TO 2

SECTION #2 : JACOBIAN EVALUATION

SECTION #2 IS OMITTED FOR NONSTIFF MODULE

JACOBIAN MATRIX IS REQUIRED ONLY IF MODULE EQUATIONS ARE STIFF
CALCULATE JACOBIAN MATRIX ON CORRECTOR PASS ONLY
JACOBIAN NEED NOT BE VERY ACCURATE, AS IT IS USED ONLY FOR CONVERGENCE
OF CORRECTOR
ONLY NONZERO ELEMENTS ARE CALCULATED, BUT ALL DIAGONAL ELEMENTS MUST
BE STORED WHETHER OR NOT THEY ARE ZERO (NORMAL OPTION)

NORMAL OPTION

IF JACOBIAN MATRIX IS NOT TRIDIAGONAL, KEYS STORAGE SCHEME IS USED
COLUMN NUMBERS OF NONZERO ELEMENTS IN ROW I ARE STORED IN
(JCOL(I,J), J=1, NUMBER OF NONZEROS IN THAT ROW)
SIMILARLY THE VALUES OF THE NONZERO ELEMENTS OF ROW I ARE
STORED IN XJACOB(I,)
REMEMBER TO STORE ALL DIAGONAL ELEMENTS EVEN IF THEY ARE ZERO

MC - MAXIMUM NUMBER OF COLUMNS IN XJACOB MATRIX
MC CAN BE LARGER THAN THE MAXIMUM NUMBER OF NONZERO ELEMENTS
IN ANY JACOBIAN ROW SINCE ADDITIONAL NONZERO ELEMENTS CAN BE
CREATED DURING THE SOLUTION. MC IS CONSTANT FOR ANY SET OF ODES
AND MAY HAVE TO BE DETERMINED BY TRIAL AND ERROR

IPIVOT - PIVOT OPTION USED IN SIMULT (1-7)

IPIVOT=1 : SIMPLE GAUSS-JORDAN ELIMINATION
IPIVOT=2 : GAUSS-JORDAN PARTIAL PIVOTING
IPIVOT=3 : GAUSS-JORDAN FULL PIVOTING
IPIVOT=4 : MINIMUM ROW-MINIMUM COLUMN
IPIVOT=5 : MINIMUM COLUMN-MINIMUM ROW
IPIVOT=6 : MAXIMUM COLUMN-MINIMUM ROW
IPIVOT=7 : MINIMUM OF ROW ENTRIES TIMES COLUMN ENTRIES

ICOL(I,J) - COLUMN NUMBER OF JTH NONZERO ELEMENT IN ROW I
XJACOB(I,J) - VALUE OF JTH NONZERO ELEMENT OF ROW I

MC=
IPIVOT=
IROW(1,1)=
XJACOB(1,1)=

·
·

IROW(N,)=
XJACOB(N,)=

TRIDIAGONAL OPTION

FOR TRIDIAGONAL JACOBIAN MATRIX,THE SUBDIAGONAL,DIAGONAL AND SUPERDIAGO
ELEMENT VALUES ARE STORED IN ARRAYS A,B AND C FROM COMMON BLOCKS SUBDI,
DIAG AND SUPERD RESPECTIVELY

N - NUMBER OF ODES

A - VALUES OF SUBDIAGONAL ELEMENTS ARE STORED IN A(2)...A(N)
A(1) IS NOT USED

B - VALUES OF DIAGONAL ELEMENTS

C - VALUES OF SUPERDIAGONAL ELEMENTS ARE STORED IN C(1)...C(N-1)
C(N) IS NOT USED

B(1)=

C(1)=

A(2)=

B(2)=

C(2)=

.

.

.

A(N-1)=

B(N-1)=

C(N-1)=

A(N)=

B(N)=

1 CONTINUE

IF TRIDIAGONAL OPTION IS BEING USED,ITRI MUST BE SET TO 1 HERE,
IF NORMAL OPTION IS USED ITRI MAY BE IGNORED

ITRI=1

2 CONTINUE

.....
SECTION #3 : DERIVATIVE CALCULATION
.....

CALCULATE DERIVATIVES

DERY(1)=

.

.

.

DERY(N)=

..

.....

C SECTION #4 : CALL DIFSUB

C*****

C CALL DIFSUB TO SOLVE ODES FOR MODULE
 C DIFSUB MAY BE CALLED MORE THAN ONCE FROM A MODULE FOR EXAMPLE IF THE
 C MODULE CONTAINS A SET OF STIFF O.D.E.S AND ANOTHER SET OF NONSTIFF
 C O.D.E.S

C ARGUMENTS : N - NUMBER OF ODES
 C Y - INDEPENDENT VARIABLE
 C DERY - DERIVATIVES

C CALL DIFSUB(N,Y,DERY)

C IF IDERY IS NOT ZERO,THE DERIVATIVES WILL BE RE-EVALUATED AND
 C RETURNED TO DIFSUB
 C ITRI MUST ALSO BE RESET IF IT IS 1

C IF(IDERY.NE.0) GO TO 1

C*****
 C SECTION #5 : STREAM OUTPUT CALCULATION
 C*****

C CALCULATE STREAM OUTPUT (STORED IN S(1, ,))

C S(1, ,)=

C .
 C .
 C .

C RETURN
 C END

3.3.1 Assumptions

The continuous distillation of a liquid mixture in either a stagewise or a continuous-contact column is a very complex phenomenon which involves heat transfer, mass transfer and fluid dynamics. To obtain complete description of such a process, one must formulate the mechanics and inter-relationships of these three transport phenomena.

The mechanics of the fluid flow requires the understanding of the column internals, the pipe sizes and arrangement, the condenser system and the reboiler system. The liquid and vapor hold-ups could be determined thereafter using some empirical relations. The next step would be to set the relationship between the vapor and the liquid at these mixing regions. Considering, the liquid holdup on a plate of the column, the composition is a function of time and position within the liquid phase on the plate. The mass transfer rate is basically a function of the difference in composition of the vapor and liquid phases at this point and also of the composition gradient within the liquid phase.

Consequently, it is apparent that a mathematical dynamic model obtained rigorously will be very complex and hard to use.

However, before modeling is attempted for a process, the objectives of such work must be established. The investment in modeling will therefore be determined by the probable return to be gained by using the model.

In the actual project, the main purposes of constructing a dynamic simulation for the distillation column are to predict the transient behavior of the column in response to a variety of types of input disturbances, to investigate the response when the column is disturbed by combinations of

possible input variables and to design feasible control strategies as well as to obtain an acceptable design of the control parameters and systems dynamic parameters. If these objectives can be achieved satisfactorily from a relatively simple model, then it is apparent that the pursuit of a completely rigorous model is unwarranted. If the model proves to be insufficient for some of the above objectives, the model could be improved by deleting the least probable assumptions.

The following assumptions have been made in developing the mathematical model of the actual column's transient behavior:

(1) There is no heat loss along the column. This assumption could be shown valid to a certain extent since the column is surrounded by a heated air jacket to minimize the heat transfer from inside the column to outside.

(2) The fluid dynamic response time is negligible compared with that of mass transfer. This assumption is justified when no substantial changes in liquid flowrates are experienced, which is very appropriate for changes in feed composition. Also, the range of input flowrate variation is found to be quite small. Moreover, the work of May (17) indicated that for small towers, the time to reach fluid equilibrium is essentially negligible compared to that for mass transfer. The diameter of the present column is 2 inches.

(3) The molar vapor holdup is small compared with that of the liquid. Huckaba and Danly (4) have shown that this assumption is perfectly valid for atmospheric distillation.

(4) The volumetric liquid holdup at each tray is not a function of time. The initial holdups are estimated by the Francis Weir relationship, using the initial liquid flowrates as the basic information. The equations are given in Appendix C.

(5) The flowing fluids are all single phase streams. The liquid and vapor entrainment are negligible.

(6) The pressure through the column is constant and equals atmospheric pressure. This assumption is valid in this case if one considers the small number of plates and the relatively small height of the liquid layers. This assumption could be deleted to make the pressure a linear function with position along the column. However, no big improvement is expected.

(7) The plate efficiencies are independent of time. The work of O'Neill (10) indicated that the efficiencies could be kept constant within the actual operating range without affecting drastically the results of the steady state simulation.

(8) The volumetric reboiler and condenser hold-ups are estimated experimentally. A 100% mixing is assumed in both holdups. The assumption for the reboiler is questionable.

(9) The liquid composition at each tray is assumed uniform. This could be valid since the diameter of the tray and the weir height are reasonably small.

Based on the above assumptions, the basic equations will be presented in the next section.

3.3.2 Basic equation derivation

3.3.2.1 Material balance equations

The basic principle of conservation has been applied to each tray including the feed tray and the solvent input tray and also to the reboiler and the condenser. All the equations have been derived using the gram-mole as the material unit. The starting point of the derivation is the generalized statement:

$$\text{Input} - \text{output} + \text{generation} - \text{disappearance} = \text{accumulation}$$

Based on the nomenclature in fig. 3.3, one can write for a ternary system:

For a normal tray:

$$\frac{dM_n}{dt} = -V_n - L_n + L_{n-1} + V_{n+1} \quad (3.3.1.a)$$

$$\frac{d(M_n x_{n,i})}{dt} = -V_n y_{n,i} - L_n x_{n,i} + L_{n-1} x_{n-1,i} +$$

$$V_{n+1} y_{n+1,i} \quad (3.3.1.b)$$

$$i = 1, 2$$

For a feed tray:

$$\frac{d}{dt} M_n = -V_n - L_n + L_{n-1} + V_{n+1} + F \quad (3.3.2.a)$$

$$\frac{d}{dt} (M_n x_{n,i}) = V_n y_{n,i} - L_n x_{n,i} + L_{n-1} x_{n-1,i} + V_{n+1} y_{n+1,i} + F x_{f,i} \quad (3.3.2.b)$$

For the condenser ($n=1$)

$$\frac{d}{dt} M_n = V_{n+1} - D - R \quad (3.3.3.a)$$

$$\frac{d}{dt} (M_n x_{n,i}) = V_{n+1} y_{n+1,i} - D x_{n,i} - R x_{n,i} \quad (3.3.3.b)$$

$$i = 1, 2$$

For the reboiler ($n = 15$)

$$\frac{d}{dt} M_n = -V_n + L_{n-1} - B \quad (3.3.4.a)$$

$$\frac{d}{dt} (M_n x_{n,i}) = -V_n y_{n,i} + L_{n-1} x_{n-1,i} - B x_{n,i} \quad (3.3.4.b)$$

$$i = 1, 2$$

For convenience, the compositions $x_{n,i}$ were used as variables of integration. Therefore, the equations (3.3.4.b) were transformed using the equations (3.3.4.a) to obtain on the left hand-side the derivative of the composition $x_{n,i}$ as a function of time.

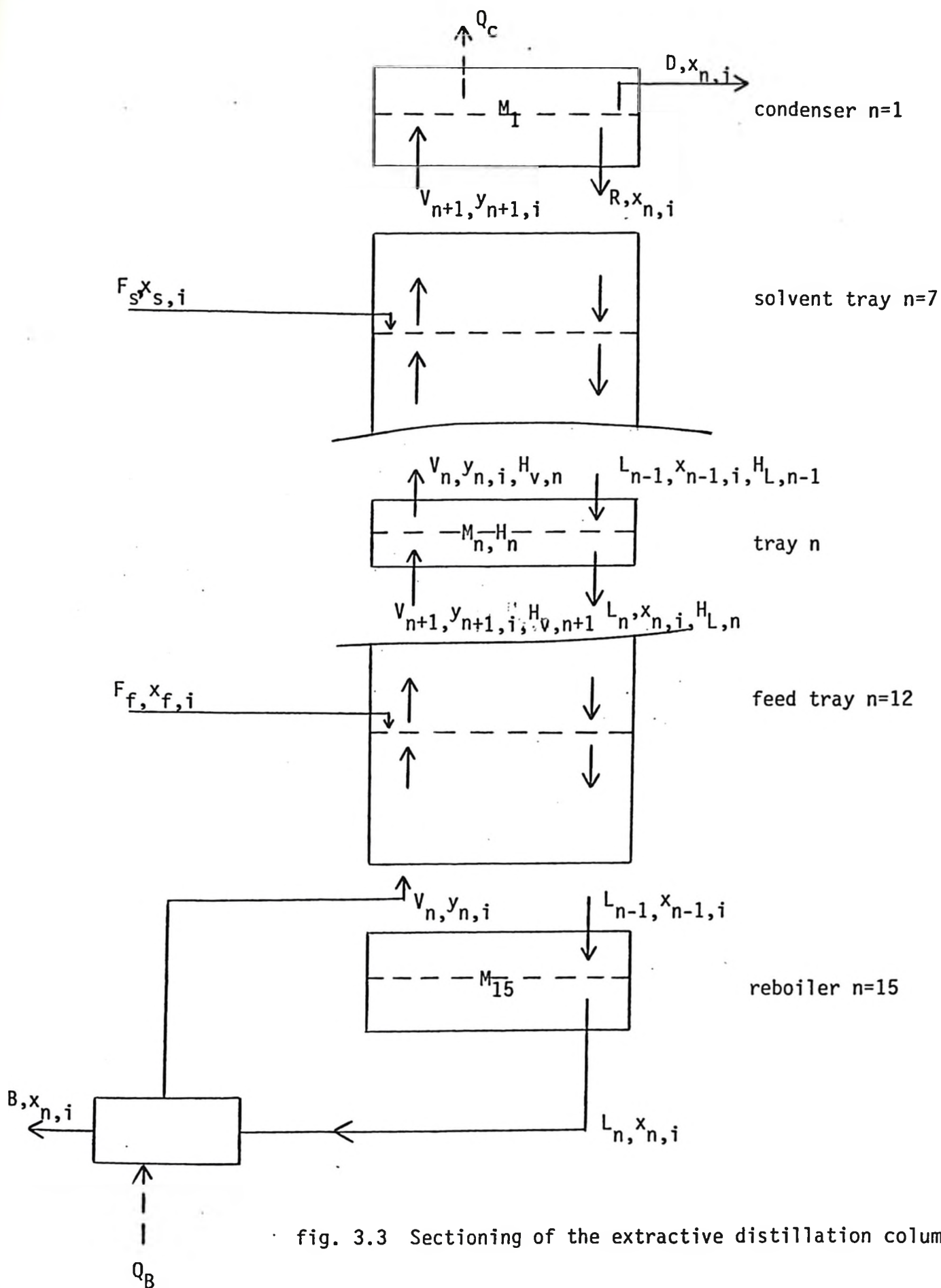


fig. 3.3 Sectioning of the extractive distillation column

After simple manipulations, the following equations were obtained:

For a normal tray:

$$\frac{d}{dt} x_{n,i} = \frac{-V_n y_{n,i} + L_{n-1} x_{n-1,i} + V_{n+1} y_{n+1,i} - x_{n,i} (-V_n + L_{n-1} + V_{n+1})}{M_n} \quad i = 1, 2 \quad (3.3.1.c)$$

For a feed tray:

$$\frac{d}{dt} x_{n,i} = \frac{-V_n y_{n,i} + L_{n-1} x_{n-1,i} + V_{n+1} y_{n+1,i} + F x_{f,i} - x_{n,i} (-V_n + L_{n-1} + V_{n+1} + F)}{M_n} \quad i = 1, 2 \quad (3.3.2.c)$$

For the condenser (n=1)

$$\frac{d}{dt} x_{n,i} = \frac{(y_{n+1,i} - x_{n,i}) V_{n+1}}{M_n} \quad i = 1, 2 \quad (3.3.3.c)$$

For the reboiler (n=15)

$$\frac{d}{dt} x_{n,i} = \frac{-V_n y_{n,i} + L_{n-1} x_{n-1,i} - x_{n,i} (-V_n + L_{n-1})}{M_n} \quad i = 1, 2 \quad (3.3.4.c)$$

The 30 equations (3.3._c) were integrated as a function of time, and the third composition (i=3) was calculated according to:

$$\sum_i x_{n,i} = 1 \quad i = 1,3 \quad (3.3.5)$$

In this simulation program, the integration was made on the acetone composition (i=1) and the methanol composition (i=2); the water composition (i=3) was obtained by difference.

3.3.2.2 Vapor-liquid equilibrium relations

The activity coefficient of each component in the liquid mixture was calculated using the enthalpic Wilson equation, extended to multi-component mixtures.

Given a liquid mixture of q components, the activity coefficient of component i in the mixture was calculated from:

$$\ln \gamma_i = - \sum_{\substack{j=1 \\ j \neq i}}^q \frac{x_j \ln(\Lambda_{ij} \Lambda_{ji})}{\left(\sum_p \Lambda_{ip} x_p \right) \left(\sum_p \Lambda_{jp} x_p \right)} \times \alpha_{ij} -$$

$$\sum_{\substack{m,j \\ m \neq j \neq i}} \frac{x_j x_m \ln(\Lambda_{jm} \Lambda_{mj})}{\left(\sum_p \Lambda_{jp} x_p \right) \left(\sum_p \Lambda_{mp} x_p \right)} \times \alpha_{ijm} \quad (3.3.6.a)$$

where

$$\alpha_{ij} = 1 + x_i \left(1 - \frac{1}{\sum_p \Lambda_{ij} x_p} - \frac{\Lambda_{ji}}{\sum_p \Lambda_{jp} x_p} \right) \quad (3.3.6.b)$$

$$\alpha_{ijm} = 1 - \Lambda_{ji} / (\sum_p \Lambda_{jp} x_p) - \Lambda_{mi} / (\sum_p \Lambda_{mp} x_p) \quad (3.3.6.c)$$

$$\Lambda_{ii} = 1 \quad (3.3.6.d)$$

$$\Lambda_{ij} = \frac{v_j}{v_i} \times \exp\left(\frac{-\lambda_{ij} - \lambda_{ii}}{RT}\right) \quad (3.3.6.e)$$

The parameters λ_{ij} for each pair of components for the present mixture of acetone-methanol-water could be found in Reference 20. Griswold and Buford (21) have tested the above equations for the ternary system mentioned above. The derivation of the enthalpic Wilson equations is presented in reference 20. The v_i 's are the molar volume of the components at temperature T in °K.

Once the activity coefficient of each component was calculated, the activity r_i could be derived by the following relation:

$$r_i = \frac{p_i}{p} \times \gamma_i, \quad p \text{ is the solution pressure} \quad (3.3.7)$$

where

$$p_i' = \exp\left(a + \frac{b}{T+c}\right), \quad p_i' \text{ is the vapour pressure} \quad (3.3.8)$$

The composition of the vapor in equilibrium with the liquid mixture y_i^*

was then calculated from:

$$y^*_i = \Gamma_i x_i \quad (3.3.9)$$

The temperature of the liquid on each tray was used as the parameter to converge the summation of the vapor component compositions to 1.

The Murphree efficiencies $E_{n,i}$ could then be applied to calculate the true composition of the vapor leaving each tray. The following relation was used for tray n :

$$y_{n,i} = y_{n+1,i} + E_{n,i} \times (y^*_{n,i} - y_{n+1,i}) \quad (3.3.10.a)$$

$n=1,14$

As no vapor enters the reboiler ($n=15$), the Murphree efficiency was defined differently by taking the composition of the liquid leaving the reboiler instead of the composition of the vapor coming to the stage. Therefore, one obtains for the reboiler:

$$y_{n,i} = x_{n,i} + E_{n,i} \times (y^*_{n,i} - x_{n,i}) \quad (3.3.10.b)$$

$n=15$

3.3.2.3. Energy equations

At the end of each time interval, the new compositions of the liquid and the vapor leaving and reaching the stage were obtained as shown in the previous sections. Then, the unsteady-state energy equation at each stage

was used to readjust the vapor and liquid flowrates.

The energy imbalance at tray n was obtained according to the following principle:

energy accumulation = energy in - energy out

$$\left(\frac{dH_n}{dt}\right)_t = (H_{L,n-1}L_{n-1} - H_{L,n}L_n + H_{V,n+1}V_{n+1} - H_{V,n}V_n + Q_n)_t \quad (3.3.11)$$

This surplus of energy was assumed to vaporize a certain quantity of liquid from the tray holdup, thus increasing the flowrate of the vapor leaving this tray. The vapor material amount was obtained from:

$$\left(\frac{dV_n}{dt}\right)_t = \frac{(dH_n/dt)_t}{(H_{V,n} - H_{L,n})_t} \quad (3.3.12)$$

Therefore, the vapor flowrates could be readjusted, starting from the reboiler up the column.

At the top of the column, due to the change in the vapor flowrates, the unbalance of the liquid flow could be computed and flowed down, trying to keep the energy equation instantaneously balanced.

3.3.3. Jacobian matrix derivation

As mentioned previously, the integration procedure requires the

Jacobian matrix of the system of ordinary differential equations, to perform the convergence of the solutions at a certain time t , in the corrector pass.

In general, for the system $\dot{y} = f(y)$, the Jacobian matrix is:

$$\underline{J} = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \dots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & & \\ \vdots & & & \\ \frac{\partial f_n}{\partial y_1} & \dots & & \frac{\partial f_n}{\partial y_n} \end{bmatrix}$$

Taking the partial derivative of the right hand side of equations (3.3.1.c) (3.3.2.c), (3.3.3.c) and (3.3.4.c) with respect to $x_{n-1,i}$ and $x_{n,i}$ successively, one could obtain for a normal tray:

$$\frac{d}{dx_{n-1,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{L_{n-1}}{M_n} \quad i = 1, 2 \quad (3.3.13.a)$$

$$\frac{d}{dx_{n,i}} \left(\frac{dx_{n,i}}{dt} \right) = - \frac{(-V_n + L_{n-1} + V_{n+1})}{M_n} \quad i = 1, 2 \quad (3.3.13.b)$$

for a feed tray:

$$\frac{d}{dx_{n-1,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{L_{n-1}}{M_n} \quad i = 1, 2 \quad (3.3.14.a)$$

$$\frac{d}{dx_{n,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{-(-V_n + L_{n-1} + V_{n+1} + F)}{M_n} \quad i = 1, 2 \quad (3.3.14.b)$$

for the condenser (n=1)

$$\frac{d}{dx_{n-1,i}} \left(\frac{dx_{n,i}}{dt} \right) = 0 \quad i = 1, 2 \quad (3.3.15.a)$$

$$\frac{d}{dx_{n,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{-V_{n+1}}{M_n} \quad i = 1, 2 \quad (3.3.15.b)$$

for the reboiler (n=15)

$$\frac{d}{dx_{n-1,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{L_{n-1}}{M_n} \quad i = 1, 2 \quad (3.3.16.a)$$

$$\frac{d}{dx_{n,i}} \left(\frac{dx_{n,i}}{dt} \right) = \frac{-(-V_n + L_{n-1})}{M_n} \quad i = 1, 2 \quad (3.3.16.b)$$

It is apparent to find that the Jacobian matrix has a tridiagonal form.

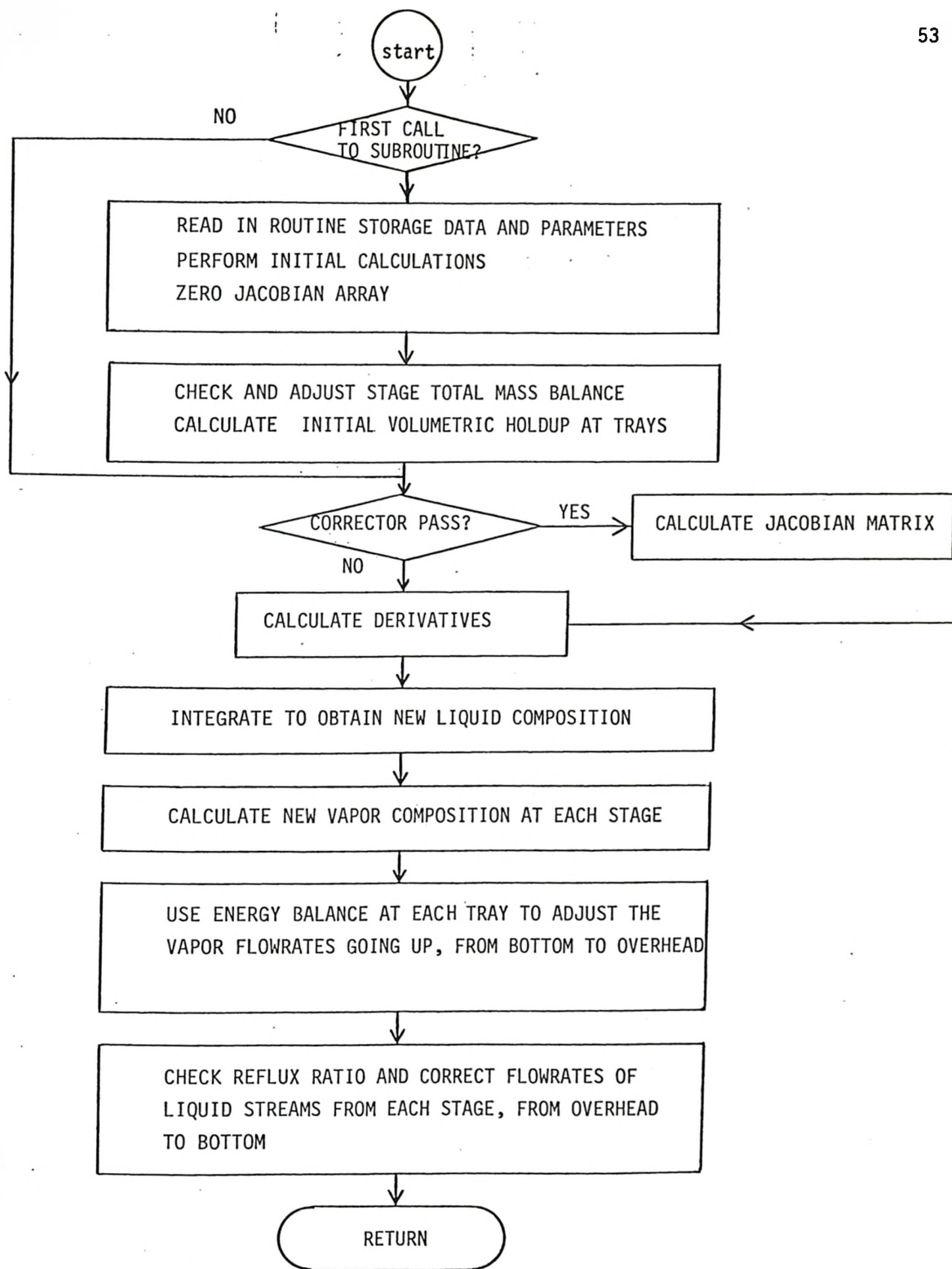


fig. 3.4 GENERAL FLOWCHART OF SUBROUTINE TYPE 1(COLUMN)

3.3.4 Simulation software

A module representing dynamically the experimental distillation column has been created and incorporated to the DYNYSYS 2.1 executive. A logic flowchart of the calculation procedure could be found on fig. 3.4.

A stand-alone steady-state program was developed by O'Neill (10) and was used to supply the starting steady-state conditions for the dynamic simulation. Information related to the utilization of the steady-state package was presented in detail in reference 10.

A data transformer program was created to adapt the output of the steady-state program to a suitable format to input into the dynamic simulation program.

The dynamic runs were performed on a CDC 6400 (McMaster University). Listings of the utility subroutines can be found in Appendix F. Listing of the main subroutine is presented in Appendix F.

CHAPTER 4

DYNAMIC RESULTS - STEP AND PULSE DISTURBANCES

The immediate objective of the work was to develop a mathematical model to represent adequately the experimental extractive distillation column. In order to evaluate the present simulation algorithm, conventional disturbances such as step changes and pulse changes, were introduced into input variables such as feed flowrate, feed composition and reflux ratio. The dynamic simulated response has been observed and compared to available experimental results obtained by D. O'Neill (10).

A presentation and analysis of the calculated and experimental results are given in the following sections, for disturbances in feed composition, feed flowrate and reflux ratio respectively.

4.1 Dynamic responses due to feed composition disturbances

In order to observe the dynamic response of the column, especially the transient behavior of the overhead product composition which generally is the controlled variable, the feed acetone composition was disturbed by a negative step change of -5.3% amplitude, a positive step change of +5.6% amplitude and a negative pulse change of -17.4% amplitude. The operating conditions of the three runs could be found on Table 4.1.

Experimentally, the column was brought initially to a certain steady-state level and the disturbance was introduced. A system of on/off valves

permits a switch of the feed line from one storage tank to another storage tank with different composition. Samples were taken from the overhead line and from the bottom line, more frequently at the beginning of the change, and were analyzed by a gas chromatograph.

Plots of experimental and simulated results with respect to time were made and presented on fig. 4.1, 4.2, 4.3. The variation of the temperature was found negligible in both experimental and simulated results. The comparison was found more consistent for the case of a pulse change. Bottom product compositions were apparently insensitive to feed composition changes as shown by experimentation and simulation.

4.2 Dynamic responses due to feed flowrate disturbances

The effects of a change in the feed flowrate were investigated. Such a change caused a perturbation in the overall mass balance of the column, therefore affecting the local and component mass balances throughout the stages.

Experimentally, a needle valve allows the manual introduction of a negative step change of -15.4% amplitude, a positive step change of +18.2% amplitude and a positive pulse change of +18.2% amplitude in the feed flowrate. The operating conditions of the three runs are presented in Table 4.2.

In the simulation, the mass change of the feed was supposed to appear instantaneously at the bottom product line, for the total mass balance to be satisfied. Therefore, sudden changes occurred for all liquid flowrates from the feed tray downward to the reboiler. Thus, the transient of the

TABLE 4.1 OPERATING CONDITIONS

FEED COMPOSITION AS DISTURBED VARIABLE

Quantity	Unit	negative step change		positive step change		negative pulse change	
		initial	final	initial	final	initial	final
F	g moles/hr	16.16	16.16	16.16	16.16	16.16	16.16
$x_{F,1}$	mol. fract.	.6076	.5753	.5753	.6076	.6067	.6076
$x_{F,2}$	mol. fract.	.3848	.4171	.4171	.3848	.3848	.3848
T_F	°C	45	45	45	45	45	45
S	g moles/hr	30.75	30.75	30.75	30.75	30.75	30.75
$x_{S,1}$	mol. fract.	0.	0.	0.	0.	0.	0.
$x_{S,2}$	mol. fract.	0.	0.	0.	0.	0.	0.
T_S	°C	70	70	70	70	70	70
RR	dimensionless	1.756	1.756	1.756	1.756	1.756	1.756
REBDT	Kcal/hr	235	235	235	235	235	235
%dist. AMPL.	dimensionless	-5.3 %		+ 5.6 %		- 17.4 %	

fig. 4.1 NEGATIVE STEP CHANGE TO FEED ACETONE COMPOSITION

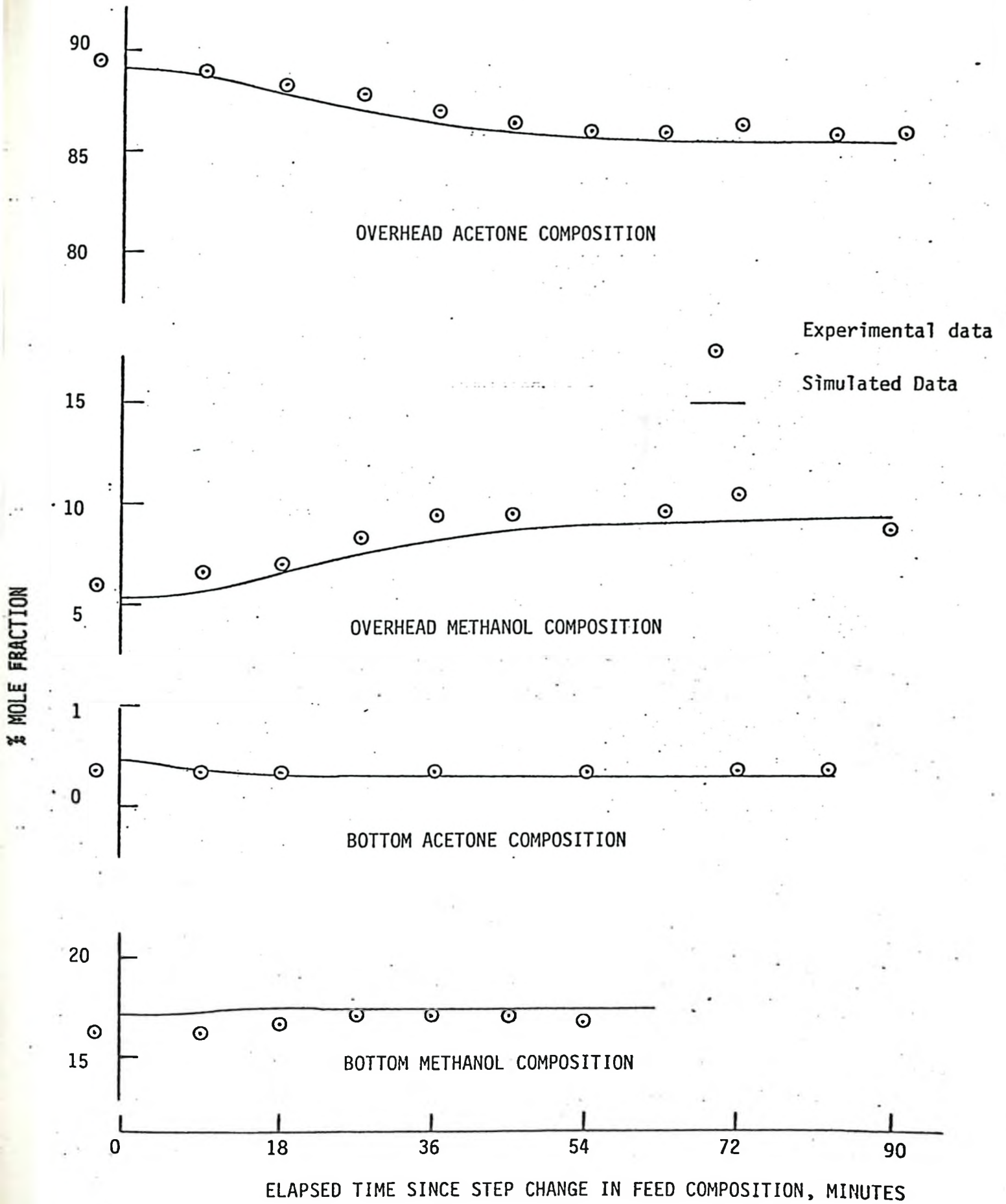


fig. 4.2 POSITIVE STEP CHANGE TO FEED ACETONE COMPOSITION

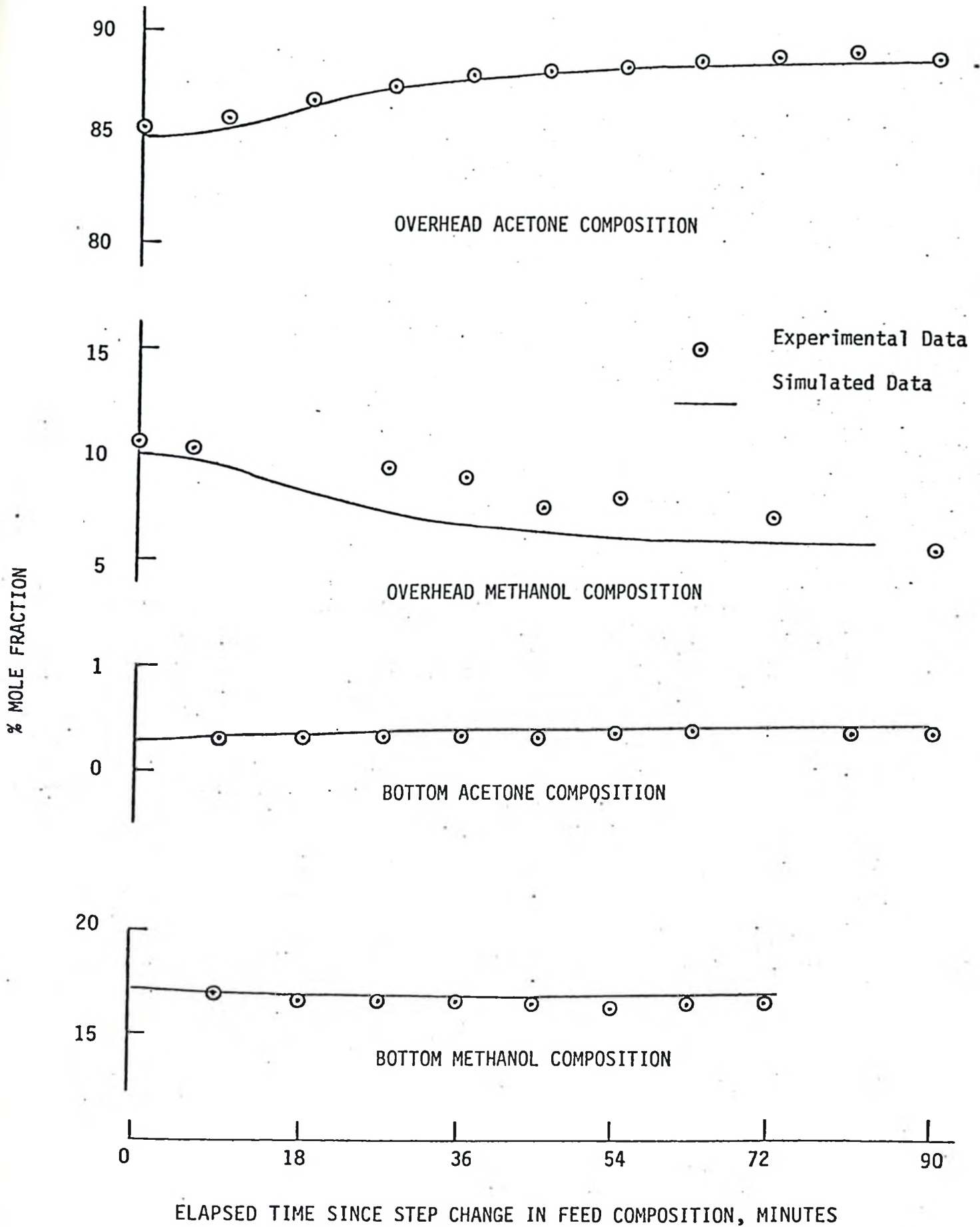
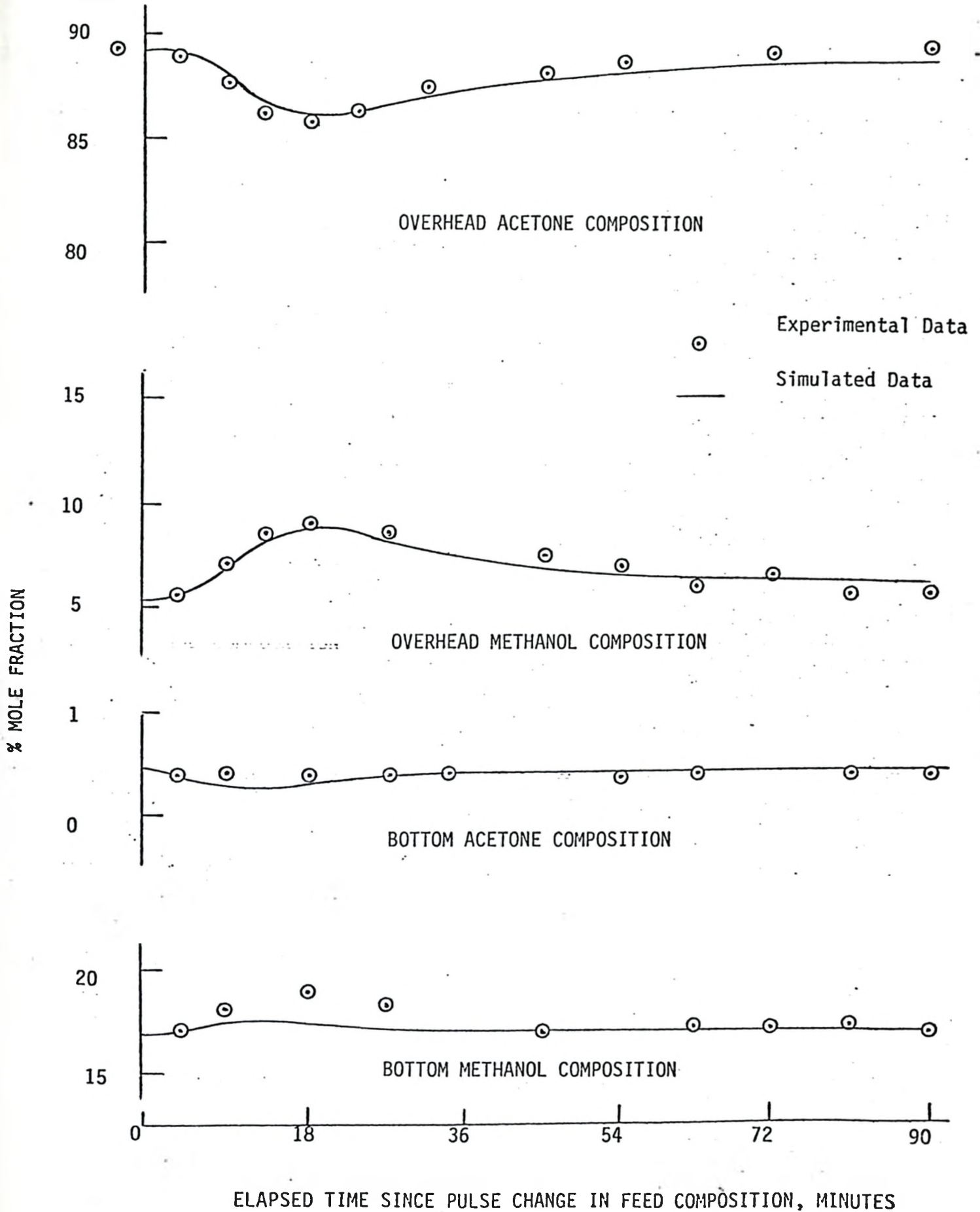


fig. 4.3 NEGATIVE PULSE CHANGE TO FEED ACETONE COMPOSITION



column resulted from the imbalance of the component mass equation for the trays between the feed and the reboiler. The fluid dynamic equilibrium time was assumed negligible compared to the equilibrium time of the temperature or composition.

The transient responses at the overhead and at the bottom were presented on fig. 4.4. 4.5, 4.6. An increase in the feed flowrate means an increase in the quantity of acetone and methanol. Since most of the acetone goes up to the condenser, the acetone mole fraction at the overhead should increase relatively to the methanol mole fraction. However, increases of both acetone mole fraction and methanol mole fraction at the reboiler could be explained by the fact that there was more acetone than methanol in the feed line.

4.3 Dynamic responses due to reflux ratio changes

An increase in the reflux ratio at the overhead implies a decrease in the overhead flowrate and vice versa. The results were simulated for the cases of a negative step change of -11.3% amplitude, a positive step change of +12.7% amplitude and a positive pulse change of +75% amplitude.

Once again, the overall mass balance of the column was affected. In the simulation, when a change in the reflux ratio occurred, the total mass balances on each stage were completed by adjusting instantaneously the liquid flowrates leaving each stage. Therefore, an imbalance of the component mass equations resulted and implied a change in the composition of the liquid.

Experimentally, a reflux divider allowed the introduction of such

TABLE 4.2 OPERATING CONDITIONS
FEED FLOWRATE AS DISTURBED VARIABLE

Quantity	unit	negative step change		positive step change		positive pulse change	
		initial	final	initial	final	initial	final
F	g moles/hr	17.53	14.83	14.83	17.53	14.83	14.83
$x_{F,1}$	mol. fract.	.6059	.6059	.6059	.6059	.6059	.6059
$x_{F,2}$	mol. fract.	.3875	.3875	.3875	.3875	.3875	.3875
T_F	°C	45	45	45	45	45	45
S	mol. fract.	30.75	30.75	30.75	30.75	30.75	30.75
$x_{S,1}$	mol. fract.	0.	0.	0.	0.	0.	0.
$x_{S,2}$	mol. fract.	0.	0.	0.	0.	0.	0.
T_S	°C	70	70	70	70	70	70
RR	dimensionless	1.784	1.784	1.784	1.784	1.784	1.784
REBDT	Kcal/hr	234	234	234	234	234	234
% dist. ampl	dimensionless	- 15.8 %		+ 18.2 %		+ 18.2 %	

fig. 4.4 NEGATIVE STEP CHANGE TO FEED FLOW RATE

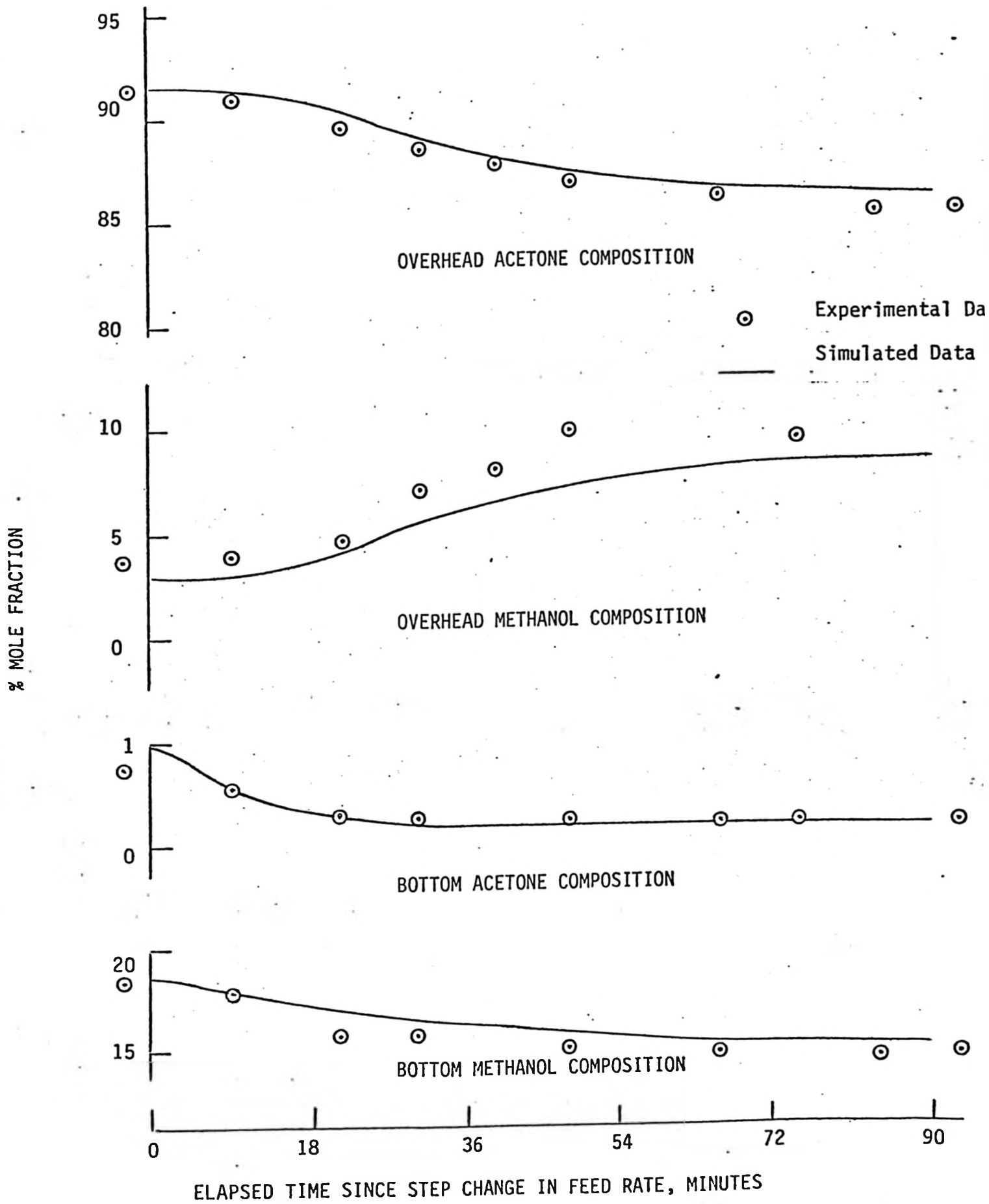


fig. 4.5 POSITIVE STEP CHANGE TO FEED FLOWRATE

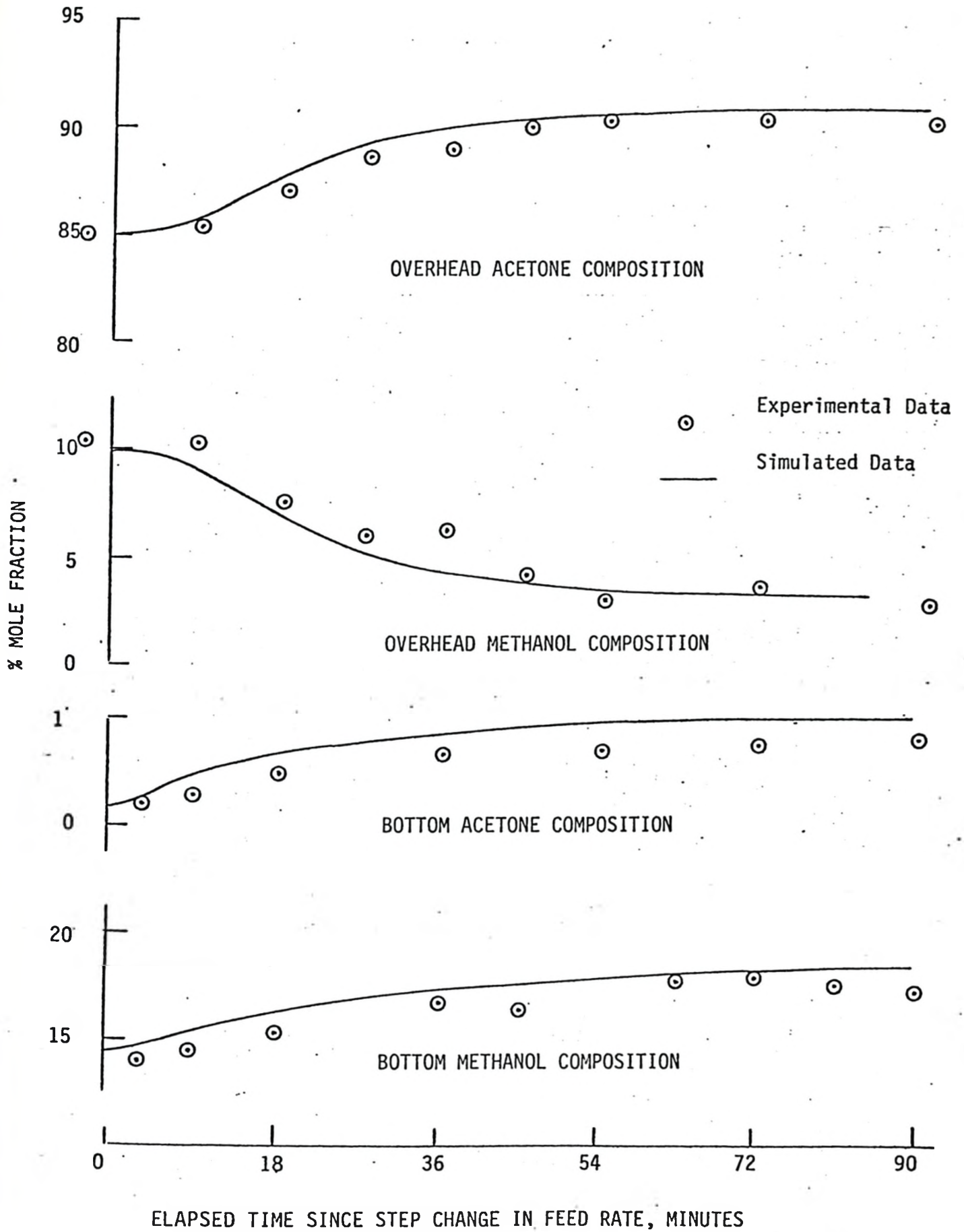


fig. 4.6 POSITIVE PULSE IN FEED FLOW RATE

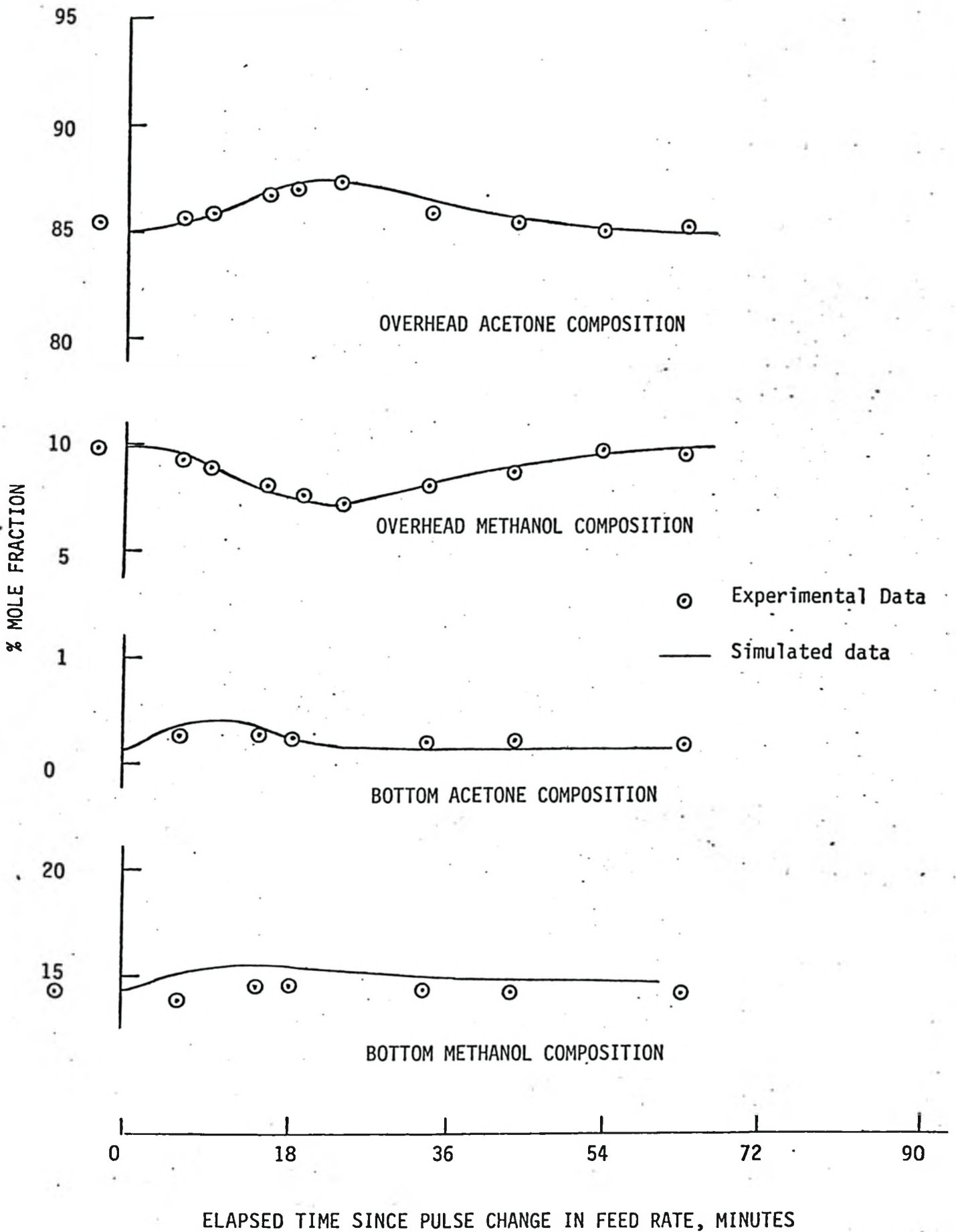


TABLE 4.3 OPERATING CONDITIONS

REFLUX RATIO AS DISTURBED VARIABLE

Quantity	unit	negative step change		positive step change		positive pulse change	
		initial	final	initial	final	initial	final
F	g moles/hr	16.37	16.37	16.37	16.37	16.37	16.37
$x_{F,1}$	mol.fract.	.5886	.5886	.5886	.5886	.5886	.5886
$x_{F,2}$	mol.fract.	.4060	.4060	.4060	.4060	.4060	.4060
T_F	°C	45	45	45	45	45	45
S	g moles/hr	30.75	30.75	30.75	30.75	30.75	30.75
$x_{S,1}$	mol. fract.	0.	0.	0.	0.	0.	0.
$x_{S,2}$	mol. fract.	0.	0.	0.	0.	0.	0.
T_S	°C	70	70	70	70	70	70
RR	dimension- less	1.756	1.558	1.558	1.756	1.756	1.756
REBDT	Kcal/hr	215	215	215	215	215	215
%Dist.ampl.	dimension- less	- 11.3 %		+ 12.7 %		+ 75%	

fig. 4.7 NEGATIVE STEP CHANGE TO REFLUX RATIO

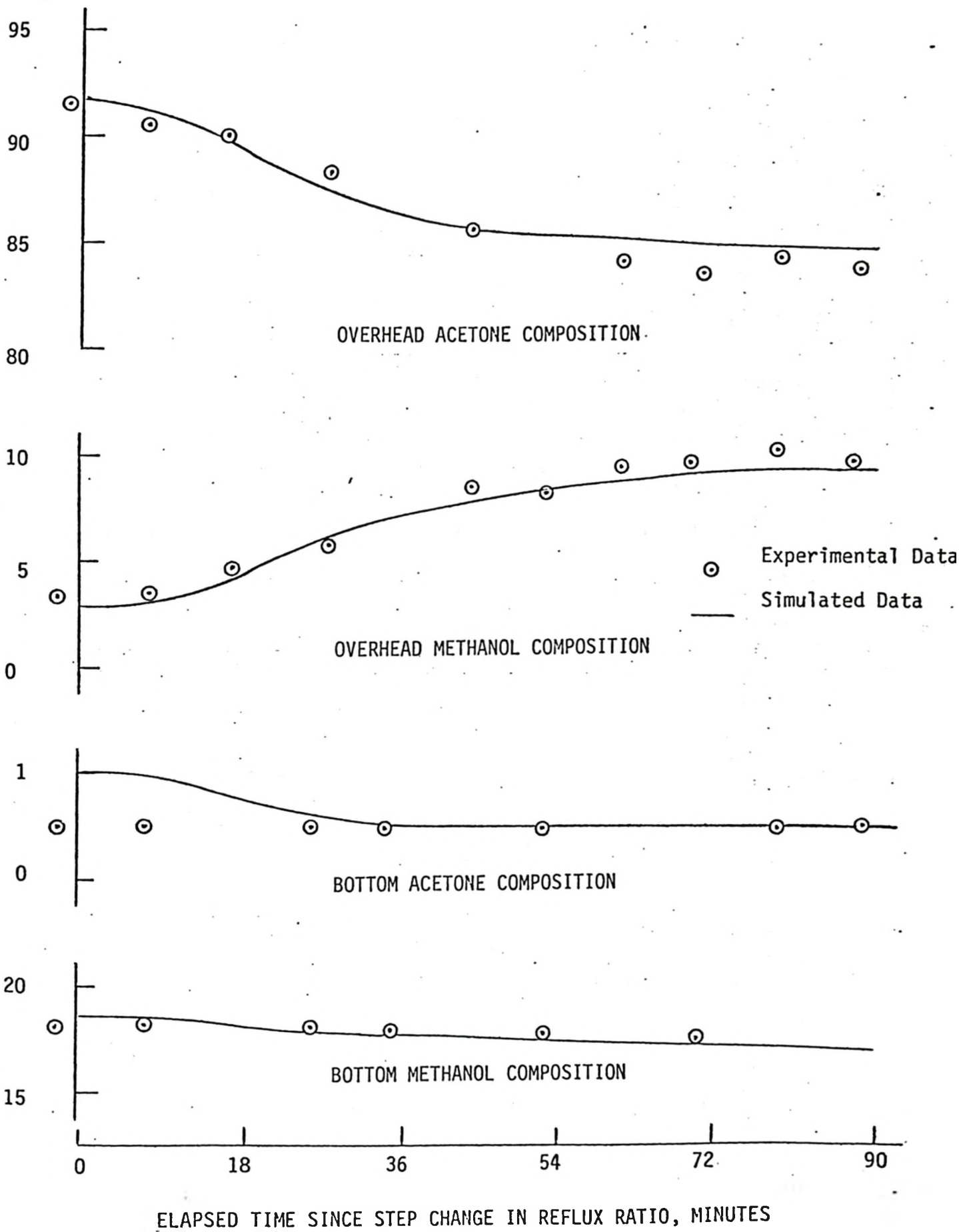


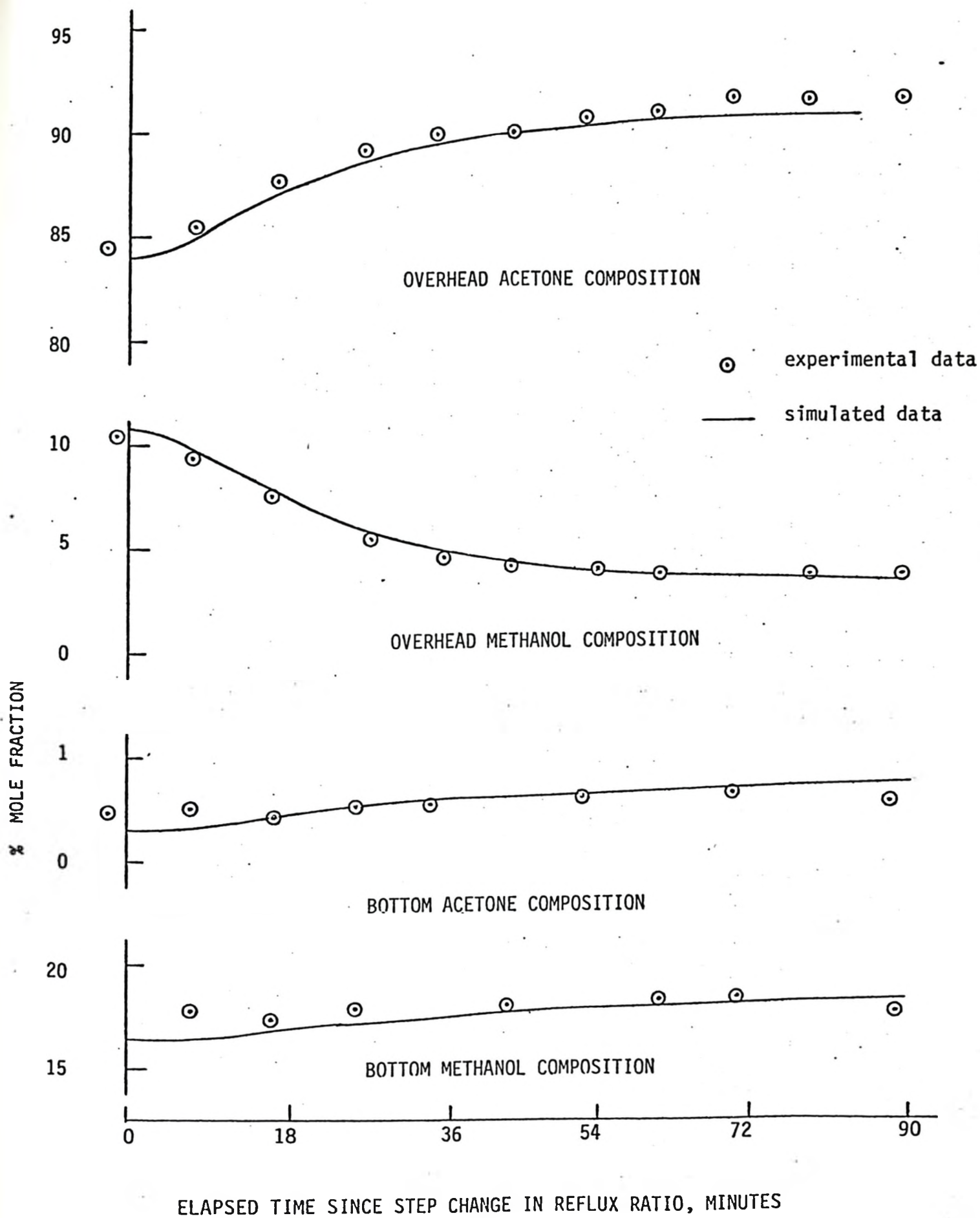
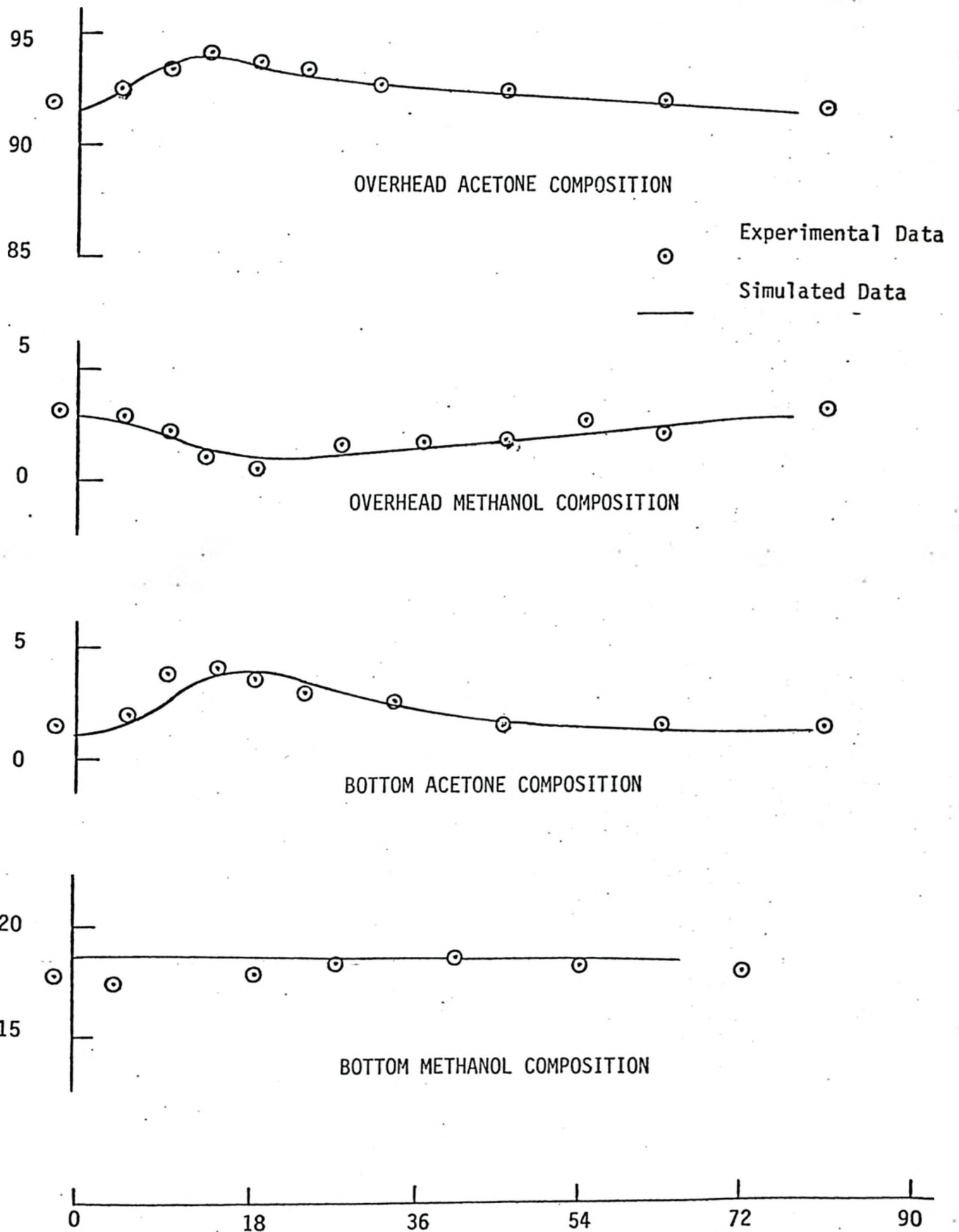
Fig. 4-8 POSITIVE STEP CHANGE IN REFLUX RATIO

fig. 4.9 POSITIVE PULSE CHANGE TO REFLUX RATIO



ELAPSED TIME SINCE PULSE CHANGE IN REFLUX RATIO, MINUTES

changes to the reflux ratio variable. The operating conditions are presented in Table 4.3.

The calculated results were compared to the available experimental data and were presented on fig. 4.7, 4.8, 4.9. A fairly good agreement was obtained at the overhead. However, inconsistencies were observed at the bottom of the column. These could be likely explained by the assumption of 100 per cent mixing the reboiler not being satisfied in practice.

4.4 Conclusion

The above study has shown that the dynamic behaviour of a fifteen-stage extractive distillation column can be described by simply laying out the basic mass, energy and equilibrium equations and by choosing an appropriate set of assumptions. The Murphree efficiencies at the stages were kept constant throughout the simulation and came from D. O'Neill's steady-state simulation work (19). The parameters in the enthalpic Wilson equation extended to multicomponent mixtures were taken from Bruin's study (20) about activity coefficient relations in miscible and partially miscible multicomponent systems. Only the parameter in the Francis weir relation was adjusted to obtain a fair consistency in the comparison of simulated data with experimental data. This relation was used to calculate the overflow height as a function of the tray characteristics and the liquid flowrate. A change in the overflow height will cause the total tray holdup to change, and a change in the total tray holdup will affect the model through the values of M_j in equations (3. .1.c), (3. .2.c), (3. .3.c) and (3. .4.c).

The most important feature of the simulation is that it describes the interactions between the fluid dynamic, heat transfer and mass transfer phenomena.

CHAPTER 5

DYNAMIC RESULTS - OSCILLATORY DISTURBANCES

This chapter presents an attempt to study the dynamic behavior of the column subject to oscillatory disturbances. The mathematical model has been found fairly adequate to represent the extractive column with disturbances such as step change and pulse change to feed variables. It was also mentioned that the model depends intimately upon the nature of the disturbance and the disturbed variable.

As a first step toward the identification technique using the black box concept, a test has been made with a square wave disturbance into the feed flowrate variable. Due to a delay in the equipment arrival and the problems encountered when hooking up the control valves as described in chapter 2, a preliminary simulation study of the effect of the frequency and the amplitude which characterize the square wave, was performed on the feed flowrate variable, using the previous simulation program with some minor modifications. The feed flowrate was chosen as the disturbed variable since experimental work could be done later to confirm the simulation study. The reason for choosing a square wave type of disturbance was to overcome the non-linearity problem of control valves in the actual operating range.

The control valves were set up and a reasonable range was determined with the adjustment of the pressure in the feed tank as mentioned in

chapter 2. Due to lack of time, only one experimental run was performed with a square wave disturbance into the feed rate variable and the results have been compared with calculated results.

A brief survey about different approaches on unsteady operation of distillation columns is presented in the following section.

5.1 Literature review

Controlled-cycling operation of columns was generally understood as operation in which periods for dense phase to flow down and light phase to flow up are repeated alternately. Schrodt (36) explained qualitatively the improvement as followed: when two phases containing a transferable substance are brought in contact, the driving force for mass transfer is initially very high, than decreases to approach zero, close to equilibrium conditions; controlled-cycling conditions involve more fresh phases brought in contact, therefore, the time-average driving force is higher. McWhirter and Cannon (37) found an efficiency increase as high as 160 per cent on experimental distillation columns operating at total reflux.

A number of investigators such as Belter and Speaker (38) considered a cycle comprising periods for dense phase flow down the column, a coalescence stage with no flow, light phase flow up the column and again a coalescence stage with no flow. Efficiencies were obtained greater than 100 per cent and throughputs were 2 to 10 times greater than the steady-state case. Reference 35 is a useful source of information on controlled-cycling literature.

A more recent approach to unsteady-state operation of distillation process was analytically done by Matsubara et al. (39). Instead of dealing with cases in which a vapor flow period and a liquid flow period are repeated

alternately, Matsubara et al. conceive an optimal cycle of operations which, basically, consisted in taking off the top product only when the composition of the more volatile component in the condenser is high and the bottom product only when the composition in the reboiler is low. The numerical study was applied to a binary distillation column with negligible vapor holdup, constant liquid holdup on each stage, identical vapor rate throughout the column, identical liquid rate throughout the enriching or the stripping sections of the column, plates with 100 per cent efficiency and with variable condenser holdup and reboiler holdup. Matsubara et al. concluded that if the maximal admissible vapor rate is large, periodic control required a much smaller number of stages relative to steady control, to attain the same separation efficiency.

Friedly (34) has also mentioned the possible improvement of non-linear processes when operated at unsteady-state conditions rather than at steady-state conditions. Lannus and Kershenbaum (33) noticed an improvement of the conversion in a tubular reactor when the inlet concentration was forced sinusoidally.

5.2 Simulation study

The extractive distillation column was simulated within the possible operating range determined by the work of D. O'Neill (10).

Any change in the feed flowrate involves a change in the fluid dynamics of the column. The same technique was used for a square wave input as was used for a step or pulse change in the feed flowrate. The flow increase was transmitted instantaneously down to the bottom output, changing the liquid flowrates coming out from the trays between the feed location and the bottom, therefore changing the holdup at the trays according

to the Francis weir relation.

Fig. 5.1.a. shows the overhead response when a square wave with a period of 0.1 hr., an amplitude of 12% was put into the feed flowrate; the response was observed during a period of time of 2 hr. and gradual stabilization to a higher steady-state level for the acetone overhead composition seemed to occur.

Simulated runs were also performed with three different periods of 0.2 hr., 0.1 hr., 0.04 hr. at a constant amplitude level of 12%, to study the effect of the period on the overhead composition response. Simulation time was limited to 1.4 hr. for economic reasons. From fig. 5.1.b, one can observe three trends:

- (1) The acetone composition did not stay at the steady-state level but increased from it substantially. The methanol mole fraction also decreased significantly.
- (2) The larger the period is the greater the deviation from the initial steady-state level.
- (3) The gradient of the deviation with respect to the period of the wave is not constant. The jump from curve C to curve B is much larger than from curve B to curve A although the increase in the period is almost the same.

The effect of the amplitude of the wave on the overhead response was also investigated by doing runs at the same period value of 0.1 hr. and three different amplitudes of 12, 9, 3 per cent successively. Effects of amplitude on the overhead response is shown in Fig. 5.1.c. It can be seen that in the range of amplitude considered (3% - 12%), the effect of amplitude is very small. This would strongly suggest that most of the improved performance possible by cycling can be obtained with only a very small amplitude (3%) and there is little incentive to go to larger amplitude.

fig. 5.1.a: OVERHEAD COMPOSITION RESPONSES TO SQUARE WAVE DISTURBANCE IN FEED FLOWRATE

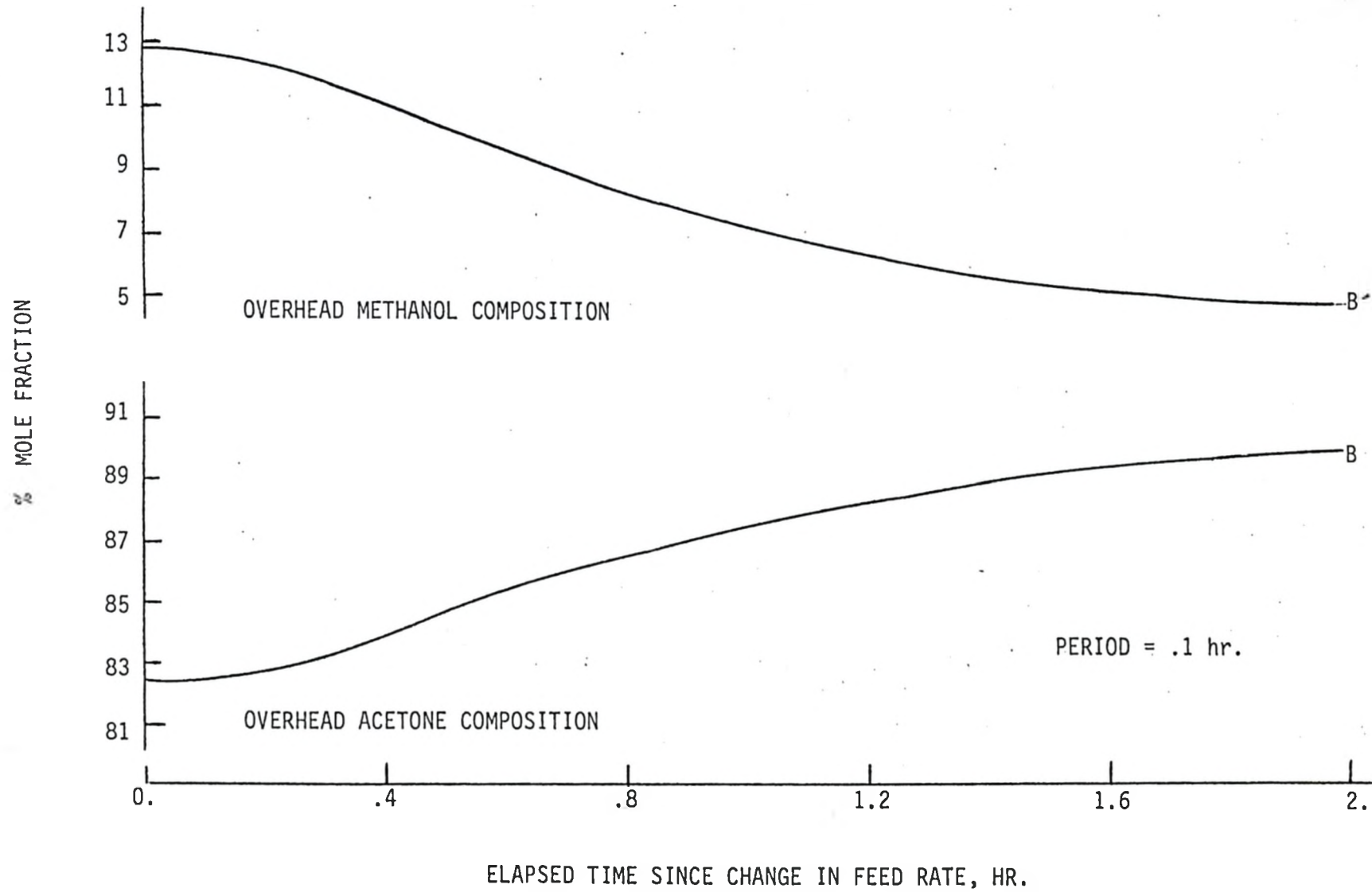


fig.5.1.b EFFECT OF FREQUENCY ON OVERHEAD COMPOSITION

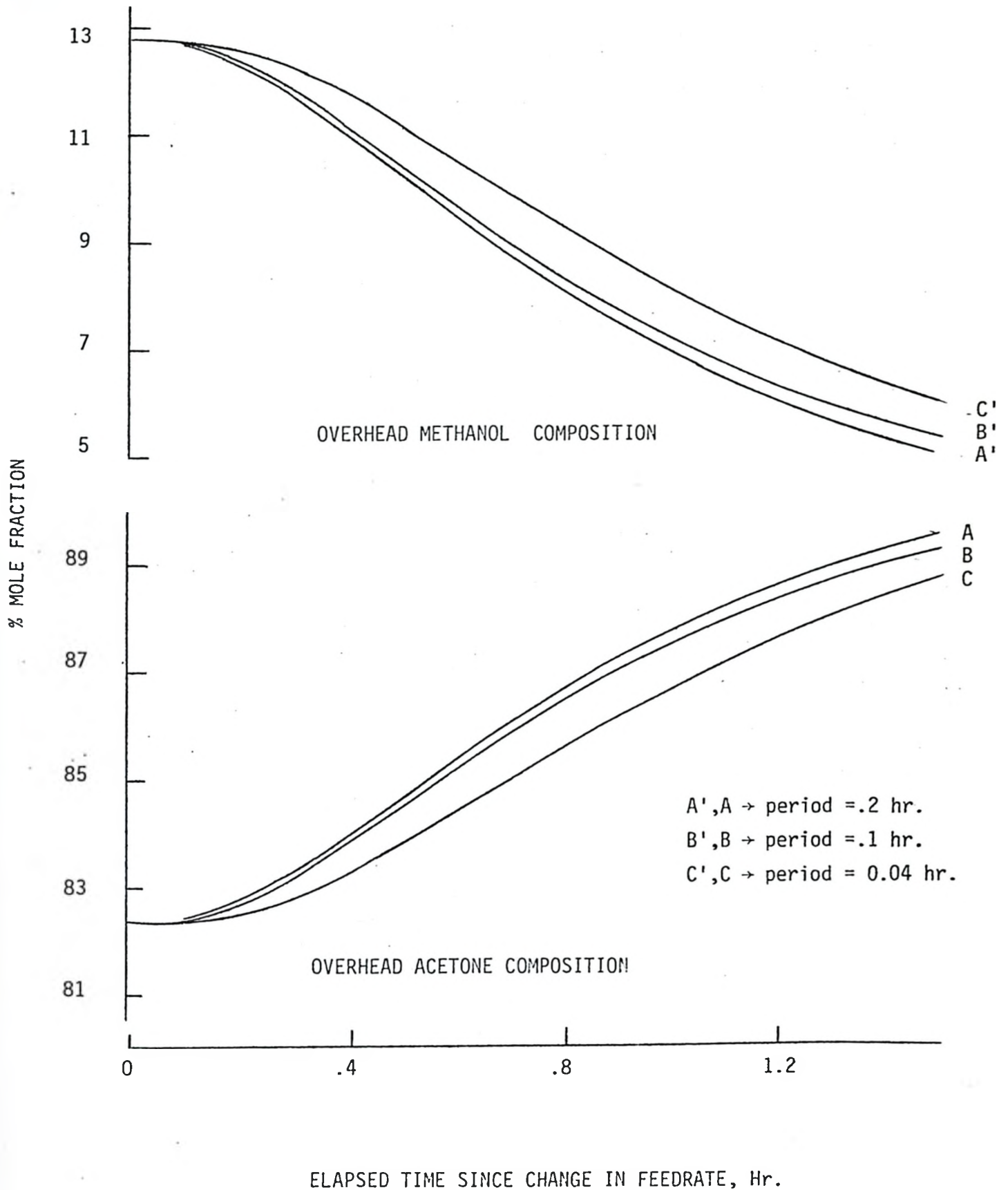
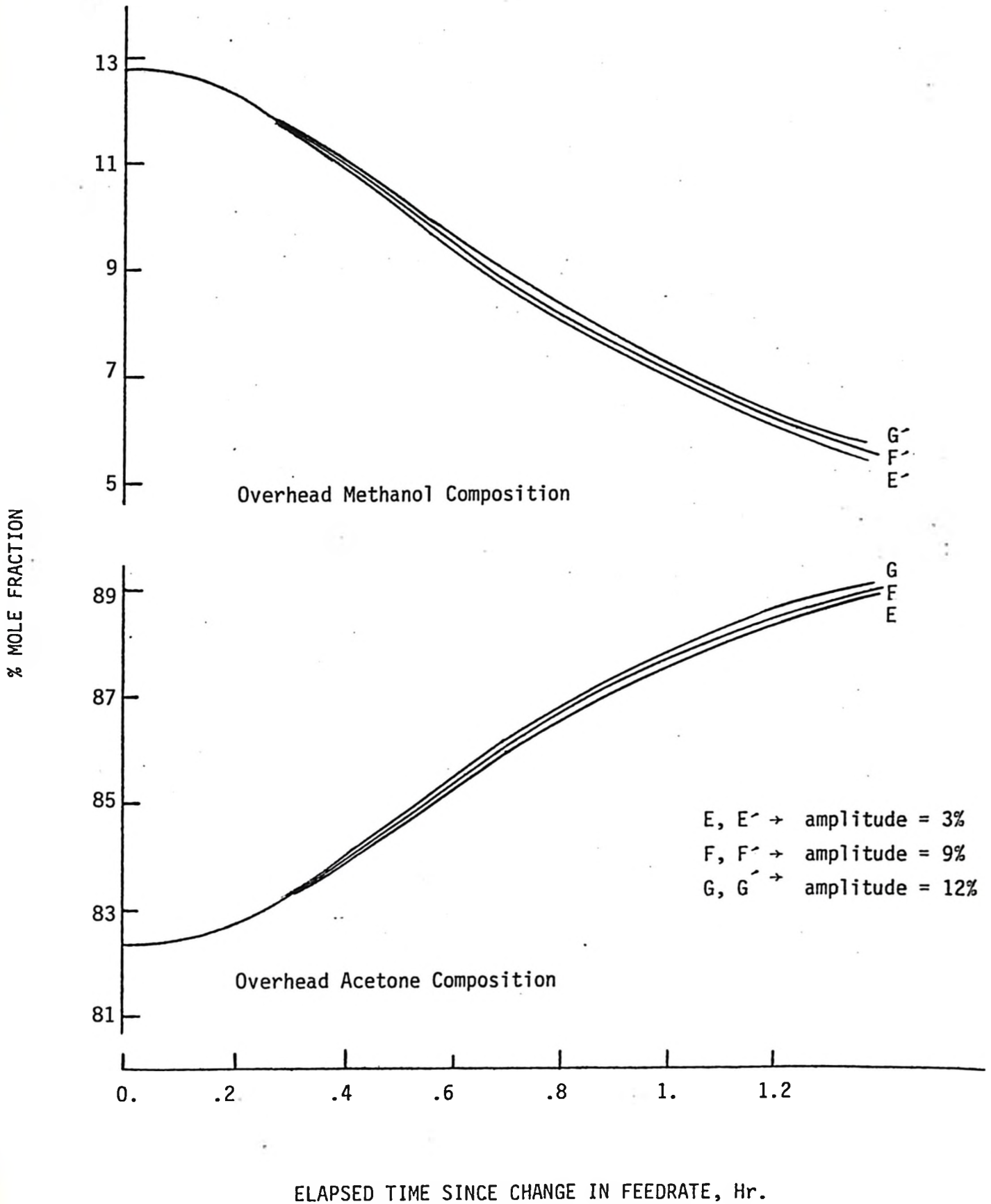


Fig. 5.1.c. Effect of Amplitude on Overhead Composition



5.3 Comparison of experimental and simulated data for the case of a square wave disturbance to the feed flowrate

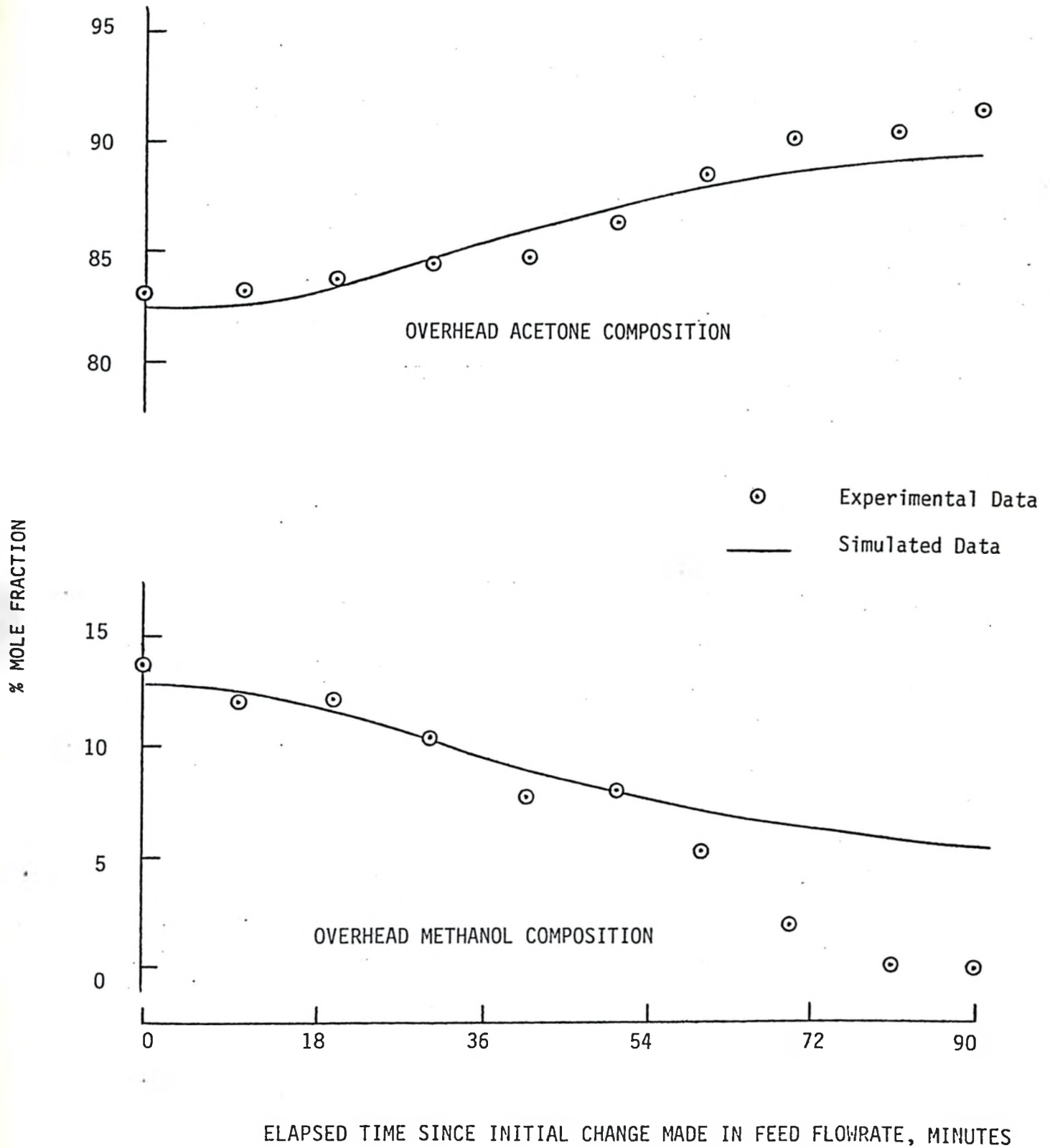
The experimental run was performed by disturbing the feed flowrate by a square wave of 12 per cent amplitude and at a period of .1 hr., through the control valve. As usual, the column was first brought to steady-state and then disturbed. Experimental conditions were presented in Appendix D. The transient response of the overhead composition was observed during a period of 1.5 hr., by taking samples every 10 minutes and analyzing with a gas chromatograph. The settings of the gas chromatograph and the integrator for the analysis can be found in Appendix E.

A comparison of the experimental data and the simulated data is presented in fig. 5.2. The following facts were observed:

(1) Experimentally, the column ceased operating at the initial steady-state level after the disturbance was put into the feed flowrate. The overhead acetone molar fraction increased in fair accordance with the simulated curve. A more detailed explanation of the response behavior by considering heat transfer, mass transfer, equilibrium, and fluid dynamics would be difficult.

(2) The experimental trend of the methanol composition agreed fairly well with the simulation during the initial period of about 1 hr., but the experiment showed that methanol almost disappeared from the overhead product at the end the response. Priming of the top trays was observed during this time. The overhead flowrate was decreasing significantly, and methanol could not reach the top due probably to tray weeping. However, water still appeared in the overhead product, which could be explained by the fact that

fig. 5.2. SQUARE WAVE DISTURBANCE TO FEED FLOWRATE



water was fed very close to the top of the column. Reboiler level increased constantly and has to be readjusted, possibly due to the fact that most of the feed was flowing down.

The simulation did not give the same results in the last section of the response since the constant holdup assumption was used throughout the simulated period of time.

It is suspected that instability of the column would have occurred if the experiment had been continued further, due to the consequences of tray weeping.

5.4 Conclusion

This chapter presented a preliminary study on the response of the column due to controlled-cycling disturbances to feed flowrate variable. The preliminary simulated results were found interesting in the sense that the efficiency seemed to improve substantially when the feed flowrate was cycled with a symmetric square oscillation.

The calculated effects of cycling the feed rate are, thus, at least qualitatively consistent with previous results found in the literature, which have shown considerable improvements in distillation column performance under oscillatory conditions. Furthermore, this work has been done on a multicomponent system as opposed to a binary system, usually mentioned in the literature. Further experimental work is needed on this effect, in particular on possible hydrodynamic instabilities introduced by the controlled-cycling of the feed flowrate (see chapter 6).

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

A mathematical model was developed to describe the dynamics of a fifteen-stage extractive distillation column using a mixture of acetone methanol and water as the solvent. The unsteady-state component material balance equations were used together with the Enthalpic Wilson equation extended to a multicomponent mixture in the equilibrium calculations. Since the fluid dynamic response of the column was rapid relative to the temperature and composition responses, a quasi-steady state assumption was made in the simulations for the step and pulse changes in feed composition, feed rate and reflux ratio variables. The technique used when the column was subject to a sudden change in the flowrate (e.g. changes in the feed flowrate variable or reflux ratio variable) consisted in satisfying, at the beginning of a change, the total tray material balances by correcting instantaneously the liquid flowrates down the column and therefore, the holdups on the trays. The comparison with available experimental data was found fairly consistent within the possible operating range of the column and showed that a reasonable simulation has been obtained from the assumptions and strategy used.

The simulation of the column was developed inside a DYNYSYS 2.1 environment which offered to the user many advantages and flexibilities, e.g. computer time savings, overhead work. Chapter 3 described the desirable features of such an approach.

The real time software developed by Jackson (11) was totally re-developed to be used with the Generalized Operating System Executive created by J.P. Tremblay (22). The new package consisted of basic data logging tasks,

unit conversion tasks, inlet temperature control tasks and inlet flowrate control tasks. A routine to perform a square wave disturbance was also available.

The rearrangement of the feed and solvent system with the addition of the control valves allows a number of possibilities for future work. One of the areas briefly investigated in this work was the study on the dynamic response of the column (overhead composition) when it was subject to controlled-cycling disturbances. A preliminary simulation study showed that the overhead composition in acetone improved significantly when the feed flowrate was disturbed by a square wave. The higher the frequency of the oscillatory disturbance, the smaller was the improvement, in the range of conditions mentioned in chapter 5. This point should be interesting for further future investigation since Lannus and Kershenbaum (33) revealed an improvement in the conversion when the inlet concentration was forced sinusoidally, in the case of a tubular reactor. Also, as stated by Friedly (34), processes which are not strictly linear can sometimes be operated better in the unsteady state than in the steady state; periodic processing takes advantage of the fact that system non linearities can make the average system output different from the steady-state values. A distillation process is one of the many non-linear systems where the non-linearity comes essentially from equilibrium relations. The effect of the amplitude of the periodic wave was also investigated and was found negligible within the operating condition range of the column.

A comparison of the simulated results with the preliminary experimental data was made in chapter 5. A fairly good agreement occurred during the first half of the response, but divergences dominated at the later times. Signs of instability were noticed experimentally, such as top tray weeping,

reduction of overhead product flowrate. Since strongly-supported experimental results were not available, the answer to the question "is instability caused by controlled-cycling disturbances in feed flowrate?" will be worth investigating later on.

The following points should be considered for future work.

- (1) As discussed in Chapter 2, the feed and solvent arrangement is very inconvenient because of the long time spent in charging the tanks through the small hole at the top. Furthermore, no feed could be added while the column is operating. The storage system should be revamped to rectify the above difficulties. Also, it is desirable that the pressures in the feed tanks and in the solvent tank can be set independently. A method of setting the desired pressure at each run is discussed in Chapter 2.
- (2) The software to control the input stream flowrates was developed. The constants of the controller could be determined by trial and error runs. Thereafter, the perturbation could be achieved with closed-loop control, in other words, just by perturbing the controller set point.
- (3) A brief review of the literature showed that unsteady-state operation of non-linear processes could improve the performance compared to the steady-state operation. This fact is of great interest for the promising results obtained by the simulation study described in Chapter 5 of this work, when the feed flowrate was disturbed by a square oscillation, and the increase in the overhead acetone composition observed. However, more experimentation must be performed to better explain and analyze the instabilities which occurred during the preliminary investigation in this project.
- (4) Since a reflux divider was used, the column, in reality, was subject to an oscillatory change in the reflux flowrate. In the simulation study on controlled-cycling changes in the feed flowrate, the frequency of the oscillation was found to affect significantly the response of the column. Therefore, the

frequency of the reflux divider cycle, which also affected, in a rigorous sense, the fluid dynamics of the column, might have an effect on the response and should be checked in future work (reflux divider period ≈ 5 sec; smallest period investigated ≈ 150 sec) of course the same reflux ratio could be achieved with different frequencies for the reflux divider cycle.

(5) It was mentioned before that the accuracy needed for a simulation model depends upon the objectives of the simulation work. However, another potential direction for further investigation of extractive distillation modeling will be the study of the effects of various assumptions on the model accuracy. As an example, constant volumetric holdup at the stages could be relaxed and the percentage inaccuracy could be analyzed.

(6) A future requirement before any significant control study can be taken will be the implementation of an on-line automatic analyzer.

An outline of the progress of this long-term project is described below:

D. Jackson (11) : - Basic process instrumentation

- Interfacing with minicomputer (Real Time Operating System, original version)

D. O'Neill (10) : - steady-state operating conditions determination

- steady-state simulation program
- preliminary study of dynamic behaviour (experimental)

Present work : - dynamic simulation for step and pulse changes in feed composition, feed flowrate and reflux ratio variables, using DYNSSYS 2.1

- Addition of control flexibility for inlet streams
- Modification of real time software to be used with GOSEX

- Preliminary dynamic and experimental study on controlled-cycling effects on column (square oscillation in feed flowrate)

Future work

anticipated

- : - Effect of reflux-divider cycling on the response of the column
- Further investigation on the effect of a square-wave disturbance in the feed flowrate (experimental and simulation studies)
- Basic assumptions checking in the model development for the extractive distillation column.

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APPENDIX A

CALIBRATION OF THE FEED AND SOLVENT LINES

Calibration curves have been obtained for the feed line and the solvent line. The pressure in the tanks was set at 15.6 psig.

For the feed line, within the possible limits of operation as determined by O'Neill (10), i.e. between 14 ml/min and 18 ml/min, the calibration curve of the feed flowrate vs the voltage read from the D.P cell, expressed in A/D units, could be described approximately a straight line, curve (2), whose equation is:

$$F = 0.1098 V - 15.7088 \quad \text{with } F \text{ in ml/min}$$

$$V \text{ in A/D units}$$

Curve (1) is the calibration curve of the valve action vs the flowrate, and could be approximated by:

$$P_F = 10.832 F^2 - 316.492 F + 2500 \quad \text{with } F \text{ in ml/min}$$

$$P_F \text{ in D/A units}$$

The same curves were obtained with the solvent line. Solvent flowrate versus the voltage from the DP cell, expressed in A/D units, is represented by curve (4) and the valve action versus the flowrate is represented by curve (3).

$$\text{for curve (4) : } S = 0.13331 V - 16.0023$$

$$\text{for curve (3) : } P_S = -5.898 S^2 + 141.457 S - 440$$

fig. A-1 CALIBRATION CURVES FOR FEED STREAMLINE

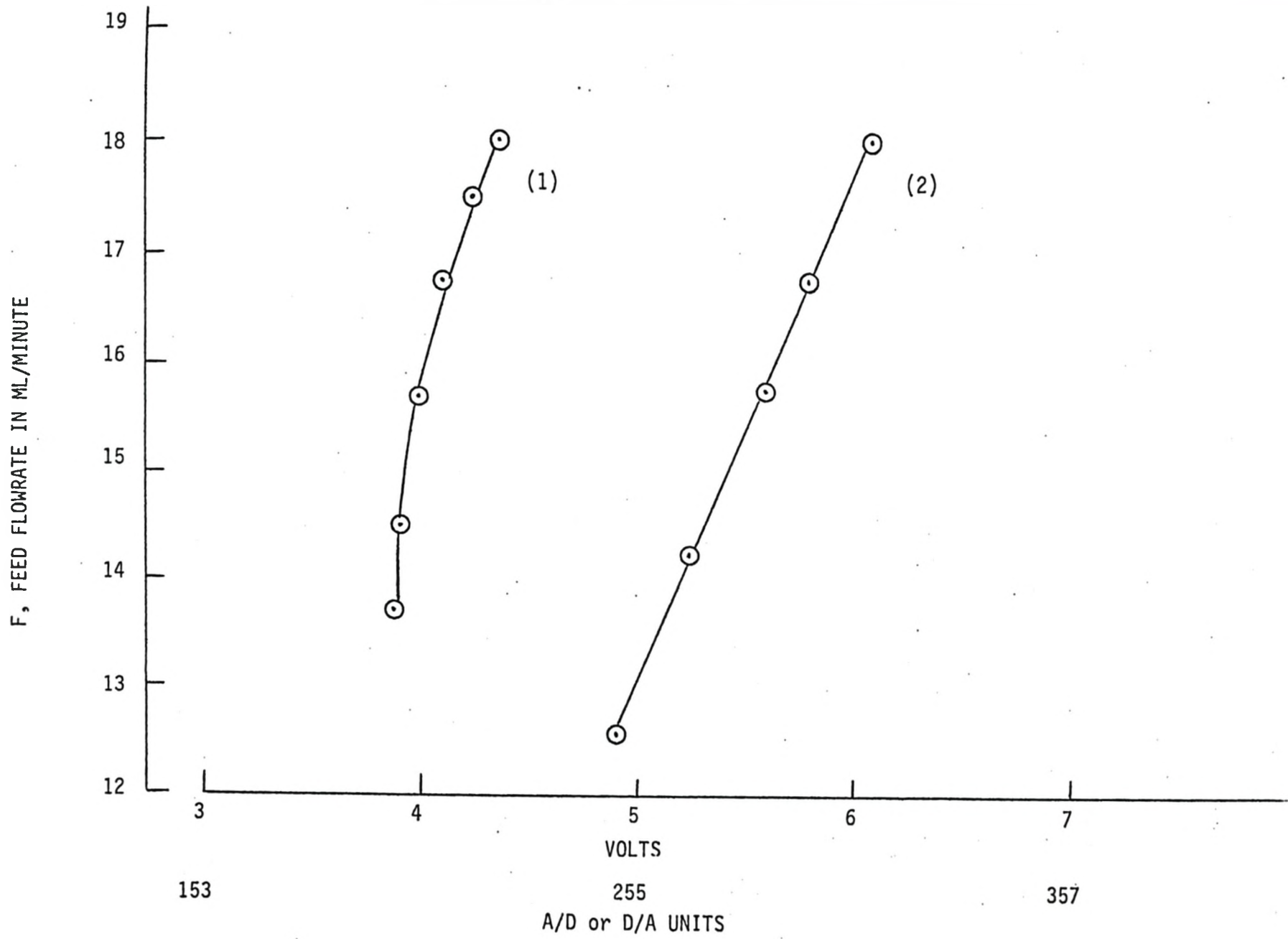
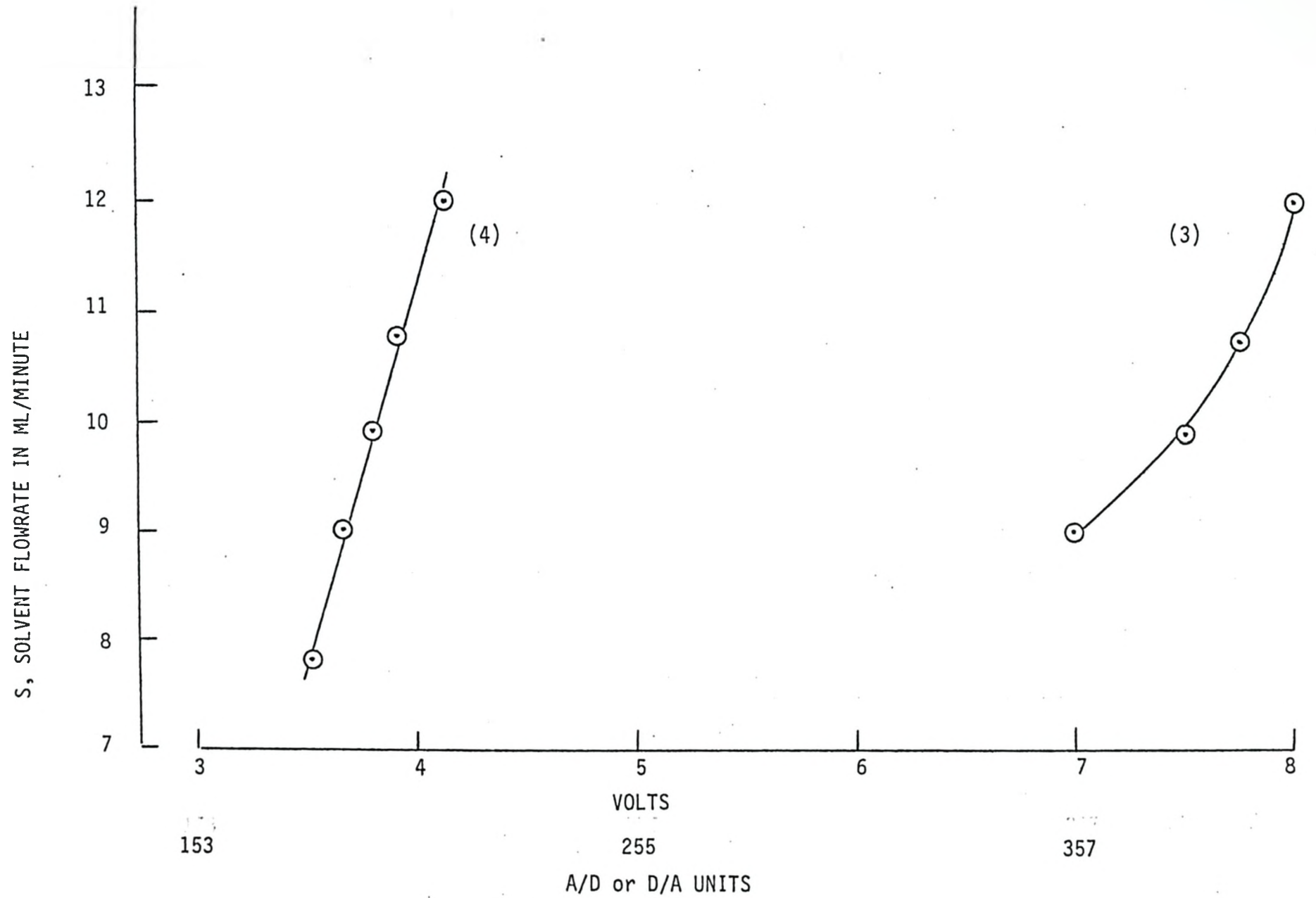


fig. A-2 CALIBRATION CURVES FOR SOLVENT STREAMLINE



- with S in ml/min

P_S in D/A units

V in A/D units

A least squares fitting technique was used.

APPENDIX BDYNSYS DATA SET1 Simulation Data

The simulation data begins with the data word "BEGIN". All cards before this are comments and are ignored by DYNSYS.

For example

IN/OUT	3.0	sets the maximum number of streams entering or leaving any module to three (default = 5)
HMAX	0.01	sets the maximum integration set size to 0.01 (default = 0.05)
TIME	3.0	sets the time of simulation to 3.0 (default = 10.0)
LIBRARY	1.0	means that one new module will be defined immediately after this card. Most common modules such as CONT1, STIR1 and VALV1 are already in a library of module names stored inside DYNSYS.
DELAY	9.0	DELAY is the new module being defined. It will be accessed as SUBROUTINE TYPE9

Other possible simulation data words are:

COMPS	X	sets the number of components to X (default = 1)
DELTAT	X	sets the initial integration step size to X (default = 0.00001)
HMIN	X	sets the minimum integration step size to X (default = 0.000001)
TOLERANCE	X	sets the error tolerance for the in- tegration to X (default = 0.001)
ORDER	X	sets the maximum permissible order of integration to X (default = 6)
NONSTIFF		causes the nonstiff option to be used (default = stiff option)
MINPIVOT	X	sets the minimum permissible pivot value for TRGB-TRGB2 to X (default = 0.000001)
PRINTING	X	causes output to be printed every X time steps (default = 1)
LINEPLOT		causes output to be printed as a line- plot (in this case additional data must be given after physical proper- ties data)
GRAPH		causes output to be printed as graph or graphs on CALCOMP plotter as well as Lineplot. LINEPLOT must also be used.

FUNCTION X causes X vectors of stream information to be read in as an input function. Stream data follows immediately.

The data word "PROCESS" signifies the beginning of the equipment data and thus the end of the simulation data.

2 Equipment Data

The data word "PROCESS" signifies the beginning of the equipment data. Here data for the various modules is written in their order of execution.

CONT1 1.0 the first module to be executed is CONT1 , referred to as module #1 in the dynamic information flow diagram.

After this, the entering and leaving stream numbers are given. A positive number indicates an input stream while a negative number indicates an output stream.

3.0 -4.0 stream 3.0 enters CONT1 and stream 4 leaves it.

The following card gives the equipment parameters for the module. This is the data which describes the individual units.

3. 1500. 1000. 2. 3.

For example, the set point for the controller is the third parameter 1000. Up to five parameters may be given. If more are required, the data word "EXTRA" X must follow and the X extra parameters appear on the following data cards.

We continue in this way for all modules. The data word "END" signifies the end of the equipment data.

3 Stream Data

The material flows between equipment are represented by material streams. Information about each stream is stored in the following vector.

position 1 - stream number
2 - flag
3 - total mass flow
4 - temperature
5 - pressure
6 - mass fraction of component 1
7 - mass fraction of component 2,
etc.

The stream flag serves the dual purpose of identifying the stream type (flags with absolute value < 10 are material flows, those > 10 are information flows) and, if negative, suppresses printing of the stream vector in the output.

The user may choose his own system of units as long as he is consistent throughout. Usually English units are employed.

STREAMS	5.	means that initial information data will be given for five streams.
EXPLICIT		means that the data will be given explicitly.

The following cards give the data. For the first stream

```
1.      1.      1000.      100.      14.7
1.
```

the stream number is 1. The stream is a material flow (the flag is less than 10). The flow rate, temperature and pressure are 1000., 100. and 14.7 respectively. There is only one component so its mass fraction is 1.0.

Data is given for five streams. The data word "END" signifies the end of the stream data.

4 Physical Properties Data

PROPERTIES -1. means that the physical properties of water are assumed.

The user may provide his own data if desired. See the DYN SYS Manual for details.

The data word "END" signifies the end of the physical properties data and in this case the end of the data set.

APPENDIX C

Francis Weir Relation Used to Calculate
the Liquid Tray Holdups

As mentioned in chapter 3, section 3.3.1 the assumption of constant volumetric holdup on the trays was made.

From the steady state simulation program, one can obtain the initial liquid molar flowrates leaving each stage. These flowrate values have been used with the Francis Weir relation to determine the initial volumetric holdups which will be kept constant throughout the dynamic simulation in this work. As described in reference 19 of Luyben, the liquid flowrate F_L is proportional to the weir length WL and to the overflow height h raised to a power of 1.5:

$$F_L = a (WL)(h)^{1.5}$$

By rearranging

$$h = \left(\frac{1}{a} \frac{F_L}{WL} \right)^{2/3}$$

with $a = 11988$

F_L in ft^3/hr , liquid flowrate
leaving the tray.

WL in ft, weir length.

h in ft, overflow height of tray
holdup.

The holdup height was then calculated:

$$H = h + WH$$

WH in ft, weir height

The volumetric holdup could be then obtained.

APPENDIX D

Run with Square Wave as Input Disturbance
in Feed FlowrateOperating conditions

Feed rate:	high level	=	18 ml/min.
	low level	=	16 ml/min.
	period of oscillation	=	6 min.
Feed composition:	60% mole acetone		
	40% mole methanol		
Solvent rate:	9.5 ml/min.		
Solvent composition:	pure water		
Reflux ratio:	1.772		
Solvent temperature:	65°C		
Feed temperature:	40°C		
Feed variac setting:	15		
Solvent variac setting:	27		
Reboiler variac setting:	70		

APPENDIX E

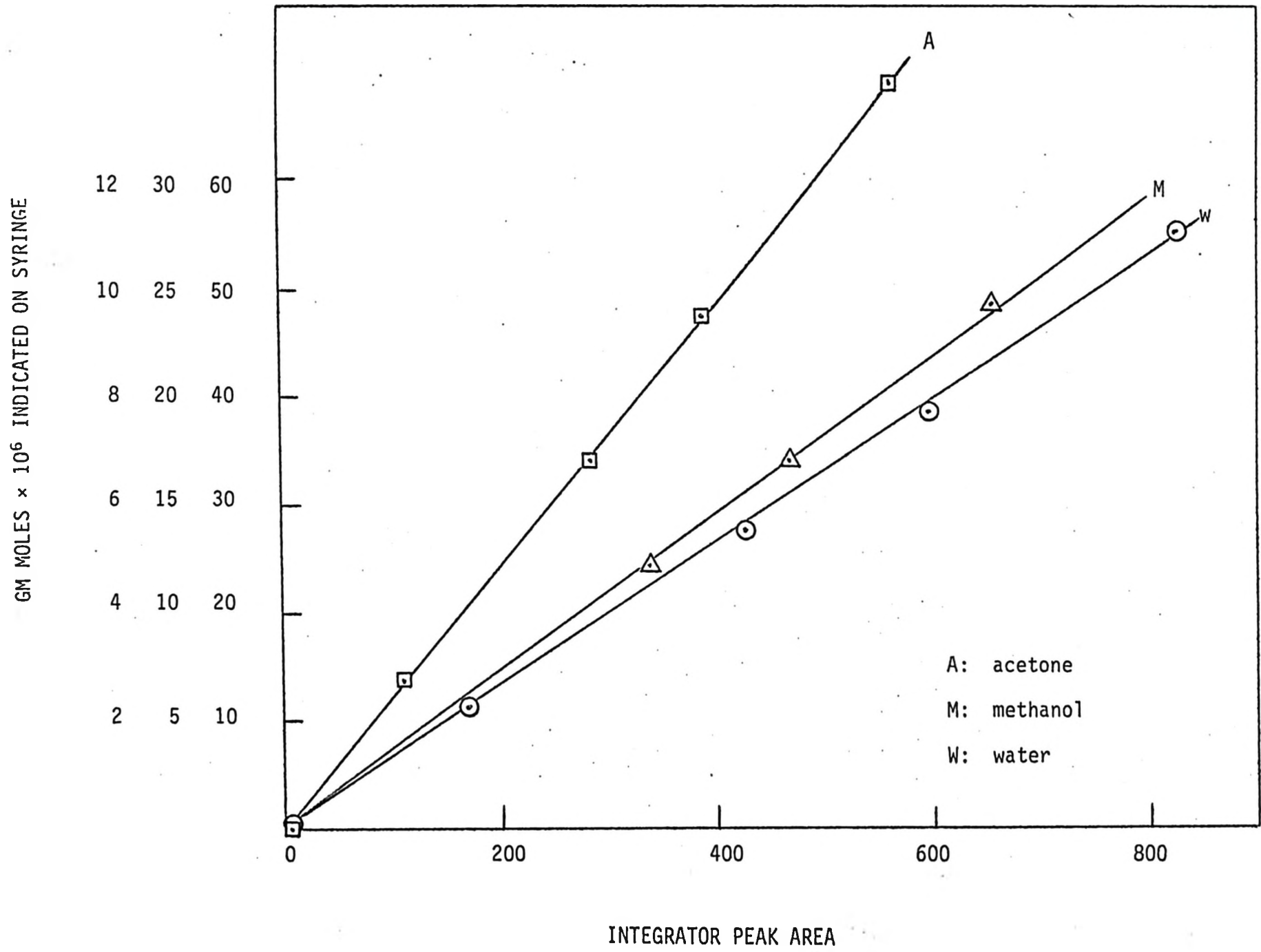
Gas Chromatograph and Integrator SettingsGas Chromatograph Varian 90-P3

- column - 6' x 1/4" O.D. stainless steel tube
 - Porapak Q, 80 mesh, packing
- carrier gas - Helium @ 65 psig
 - carrier flowrate = 60 ml/min.
 - reference flowrate = 20 ml/min.
- dial settings - column power = 55
 - detector power = 45
 - injector power = 50
 - attenuator = 1
- operating temperatures - column - 175°C
 - detector - 240°C
 - injector - 216°C
 - collector - 212°C

Integrator Hewlett-Packard 3370B

- settings - noise suppression - maximum
 - slope sensitivity - up = 0.03
 - down = 0.03

A M W



- B.L. reset delay = 0.5 minutes
- area threshold = 100
- shoulder control - front - on
 - rear = 100 mV

APPENDIX F

Dynamic Simulation Programs

A number of utility routines have been developed to assist the dynamic simulation in this work.

- ENTHV: this function calculates the enthalpy of a vapor stream at a specified temperature, pressure and composition
- ENTHL: this function calculates the enthalpy of a liquid stream at a specified temperature, pressure and composition, for the mixture of acetone-methanol-water, taking into account the heat of mixing of the components
- ACTY: this function calculates the coefficient of activity of each component in a mixture of three component using the enthalpic Wilson equation extended to multicomponent mixtures, as described in section 3.3.2.2.
- KVAL: this function calculates the activity of each component in a mixture of components, as described in section 3.3.2.2.

The listings of the above utility programs and the main subroutine Type 1 are presented on the following pages.

STREAM DATA

S(, ,1) STREAM NUMBER
 S(, ,2) STREAM FLAG
 S(, ,3) TOTAL MOLAR FLOW (GMOLES/HR)
 S(, ,4) TEMPERATURE (OC)
 S(, ,5) PRESSURE (MM HG)
 S(, ,6) MOLE FRACTION ACETONE
 S(, ,7) MOLE FRACTION METHANOL
 S(, ,8) MOLE FRACTION WATER

SYSTEM STORAGE SPACE

REAL MH
 COMMON/MAT/MP(5,8),EP(5,5),S(2,50,10),EX(100)
 COMMON/CON/IG, NCOMP, NC5, H, NE, NS, NPR, NPOL, TMAX, IORDER, NGRAPH
 COMMON/UNIT/IM, NMP
 COMMON/GEAR2/EPS, TIME, KFLAG, JSTART, NBVMAX, ICONV, ISTIFF
 COMMON/MODULE/IDERY, ITER, ITRI, MC, IPIVOT
 COMMON/SUBDI/A(50)
 COMMON/DIAG/B(50)
 COMMON/SUPERD/C(50)

SUBROUTINE STORAGE SPACE

DIMENSION VHUP(20), HUP1(20)
 DIMENSION ETHBAL(20), VOIF(20)
 DIMENSION Y(100), DERY(100)

SECTION 1

INITIATION AND PARAMETER CALCULATION

USE NEWTON-RAPHSON ITERATION WITH STIFF OPTION(ITER=1)

ITER=1
 IF(JSTART .NE. 0 .OR. IG .EQ. 1) GO TO 200

TRANSFER INFORMATION INTO SUBROUTINE SPACE

VHUP(15)	REBOILER VOLUMETRIC HOLDUP
VHUP(1)	CONDENSER VOLUMETRIC HOLDUP
WH	WEIR HEIGHT
WL	WEIR LENGTH
DIA	TRAY DIAMETER
RR	REFLUX RATIO
NT	TOTAL NUMBER OF TRAYS
NFT	FEED TRAY
NST	SOLVENT TRAY


```

..
DO 27 IK=J,NT
S(2,IK+20,3)=S(2,IK+20,3)+BAL
27 CONTINUE
17 CONTINUE
C
C CHECK FOR CONDENSER
C
S(2,16,3)=S(2,2,3)/(PR+1.)
BAL=S(2,2,3)-S(2,16,3)-S(2,21,3)
DO 37 IK=1,NT
37 S(2,IK+20,3)=S(2,IK+20,3)+BAL
CONTINUE
C
C CALCULATION OF INITIAL HOLD UP USING THE FRANCIS WEIR RELATION
C GIVEN THE INITIAL LIQUID FLOW RATE FROM EACH TRAY
C START CALCULATION FROM THE BOTTOM(EXCLUDING THE REBOILER AND T
C CONDENSER
C
NTM2=NT-2
DO 1 II=1,NTM2
I=NT-II
III=I+20
P=MW(IG,III)
Q=DENS(IG,III)
C
C CALCULATE THE OVERHEIGHT(IN FEET)
C
FLOW =S(IG,III,3)*P/Q*3.5314*.00001
H=(FLOW /11988./WL)**.66667
HH=H+WH
C
C CALCULATE THE MOLAR HOLD UP(IN GMOLES)
C
VHUP(I)=HH*30.48*TAREA
HUP1(I)=VHUP(I)*Q/P
1 CONTINUE
C
C TRANSFER THE VARIABLES INTO WORKING AREA FOR INTEGRATION
C
DO 5 I=1,NT
II=I+20
C MOLE FRACTION ACETONE
NN=NT+1-I
Y(NN)=S(IG,II,6)
C MOLE FRACTION METHANOL
N=NN+NT
Y(N)=S(IG,II,7)
5 CONTINUE
DO 30 I=3,8
S(1,17,I)=S(IG,17,I)
S(1,18,I)=S(IG,18,I)
30 CONTINUE
C
200 CONTINUE
C

```



```

C
C
300 CONTINUE
ITRI=1

C
C
C SECTION 3
C CALCULATION OF THE DERIVATIVES
C THIS SEGMENT OF PROGRAM APPLIES FOR THE CASE OF 3 COMPONENT SYSTEM
C
C
DO 20 I=2,NTM1
N=NT+1-I
IF(N.EQ.NFT)GO TO 21
IF(N.EQ.NST)GO TO 22
C FOR NORMAL TRAY
ADD4=0.
ADD5=0.
ADD6=0.
GO TO 23
21 CONTINUE
C FOR FEED TRAY
ADD4=S(IG,18,3)
ADD5=S(IG,18,3)*S(IG,18,6)
ADD6=S(IG,18,3)*S(IG,18,7)
GO TO 23
22 CONTINUE
C FOR SOLVENT TRAY
ADD4=S(IG,17,3)
ADD5=S(IG,17,3)*S(IG,17,6)
ADD6=S(IG,17,3)*S(IG,17,7)
GO TO 23
23 CONTINUE
C VARIATION OF ACETONE COMPOSITION
LL TRANSFER STATEMENT -- TRANSFER IGNORED
L1=I
DERY(L1)=(-S(IG,N,3)*S(IG,N,6)+S(IG,N-1+20,3)*Y(L1+1)+
1S(IG,N+1,3)*S(IG,N+1,5)-Y(L1)*(-S(IG,N,3)+S(IG,N-1+20,3)+S(IG
1,N+1,3)+ADD4)+ADD5)/HUP1(N)
C VARIATION OF METHANOL COMPOSITION
L2=15+I
DERY(L2)=(-S(IG,N,3)*S(IG,N,7)+S(IG,N-1+20,3)*Y(L2+1)+
1S(IG,N+1,3)*S(IG,N+1,7)-Y(L2)*(-S(IG,N,3)+S(IG,N-1+20,3)+S(IG
1,N+1,3)+ADD4)+ADD6)/HUP1(N)
GO TO 20
20 CONTINUE

C
C
C VARIATION OF THE MOLE COMPOSITION AT THE REBOILER
LL TRANSFER STATEMENT -- TRANSFER IGNORED
DERY(1)=(-S(IG,15,3)*S(IG,15,6)+S(IG,34,3)*Y(2)-S(IG,35,3)*
1Y(1))/ (VHUP(15)*DENS(IG,35)/MW(IG,35))
DERY(16)=(-S(IG,15,3)*S(IG,15,7)+S(IG,34,3)*Y(17)-S(IG,35,3)*
1Y(16))/ (VHUP(15)*DENS(IG,35)/MW(IG,35))

C
C
C VARIATION OF THE MOLE COMPOSITION AT THE CONDENSER

```

```

C
C
  DERY(15)=(S(IG,2,3)*(S(IG,2,6)-Y(15)))/(VHUP(15)*
1DENS(IG,21)/MW(IG,21))
  DERY(30)=(S(IG,2,3)*(S(IG,2,7)-Y(30)))/(VHUP(15)*
1DENS(IG,21)/MW(IG,21))
C
C
  SECTION 4
INTEGRATE
  CALL DIFSUB(NEQ,Y,DERY)
  IF(IDERY .NE. 0) GO TO 300
C
C
  SECTION 5
OUTPUT MANIPULATIONS
C
C
  MANIPULATION 1
TRANSFER VARIABLES INTO SYSTEM STORAGE
997 CONTINUE
  DO 8 I=1,NT
  II=I+20
  NN=NT+1-I
  S(1,II,6)=Y(NN)
  N=NN+NT
  S(1,II,7)=Y(N)
  S(1,II,8)=1.-Y(NN)-Y(N)
  8 CONTINUE
  DO 31 I=1,35
  DO 32 J=4,5
  S(1,I,J)=S(IG,I,J)
  32 CONTINUE
  31 CONTINUE
C
C
  MANIPULATION 2
CALCULATION OF THE MOLECULAR HOLD UP
  DO 43 II=1,NTM2
  I=NT-II
  III=I+20
  P=MW(1,III)
  Q=DENS(1,III)
  HUP1(I)=VHUP(I)*Q/P
  43 CONTINUE
C
C
  MANIPULATION 3
CALCULATION OF THE COMPOSITION OF THE VAPOR LEAVING EACH TRAY
AT THE REBOILER
  III=NT
  II=NT+20
  DUM=EQUIL(1,II,III)
  TRUE SEPARATION AT REBOILER
  S(1,III,7)=EX(MP(IH,NMP+1)+NT-1)*S(1,III,7)+S(1,II,7)*(1.-
1EX(MP(IH,NMP+1)+NT-1))

```



```

      HVOUT=ENTHV(1 , III)
      IF(III.EQ.NFT) GO TO 87
      IF(III.EQ.NST) GO TO 81
C
80  NORMAL TRAY
      CONTINUE
      ADD=0.
      GO TO 82
C
C  FOR FEED AND SOLVENT TRAYS
C
87  CONTINUE
      ADD=S(1 , 18, 3)*ENTHL(1 , 18)
      GO TO 82
81  CONTINUE
      ADD=S(1 , 17, 3)*ENTHL(1 , 17)
      GO TO 82
82  CONTINUE
ULL TRANSFER. STATEMENT -- TRANSFER IGNORED
      ETHBAL(III)=S(IG, III+1, 3)*HVIN+S(IG, II-1, 3)*HLIN-S(IG, II, 3)
      1*HLOUT-S(IG, III, 3)*HVOUT +ADD
      VDIF(III)=ETHBAL(III)/(HVOUT-HLOUT)
C
C  REINITIATE FOR NEXT TRAY CALCULATION
C
      HVIN=HVOUT
      HLOUT=HLIN
      3  CONTINUE
C
C  VAPOUR FLOWPATES
C
      TVAP=0.
      DO 33 I=1, NTM1
      III=NT+1-I
      TVAP=TVAP+VDIF(III)
      S(1, III, 3)=S(IG, III, 3)+TVAP
33  CONTINUE
C
C  . FOR THE CONDENSER
      S(1 , 16, 3)=S(1 , 2, 3)/(RR+1.)
      TLIQ=S(1, 2, 3)-S(1, 16, 3)-S(IG, 21, 3)
      S(1, 21, 3) =S(1, 21, 3)+TLIQ
      TVAP=TLIQ
      DO 34 I=2, NT
      TVAP=TVAP-VDIF(I)
      S(1, I+20, 3)=S(IG, I+20, 3)+TVAP
34  CONTINUE
C
C
105  RETURN
      CONTINUE
      PRINT 500
500  FORMAT(10X, '*****ERROR AT REBOILER*****')
      STOP
      END

```

FUNCTION ACTY(IG,IS)

THIS PROGRAM CALCULATES THE COEFFICIENT OF ACTIVITY OF EACH COMPONENT IN A ACETONE-METHANOL-WATER MIXTURE, USED WITH DYNYSYS 2.1

```

COMMON/MAT/MP(5,8),EP(5,5),S(2,50,10),EX(100)
COMMON/PTAB/IGFLAG,PP(10,20)
COMMON /CON/ IU, NCOMP, NC5, H, NE, NS, NPR, NPOL, TMAX, IORDER, NGRAPH
COMMON/KVALU/HKK(10)
DIMENSION A(3),B(3),C(3),AA(3),BB(3),CC(3),X(3),GAM(3,3)
1 ,ACT(3),LAM(3,3),Y(3),V(3),VV(3),Y2(3)
DIMENSION ALP(3,3),ALP1(3,3,3),SUMGX(3)
REAL LAM
DATA AA/56.8622,21.795,22.8876/,BB/8.4555E-3,4.9507E-2,-3.642E-2/,
1 CC/1.65E-4,5.68E-5,6.856E-5/
LAM(1,2)=-216.966
LAM(2,1)=506.093
LAM(1,3)=-436.468
LAM(3,1)=1185.436
LAM(2,3)=-208.7681
LAM(3,2)=571.3078
ENTHALPIC WILSON EQUATION TO PREDICT VAPOUR MOL FRACTION IN EQUILIBRIUM
WITH GIVEN LIQUID CONCENTRATION
BINARY COEFFICIENTS FOR WILSON EQUATION, VAPOUR PRESSURE ANTOINE
COEFFICIENTS AND LIQUID MOLAR VOLUMES FROM
ACETONE -1, METHANOL -2, WATER -3
TK=S(IG,IS,4)+PP(1,20)
ACTY=0.

CALCULATE THE GAMMA#S BY (15-B)

DO 20 J=1,3
GAM(J,J)=1.
DO 10 I=1,3
IF(I.EQ.J) GO TO 10
FC=EXP(-LAM(I,J)/(1.987*TK))
V(J)=AA(J)+(BB(J)+CC(J)*TK)*TK
VV(I)=AA(I)+(BB(I)+CC(I)*TK)*TK
GAM(I,J)=V(J)/VV(I)*FC
10 CONTINUE
20 CONTINUE

READ IN THE PROPERTIES OF THE STREAMS

DO 70 I=6,NC5
N=I-5
X(N)=S(IG,IS,I)
70 CONTINUE
DO 107 I=1,3
SUMGX(I)=0.0
DO 101 IP=1,3
101 SUMGX(I)=SUMGX(I)+GAM(I,IP)*X(IP)
107 CONTINUE
DO 102 I=1,3
DO 102 J=1,3
102 ALP(I,J)=1.0+X(I)*(1.0-1.0/SUMGX(I)-GAM(J,I)/SUMGX(J))
DO 106 I=1,3
DO 105 J=1,3
IF(I.EQ.J) GO TO 105
DO 103 M=1,3
IF(M.EQ.I .OR. M.EQ.J) GO TO 103
ALP1(I,J,M)=1.0-GAM(J,I)/SUMGX(J)-GAM(M,I)/SUMGX(M)
103 CONTINUE
105 CONTINUE
106 CONTINUE
DO 60 I=1,3
SUM1=0.0

```

```

DO 30 J=1,3
SUM1=SUM1+X(J)*ALOG(GAM(I,J)*GAM(J,I))*ALP(I,J)/(SUMGX(I)*SUMGX
1 (J))
30 CONTINUE
SUM2=0.0
DO 50 M=1,3
IF(M.EQ.I) GO TO 50
DO 55 J=1,3
IF(J.EQ.I .OR. J.EQ.M) GO TO 55
SUM2=SUM2+X(J)*X(M)*ALOG(GAM(J,M)*GAM(M,J))*ALP1(I,J,M)/
1 (SUMGX(J)*SUMGX(M))
55 CONTINUE
50 CONTINUE
PP(I,9)=EXP(-SUM1-SUM2)
60 CONTINUE
RETURN
END

```

REAL FUNCTION KVAL(IG,IL,IV)

THIS PROGRAM CALCULATES THE ACTIVITY OF EACH COMPONENT IN A MIXTURE

```

COMMON/MAT/MP(5,8),EP(5,5),S(2,50,10),EX(100)
COMMON/CON/IU, NCOMP, NC5, H, NE, NS, NPR, NPOL, TMAX, IORDER, NGRAPH
COMMON/PTAB/IGFLAG, PP(10,20)
COMMON/KVALU/HKK(10)
DUMMY STATEMENT
KVAL=0.0
T=S(IG,IL,4)+PP(1,20)
P=S(IG,IL,5)
DUM=ACTY(IG,IL)
DO 1 I=1, NCOMP
HKK(I)=10.**((PP(I,6)-PP(I,7)/(PP(I,8)+T-273.))*PP(I,9)/P
1 CONTINUE
RETURN
END

```

FUNCTION ENTHV(IG,IS)

ETV

THIS PROGRAM CALCULATES THE ENTHALPY OF A VAPOUR MIXTURE, USED WITH DYNYSYS 2.1

```

COMMON/MAT/MP(5,8),EP(5,5),S(2,50,10),EX(100)
COMMON/CON/IU, NCOMP, NC5, H, NE, NS, NPR, NPOL, TMAX, IORDER, NGRAPH
COMMON/PTAB/IGFLAG, PP(10,20)
T=S(IG,IS,4)
HV=0.
DO 10 I=1, NCOMP
HV=HV+S(IG,IS,I+5)
K K +((((((PP(I,15)*T+PP(I,14))*T+PP(I,13))*T
+PP(I,12))*T+PP(I,11))*T+PP(I,10))
ENTHV=HV
RETURN
END

```

FUNCTION ENTHL(IG,IS)

THIS PROGRAM CALCULATES THE ENTHALPY OF A LIQUID MIXTURE
OF ACETONE-METHANOL-WATER, USED WITH DYNYSYS 2.1

COMMON/HAT/MP(5,8),EP(5,5),S(2,50,10),EX(100)
COMMON/CON/IU,NCOMP,NC5,H,NE,NS,NP,NPOL,TMAX,IORDER,NSGRAPH
COMMON/PTAB/IGFLAG,PP(10,20)
DIMENSION X(3)
HACEL(T)=30.6E-3*T
HMETL(T)=19.74E-3*T
HWATL(T)=18.016E-3*T

FORMULATION OF HEAT OF MIXING
THE PARAMETERS ARE GIVEN BY A LEAST SQUARE FITTING

HMI XWA(XC)=-6.00506E-3+0.368503*XC-2.1499*XC**2+5.30655*XC**3
1-3.50732*XC**4
HMI XMA(XC)=2.01772E-3-0.753418*XC+0.94409*XC**2-0.192395*XC**3
HMI XWM(XC)=6.05874E-3+0.171893*XC+0.646148*XC**2-0.813034*XC**3

SET THE NECESSARY VARIABLES FROM THE STREAMS

T=S(IG,IS,4)
DO 10 I=1,3
II=I+5
X(I)=S(IG,IS,II)
CONTINUE
ENTHL=HACEL(T)*X(1)+HMETL(T)*X(2)+HWATL(T)*X(3)
IF(X(1).EQ.1. .OR.X(2).EQ.1..OR.X(3).EQ.1.) GO TO 1
X1B=X(1)+X(2)
X1A=X(2)/X1B
X2B=X(3)+X(2)
X2A=X(3)/X2B
X3B=X(3)+X(1)
X3A=X(3)/X3B
ENTHL=ENTHL-X1B*HMI XMA(X1A)-X2B*HMI XWM(X2A)-X3B*HMI XWA(X3A)
CONTINUE
RETURN
END

APPENDIX G

Distillation Control Programs

The control software of the extractive distillation column has been developed under the GOSEX created by J.P. Tremblay (22). The minicomputer NOVA/2 in the Chemical Engineering computer room was equipped with necessary peripheral devices (A/D converter, D/A converter, relays, contact sense, one operator console and one data logging line printer) and could be used to run the column.

The user must provide:

- (1) a symbol table to facilitate duties as parameter change, variable logging...
(SYMBOL OF TAPE #2 OF 2)
- (2) a disk file containing user messages (MESSG.TR)
- (3) user control programs (INFCE, FSCON, SWAVE, SSAMP)

The listings are presented on the following pages with explanations.

The listings of GOSEX parameter tape, symbol table and executive message file (see reference 22) are also presented.

A loading map could be found at the end of Appendix G, and the loading procedure is detailed in reference 22.

INFCF

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```

      .TITL INFCF
      ; INTERFACE TO THE GOSEX EXECUTIVE
      ; DECEMBER, 1975
      ; MCMASTER UNIVERSITY
      ; CHEMICAL ENGINEERING DEPARTMENT
      ;
      ;
      . ENT OVLAY, ALARM, DATUM, RELAY, SENSE
      . ENT SCAN, CLOOP, SUPRS, TASKS, UDEF
      . EXTN FEEFT, SOLFT
      . EXTN SOLFM, SOLVB, FEEFM, FEEFB
      . EXTN FEETC, SOLTC
      . EXTN TRAP, SSAMP
      . EXTD TIMER
000001 . TXTM 1
      . NREL
      ; OVERLAY FILENAME DEFINITION
000'000002"OVLAY: . +1*2
      . TXT @DISTIL.OL@
001'042111
002'051524
003'044514
004'027117
005'046000
      ; ALARM TABLE DEFINITION
006'000010 ALARM: 10 ; # OF ALARMS IN TABLE
      . BLK 10
      000010 . BLK 10
      000012 DATUM: . BLK ATODS ; A/D CHANNELS
      000012 RELAY: . BLK RLAYS ; RELAYS
0033'177777 SENSE: TRAP
0044'000043' TRAP
0055'000044' TRAP
0066'000045' TRAP
0077'000046' TRAP
0088'000047' TRAP
0099'000048' TRAP
0100'000049' TRAP
0111'000050' TRAP
0122'000051' TRAP
0133'000052' TRAP
0144'000053' TRAP
      ; MULTIFLEXER SCAN RATE
0155'000002 SCAN: 2 ; 2 TIMES PER SECOND
      ; PID CONTROL LOOP DEFINITION
0166'177777 CLOOP: SOLFM ; SOLVENT LOOP
0177'177777 SOLVB
0188'177777 FEEFM ; FEED LOOP
0199'177777 FEEFB
0200'100000 IBO
      ; USER SHUTDOWN ROUTINE
0211'054407 SUPRS: STA 3 . +7
0222'126420 SUBZ 1 1 ; ZERO AC1
0233'044752 STA 1 RELAY+6 ; TURN OFF FEED HEATER
0244'044750 STA 1 RELAY+5 ; TURN OFF SOLVENT HEATER
0255'024001 LDA 1 TIMER ; WAIT FOR RELAYS TO BE SET
0266'006017 . SYSTEM
0277'010400 . DELAY
0288'000000 0
0299'002777 JMP @ -1
      ; USER TASK DEFINITION TABLE
0300'177777 TASKS: FEETC ; FEED TEMP. MONITOR

```

```

IINPCE
50000110      110      ; PRIORITY
60000100      100      ; IDENTIFICATION
70000000      180
00177777      SOLTD    ; SOLVENT TEMP MONITOR
10000110      110
20000110      110
30000000      180
40000056      SOLFM    ; SOLVENT RATE MONITOR
50000110      110
60000120      120
70000000      180
00000060      FEEFM    ; FEED RATE MONITOR
10000110      110
20000130      130
30000000      180
40177777      SSAMP    ; SAMPLING MONITOR(OVERHEAD AND BOTTOM)
50000110      110
60000140      140
70000000      180
00177777      FEEFT    ; SQUARE WAVE IN FEED RATE ROUTINE
10000110      110
20000150      150
30000000      180
40177777      SOLFT    ; INPUT FLOWRATES SETTING ROUTINE
50000110      110
60000160      160
70000000      180
00100000      180
00000000 UDEF:  0
                .END

```

```

TITL F$CON
; CONTROL PROGRAM HAS 4 TASKS
; FEETC
;
; ON/OFF CONTROL OF FEED TEMPERATURE
; AND CONVERT DATA TO ENG UNITS
; FNOFF CONTROL PERIOD
; FTSET SET POINT
;
;
; SOLTC
;
; ON/OFF CONTROL OF SOLVENT TEMPER
; AND CONVERT DATA TO ENG UNITS,
; ALSO CONVERT 3 OTHER TEMP READ-
; INGS TO ENG UNITS
; SNOFF CONTROL PERIOD
; STSET SET POINT
;
;
; SOLFM
;
; PID CONTROL FOR SOLVENT RATE
; AND CONVERSION OF DATA INTO ENG UNITS
;
; FEERM
;
; PID CONTROL FOR FEED RATE AND
; CONVERSION OF DATA INTO ENG UNITS
;
;
; DECEMBER, 1975
; MCMASTER UNIVERSITY
; CHEMICAL ENGINEERING DEPARTMENT
;
;
; ENT SOLFM, SOLVB, FEERB, FEERM
; ENT FEETC, SOLTC
; ENT FNOFF, FTSET, ADFTC, FTEMP
; ENT SNOFF, STSET, ADSTE, STEMP
; ENT FLOW, OFEAF, FFOON
; ENT SLOW, OFERS, SFOON
; EXTN CONTC, GUAD, ONVRS, NTPLY
; ENT CONVB, ADT
; EXTN LNEAR, LNVRB
; EXTD TIMER
; ENT FEETB, SOLTB
; ENT OUTBS, OUTBF
; NREL
;
; FEED TEMPERATURE CONTROL ROUTINE
;
00'034434 FEETC LDA 3 FEETB-1
01'054016 STA 3 USR
02'026427 LDA 1 @OUTUM4
03'022427 LDA 0 @OUTUM5
04'106400 SUB 0 1
05'044420 STA 1 ADFTC
06'020447 LDA 0 ACORB
07'006424 JSR @AGUAD
08'050437 LDA 2 AGNT
09'045004 STA 1 4 2
10'020414 LDA 0 FTSET
11'030414 LDA 2 FHSW
12'024411 LDA 1 ADFTC
13'122433 SUBZ# 1 0 SMC
14'152400 SUB 2 2
15'052411 STA 2 @RLWF
16'024403 LDA 1 FNOFF
17'006017 SYSTM
18'010400 DELAY

```

```

; GET RAW FEED TEMP READING
; GET REFERENCE READING
; A/D-AVD REFERENCE
; STORE FEED TEMP (IN A/D UNITS)

```

```

; GET SET POINT TEMP
; GET RELAY SWITCH WORD
; GET FEED TEMP
; SKIP IF TEMP <= SET POINT TEMP

```

```

; INSTALL RELAY WORD
; GET WAIT PERIOD

```



```

FSDON
23'000764 FNOFF: 500
24'000756 JMP FEETC+2

25'000000 ADFTE: 0
26'000000 FTSET: 0
27'001000 FHSW: 1000
    000003 RLWF: GADD RELAY, 3
    000004 DTUM4: GADD DATUM, 4
    000005 DTUM5: GADD DATUM, 5
33'177777 @AQUAD: @AQUAD
34'000035 FEETB: FEETB
    000012 FEETB: .BLK 10..
47'000050 AENT: ENTAB
50'000000 ENTAB: 0
51'000000 0
52'000000 0
53'000000 STEMP: 0
54'000000 FTEMP: 0
55'000056 ACONB: CONVB
56'175710 CONVB: -1080.
57'076272 +31930.
60'000000 +0

```

; BIT 6

; TABLE IN ENG. UNITS

; SOLVENT TEMPERATURE ROUTINE

```

61'034470 SOLTC: LDA 3 SOLTB-1
62'054016 STA 3 USF
63'026447 LDA 1 @DTUM3
64'022746 LDA 0 @DTUM5
65'106400 SUB 0 1
66'044445 STA 1 ADSTE
67'020766 LDA 0 ACONB
70'006743 JSR @AQUAD
71'030756 LDA 2 AENT
72'045003 STA 1 3 2
73'020441 LDA 0 STSET
74'030442 LDA 2 SHSW
75'024436 LDA 1 ADSTE
76'122433 SUBZ# 1 0 SNC
77'152400 SUB 2 2
80'052435 STA 2 @RLNS
81'024436 LDA 1 C3
82'044436 STA 1 CNT
83'024441 LDA 1 ADT
84'044441 STA 1 ADT1
85'024742 LDA 1 AENT
86'044435 STA 1 AENT1
87'024432 LDA 1 DTUM0
88'044432 STA 1 CNT1
89'026431 LDA 1 @CNT1
90'022720 LDA 0 @DTUM5
91'106400 SUB 0 1
92'046431 STA 1 @ADT1
93'020740 LDA 0 ACONB
94'006715 JSR @AQUAD
95'046424 STA 1 @AENT1
96'010433 ISZ AENT1

```

; CONVERSION

; CONTROL ACTION

; INSTALL RELAY

; CONVERSION OF OTHER TEMP

; A/D-A/D REFERENCE

; STORE RESULT IN A/D TABLE

```

PACON
21 010424      ISZ ADT1
22 010420      ISZ CNT1
23 014415      DSZ CNT
24 000765      JMP  -13
25 024403      LDA 1 SNOFF          ;GET WAIT PERIOD
26 006017      .SYSTM
27 010400      .DELAY
30 000764      SNOFF      500
31 000732      JMP  SOLTC+2
   000003      DTUM3:    .GADD DATUM, 3
33 000000      ADSTE:    0
34 000000      STSET:    0
   000002      RLWS:    .GADD RELAY, 2
36 002000      SHSW:    2000          ;BIT 5
37 000003      C3:      3
40 000000      CNT:      0
   000000      DTUM0:    .GADD DATUM, 0
42 000000      CNT1:    0
43 000000      AENT1:    0
44 000146      AADT:    ADT
45 000000      ADT1:    0
46 000000      ADT:      0          ;TABLE OF TEMP. IN A/D UNITS
47 000000      0
50 000000      0
51 000152      SOLTB
   000012      SOLTB:    .BLK 10

```

;PID CONTROLLER FOR SOLVENT FLOWRATE

```

64 034435      SOLFM:    LDA 3 SOLVE-1          ;GET CONTROLLER BLOCK ADDRESS
65 054016      STA 3 USF
66 023427      LDA 0 @VARBLE 3          ;GET RAW DATA
67 041423      STA 0 SMOTH 3          ;STORE
70 177777      CONTL          ;CALL CONTROLLER
;CONVERSION TO ENG UNITS FOR OUTPUT
71 021450      LDA 0 SPCON 3          ;CONVERT INPUT VARIABLE
72 025423      LDA 1 SMOTH 3
73 007451      JSR @SPACE 3
74 044416      STA 1 SFLOW
75 021454      LDA 0 MINCON 3          ;CONVERT OUTPUT ACTION
76 025422      LDA 1 OUTPT 3
77 007455      JSR @MNAZE 3
80 044413      STA 1 OPERS
81 025442      LDA 1 DELAY 3
82 030015      LDA 2 TIMER
83 177777      MTPLY
84 101004      MOV 0 0 SZR
85 126000      ADC 1 1
86 006017      .SYSTM
87 010400      .DELAY
89 000000      0
91 000757      JMP  SOLFM+4
92 000000      SFLOW:    0
93 000000      OPERS:    0
94 177502      SPCON:    -190          ;A*10**5
95 003136      +1630          ;B*10**5
96 175210      -1400          ;C*10
97 000000      OUTBS:    0          ;TRUE A *10 **5
99 000000      0          ;TRUE B*10
;CONTROLLER DATA BLOCK FOR SOLVENT RATE MONITORING

```

```

FSDON
011'000222' SOLVE
000026 SOLVB: BLK 22
50'000000 0 ; FILTER
000006 GADD DATUM, 6 ; ADDRESS OF INPUT DATA
52'000000 0 ; INPUT HIGH ALARM LIMIT
53'000000 0 ; INPUT LOW ALARM LIMIT
54'000000 0 ; HI ALARM MESSAGE NUMBER
55'000001 1 ; LO ALARM MESSAGE NUMBER
56'000002 2 ; TIME INTER. FOR SUCC ALARM DISPL
57'000000 0 ; SET POINT IN A/D UNITS
60'000000 0 ; KP
61'000000 0 ; KPD
62'000000 0 ; KPI
63'000000 0 ; SCALE
64'000001 1 ; DELAY
65'000000 0 ; DIRECT OR CASCADE CONTROL
66'000000 0 ; D/A CHANNEL NUMBER
67'000000 0 ; UPPER LIMIT ON OUTPUT ACTION
70'000000 0 ; LOWER LIMIT ON OUTPUT ACTION
71'000000 0 ; MEAN VALUE OF OUTPUT ACTION
72'000214' SPCON ; ADDRESS OF CONSTANT BLOCK FOR CONV.
73'000033' DUAD ; ADDRESS OF CONV. ROUTINE
74'177777 QNVR ; INVERSE CONVERSION
75'000144 100
76'000217' OUTBS
77'177777 LNEAR
80'177777 LNVR
911'000145 101
92'000146 102
; PID CONTROLLER FOR FEED FLOWRATE
93'034435 FEEFM: LDA 3 FEEFB-1 ; GET CONTROLLER BLOCK ADDRESS
94'054016 STA 3 USF
95'023427 LDA 0 @VRBLE 3 ; GET RAW DATA
96'041423 STA 0 SMOOTH 3
97'000170' CONTL ; CALL CONTROLLER
; CONVERSION TO ENG. UNITS FOR OUTPUT
00'021450 LDA 0 SPCON 3 ; CONVERT INPUT VARIABLE
01'025423 LDA 1 SMOOTH 3
02'007451 JSR @SPACE 3
03'044416 STA 1 FFLOW
04'021454 LDA 0 MNCON 3 ; CONVERT OUTPUT ACTION
05'025422 LDA 1 OUTPT 3
06'007455 JSR @MNAZE 3
07'044413 STA 1 OPERF
08'025442 LDA 1 DELAY 3
09'030015 LDA 2 TIMER
12'000203' MTPLY
13'101004 MOV 0 0 SZR
14'126000 ADC 1 1
15'006017 SYSTM
16'010400 DELAY
17'000000 0
18'000757 JMP FEEFM+4
19'000000 FFLOW: 0
20'000000 OPERF: 0
23'176650 FPCON: -600 ; A*10**5
24'005132 2650 ; B*10**3
25'176042 -990 ; C*10
26'000000 OUTBF: 0 ; TRUE A *10 **3

```

```

FEEDON
0000000 0 ;TRUE 5 *10
;CONTROLLER DATA BLOCK FOR FEEDRATE
;MONITORING
0000341 FEEFB
000026 FEEFB: BLK 22
0000000 0 ;FILTER
000007 GADD DATUM, 7 ;ADDRESS OF INPUT DATA
0000000 0 ;INPUT HIGH ALARM LIMIT
0000000 0 ;INPUT LOW ALARM LIMIT
0000002 2 ;HI ALARM MESSAGE NUMBER
0000003 3 ;LO ALARM MESSAGE NUMBER
0000002 2 ;TIME INTER. FOR SUCC ALARM DISP
0000000 0 ;SET POINT IN A/D UNITS
0000000 0 ;KP
0000000 0 ;KPD
0000000 0 ;KPI
0000000 0 ;SCALE
0000001 1 ;DELAY
0000000 0 ;DIRECT OR CASCADE CONTROL
0000001 1 ;D/A CHANNEL NUMBER
0000000 0 ;UPPER LIMIT ON OUTPUT ACTION
0000000 0 ;LOWER LIMIT ON OUTPUT ACTION
0000000 0 ;MEAN VALUE OF OUTPUT ACTION
0000333 FFCOIN ;ADDRESS OF CONSTANT BLOCK FOR CONV
000273 QUAD ;ADDRESS OF CONV ROUTINE
000274 DNVS ;INVERSE CONV
000144 100
000336 OUTBF
000277 LNEAR
000300 LNVS
000145 101
000147 103
END

```

SSAMP

```

TITL SSAMP
; ROUTINE TO ACKNOWLEDGE CHANGES OCCURRED AT PROCESS
; SITE AND TO PRINT OUT AN APPROPRIATE MESSAGE
; RELAY BIT 0 AND CONTACT SENSE BIT 0 FOR OVERHEAD CHANGE
; RELAY BIT 1 AND CONTACT SENSE BIT 1 FOR BOTTOM CHANGE
; DECEMBER, 1975
; MONASTER UNIVERSITY
; CHEMICAL ENGINEERING DEPARTMENT
;
;

```

```

EXTN REC
ENT SSAMP, TRAP
NREL
0*034443 SSAMP: LDA 3 SSAMB-1
1*054016 STA 3 USP
2*102400 SUB 0 0
3*040454 STA 0 TRAP
4*020452 LDA 0 TRAP-1
5*177777 .REC
6*020452 LDA 0 MASK
7*123420 ANDZ 1 0 ; MASK UNWANTED BITS
0*152520 SUBZL 2 2 ; PUT 1 IN AC2
1*112414 SUB# 0 2 SZR ; SKIP IF BOTTOM SIGNAL OCCURS
2*000415 JMP OVERH
3*125113 MOVL# 1 1 SNC ; SKIP IF SIGNAL ON
4*000406 JMP BTOPE ; GO TO SIGNAL OFF
5*052444 STA 2 @BTRLA ; SET RELAY BIT ON
6*052444 STA 2 @BTDN ; PRINT MESSAGE
7*152400 SUB 2 2 ; PUT 0 IN AC2
0*052443 STA 2 @BTDF
1*000763 JMP SSAMP+4
2*176400 BTOPE: SUB 3 3
3*056436 STA 3 @BTRLA ; CLEAR RELAY BIT
4*052437 STA 2 @BTDF ; PRINT MESSAGE
5*056435 STA 3 @BTDN
6*000756 JMP SSAMP+4
7*125113 OVERH: MOVL# 1 1 SNC ; SKIP IF SIGNAL ON
0*000406 JMP OVDPE
1*052433 STA 2 @OVRLA ; SET RELAY BIT
2*052433 STA 2 @OVEDN ; PRINT MESSAGE
3*152400 SUB 2 2
4*052432 STA 2 @OVEDF
5*000747 JMP SSAMP+4
6*176400 OVDPE: SUB 3 3
7*056425 STA 3 @OVRLA ; CLEAR RELAY BIT
0*052426 STA 2 @OVEDF ; PRINT MESSAGE
1*056424 STA 3 @OVEDN
2*000742 JMP SSAMP+4

3*000044 SSAMB
000012 SSAMB: .BLK 10.
3*000057 TRAP
7*000000 TRAP: 0
0*000017 MASK: 17
000001 BTRLA: GADD RELAY, 1
000006 BTDN: GADD ALARM, 6
000007 BTDF: GADD ALARM, 7
000000 OVRLA: GADD RELAY, 0

```

SSAMP

000004 DVEDN: GADD ALARM, 4

000005 DVEDF: GADD ALARM, 5

END

```

TITL SNAVE
DECEMBER, 1975
MCMASTER UNIVERSITY
CHEMICAL ENGINEERING DEPARTMENT

```

```

ENT SOLFT, FFLO1, SFL01, WAIT, TWAIT
ENT FEFT, FHL, FLL, FLG
EXTN LNEAR, MTPLY
EXTD TIMER

```

```

NREL
PROGRAM TO SET FEED AND SOLVENT FLOWRATES
AND TO READ FLOWRATES FROM DP CELLS, AND
CONVERT THE READINGS INTO ML/MIN DATA FOR
DISPLAY.

```

```

;CHANS          D/A CHANNEL FOR SOLVENT VALVE
;CHANF          D/A CHANNEL FOR FEED VALVE
;SOLFR          STTING OF SOLVENT RATE IN D/A UNITS
;FEEFR         SETTING OF FEED RATE IN D/A UNITS
;SFL01         CURRENT SOLVENT RATE IN ML/MIN
;FFLO1         CURRENT FEED RATE IN ML/MIN

```

```

10 034431 SOLFT: LDA 3 SOLF-1
11 054016 STA 3 USP
12 020442 LDA 0 CHANS ;SET POINT TO SOLVENT RATE
13 024442 LDA 1 SOLFR
14 062023 DOB 0 DACV
15 065023 DOA 1 DACV
16 020440 LDA 0 CHANF
17 024440 LDA 1 FEEFR
18 062023 DOB 0 DACV
19 065023 DOA 1 DACV
20 026436 LDA 1 @SOLAD
21 020436 LDA 0 SCON-1
22 006444 JSR @LINEA ;CONVERSION
23 044444 STA 1 SFL01
24 026436 LDA 1 @FEEAD
25 020436 LDA 0 FCON-1
26 006440 JSR @LINEA ;CONVERSION
27 044441 STA 1 FFLO1
28 024405 LDA 1 WAIT
29 030001S LDA 2 TIMER
30 177777 MTPLY
31 006017 SYSTM
32 010400 DELAY
33 000005 WAIT: JMP READ
34 000762 SOLF
35 000032 BLK 10
36 00012 SOLFT:
37 000000 CHANS: 0
38 000600 SOLFR: 384.
39 000001 CHANF: 1
40 000321 FEEFR: 209
41 000006 SOLAD: GADD DATJM, 6
42 000052 SCON
43 000202 SCON: 130

```

```

SWAVE
333'177540      -160
      000007 FEEAD:  GADD DATUM. 7
335'000056      FCON
336'000156 FCON:  110
337'177543      -157
339'177777 LINEA:  LNEAR
311'000000 SFL01:  0
312'000000 FFL01:  0

; PROGRAM TO SHIFT THE FEED FLOWRATE TO A HIGH
; LEVEL (FHL) AND TO A LOW LEVEL (FLL) ALTERNA-
; TIVELY.
; TWAIT          WAITING HALF PERIOD IN SEC.
; FHL AND FLL ARE IN D/A UNITS
;
;
533'034421 FEEFT:  LDA 3 FEEVB-1
534'054016      STA 3 USF
535'020433      LDA 0 FHL          ; GET HIGH LEVEL
536'024431      LDA 1 FLG          ; GET FLAG VALUE
537'124005      COM 1 1 SNR        ; HI-LO?
700'020431      LDA 0 FLL          ; IF FLAG=0, GET LOW LEVEL
711'030755      LDA 2 CHANF
712'072023      DOB 2 DACV        ; SET D/A CHANNEL
713'061023      DOA 0 DACV
714'044423      STA 1 FLG          ; SAVE FLAG VALUE
715'024405      LDA 1 TWAIT
716'030001$     LDA 2 TIMER
717'000024      MTPLY
000'006017      . SYSTM
001'010400      . DELAY
002'000264 TWAIT:  180.
003'000762      JMP FEEFT+2
004'000105      FEEVB
      000012 FEEVB:  . BLK 10.
117'000000 FLG:  0
210'000426 FHL:  278.
211'000274 FLL:  188
      . END

```


USERS OF THE GSEX EXECUTIVE MUST CONFIGURE ALL OF THE EXECUTIVE PROGRAMS WITH THIS PARAMETERS TAPE THE USER MAY SPECIFY THE VALUE OF A CERTAIN NUMBER OF THE PARAMETERS HEREIN. THESE PARAMETERS ARE:

NVARS
LPTS
TTYS
PTPS
CASS
ATODS
PTRS
CNTCT
RLAYS
DIOAS
FORT4

ON NO ACCOUNT SHOULD OTHER PARAMETER VALUES BE CHANGED

DISPLACEMENTS IN THE GENERAL WORK SPACE

WUSR GENRL= 10. ; SIZE OF GENERAL WORK SPACE
WUSR RETUR= 0 ; RETURN ADDRESS STORAGE
WUSR RETAD= 1 ; RETURN ADDR STORAGE
WUSR BYTEP= 2 ; BYTE POINTER STORAGE
WUSR COUNT= 3 ; COUNTER
WUSR KOUNT= 4 ; COUNTER
WUSR WORD1= 5 ; TEMPORARY STORAGE
WUSR WORD2= 6 ; TEMPORARY STORAGE
WUSR WORD3= 7 ; TEMPORARY STORAGE
WUSR WORD4= 8 ; TEMPORARY STORAGE
WUSR WORD5= 9 ; TEMPORARY STORAGE

DISPLACEMENTS USED FOR THE LOG AND PLOT ROUTINES

WUSR LOOP1= GENRL ; LOOP COUNTER
WUSR LOOP2= GENRL+1 ; LOOP COUNTER
WUSR SPOT1= GENRL+2 ; POINTER
WUSR SPOT2= GENRL+3 ; POINTER
WUSR NDATA= GENRL+4 ; # DATA TO LIST
WUSR INTVL= GENRL+5 ; # SECS BETWEEN RECORDS
WUSR CHANL= GENRL+6 ; CHANNEL # USED FOR OUTPUT
WUSR LNCNT= GENRL+7 ; PAGE LINE COUNT
WUSR HOUR= GENRL+8. ; STARTING HOUR OF RECORD
WUSR MIN= GENRL+9. ; STARTING MINUTE OF RECORD
WUSR SEC= GENRL+10. ; STARTING SECOND OF RECORD
WUSR TMSHO= GENRL+11. ; COUNTER FOR TIME OF DAY DISPLAY
WUSR MNSIZ= GENRL+12. ; LOWER RANGE VALUE OF PLOT
WUSR MXSIZ= GENRL+13. ; UPPER RANGE VALUE OF PLOT
WUSR DNAME= GENRL+14. ; BYTE POINTER OF DEVICE FILENAME
WUSR UNIT= GENRL+15. ; DEVICE UNIT #
WUSR ADSYM= GENRL+16. ; ADDR OF POINTER TO SYMBOLS LIST
WUSR ADVAL= GENRL+17. ; ADDR OF POINTER TO VALUES TABLE
WUSR ADBUF= GENRL+18. ; BYTE POINTER TO WRITTING BUFFER
WUSR NVARS= 20. ; # VARIABLES TO BE LOGGED OR PLOTTED
WUSR IDCOD= 0 ; OUTPUT TASK DEFINITION CODE
WUSR TABSA= 1 ; DEVICE STORAGE BLOCK S. A
WUSR IDENT= 2 ; TASK IDENTIFICATION NUMBER
WUSR PRIOR= 3 ; TASK PRIORITY

OUTPUT TASK DEFINITION CODES

```

WSR LOGIT= 180+321
WSR LOGPN= 180+331
WSR LOGOK= 180+341
WSR LOGOS= 180+351
WSR FLTCL= 180+302
WSR FLTLF= 180+312
WSR FLTTT= 180+322
WSR FLTFN= 180+332
WSR FLTDK= 180+342
WSR FLTOS= 180+352

```

CONSTANTS WHICH ARE USED TO DEFINE DISPLACEMENTS
FOR THE DISK MESSAGE ROUTINE

```

WSR TMESS= GENRL ; TOTAL NUMBER OF MESSAGES IN DISK FILE
WSR MXLGT= GENRL+1 ; MAXIMUM MESSAGE LENGTH PERMITTED
WSR DSKCL= GENRL+2 ; CHANNEL # TO DISK FILE
WSR DSKNM= GENRL+3 ; BYTE POINTER TO DISK FILE NAME
WSR DEVCL= GENRL+4 ; CHANNEL # TO OUTPUT DEVICE
WSR DEVNM= GENRL+5 ; BYTE POINTER TO OUTPUT DEVICE NAME
WSR BUFR= GENRL+6 ; BYTE POINTER TO BUFFER AREA OF LENGTH MXLGT
WSR HIBYF= 0 ; HIGH ORDER BYTE POINTER TO MESSAGE
WSR LOBYF= 1 ; LOW ORDER BYTE POINTER TO MESSAGE
WSR LNGTH= 2 ; MESSAGE LENGTH IN BYTES

```

DISPLACEMENTS IN THE USER TASKS DEFINITION BLOCKS.
EACH BLOCK IS FOUR WORDS LONG AND EACH USER TASK HAS
ONE BLOCK DEFINING ITS NECESSARY ATTRIBUTES.

```

WSR TSKSA= 0 ; S. A. OF THE TASK
WSR TSKPR= 1 ; PRIORITY OF THE TASK (1 TO 377-NEVER 0)
WSR TSKID= 2 ; TASK IDENTIFICATION CODE-1 TO 300,  
; NEVER 0 OR ABOVE 300
WSR TSKIL= 3 ; TASK'S KILL FLAG
THE TASK DEFINITION BLOCK IS EXTENDED BY ONE WORD  
IF THE FORT4 PARAMETER, DEFINED BELOW IS NON-ZERO
WSR TSKMD= 4 ; TASK MODE-IF FORTRAN IV TASK, ZERO  
; -IF ASSEMBLER ONLY, NON-ZERO

```

THE FOLLOWING CONSTANTS DEFINE THE SYSTEM CONFIGURATION
ZERO: DEVICE NOT IN THE SYSTEM
NON-ZERO: NUMBER OF DEVICES CONFIGURED IN SYSTEM

```

WSR LPTS= 1 ; LINE PRINTER
WSR TTYS= 1 ; # TELETYPES ON CPU
WSR PTPS= 0 ; PAPER TAPE PUNCH
WSR CASS= 0 ; CASSETTE FILE
WSR ATODS= 10 ; ANALOG TO DIGITAL CONVERTER
WSR PTRS= 0 ; PAPER TAPE READER
WSR CNTCT= 10 ; CONTACT SENSE
WSR RLAYS= 10 ; RELAYS
WSR DTDAS= 10 ; DIGITAL TO ANALOG CONVERTER

```

DOS DISPLACEMENTS USED BY THE GOSEX PACKAGE

```

WSR USTP= 12 ; POINTER TO CURRENT PROGRAM'S UST
WSR TID= 12 ; TASK ID IN TASK'S TCB
WSR USTCT= 14 ; CURRENT TCB POINTER TO PROGRAM'S UST
WSR USTIN= 17 ; START OF USER NREL CODE IN UST

```

FORTRAN IV PARAMETER

WHEN ZERO, ALL TASKS MUST BE IN ASSEMBLER
WHEN NON-ZERO, THIS PARAMETER SPECIFIES THE MAXIMUM NUMBER OF
PARALLEL FORTRAN IV TASKS THAT MAY RUN AT ONE TIME THE

CONTROLLER BLOCK DISPLACEMENTS

```

UJSR WKS:SP= GENRL ;WORK SPACE-2 WORDS
UJSR SIGN= GENRL+2 ;SIGN STORAGE
UJSR EROR0= GENRL+3 ;ERROR AT T
UJSR EROR1= GENRL+4 ;ERROR AT T-1
UJSR EROR2= GENRL+5 ;ERROR AT T-2
UJSR EROR3= GENRL+6 ;ERROR AT T-3
UJSR TSUM= GENRL+7 ;INTEGRAL SUM STORAGE
UJSR OUTPT= GENRL+8 ;CURRENT OUTPUT ACTION
UJSR SMOTH= GENRL+9 ;FILTERED DATA STORAGE
UJSR CNTHI= GENRL+10 ;HIGH LIMIT ALARM COUNTER
UJSR CNTLO= GENRL+11 ;LOW LIMIT ALARM COUNTER
UJSR FILTR= GENRL+12 ;FILTER CONSTANT
UJSR VRBLE= GENRL+13 ;ADDR OF RAW DATA
UJSR INHI= GENRL+14 ;INPUT HIGH LIMIT
UJSR INLO= GENRL+15 ;INPUT LOW LIMIT
UJSR MESSHI= GENRL+16 ;MESSAGE # FOR HIGH LIMIT ALARM IN MESSG. MG
UJSR MESSLO= GENRL+17 ;MESSAGE # FOR LOW LIMIT ALARM IN MESSG. MG
UJSR AWAIT= GENRL+18 ;INTERVAL BETWEEN SUCCESSIVE ALARMS
UJSR SETPT= GENRL+19 ;SET POINT
UJSR KP= GENRL+20 ;PROPORTIONAL GAIN
UJSR KPD= GENRL+21 ;PROPORTIONAL DERIVATIVE GAIN
UJSR KPI= GENRL+22 ;PROPORTIONAL INTEGRAL GAIN
UJSR SCALE= GENRL+23 ;SCALE FACTOR WITH ACTION DIRECTION
UJSR DELAY= GENRL+24 ;TIME INTERVAL BETWEEN CONTROL ACTIONS
UJSR CASCD= GENRL+25 ;CASCADE FLAG
UJSR DESTN= GENRL+26 ;ADDR OF DESTINATION DATA BLOCK OR
;D/A CHANNEL #
UJSR DUTHI= GENRL+27 ;HIGH LIMIT ON OUTPUT
UJSR OUTLO= GENRL+28 ;LOW LIMIT ON OUTPUT
UJSR MEAN= GENRL+29 ;MEAN OUTPUT VALUE
UJSR SPCDN= GENRL+30 ;ADDR OF CONSTANT BLOCK FOR SETPT CONVERSION
UJSR SPAZE= GENRL+31 ;ADDR OF ROUTINE TO CONVERT FROM
;A/D TO ENGINEERING UNITS
UJSR SPEZA= GENRL+32 ;ADDR OF ROUTINE TO CONVERT FROM
;ENGINEERING TO A/D UNITS
UJSR SPCAP= GENRL+33 ;MESSAGE # FOR SETPT CAPTION IN OPCOM. MG
UJSR NINCON= GENRL+34 ;ADDR OF CONSTANT BLOCK FOR MEAN CONVERSION
UJSR NINAZE= GENRL+35 ;ADDR OF ROUTINE TO CONVERT FROM
;D/A (OR A/D) TO ENGINEERING UNITS
UJSR NINEZA= GENRL+36 ;ADDR OF ROUTINE TO CONVERT FROM
;ENGINEERING TO D/A (OR A/D) UNITS
UJSR NINCAP= GENRL+37 ;MESSAGE # FOR MEAN CAPTION IN OPCOM. MG
UJSR LPNES= GENRL+38 ;LDDP'S DESCRIPTIVE MESSAGE # IN OPCOM. MG

```

.EOT ;END OF GOSSEX PARAMETER TAPE

. TITL SYMBL

```
;SYMBL TAPE # 1 OF 2
;USER BUILT SYMBOL TABLE
;THIS TAPE-GOSEX SYMBOLS
```

. ENT USST, UEST

; EXECUTIVE FUNCTION SYMBOLS

```
. EXTN START, CEASE, STATS, ENDDIO, ENDAL, CLEAR, CHNGE, PARAM
. EXTN TUNER, LOG, PLOT, READY, RELSE, RETRN, CLOCK, PROFL
```

; DEVICE SYMBOLS

. EXTN CONSL, PRINT, TTYPE, PUNCH, DISK, CASSET, READR

. NREL

; USER MUST DECLARE THE FOLLOWING AT THE END OF TAPE # 2

; SST: LAST SYMBOL-CODE WORD # 1

; UEST= EST

; USST= SST

```
;ALSO, THE USER MUST INCLUDE THE APPROPRIATE EXTN
;DECLARATIONS FOR TAPE # 2 THIS MAY BE DONE IN TAPE # 2 ITSELF
;IN THIS INSTANCE, IT IS NECESSARY THAT THE EXTERNAL
;DECLARATIONS 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
; S
; T
; U
; V
; W
; X
; Y
; Z
; 28.
; 29.
; 30.
; 31.
; 32.
; 33.
; 34
; 35.
; 36.
; 37.

; EXAMPLE OF CODING:

; SYMBOL "ABCDE" MAY BE ENCODED BY THE USER IN THE FOLLOWING WAY
; [DJ*40. +LEJ*32. ; SYMBOL CODE WORD # 2
; [AJ*40. +CEJ*40. +[C] ; SYMBOL CODE WORD # 1

; WHERE [#J 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

01003 SYMBI

00000'000000'EST:

; EXECUTIVE FUNCTIONS LIST

00001'177777	START	; SYMBOL VALUE-USUALLY ESTABLISHED AT LOAD
00002'107700	36800	; SYMBOL CODE WORD # 2
00003'134773	47611	; SYMBOL CODE WORD # 1
00004'177777	CEASE	
00005'111340	37600	
00006'051643	21411	
00007'177777	STATS	
00010'114640	39328	
00011'134773	47611	
00012'177777	ENDIO	
00013'061040	25120	
00014'060616	24974	
00015'177777	ENDAL	
00016'034700	14784	
00017'060616	24974	
00020'177777	CLEAR	
00021'035200	14976	
00022'052277	21695	
00023'177777	CHNGE	
00024'053340	22240	
00025'052050	21544	
00026'177777	PARAM	
00027'034740	14816	
00030'122124	42068	
00031'177777	TUNER	
00032'047200	20096	
00033'140160	49264	
00034'177777	LOG	
00035'000000	0	
00036'106571	36217	
00037'177777	PLDT	
00040'113000	38400	
00041'123011	42505	
00042'177777	READY	
00043'045140	19040	
00044'130543	45411	
00045'177777	RELSE	
00046'111340	37600	
00047'130556	45422	
00050'177777	RETRN	
00051'107400	36608	
00052'130566	45430	
00053'177777	CLOCK	
00054'041640	17312	
00055'052311	21705	
00056'177777	FRDFL	
00057'051300	21184	
00060'123371	42745	

; DEVICES LIST

00061'177777	CONSL
00062'111700	37824
00063'052500	21824
00064'177777	PRINT
00065'075700	31680
00066'123363	42739

00004 SYMBL
 00067 177777
 00070 101740
 00071 140123
 00072 177777
 00073 041500
 00074 123560
 00075 177777
 00076 064400
 00077 055225
 00100 177777
 00101 047300
 00102 051425
 00103 177777
 00104 044600
 00105 130543

TTYFE
 33760
 49235
 FUJNH
 17216
 42864
 DISK
 26880
 23189
 CASET
 20160
 21269
 READR
 18816
 45411

CONTROLLER PARAMETERS LIST-VALUE SPECIFIED IN PARAMETER TAPE

00106 000026
 00107 114600
 00110 063416
 00111 000030
 00112 057400
 00113 075222
 00114 000031
 00115 076400
 00116 075226
 00117 000035
 00120 102700
 00121 133666
 00122 000036
 00123 000000
 00124 103520
 00125 000037
 00126 000000
 00127 103536
 00130 000040
 00131 000000
 00132 103543
 00133 000041
 00134 067740
 00135 133523
 00136 000042
 00137 035540
 00140 054756
 00141 000045
 00142 056140
 00143 120466
 00144 000046
 00145 070440
 00146 120466
 00147 000047
 00150 074000
 00151 111043

FILTR
 39296
 26362
 INHI
 24320
 31378
 INLD
 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

```

;SYMBOL OF TAPE #2 OF 2
;EXTN SOLFT,FFLOW,SFLWL,SFLDL,WAIT,TWAIT
;EXTN FEFT,FHL,FLL,FLS
;EXTN FEETC,FNOFF,FTSET,ADLTE
;EXTN SOLTC,SNOFF,STSET,ADSTE
;EXTN FFLOW,OPERS,FFCON,FTMP
;EXTN SFLWM,FEFPM,SFCON,STEMP
;EXTN DATUM,SCAN
;EXTN DJTBS,OUTCF
;EXTN SSAMP

```

```

;FEED TEMPERATURE CONTROL LOOP PARAMETERS

```

```

FEETC
30 *40 +13 *32.
16 *40 +15 *40 +15.
FNOFF
16 *40 +26 *32
16 *40 +24 *40 +25.
FTSET
15 *40 +30 *32.
16 *40 +30 *40 +29.
ADLTE
30 *40 +15 *32
11 *40 +14 *40 +16.
FTMP
23 *40 +26 *32
16 *40 +30 *40 +15.

```

```

;SOLVENT TEMPERATURE CONTROL LOOP PARAMETERS

```

```

SOLTC
30 *40 +13 *32
29 *40 +25 *40 +22.
SNOFF
16 *40 +26 *32
29 *40 +24 *40 +25.
STSET
15 *40 +30 *32
29 *40 +30 *40 +29
ADSTE
30 *40 +15 *32
11 *40 +14 *40 +29
STEMP
23 *40 +26 *32.
29 *40 +30 *40 +15.
ADT
0 *40 +0 *32
11 *40 +14 *40 +30

```

```

;FLOWRATES(FEED AND SOLVENT)CONTROL LOOP PARAMETERS

```

```

SFLWL
25 *40 +33 *32
29 *40 +16 *40 +22.
OPERS
28 *40 +29 *32
25 *40 +26 *40 +15.
SFCON
25 *40 +24 *32
29 *40 +16 *40 +13.
FFLOW
25 *40 +33 *32.

```



```

0006  SYMBI
00226'063226  16. *40 +16. *40. +22
00227'177777  DPERF
00230'107000  28. *40 +16. *32
00231'120137  25 *40 +26. *40 +15
00232'177777  PFLON
00233'100000  25. *40. +24. *32
00234'063215  16. *40 +16 *40. +15
00235'177777  SOLFM
00236'051340  16. *40 +23. *32
00237'134476  29. *40 +25. *40 +22
00240'177777  FEEFN
00241'051340  16. *40. +23. *32
00242'063147  16. *40. +15. *40 +15
00243'177777  DUTES
00244'037640  12 *40 +29. *32
00245'120466  25 *40 +31. *40. +30.
00246'177777  DUTBF
00247'037000  12 *40. +16. *32
00250'120466  25. *40. +31. *40. +30.
00251'177777  DATJM
00252'116740  31. *40. +23. *32
00253'054526  14. *40. +11. *40 +30.
00254'177777  SCAN
00255'074000  24. *40. +0. *32
00256'133523  29. *40. +13. *40 +11
00257'177777  CONVE
00260'120600  32 *40. +12 *32
00261'052500  13. *40. +25. *40. +24
; SQUARE WAVE TO FEED RATE ROUTINE
00262'177777  FEFT
00263'051700  16. *40 +30. *32.
00264'063147  16. *40. +15. *40 +15.
00265'177777  FHL
00266'000000  0. *40. +0. *32.
00267'063346  16. *40. +18. *40 +22
00270'177777  FLL
00271'000000  0. *40. +0. *32.
00272'063606  16. *40. +22. *40. +22.
00273'177777  FLG
00274'000000  0. *40. +0. *32.
00275'063601  16 *40. +22 *40. +17.
00276'177777  SOLFT
00277'051700  16 *40 +30 *32
00300'134476  29. *40. +25 *40. +22
00301'177777  FFLD1
00302'076500  25 *40. +2 *32
00303'063226  16. *40 +16. *40. +22
00304'177777  SFLD1
00305'076500  25 *40. +2 *32
00306'135726  29. *40. +16 *40 +22
00307'177777  WAIT
00310'113000  30. *40. +0. *32
00311'150013  33. *40 +11. *40. +19.
00312'177777  TWAIT
00313'061300  19. *40 +30 *32
00314'140263  30 *40 +33. *40. +11
; SAMPLING MONITOR ROUTINE
00315'177777  SSAMP
00316'073100  23 *40 +26 *32

```

0007 SYMBL
00317'134723 SST: 29. *40. +29. *40. +11.
000000'UEST=EST
000317'USST=SST
. END

```

LINE # LINE AS READ FROM SOURCE FILE
0000 <15><12>
0001 <12>NOT AN EXECUTIVE FUNCTION
0002 <12>EXECUTIVE FUNCTION NOT AVAILABLE
0003 <12>TASK NAME:
0004 <12>NOT A USER TASK<15>
0005 <12>USER TASK CREATED
0006 <12>TASK IS ALREADY ACTIVE
0007 <12>USER TASK KILLED
0008 <12>TASK IS ALREADY INACTIVE
0009 <12>TASK IS INACTIVE
0010 <12>TASK IS ACTIVE
0011 <12>DEVICE NAME:
0012 <12>NOT A SYSTEM DEVICE<15>
0013 <12>DEVICE NOT CONFIGURED FOR USE
0014 <12>SPECIFIED DEVICE DEACTIVATED
0015 <12>DEVICE NOT IN USE
0016 <12>ALL CONFIGURED DEVICES DEACTIVATED
0017 <12>DISK DIRECTORY & FILENAME:
0018 <12>DELETION CONFIRMED
0019 <12>FILENAME ERROR<15>
0020 <12>CURRENT DISPLAY INTERVAL(SECONDS):
0021 <12>RESET DISPLAY INTERVAL(SECONDS):
0022 <12>CHANGE CONFIRMED
0023 <12>INTERVAL IMPROPERLY SPECIFIED<15>
0024 <12>INTERVAL TOO LONG FOR CURRENT RTC FREQUENCY<15>
0025 <15><12><40>*?*.
0026 <15><12><40>.
0027 <15><12>LOOP NAME:
0028 <12>NOT A CONTROLLER LOOP<15>
0029 FILTER CONSTANT(0 TO +1000.)/<40>
0030 INPUT HIGH ALARM LIMIT-
0031 INPUT LOW ALARM LIMIT-
0032 CURRENT SET POINT-
0033 PROPORTIONAL GAIN(+VE)/<40>
0034 PROPORTIONAL-DERIVATIVE GAIN(+VE)/<40>
0035 PROPORTIONAL-INTEGRAL GAIN(+VE)/<40>
0036 SCALE FACTOR & DIRECTION OF ACTION/<40>
0037 CONTROL INTERVAL(SECONDS)/<40>
0038 OUTPUT HIGH LIMIT-
0039 OUTPUT LOW LIMIT-
0040 OUTPUT MEAN-
0041 <15><12>CONVERSION ERROR
0042 <15><12><40>*?*<15><12>
0043 <12>FILE IN USE
0044 <12>DELETION NOT POSSIBLE, CODE<40>
0045 <12>VARIABLES LIST-MAX:
0046 <12>DEVICE IN USE
0047 <12>DEVICE NOT EQUIPPED FOR LOGGING
0048 <12>DISPLAY MODE:
0049 <12>NO LIST<15>
0050 <12>END OF LIST<15>
0051 <12>LOGGING INTERVAL(SECONDS):
0052 <12>OUTPUT TASK CREATED
0053 <12>UNABLE TO INITIATE OUTPUT TASK
0054 <12>CASSETTE UNIT & FILE #:
0055 <12>DEVICE NOT EQUIPPED FOR PLOTTING
0056 <12>SCALE FACTOR:
0057 <12>PLOTTING INTERVAL(SECONDS):
0058 <12>MIN RANGE OF PLOT:

```

```

00059 <12>MAX RANGE OF PLOT:
00060 <15><12>USER IN BACKGROUND
00061 <15><12>USER IN FOREGROUND
00062 <15><12>USER BUILT SYMBOL TABLE NOT DEFINED<15><12>
00063 <15><12>RELAY BIT STATUS TABLE NOT DEFINED<15><12>
00064 <15><12>A/D READ DATA STORAGE NOT DEFINED<15><12>
00065 <15><12>USER CLOCK SET TO RTC FREQUENCY<15><12>
00066 <15><12>USER CLOCK NOT DEFINED<15><12>
00067 <15><12>CONTACT SENSE DISPATCH TABLE NOT DEFINED<15><12>
00068 <15><12>USER SHUTDOWN ROUTINE NOT DEFINED<15><12>
00069 <15><12>USER TASK DEFINITION TABLE NOT DEFINED<15><12>
00070 <15><12>ERROR DETECTED IN USER TASK DEFINITION TABLE<15><12>
00071 <15><12>USER ALARM DEFINITION TABLE NOT DEFINED<15><12>
00072 <15><12>USER MESSAGE FILE NOT DEFINED<15><12>
00073 <15><12>EXECUTION ABORTED<15><12>
00074 <15><12>AOK-TO RUN, STRIKE ANY KEY<15><12>
00075 <12>DIRECTORY OR DEVICE NAME:
00076 <12>DIRECTORY OR DEVICE INITIALIZED
00077 <12>DIRECTORY OR DEVICE ALREADY INITIALIZED
00078 <12>INITIALIZATION NOT POSSIBLE, CODE<40>
00079 <12>DIRECTORY OR DEVICE RELEASED
00080 <12>DIRECTORY OR DEVICE IN USE
00081 <12>RELEASE NOT POSSIBLE, CODE<40>
00082 <15><12>USER SPACE RELEASED<15><12>
00083 <15><12>CONTROL LOOP DEFINITION TABLE NOT DEFINED<15><12>
00084 <15><12>ERROR DETECTED IN CONTROL LOOP DEFINITION TABLE<15><12>
00085 <15><12>ERROR DETECTED IN CONTACT SENSE DISPATCH TABLE<15><12>
00086 <12>AXIAL POSITION:
00087 <15><12>DEF EXECUTIVE FUNCTION LIST EXTENSION NOT DEFINED<15><12>
00088 UNUSED
00089 UNUSED
00090 UNUSED
00091 UNUSED
00092 UNUSED
00093 UNUSED
00094 UNUSED
00095 UNUSED
00096 UNUSED
00097 UNUSED
00098 UNUSED
00099 UNUSED
00100 MILLIMETERS*10./MINUTE<40>
00101 XVALVE OPEN<40>
00102 <12>SOLVENT FLOWRATE CONTROL LOOP<15>
00103 <12>FEED FLOWRATE CONTROL LOOP<15>

```

HESSG:

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```
LINE # LINE AS READ FROM SOURCE FILE
01000 <12>SOLVENT RATE NEAR MAXIMUM<15>
01001 <12>SOLVENT RATE NEAR MINIMUM<15>
01002 <12>FEED RATE NEAR MAXIMUM<15>
01003 <12>FEED RATE NEAR MINIMUM<15>
01004 <12>OVERHEAD SIGNAL ON <15>
01005 <12>OVERHEAD SIGNAL OFF <15>
01006 <12>BOTTOM SIGNAL ON <15>
01007 <12>BOTTOM SIGNAL OFF <15>
```

UTIL SV LOADED BY RLDR REV 03 AT 12:29:51 10/12/75

WFCE
SDDN
SAMP
WAVE
WMBL
WTRF
WYED
WDER
WNVY

006002
000,000 START
CEASE
STATS 000216
000,001 ENDID
ENDAL
CLEAR
CHNGE 000502
000,002 PARAM 000560
000,003 TUNER 000613
000,004 LOG 000455
000,005 HEADL 000320
000,006 PLOT 000502
000,007 HEADP 000314
000,010 PREP 000536
000,011 READY
RELSE
RETRN
CLOCK 000263
000,012 PROFL 000506
000,013 PROHD 000274
007002

WGER
WTER
WFILE
WJNS
WVLY
WTRM
WACAL
WXNT
WPRI
WIDC
WUND

WCONTL 001274
WOTCK 011071

NMAX 012076
ZMAX 000123
CSZE 000000
EST 000000
SST 000000

TIMER 000056
PCTMP 000101
TSAV 000102
TMIN 000103
CTCB 000104
OVLAY 000633
ALARM 000641
DATUM 000652
RELAY 000664
SENSE 000674

SCAN 000710
CLOOF 000711
SUNRS 000716
TASKS 000727
UDEF 000764
FEETC 000765
FNDFP 001010
ADFTE 001012
FTSET 001013
FEETB 001022
STEMF 001040
FTEMP 001041
CONVB 001043
SOLTC 001046
SNDFP 001115
ADSTE 001120
STSET 001121
ADT 001133
SOLTB 001137
SOLFM 001151
SFLOW 001177
OPERS 001200
SFCON 001201
OUTBS 001204
SOLVB 001207
FEEFM 001270
FFLOW 001316
OPERF 001317
FFCON 001320
OUTBF 001323
FEEFB 001326
. UIEX 001400
. UPEX 001400
. UCEX 001400
SSAMP 001407
TRAP 001466
SOLFT 001476
WAIT 001525
SFLD1 001557
FFLD1 001560
FEEFT 001561
TWAIT 001600
FLG 001615
FHL 001616
FLL 001617
UEST 001620
USST 002137
INTRP 002140
MODE 002244
START 002270
CEASE 002273
STATS 002276
ENDIO 002301
ENDAL 002304
CLEAR 002307
CHNGE 002312
PARAM 002315
TUNER 002320
LOG 002323
PLOT 002326
READY 002331
RELSE 002334
RETRN 002337
CLOCK 002342
BEDEL 002345

002355
MESS 002355
MINITR 002412
MTFLX 003154
ADDCT 003221
CTDCT 003260
IDEVCE 003335
CONSL 004207
RPRINT 004213
TTYPE 004217
RPNCH 004220
DISK 004221
ICASET 004233
IREADR 004234
IOPCOM 004235
MESSG 004243
.. BDEC 004750
.. BDC 005001
.. DBIN 005102
.. DBIN 005150
.. BFLT 005217
.. FBIN 005412
IEXC01 006002
IEXC04 006002
IEXC08 006002
IEXC09 006002
EXC10 006002
EXC12 006002
EXC14 006002
EXC15 006002
EXC17 006002
EXC11 006004
EXC13 006004
EXC20 006004
ERROR 006050
DSKMG 006051
MTPLY 006052
MTPLA 006053
DIVID 006054
EXC16 006054
ROUND 006055
KEYED 006057
DECD 006060
ENCD 006061
LOCAT 006062
RETRV 006063
RANGE 006064
BDEC 006065
EXC02 006065
BDC 006066
DBIN 006067
OBIN 006070
BFLT 006071
FBIN 006072
. DVKI 006073
. TDVL 006074
. DVRE 006075
. DVEX 006076
. KILL 006077
. TASK 006100
. AKIL 006105
. ASIJS 006106
. AFEN 006106
. ARDY 006107
. AUNP 006107
. IXMT 006110

ALL 000111
XMTW 006112
REC 006113
PRI 006114
IDST 006115
TIDS 006116
TIDR 006117
TIDK 006120
TIDP 006121
SMSK 006122
IEXC17 006125
IEXC05 006127
IEXC03 006150
IEXC18 006155
IEXC06 006232
IEXC07 006341
ILDGER 007002
IPAUZE 007203
TFORM 007301
DATER 007327
IPLTER 007401
PTEXT 007414
CLEAN 007633
NUMBS 007652
FFILE 007733
QUAD 010245
LNEAR 010246
QNVRS 010317
LNVRS 010320
QVWRT 010650
TMAX 010763
TNXT1 011007
QTCNT 011067
LQTSC 011070
SYST2 011077
SYST1 011102
TLINK 011115
LNKPR 011155
TREL 011162
INHB 011170
TIJNLK 011200
TSKER 011331
TERCM 011332
TIDSR 011355
XSRH 011622
TFR01 011675
CONTL 177777
BTCK 177777
QVY01 000,000
QVY02 000,000
QVY03 000,000
QVY04 000,001
QVY05 000,001
QVY06 000,001
QVY07 000,001
QVY08 000,002
QVY09 000,003
QVY10 000,004
QVY11 000,005
QVY12 000,006
QVY13 000,007
QVY14 000,010
QVY15 000,011
QVY16 000,011
QVY17 000,011
QVY18 000,011

DVT14 000, 012
DVT20 000, 013
